NUMERICAL SIMULATION OF BLUNT BODY GENERATED DETONATION WAVE RAMJET FLOWFIELDS

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
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University of Toronto

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Abstract

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Blunt body generated detonation wave ramjet flowfields have been studied numerically for a stoichiometrically premixed air-hydrogen gas mixture involving 13 species. Three different blunt body diameters are examined within a domain at fixed height and length, creating the channel blockage ratios of 16%, 25% and 33%.

For this an implicit numerical method based on the \textit{Lower-Upper Symmetric Gauss-Seidel} scheme and a \textit{Roe flux difference splitting} scheme was developed and thoroughly validated for laminar flows with non-equilibrium chemistry on structured multi-block grids.

Blunt body generated combustion is superior over wedge generated combustion for low inflow temperatures, since ignition can be achieved within a domain of significantly smaller size.

With increasing channel blockage ratio the losses of total pressure and momentum increase, while the heat added slightly decreases. This makes the smallest channel blockage ratio the favourable.
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# Contents

<table>
<thead>
<tr>
<th>Notation</th>
<th>viii</th>
</tr>
</thead>
</table>

## 1 Introduction

1.1 General Background ........................................... 1
1.2 Scope of Study ................................................. 4
1.3 Solution Approach .............................................. 6

## 2 Governing Equations

2.1 Overview and Physical Model .................................. 8
2.2 Basic Vectors .................................................... 9
2.3 Point Chemistry Equations ..................................... 10
2.4 Euler Equations .................................................. 10
2.5 Navier-Stokes Equations ....................................... 11
2.6 Flow and Thermodynamic Variables in Detail .................. 11
2.7 Thermodynamic Species Properties ............................ 14
2.8 Species Transport Properties ................................... 15
2.9 Thermodynamic and Transport Properties for the Gas Mixture .... 18
2.10 Temperature Calculation ....................................... 19
2.11 Ideal Single Species Gas ...................................... 20
2.12 Propulsion Performance Analysis ............................. 21
  2.12.1 Mass Flux Balance ........................................ 21
  2.12.2 Momentum Balance ......................................... 22
  2.12.3 Enthalpy Balance ........................................... 23
  2.12.4 Entropy Increase .......................................... 25
  2.12.5 Total Pressure Loss ....................................... 26
## 3 Boundary Conditions

3.1 Inflow and Outflow ............................................. 27
3.2 Symmetry and Inviscid Wall ..................................
3.3 Viscous Wall ..................................................... 29

## 4 Spatial Discretization

4.1 Inviscid Fluxes ................................................... 31
4.2 Viscous Fluxes .................................................... 32
4.3 Implementation of Boundary Conditions ...................... 34
4.4 Artificial Dissipation ............................................ 35

## 5 Temporal Discretization

5.1 Explicit Time-Marching Methods .............................. 39
5.2 Implicit Time-Marching Methods ............................. 41
5.3 Time Step Calculation .......................................... 45

## 6 Grid Generation

6.1 Boundary Definition ............................................. 47
6.1.1 NURBS .......................................................... 48
6.1.2 Spline Interpolation ......................................... 49
6.1.3 Boundary Point Distribution ............................... 50
6.2 Transfinite Interpolation ....................................... 54
6.3 Elliptic Grid Generation ........................................ 56
6.3.1 Governing Equations ....................................... 56
6.3.2 Line and Point Clustering .................................. 57
6.3.3 Orthogonality ................................................ 58
6.4 Grids for Test Cases ............................................. 64
6.4.1 Free Stream Flow ............................................ 64
6.4.2 Flat Plate Flow ............................................... 65
6.4.3 Wedge Flow ................................................... 65
6.4.4 Channel Flow ................................................ 67
6.4.5 Blunt Body Flow ............................................. 67
6.5 Grids for Thesis Cases ......................................... 69
# Test Cases

- **7.1** Point Chemistry
  - **7.1.1** Initial Conditions
  - **7.1.2** Oxygen-Hydrogen, 8 Species and 17 Reactions
  - **7.1.3** Air-Hydrogen, 9 Species and 19 Reactions
  - **7.1.4** Air-Hydrogen, 13 Species and 33 Reactions
  - **7.1.5** Ignition Delay Times

- **7.2** Freestream
  - **7.2.1** Supersonic Combustion
  - **7.2.2** Diffusive Mixing

- **7.3** Flat Plate Flow

- **7.4** Wedge
  - **7.4.1** Oblique Shock
  - **7.4.2** Corner Flow
  - **7.4.3** Reactive Wedge Flow

- **7.5** Viscous Flow in Channel

- **7.6** Blunt Body Flow

- **7.7** Test Cases Overview

# Thesis Cases

- **8.1** Geometrical and Physical Setup
  - **8.1.1** Channel Blockage Ratio 16%
  - **8.1.2** Channel Blockage Ratio 25%
  - **8.1.3** Channel Blockage Ratio 33%
  - **8.1.4** Comparative Wedge Flow
  - **8.1.5** Overview

# Propulsive Performance Analysis

# Outlook

# A Source Term Jacobi Matrix

- **A.1** Numerical Source Term Jacobi Matrix
- **A.2** Analytical Source Term Jacobi Matrix
Notation

Scalar Quantities

\( a \)  
  sound speed

\( a_\chi \)  
  polynomial coefficients (\( \chi \) is an arbitrary subscript)

\( A_{0,l} \)  
  constant for forward reaction speed reaction \( l \) (modified Arrhenius equation)

\( c_p \)  
  specific heat coefficient (constant pressure)

\( c_v \)  
  specific heat coefficient (constant volume)

\( CBR \)  
  channel blockage ratio

\( d \)  
  blunt body diameter

\( D \)  
  diffusion constant

\( e \)  
  internal energy per unit mass

\( E \)  
  total energy per unit mass

\( E_{A,l} \)  
  activation energy for forward reaction speed reaction \( l \) (modified Arrhenius equation)

\( g \)  
  free enthalpy, Gibb’s energy, per unit mass

\( h \)  
  enthalpy per unit mass

\( k_{f,l} \)  
  forward reaction speed reaction \( l \)

\( k_{b,l} \)  
  backward reaction speed reaction \( l \)

\( K_{c,l} \)  
  equilibrium constant reaction \( l \), related to concentration

\( K_{g,l} \)  
  molar equilibrium constant reaction \( l \)

\( M_i \)  
  molar mass component \( i \)

\( [M_i] \)  
  concentration component \( i \)

\( [M'_l] \)  
  concentration third body efficiency reaction \( l \)

\( N_{c_p} \)  
  number of coefficients for \( c_p \) calculation

\( N_D \)  
  number of coefficients for \( D \) calculation
$N_r$  number of reactions
$N_s$  number of species
$N_\lambda$  number of coefficients for $\lambda$ calculation
$N_\mu$  number of coefficients for $\mu$ calculation
$p$  pressure
$R_m$  gas constant
$s$  entropy per unit mass
$\Delta s_x$  cell side length
$\Delta t$  time step
$T$  temperature
$u$  $x$-component velocity
$v$  $y$-component velocity
$x$  $x$ coordinate
$X_i$  molar fraction of component $i$
$y$  $y$ coordinate
$Y_i$  mass fraction of component $i$
$\alpha_{l,i}$  third body efficiency component $i$ in reaction equation $l$
$\tilde{\alpha}_l$  temperature exponent for forward reaction speed reaction $l$ (modified Arrhenius equation)
$\delta_m$  mixing layer thickness
$\Delta$  standoff distance
$\epsilon$  molecular potential
$\dot{\epsilon}$  entropy correction coefficient
$\gamma$  specific heat ratio
$\lambda$  heat conductivity mixture
$\lambda_i$  heat conductivity component $i$
$\mu$  viscosity mixture
$\mu_i$  viscosity component $i$
$\nu_{i,l}$  overall stoichiometric coefficient, species $i$, reaction $l$
$\nu_{i,l}'$  stoichiometric coefficients reactants, species $i$, reaction $l$
$\nu_{i,l}''$  stoichiometric coefficients products, species $i$, reaction $l$
$\phi$  correction factor (mixture properties)
$\rho$  density
$\sigma$  collision diameter
\[ \tau \] shear tension

\[ \omega_i \] chemical production component \( i \)

\( \Omega^{(1,1)} \), \( \Omega^{(2,2)} \) collision integrals

**Vector Quantities**

\( f \) field force (e.g. gravitation)

\( g \) flux limiter

\( G_c \) convective flux in \( x \)-direction

\( G_d \) diffusive flux in \( x \)-direction

\( H_c \) convective flux in \( y \)-direction

\( H_d \) diffusive flux in \( y \)-direction

\( i \) diffusion mass flux component \( i \)

\( Q \) vector of conserved variables

\( R \) residual vector (right hand side)

\( S \) chemical source vector

\( \alpha \) flux correction vector

\( \xi \) energy flux

\( \Phi \) flux limiter related vector

**Matrix Quantities**

\( \hat{D}, \hat{k}, \hat{U} \) factors for LU-SGS scheme

\( \hat{L} \) source term Jacobi matrix

\( \hat{L} \) unity matrix

\( \hat{\Lambda} \) spectral radii matrix

**Subscripts**

\( i, j, k, l \) indices

\( su \) Sutherland’s law related quantities

\( t \) total thermodynamic variables

wall wall related quantities

\( \xi, \eta \) metrical values
Superscripts

$x^*$ molar quantity

Operators

$\nabla$ gradient

$\times$ vector product

$\otimes$ tensor product
Chapter 1

Introduction

1.1 General Background

The means of propulsion predominantly used for atmospheric and space flight are gas turbines and rocket engines, while piston engines for low speed and electrical plasma-jet engines for orbit applications play a less significant role.

Since within the area of hypersonic flight piston and electrical plasma-jet engines are not used, we can focus on gas turbines and rocket engines. Gas turbines present an air-breathing form of propulsion, while rocket engines are completely independent of the atmosphere because both the fuel and the oxidizer have to be carried by the rocket. Obviously, this has a direct impact on the operating costs. An improvement to the situation would be the combination of a rocket engine with an air-breathing type of propulsion. Here the usefulness of the gas turbine is limited since it becomes inefficient at hypersonic flight Mach numbers. The temperature in the compressor would raise to a point where extensive cooling is required, which is usually only applied to turbine stages. Therefore, only the kinetic energy in the incoming fluid should be used for the compression in this case, which leads to the concept of ramjets and scramjets.

An overview of the propulsion concepts introduced above, with an emphasis on hypersonic propulsion, can be found in [4] and [10]. Their specific impulses and operational Mach number ranges are given in Fig. 1.1. Apart from demonstrators, such as the French Leduc 010, 016 and 021, the Griffon II and the American Lockheed F-80 with Marquardt ramjets and the X-7 research vehicles (see [10]), ramjets and scramjets have not really become widespread so far and are still in a somewhat experimental stage with research efforts ongoing. As can be seen in Fig. 1.1 the ramjet covers inflow Mach numbers from
2.5 to 6 while the scramjet works from an inflow Mach number of about 5. However, the key difference is that the first operates with subsonic, and the latter with supersonic combustion.

A typical design of a ramjet can be found in Fig. 1.2. The flame holders create a recirculation zone by which the flame is stabilized. Within the ramjet the fuel starts to burn after the flame holder. In contrast to a ramjet the scramjet lacks a normal shock wave at the entrance of the combustion chamber since the flow velocity remains supersonic. Its design is given in Fig. 1.3. Critical points in scramjet design are fuel-air mixing and combustion initiation. It is obvious, that the mixing quality at the inflow of the combustor and its design strongly influence the ignition delay. Under the assumption of perfectly premixed gas inflow to the combustor, the research interest can be focused on finding a geometrical design for the combustor, that allows stable and efficient combustion.

Shock induced combustion has therefore been a key interest of research in the propulsion group at the University of Toronto Institute for Aerospace Studies (UTIAS) (see [24]), leading to the shock induced combustion ramjet (see Fig. 1.4). In particular, a wedge flow of a fully premixed reactive fuel-air gas mixture within the combustion
chamber was studied extensively. For each set of inflow conditions there is an optimum wedge angle creating Chapman-Jouguet conditions. In this case, combustion occurs at optimum conditions, which implies minimum increase in entropy and maximum heat release. Unfortunately there is not only one fixed inflow condition during flight and the Chapman-Jouguet condition is sensitive to many parameters. Placing rods within the combustion chamber promises certain ignition for a wide range of inflow conditions due to the normal shock in front of the blunt body. This concept is somewhat similar to that of a flame holder in a ramjet and a recirculation region is to be expected behind the rods. However, here the combustion is already started in front of the blunt body since the high temperature and pressure between the shock wave and the stagnation point significantly reduce the ignition delay of the premixed gas.

It can be expected that rods produce higher losses than a wedge flow at Chapman-
Jouguet conditions, since a normal shock implies higher entropy increase than an oblique shock. The same is valid for a recirculation region, where vortices increase the entropy of the flow. Therefore, the scope of this study is to gain first insights into the quality and quantities of such losses and evaluate the performance of this concept. A detailed problem description is given in the next Section.

1.2 Scope of Study

As mentioned above, the main goal in this study is to evaluate the efficiency of the combustion started by rods instead of by a wedge. A comparison of the geometric setup is given in Figs. 1.5 and 1.6. The assumption of the combustion chamber being much wider than high leads to the approximation of the given problem to be two-dimensional. This means that the effects of the side walls are neglected and the problems presented in Figs. 1.7 and 1.8 are to be solved. Even for the two-dimensional setup there are many
unanswered questions. What is the optimum ratio of blunt body diameter and number for a given channel height? What is the best shape for the blunt bodies? Is a cylindrical or a droplet type of shape preferable? How does the overall performance of blunt body generated combustion compare to that generated by a wedge? While the question of the most efficient shape for the blunt bodies remains unapproached, this study tries to gain some first insight into the influence of the channel blockage ratio, that is the ratio of blunt body diameter to channel height, and the performance compared to wedge induced combustion.

One key element of such a study is the proper solution of the resulting blunt body generated detonation wave ramjet flowfield. Within this study laminar flow with non-equilibrium chemistry is solved to obtain solutions to the physical problem. The restriction to laminar flow seems somewhat unsatisfactory but unavoidable since the accurate modelling of turbulent combustion is still a topic of discussion. Additionally its numerical computation with methods known today is exceptionally demanding and by far beyond the scope of this work. In order to save computational resources the problem presented in Fig. 1.8 is reduced by the application of symmetry conditions as shown in Fig. 1.9. This particular problem is characterized by supersonic inflow and outflow, symmetry lines at both the top and the bottom of the flow domain and a solid wall due to the cylinder. The temperature of the wall is kept constant, which requires a specific amount of cooling from the inside of the cylinder.
1.3 Solution Approach

With the given physical problem description the tools for its solution have to be developed. There are several components required to make a numerical solution possible: discretization of the geometrical domain, definition of physical and chemical behaviour of the gas components and last, but not least, the actual solution algorithm to obtain the correct flow field.

The discretization of the domain is achieved by a structured multi-block approach. This is a compromise between a structured single-block attempt, which is clearly un-applicable due to the geometry to be examined, and an unstructured grid, which would have been to cumbersome at this stage, although it might be feasible in the future. However, the multi-block approach is well established and is a reasonable choice to make. The grid generation is straight forward and there is a wide variety of literature available (see [28] for an overview).

The physical and chemical behaviour can be modelled in many ways. Here the specific heats, entropy and enthalpy are described by polynomials utilizing data tables (see [18],...
Transport coefficients such as viscosity, heat conductivity and diffusion coefficients are calculated by means provided by the kinetic gas theory (statistical thermodynamics, see [12], [29] and [6]). This is in accordance with many other researchers within the field. For 'simple' and 'fast' single species computations Sutherland's law is applied to obtain values for viscosity and heat conductivity. Also, there are many reaction schemes to model non-equilibrium chemistry. The most important reaction scheme within this work describes the behaviour of an air-hydrogen gas mixture, including 13 species, with 33 reactions (see [14]). Although for reasons of versatility explicit time marching schemes in form of the Runge-Kutta type are being made available, the baseline numerical methods are implicit, namely the Euler implicit first order, trapezoidal and Gear second order schemes (see [11]). They are solved with the lower upper symmetric Gauß Seidel (LUSGS) scheme (see [7] and [24]), which in its original form clearly destroys any time accuracy due to its inherent factorization error. The chemical source term and the inviscid fluxes are treated implicitly to a second order accuracy by the utilization of analytical Jacobian matrices (see [23]). In combination with the spatial cell centred finite volume discretization, a Roe type of flux splitting with entropy correction is used to ensure stability (see [11], [5] and [32]). This splitting can be made second order accurate with the application of nonlinear flux limiter functions.

Before the numerical code is applied to any thesis case a thorough validation is undertaken utilizing a number of test cases to ensure proper functioning of its components.
Chapter 2

Governing Equations

2.1 Overview and Physical Model

In this Chapter the focus is on the presentation of the governing equations for two dimensional compressible laminar flows with non-equilibrium chemistry. All steps required to describe the equations and to calculate relevant species properties and transport properties for the examined gas mixture are described in detail. The definitions of species heat coefficients, enthalpy, entropy, viscosity, heat conductivity and diffusion coefficients are given. In addition equations to determine properties for a gas mixture are defined as well as those required for a single species gas.

Detailed information about the treatment of boundaries, both from the physical and numerical point of view, is presented later. Also the numerical implementation of the governing equations can be found in subsequent Chapters.

The first step undertaken is the definition of vectors for conserved variables, source terms, convective and diffusive fluxes. These allow to define the governing equations at different ‘levels’, from point chemistry equations to the full Navier-Stokes equations. All variables utilized within these equations are then explained in further detail, their definitions and derivations are presented for multi-species and single species gas flows. The Chapter ends with the definition of quantities used for the analysis of the ‘propulsive performance’, addressing the momentum balance, loss of total pressure, increase of entropy and enthalpy.

Equivalent presentations of the governing equations for multi-species and single species gas flows can be found in [7] and [11], respectively.


2.2 Basic Vectors

The basic set of thermodynamic variables used to describe the conserved variables are density \( \rho \), velocities \( u \) and \( v \), total energy \( E \) and the mass fractions \( Y_i \) (with \( i = 1, \ldots, N_s - 1 \)). The number of species \( N_s \) depends on the chemical model that is used and has the minimum value of 1 for single species flows. The production or destruction of a species is controlled by the source terms \( \omega_i \). With this the vector of conserved variables \( Q \) and the source term \( S \) can be given as:

\[
Q = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho E \\
\rho Y_1 \\
\vdots \\
\rho Y_{N_s-1}
\end{bmatrix} \quad (2.1) \quad S = \begin{bmatrix}
0 \\
0 \\
0 \\
\omega_1 \\
\vdots \\
\omega_{N_s-1}
\end{bmatrix} \quad (2.2)
\]

In addition to the variables already explained the pressure \( p \) is needed for the convective flux vectors \( G_c \) and \( H_c \):

\[
G_c = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
u (\rho E + p) \\
\rho u Y_1 \\
\vdots \\
\rho u Y_{N_s-1}
\end{bmatrix} \quad (2.3) \quad H_c = \begin{bmatrix}
\rho v \\
\rho uv \\
\rho v^2 + p \\
v (\rho E + p) \\
\rho v Y_1 \\
\vdots \\
\rho v Y_{N_s-1}
\end{bmatrix} \quad (2.4)
\]

The viscous flux vectors \( G_d \) and \( H_d \) consist of shear tensions \( \tau_{ij} \), energy fluxes \( \epsilon_i \) and diffusive fluxes \( j_{i,k} \), where \( i \) and \( j \) indicate coordinates (\( x \) or \( y \)) and \( k \) a species (\( k = 1, \ldots, N_s - 1 \)).
2.3 Point Chemistry Equations

The most simple system of equations is given by the point chemistry equations. There is no need for spatial discretization, the equations have to be integrated in time only. This can already be used to validate the non-equilibrium chemistry with respect to species properties and reaction scheme. Furthermore an extended overview of a specific chemical reaction scheme can be obtained computationally inexpensively. The point chemistry is referred to as zero-dimensional analysis in the relevant literature (see [17]) and its equations are presented in differential and integral formulation.

\[
\begin{align*}
G_d &= \begin{bmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
u\tau_{xx} + v\tau_{xy} - \epsilon_x \\
-j_{x1} \\
\vdots \\
-j_{xN_x-1}
\end{bmatrix} \\
H_d &= \begin{bmatrix}
0 \\
\tau_{yx} \\
\tau_{yy} \\
u\tau_{xy} + v\tau_{yy} - \epsilon_y \\
-j_{y1} \\
\vdots \\
-j_{yN_y-1}
\end{bmatrix}
\end{align*}
\]  

(2.5)  

(2.6)

2.4 Euler Equations

With respect to the point chemistry equations and the Navier-Stokes equations the intermediate level of difficulty and computational cost is presented by the Euler equations. In the presented form they model inviscid reactive flows in two dimensions, which implies the need for a spatial discretization in addition to the time marching method. Again, the equations are given in differential and integral formulation.

\[
\begin{align*}
\frac{\partial}{\partial t} Q &= S \\
\iint_A \frac{\partial}{\partial t} Q \, dA &= \iint_A S \, dA
\end{align*}
\]  

(2.7)  

(2.7a)

\[
\begin{align*}
\frac{\partial}{\partial t} Q + \frac{\partial}{\partial x} G_c + \frac{\partial}{\partial y} H_c &= S \\
\iint_A \frac{\partial}{\partial t} Q \, dA + \oint \left[ \begin{array}{c} G_c \\ H_c \end{array} \right] \, dl &= \iint_A S \, dA
\end{align*}
\]  

(2.8)  

(2.8a)
2.5 Navier-Stokes Equations

The Navier-Stokes equations include viscous fluxes in addition to the convective fluxes, which makes them computationally most expensive to solve with respect to those presented in this work. As the previous equations, they are presented in both differential and integral formulation.

\[
\frac{\partial}{\partial t} Q + \frac{\partial}{\partial x} (G_c - G_d) + \frac{\partial}{\partial y} (H_c - H_d) = S
\]  
(2.9)

\[
\int \int_A \frac{\partial}{\partial t} Q dA + \int \int \left[ \frac{G_c - G_d}{H_c - H_d} \right] d\ell = \int \int_S S dA
\]  
(2.9a)

2.6 Flow and Thermodynamic Variables in Detail

With the governing equations as framework we can look further into details of the computation of the required quantities. In multi-species flows obviously the mass and molar fractions play an important role to characterize the composition of the gas mixture. The summation of mass fractions \( Y_i \) and molar fractions \( X_i \) over all species always yields to 1:

\[
\sum_{i=1}^{N_s} Y_i = 1
\]  
(2.10)

\[
\sum_{i=1}^{N_s} X_i = 1
\]  
(2.11)

With given molecular weight of the species \( M_i \) and species mass fraction the molecular weight of the gas mixture can be calculated. Its reciprocal value is given by

\[
\frac{1}{M} = \sum_{i=1}^{N_s} \frac{Y_i}{M_i}
\]  
(2.12)

Now we can relate the mass fractions \( M_i \) to the mol fractions \( X_i \) and the concentrations \([M_i]\) via the molecular weight of the gas mixture and the density. This yields

\[
X_i = \frac{Y_i}{M_i} M
\]  
(2.13)

\[
[M_i] = \frac{1}{M_i} \rho Y_i = X_i \frac{\rho}{M}
\]  
(2.14)
Under the assumption that the gas mixture can be approximated by the ideal gas equation \( p = \rho RT \), the following equations hold:

\[
p = \rho RT = \rho \frac{R_m}{M} T = \rho R_m T \sum_{i=1}^{N_s} Y_i M_i \]

\[
E = \sum_{i=1}^{N_s} Y_i h_i - \frac{p}{\rho} + \frac{1}{2} (u^2 + v^2)
\]

\[
\rho E = \rho \sum_{i=1}^{N_s} Y_i h_i - p + \frac{\rho}{2} (u^2 + v^2)
\]

This relates the pressure \( p \), the density \( \rho \), the velocities \( u \) and \( v \) and the total energy \( E \) and is fundamental to close the system of Navier-Stokes equations. The enthalpy for a species is given as \( h_i \) and the universal gas constant as \( R_m \).

Another important component of the Navier-Stokes equations, the viscous fluxes, require the calculation of the shear tensions \( \tau_{ij} \). They are defined by the velocity gradients and viscosity \( \mu \) as given in the following:

\[
\tau_{xx} = \frac{2}{3} \mu \left( 2 \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)
\]

\[
\tau_{yy} = \frac{2}{3} \mu \left( 2 \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} \right)
\]

\[
\tau_{xy} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)
\]

Additional components of the viscous fluxes, the vectors of the diffusion fluxes for the species, are given in their most general form by

\[
\dot{j}_i = \begin{bmatrix} j_{x,i} \\ j_{y,i} \end{bmatrix} = \begin{bmatrix} j^d_i \\ j^p_i \\ j^m_i \\ j^T_i \end{bmatrix} = \frac{\rho}{M^2} \sum_{k=1}^{N_s} M_i M_k D_{i,k} \left[ \nabla X_k + (X_k - Y_k) \frac{1}{p} \nabla p + \frac{\rho_k}{p} \left( f_k - \sum_{j=1}^{N_s} Y_i f_{i,j} \right) \right] - D_i^T \frac{1}{T} \nabla T
\]

In this work we will only concentrate on diffusion due to concentration gradients since diffusion due to pressure and temperature gradient are of minor importance in most
combustion problems (see [29]). Furthermore, the double summation is a computationally very expensive procedure so that an additional simplification in form of Fick's law for diffusion suggests decreased computational cost at comparable accuracy. According to Fick's law the diffusion flux of a species $i$ is being calculated via mass fraction gradient and an averaged diffusion coefficient $D_{i,mix}$:

$$j_i = \rho D_{i,mix} \nabla Y_i$$  \hspace{1cm} (2.22)

This averaged diffusion coefficient still requires the calculation of the binary diffusion coefficients $D_{i,j}$ and its definition is given in a later Subsection.

The vector of the energy flux for a species due to heat conduction, enthalpy diffusion and Dufour effect is, again in its most general form:

$$\mathbf{\epsilon} = \begin{bmatrix} \epsilon_x \\ \epsilon_y \end{bmatrix} = \mathbf{j} + \frac{j_d}{\rho} + \frac{j_D}{Y_i - Y_j}$$

$$= \quad \text{heat conduction} \quad \text{enthalpy diffusion} \quad \text{Dufour effect}$$

$$= -\lambda \nabla T + \sum_{i=1}^{N_s} h_i j_i + \frac{P_{mT}}{\rho} \sum_{i=1}^{N_s} \sum_{j=1}^{N_s} \frac{X_j D_{i,j}^{T}}{M_i D_{i,j}} \left( \frac{j_i}{Y_i} - \frac{j_j}{Y_j} \right)$$ \hspace{1cm} (2.23)

Again, the Dufour effect is neglected within this work, which leads to this simplified expression for the energy flux:

$$\mathbf{\epsilon} = \quad -\lambda \nabla T + \sum_{i=1}^{N_s} h_i j_i$$ \hspace{1cm} (2.24)

Of great importance for any reactive flow is the production or destruction of a species, given by the following source term:

$$\omega_j = M_j \sum_{l=1}^{N_r} \left( [M]_l \cdot (\nu''_{j,l} - \nu'_{j,l}) \cdot \left( \frac{k_{f,l}}{\rho} \prod_{i=1}^{N_s} [M]_l^{\nu''_{j,l} - \nu'_{j,l}} \prod_{i=1}^{N_s} [M]_l^{\nu''_{j,l}} \right) \right)$$ \hspace{1cm} (2.25)

where the third body efficiency $[M]_l$ for reaction $l$ can be expressed as

$$[M]_l = \alpha_{l,0} + \sum_{k=1}^{N_r} \alpha_{l,k} [M_k]$$ \hspace{1cm} (2.26)

$$\alpha_{l,0} = \begin{cases} 1 & \text{for } \max(\alpha_{l,1}, \ldots, \alpha_{l,N_r}) = 0 \\ 0 & \text{otherwise} \end{cases}$$ \hspace{1cm} (2.27)

The stoichiometric coefficients $\nu''_{j/l,i,l}$ and $\nu'_{j/l,i,l}$ are used to describe the reaction scheme applied for the study. The forward reaction speed for reaction $l$ $k_{f,l}$ is calculated using
the extended Arrhenius equation and the backward reaction speed \( k_{b,l} \) is determined by forward reaction speed and the equilibrium constant \( K_{c,l} \) related to the concentration:

\[
k_{f,l} = A_0 l T^{\delta_l} \exp \left( -\frac{E_{A_l}}{R_m T} \right) \tag{2.28}
\]

\[
k_{b,l} = \frac{k_{f,l}}{K_{c,l}} \tag{2.29}
\]

The reaction activation energy \( E_{A_l} \) and the temperature exponent \( \delta_l \) are parameters within the extended Arrhenius equation that determine the forward reaction speed for reaction \( l \). While the activation energy and the temperature exponent have to be determined in the context of the reaction scheme used, that means that for each scheme these parameters have to be known for all elementary reaction equations, the equilibrium constant depends on the species properties. The calculation of those will be the topic in the next Section.

### 2.7 Thermodynamic Species Properties

One of the most important aspects of multi-species flows is the accurate modelling of the species properties, within this work foremost the specific heat coefficient at constant pressure, the enthalpy and the entropy. Other quantities, such as specific heat at constant volume, specific heat ratio, internal energy or equilibrium constants, can be derived subsequently.

The specific heat coefficient at constant pressure for species \( i \) \( c_{p_i} \) is defined using a polynomial and appropriate coefficients. This is in conformance with the methodology of the NASA Lewis chemical equilibrium program. Also the coefficients (see Appendix) are taken from the widely used NASA tables (see [19], [27] and [18]). Exceeding the standard form of the polynomials with five coefficients (1191) within this work a more flexible approach is used allowing an arbitrary number of coefficients for the molar specific heat coefficient at constant pressure:

\[
c_{p_i}^{*} = \frac{\sum_{k=1}^{N_{ip}} a_{k, l} T^{k-1}}{R_m} \tag{2.30}
\]

Therefore new, more detailed species data could be used without complications when it becomes available. The previous definition is then applied and extended to calculate the
molar enthalpy \( h_i^* \) and molar entropy \( s_i^* \) for a species \( i \)

\[
\frac{h_i^*}{R_m} = a_{h,i}^* + \int \frac{c_{p,i}^*}{R_m} dT = a_{h,i}^* + \sum_{k=1}^{N_{cp}} a_{k,i}^* \frac{T_k}{k}
\]

\[
\frac{s_i^*}{R_m} = a_{s,i}^* + \int \frac{c_{p,i}^*}{R_m T} dT = a_{s,i}^* + a_{s,i}^* \ln T + \sum_{k=2}^{N_{cp}} a_{k,i}^* \frac{T_{k-1}}{k-1}
\]

With the current form of information available for the thermodynamic species properties it is mandatory to have several different sets of coefficients for given temperature intervals. With known enthalpy and entropy the molar equilibrium constant and that related to the concentration, used to calculate the backward reaction speed, can be determined according to:

\[
K_{\theta,r} (p_0, T) = \exp \left( \frac{-1}{R_m T} \sum_{k=1}^{N_r} \nu_{k,r} g_k^* \right) = \\
\exp \left( -\sum_{k=1}^{N_r} \nu_{k,r} \left[ \frac{h_k^*}{R_m T} - \frac{s_k^*}{R_m} \right] \right)
\]

\[
K_{\theta,r} (p, T) = K_{\theta,r} (p_0, T) \cdot \left( \frac{p_0}{p} \right)^{\sum_{k=1}^{N_r} \nu_{k,r}}
\]

\[
K_{c,r} (T) = K_{\theta,r} (p_0, T) \cdot \left( \frac{p_0}{R_m T} \right)^{\sum_{k=1}^{N_r} \nu_{k,r}}
\]

The molar free enthalpy \( g_k^* \) and stoichiometric coefficient \( \nu_{k,r} \) for species \( k \) and reaction \( r \) are used to calculate the molar equilibrium constant. The reference pressure \( p_0 \) is not independent from the coefficients for the polynomials and therefore has to be provided with them. In this work \( p_0 = 1 \text{bar} = 1 \cdot 10^5 \text{Pa} \) is used.

### 2.8 Species Transport Properties

While the definition of thermodynamic species properties is already sufficient for point chemistry equations and Euler equations, in the case of Navier-Stokes equations the species transport properties have to be calculated in addition. They can be evaluated by the means of kinetic gas theory (see [12]) in combination with ‘real gas’ corrections or with polynomials as the thermodynamic species properties. Additional information can be found in [29].
The corrections used in combination with the means of kinetic gas theory utilize a reduced collision integral which is based on the Lennard-Jones-6-12 potential. The two reduced collision integrals $\Omega^{(1,1)^*}$ and $\Omega^{(2,2)^*}$ are a function of the reduced temperature $T^*$.

\[
\Omega^{(1,1)^*} = \Omega^{(1,1)^*}(T^*) = \sum_{k=1}^{N_{\Omega^{(1,1)^*}}} a_{k,\Omega^{(1,1)^*}} T^{*k-1}
\]

\[
\Omega^{(2,2)^*} = \Omega^{(2,2)^*}(T^*) = \sum_{k=1}^{N_{\Omega^{(2,2)^*}}} a_{k,\Omega^{(2,2)^*}} T^{*k-1}
\]

\[
T^* = \frac{kT}{\epsilon}
\]

where $\epsilon$ is the potential parameter of the molecule and $k$ the Boltzmann constant. Alternatively, by introducing $A^*$, $\Omega^{(2,2)^*}$ can be calculated using

\[
A^* = \sum_{k=1}^{N_{A^*}} a_{k,A^*} T^{*k-1}
\]

\[
\Omega^{(2,2)^*} = A^* \cdot \Omega^{(1,1)^*}
\]

As in the case of the thermodynamic species properties the coefficients for the polynomials above are given for specific temperature intervals. With this the viscosity $\mu_i$ for species $i$ can be evaluated according to:

\[
\mu_i = 2.6693 \cdot 10^{-28} \frac{\sqrt{M_i T^*}}{\sigma^2 \Omega^{(2,2)^*}}
\]

The dimension of the viscosity is $[\mu] = kg/m \cdot s$ and all other variables have to be used in SI-units ($kg, m, s, K$). For a pure monoatomic gas the heat conductivity $\lambda_i$ for species $i$ is defined as

\[
\lambda_{i\text{monoatomic}} = 8.323 \cdot 10^{-22} \frac{\sqrt{T/M_i}}{\sigma^2 \Omega^{(2,2)^*}} =
\]

\[
= \frac{15}{4} \frac{R_m}{M_i} \mu_i
\]

where $\sigma$ is the collision diameter. Again all variables used have to be prescribed in SI-units. For a polyatomic gas a modified Eucken correction increases accuracy, which is given by

\[
\lambda_i = \lambda_{i\text{monoatomic}} \left(0.115 + 0.354 \frac{C_F}{R_m}\right)
\]
The last missing transport property is the binary diffusion coefficient $D_{i,j}$ for the species $i$ and $j$, which is defined as

$$D_{i,j} = 1.8583 \cdot 10^{-22} \frac{\sqrt{T^*_{i,j}}}{\rho \sigma_{i,j}^2 \Omega(1.1)^* (T^*_{i,j})}$$  

with all variables used in SI-units. The reduced temperature $T^*_{i,j}$ can be calculated using the combined parameters $\sigma_{i,j}$ and $\epsilon_{i,j}$ for for the binary collision diameter and potential, respectively:

$$\sigma_{i,j} = \frac{\sigma_i + \sigma_j}{2}$$  
$$\epsilon_{i,j} = \sqrt{\epsilon_i \epsilon_j}$$

The thermo diffusion coefficient $D^T_i$ for a multi-component gas mixture is very difficult to calculate (see p. 543 [12]) and, as already mentioned, its effect in most combustion problems negligible (see [29]).

An alternative is to calculate the transport coefficients using polynomial expressions as for the specific heat at constant pressure.

$$\lambda_i = \sum_{k=1}^{N_1} a_{\lambda_k,i} T^{k-1}$$

$$\mu_i = \sum_{k=1}^{N_2} a_{\mu_k,i} T^{k-1}$$

$$D^*_{i,j} = \sum_{k=1}^{N_D} a_{D_{k,i,j}} (\ln T)^{k-1}$$

$$D_{i,j} = \frac{D^*_{i,j}}{p}$$

This is very cumbersome especially for the diffusion coefficient because the coefficients $a_{D_{k,i,j}}$ have to be provided for each species with respect to each other species within the gas mixture. Hence, for practical reasons the computation of transport properties for multi-species gases is not used and only presented for completeness.
2.9 Thermodynamic and Transport Properties for the Gas Mixture

With all species and transport properties known the mixture properties can be calculated. Again, [29] is recommended as a reference worth while consulting. Firstly, the point of interest is the calculation of the thermodynamic properties. Generally these coefficients are calculated summarizing the thermodynamic species properties weighted with the relevant mass fraction. For the specific heat at constant pressure $C_p$, at constant volume $C_v$, the ratio of heat coefficients $\gamma$ and the gas constant this yields to:

$$C_p = \sum_{i=1}^{N_s} Y_i C_{p_i}$$

$$C_v = \sum_{i=1}^{N_s} Y_i C_{v_i} = C_p - R = \sum_{i=1}^{N_s} Y_i \left( C_{p_i} - \frac{R_m}{M_i} \right)$$

$$\gamma = \frac{C_p}{C_v} = \frac{C_p}{C_p - R}$$

$$R = R_m \sum_{i=1}^{N_s} \frac{Y_i}{M_i} = \frac{R_m}{M}$$

Secondly, the transport properties for the gas mixture need to be calculated. For viscosity, heat conductivity for the gas mixture and the averaged diffusion coefficients for a species this yields:

$$\mu = \sum_{k=1}^{N_s} \sum_{j=1}^{N_s} X_k \mu_k \frac{X_j \phi_{k,j}}{\sum_{j=1}^{N_s} X_j \phi_{k,j}}$$

$$\lambda = \sum_{k=1}^{N_s} \sum_{j=1}^{N_s} X_k \lambda_k \frac{X_j \phi_{k,j}}{\sum_{j=1}^{N_s} X_j \phi_{k,j}}$$

$$D_{k,\text{mix}} = \frac{1 - X_k}{\sum_{j=1, j \neq k}^{N_s} X_j \frac{\phi_{j,k}}{\phi_{k,j}}}$$

Here $\phi_{i,k}$ is a correction factor needed to improve the accuracy of the viscosity $\mu$ and heat conductivity $\lambda$:

$$\phi_{i,k} = \left[ 8 \left( 1 + \frac{M_i}{M_k} \right) \right]^{-\frac{1}{2}} \cdot \left[ 1 + \left( \frac{\mu_i}{\mu_k} \right)^\frac{1}{2} \cdot \left( \frac{M_i}{M_k} \right)^\frac{1}{4} \right]^2$$
2.10 Temperature Calculation

For multi-species gases with temperature dependent specific heat coefficients the calculation of the temperature with the conserved variables given is more involved, since it can only be determined iteratively. This is caused by the fact that the total energy is a function of mass fractions, species enthalpies, pressure, density and the velocities. The species enthalpies and the pressure both depend on the temperature so that for the given mass fractions, density and velocities a temperature has to be found so that Eq. 2.16 is fulfilled. Using the expression for the total energy $E$ presented previously (2.16)

\[ E = \sum_{i=1}^{N_s} Y_i h_i - \frac{p}{\rho} + \frac{1}{2} (u^2 + v^2) \]

with $p = \rho RT = \rho \frac{R_m}{M} T$ and $h_i = \frac{h_i^*}{M_i}$ follows

\[ E = \sum_{i=1}^{N_s} Y_i \frac{h_i^*}{M_i} - \frac{R_m}{M} T + \frac{1}{2} (u^2 + v^2) = \]

\[ = \sum_{i=1}^{N_s} Y_i \left( a_{h,i}^* + \sum_{j=1}^{N_{sp}} a_{j,i}^* \frac{T^j}{j} \right) - \frac{R_m}{M} T + \frac{1}{2} (u^2 + v^2) \]

Assume $E$, $u$ and $v$ given and constant for the iteration procedure to obtain the temperature the function $f$ can be defined and subsequently the temperature calculated as follows

\[ f(T) = \sum_{i=1}^{N_s} Y_i \frac{R_m}{M_i} \left( a_{h,i}^* + \sum_{j=1}^{N_{sp}} a_{j,i}^* \frac{T^j}{j} \right) - \frac{R_m}{M} T + \frac{1}{2} (u^2 + v^2) - E \]

\[ \frac{df(T)}{dT} = \sum_{i=1}^{N_s} Y_i \frac{R_m}{M_i} \left( \sum_{j=1}^{N_{sp}} a_{j,i}^* T^{j-1} \right) - \frac{R_m}{M} \]

\[ T^{n+1} = T^n - \frac{f(T)}{\frac{df(T)}{dT}} \]

Depending on the initial guess of the temperature this iteration scheme usually converges very fast. In most cases of numerical instabilities for multi-species gas flow computations, however, problems with the iterative temperature calculation are their first indicator.
2.11 Ideal Single Species Gas

For ideal single species gas with constant and given ratio of specific heats $\gamma$ and molecular weight $M$ all the calculations above can be greatly simplified. It yields to the equations given below for specific heat at constant pressure and volume

$$C_{p_{single}} = \frac{\gamma}{\gamma - 1} \cdot \frac{R_m}{M}$$

(2.62)

$$C_{v_{single}} = \frac{1}{\gamma - 1} \cdot \frac{R_m}{M}$$

(2.63)

with the gas constant

$$R_{single} = \frac{R_m}{M}$$

(2.64)

For viscosity $\mu_{single}$ and heat conductivity $\lambda_{single}$ Sutherland’s Law is applied. A reference temperature $T_{0,su}$, reference viscosity $\mu_{0,su}$ and heat conductivity $\lambda_{0,su}$ have to be given as well as two functional constants $S_{su}$ and $A_{su}$. Then the two transport properties can be calculates as

$$\mu_{single} = \mu_{0,su} \left( \frac{T}{T_{0,su}} \right)^{\frac{3}{2}} \frac{T_{0,su} + S_{su}}{T + S_{su}}$$

(2.65)

$$\lambda_{single} = \lambda_{0,su} (1 + A_{su}T) \frac{\mu_{single}}{\mu_{0,su}}$$

(2.66)

Within this work, for air the reference values and constants used are:

$$\gamma = 1.4$$

$$M = 28.97 \frac{kg}{kmol}$$

$$T_{0,su} = 273K$$

$$\mu_{0,su} = 17.1 \cdot 10^{-6} \frac{kg}{m \cdot s}$$

$$\lambda_{0,su} = 0.0242 \frac{W}{m \cdot K}$$

$$S_{su} = 110K$$

$$A_{su} = 1.54341 \cdot 10^{-4} \frac{1}{K}$$

Obviously for this type of flow the diffusion does not play any role. For conversions between primitive and conservative variables the energy term $\rho E$ can be expressed in primitive variables as

$$\rho E = \frac{p}{\gamma - 1} + \frac{\rho}{2} \left( u^2 + v^2 \right)$$

(2.67)
and the pressure $p$ in terms of conservative variables as

$$p = (\gamma - 1) \left[ \rho E - \frac{1}{2\rho} ((\rho u)^2 + (\rho v)^2) \right]$$  \hspace{1cm} (2.68)

Finally, the temperature $T$ is calculated utilizing the ideal gas law:

$$T = \frac{pM}{\rho R_m}$$  \hspace{1cm} (2.69)

### 2.12 Propulsion Performance Analysis

In this Section several quantities for the analysis of propulsive performance are presented (see also [21] for additional information). Among those quantities the most obvious performance indicator for any propulsion system is the momentum balance, since it provides information about the forces created by the engine. Especially for combustion processes the heat released is another vital point of interest. Therefore the enthalpy balance and the heat of reaction have to be calculated to allow insight into the thermodynamic and chemical characteristics of the examined test case. But the knowledge of the forces created and heat released alone is not of much use, and in addition the 'cost' must be found. This is achieved by calculating the increase of entropy and the loss of total pressure for the given system, which, in combination with the quantities mentioned before, allows a conclusive statement about the propulsive performance.

In three geometrical dimensions we can assign a length ($x$-coordinate), a height ($y$-coordinate) and a depth ($z$-coordinate) to the different geometrical directions. As already stated in the Introduction the three-dimensional problem is approximated by a two-dimensional problem. To calculate actual forces and mass fluxes we assume the depth to be 1m, which is equivalent to a normalization of the dimensions in the $z$-coordinate direction.

#### 2.12.1 Mass Flux Balance

Although the mass flux alone is not of any use in performance analysis, it can be used to validate one of the most important aspects of numerical computations, the conservation of the mass. The continuity equation is, with respect to the presentation of governing equations above, the first equation of the Navier-Stokes equations:

$$\iint \frac{\partial}{\partial t} \rho \, dA + \oint \rho u \cdot n \, dl = 0$$  \hspace{1cm} (2.70)
Separating inflow and outflow boundaries it can be rewritten for steady state problems as

\[ \sum_{\text{inflow}} \int \rho u \cdot n \, dl + \sum_{\text{outflow}} \int \rho u \cdot n \, dl = 0 \]  

(2.71)

Obviously, there is no mass flux through boundaries such as solid walls or lines of symmetry. The direction of integration for the equation above is prescribed, since the control volume must be a simply connected region. Now we define the mass flux \( \dot{m} \) as the absolute value of either all inflow or all outflow boundary mass fluxes.

\[ \dot{m} = \left| \sum_{\text{inflow}} \int \rho u \cdot n \, dl \right| \cdot 1m = \left| \sum_{\text{outflow}} \int \rho u \cdot n \, dl \right| \cdot 1m \]  

(2.72)

This result will be used further on to calculate specific values for entropies and enthalpies.

### 2.12.2 Momentum Balance

Based on the momentum equations, which are a part of the Navier-Stokes equations, the forces on the engine or particular engine components can be calculated. This is achieved by defining the whole flow domain as control volume and evaluating the appropriate integrations over the volume and its boundary surfaces. Obviously, for two-dimensional problems the integrations degrade to area and line integrals. Hence,

\[ \iiint_A \frac{\partial}{\partial t} \begin{bmatrix} u \\ v \end{bmatrix} \, dA + \oint \begin{bmatrix} \rho u (u) + p (1 - (\tau_{xx} \tau_{xy} \tau_{xv} \tau_{yy}) \end{bmatrix} \cdot n \, dl = 0 \]  

(2.73)

is the resulting system of equations. For steady problems the differential with respect to time becomes zero, which allows rewriting the equations in the following form,

\[ \int \rho u \begin{bmatrix} u \\ v \end{bmatrix} \, dy - \int \rho v \begin{bmatrix} u \\ v \end{bmatrix} \, dx + \int pn \, dl - \int \begin{bmatrix} \tau_{xx} & \tau_{xy} \\ \tau_{xy} & \tau_{yy} \end{bmatrix} \cdot n \, dl = 0 \]  

(2.74)

where \( n \) is the outward facing normal vector \( n = \frac{1}{\sqrt{dx^2 + dy^2}} \cdot [dy, -dx] \). From the mathematical point of view it is important to mention that the control volume must be a
simply connected region, which means that the direction of the line integration around the control volume is prescribed.

The next step is to separate the forces acting on the walls from the momentum contributions of the fluid entering and leaving the domain of interest.

\[
\sum_{\text{in-/outflow}} \left( \int \rho u \left[ \begin{array}{c} u \\ v \end{array} \right] dy - \int \rho v \left[ \begin{array}{c} u \\ v \end{array} \right] dx + \int p \, dl \right) = - \sum_{\text{wall}} \left( \int p \, dl - \int \left[ \begin{array}{cc} \tau_{xx} & \tau_{xy} \\ \tau_{xy} & \tau_{yy} \end{array} \right] \cdot n \, dl \right)
\]

(2.75)

Identifying the right hand side of the above equation as the force acting on the fluid, the force acting on the structure of the engine, which is equivalent with the 'combustor thrust', is given by:

\[
E_{\text{combustor thrust}} = - \sum_{\text{in-/outflow}} \left( \int \rho u \left[ \begin{array}{c} u \\ v \end{array} \right] dy - \int \rho v \left[ \begin{array}{c} u \\ v \end{array} \right] dx + \int p \, dl \right) \cdot 1m
\]

\[
= \sum_{\text{wall}} \left( \int p \, dl - \int \left[ \begin{array}{cc} \tau_{xx} & \tau_{xy} \\ \tau_{xy} & \tau_{yy} \end{array} \right] \cdot n \, dl \right) \cdot 1m
\]

(2.76)

Usually the terms un-installed and installed thrust are used within the engine concept (see [21]), where additive and external drag decrease the un-installed thrust to yield the installed thrust. In this first study we are concerned with combustor flowfields where the external drag is not known. But even if this external drag is known for an engine, there would be the difficulty in assessing which part of that drag is due to the combustor and which part of it due to other engine components. Therefore the definition of the combustor thrust makes sense, as long as these facts are kept in mind. To conclude, the combustor thrust \(E_{\text{combustor thrust}}\) will be used for assessing the force generated by the cases of interest. The evaluation of both the forces acting on the walls and the momentum of inflow and outflow allow a control of the momentum components as they should balance.

### 2.12.3 Enthalpy Balance

From the first law of thermodynamics for open systems it is known, that the total energy of a system changes with heat or work from outside added to or subtracted from the system. At the same time the total energy of that system consists of internal, kinetic
and potential energy. Since the potential of any gravitational or electrical field is not of interest in this work, the first law of thermodynamics for steady flow processes between two states 1 and 2 can be written in specific quantities as

\[ w_{12} + q_{12} = h_2 - h_1 + e_{\text{kin,2}} - e_{\text{kin,2}} \]  

(2.77)

where \( q_{12} \) and \( w_{12} \) are the specific heat and work added to or subtracted from the system between stages 1 and 2. The specific quantities have to be calculated by an integration along the boundary according to

\[ h = \frac{1}{m} \int \rho u \cdot n \sum \ Y_i h_i \ dl \]  

(2.78)

\[ e_{\text{kin}} = \frac{1}{m} \int \rho u \cdot n \left( \frac{1}{2} u^2 \right) \ dl \]  

(2.79)

This analysis allows to differentiate between enthalpy changes, kinetic energy changes and heat that is being extracted due to cooling of the walls in case of a fixed wall temperature and work imposed on the fluid by the shear layer on the walls. For inviscid flows the left hand side is zero since no shear stresses or heat transfers occur. Then the change in enthalpy is balanced by the change of the kinetic energy.

Another quantity, from the combustion point of view more important, is the specific heat of reaction \( \Delta h_r \). It is defined as the amount of (positive) heat interaction required to bring the products back to the same temperature as the reactants. This is a ‘theoretical’ process which occurs under constant pressure and with frozen chemistry (see [21]). Therefore the products will not change their chemical composition, that means the mass fractions will remain the same even when the temperature decreases. Hence,

\[ \Delta h_r = \frac{1}{m} \left\{ \sum_{\text{outflow}} \rho u \cdot n \sum_{i=1}^{N_F} Y_i h_i \left(T_{\text{inflow}}\right) dl - \sum_{\text{inflow}} \rho u \cdot n \sum_{i=1}^{N_F} Y_i h_i \left(T_{\text{inflow}}\right) dl \right\} \cdot 1m \]  

(2.80)

As an alternative the specific standard heat of formation of reactants and products can be used to find an approximation for the heat released by the combustion. The heat of formation is defined as the (positive) heat interaction required to form a compound from its elements at constant pressure and prescribed temperature (again, see [21]). Standard conditions are given at a pressure of \( p_{\text{standard}} = 101300 Pa \) and a temperature of \( T_{\text{standard}} = 298.15 K \), which suggests that the standard enthalpy of formation has to
be calculated under these conditions. However, this would be very difficult for the given problem since pressure and temperature change within the domain of interest. Therefore the composition of the gas mixture at the inflow and outflow boundaries are thought to be frozen during a process that transfers the actual states to standard states. Afterwards the difference in standard heat of formation $\Delta h^0_f,i$ between products and reactants under standard conditions is calculated according to

$$
\Delta h_f = \frac{1}{m} \left\{ \sum_{\text{outflow}} \int \rho u \cdot n \sum_{i=1}^{N_s} Y_i \Delta h^0_{f,i} (T_{\text{standard}}) \, dl \right. \\
- \sum_{\text{inflow}} \int \rho u \cdot n \sum_{i=1}^{N_s} Y_i \Delta h^0_{f,i} (T_{\text{standard}}) \, dl \right\} \cdot 1m
$$

(2.81)

With the enthalpy related quantities presented in this Subsection a first insight into the heat released within the combustion is possible.

### 2.12.4 Entropy Increase

Very similar to the calculation of the specific enthalpy the entropy for inflow and outflow boundaries is calculated.

$$
s = \frac{1}{m} \int \rho u \cdot n \sum_{i=1}^{N_s} Y_i s_i \, dl \cdot 1m
$$

(2.82)

In thermodynamic considerations the entropy is usually employed as the criterion for the thermodynamic quality of the process, and therefore especially important for propulsion problems. As for internal energy and enthalpy, in the case of the entropy the change of the quantity is meaningful, not its absolute value. Therefore we are interested in the change of the specific entropy $\Delta s$, which can be given as

$$
\Delta s = \frac{1}{m} \left\{ \sum_{\text{outflow}} \int \rho u \cdot n \sum_{i=1}^{N_s} Y_i s_i \, dl \right. \\
- \sum_{\text{inflow}} \int \rho u \cdot n \sum_{i=1}^{N_s} Y_i s_i \, dl \right\} \cdot 1m
$$

(2.83)

For future research the calculation of the entropy change based on an integration along stream lines might be of interest and increased accuracy can be expected. At this stage, however, the change of entropy is calculated using a mass flux averaging of the species entropies obtained from the polynomials discussed in an earlier Section.
The total pressure is defined by (see [10])

\[
pt = p \left(1 + \frac{\gamma - 1}{2} Ma^2\right)^{\gamma/(\gamma - 1)}
\]  

(2.84)

which will allow calculating the total pressure losses in several different ways. The first method applied used mass flux averaging, which reads as

\[
\Delta p_{tm} = \frac{1}{m} \left\{ \sum_{\text{outflow}} \int \rho \mathbf{u} \cdot \mathbf{n} \, pt \, dl - \sum_{\text{inflow}} \int \rho \mathbf{u} \cdot \mathbf{n} \, pt \, dl \right\} \cdot 1m
\]  

(2.85)

The second way presented here is the area average of the total pressure on the inflow and outflow boundaries. This yields

\[
\Delta p_{ta} = \left\{ \sum_{\text{outflow}} \frac{1}{\int \, dl} \, \int pt \, dl - \sum_{\text{inflow}} \frac{1}{\int \, dl} \, \int pt \, dl \right\} \cdot 1m
\]  

(2.86)

and is compared to the mass averaged total pressure loss for the thesis cases examined at a later stage.
Chapter 3

Boundary Conditions

The general approach to ensure the fulfilment of boundary conditions in this work is characterised in the following. Instead of creating 'dummy'-cells around block boundaries we store values of the conserved (and consequently the primitive) variables on the cell sides which represent the boundary of the flow domain. Based on the primitive variables these values are prescribed or extrapolated from within the flowfield, depending on the type of the boundary condition and the direction of the local characteristics. Once the primitive variables are updated the conserved variables are calculated based upon them. It is important to note that this implies an explicit coupling of the boundary conditions. This update is also done within the stages of the explicit multi-stage Runge-Kutta schemes (see later Chapters) to ensure proper physical behaviour. In the following sections the specific types of boundary conditions are dealt with. Block to block connections are not considered as boundary conditions since the data handling and the index lists generated within the code ensure that the algorithm does not 'realize' that a neighbouring cell is within another block. Even for the lower-upper symmetric Gauss-Seidel scheme (LUSGS) described in detail within a later chapter there are no 'real' block to block boundaries where additional updating of values might be required.

3.1 Inflow and Outflow

Inflow and outflow boundary conditions are dictated by the characteristics of the boundary values. The direction of a characteristic determines the 'flux' of information and therefore where a value associated with that specific characteristic has to come from. For an inflow boundary that means that for each characteristic entering the flow domain a
value has to be prescribed and for each characteristic leaving the flow domain a value has to be extrapolated from within the flowfield. Subsequently for the outflow boundary characteristics leaving the flow domain imply that values have to be extrapolated from within the flowfield and in the other case values have to be specified at the outflow boundary. With the focus on supersonic flow this leads to a situation where all values are prescribed at the inflow and all values are extrapolated from within the flowfield. In the case of subsonic flow one characteristic goes in the opposite direction of the flow. Hence, at the inflow boundary one primitive variable (preferably the pressure $p$) would be extrapolated from within the flowfield, others specified and at the outflow boundary one primitive variable would be specified (again the pressure $p$) and all others extrapolated from within the flowfield. Another approach calculates Riemann invariants for the boundaries and calculates these accordingly instead of the primitive variables. This might be favourable especially for external flows where the far field boundary condition has to be dealt with.

3.2 Symmetry and Inviscid Wall

In the case of a symmetry or inviscid wall one has to ensure tangential flow by calculating the velocity on the wall as

$$\mathbf{u}_{\text{wall}} \cdot \mathbf{n} = 0$$

(3.1)

The density $\rho$, pressure $p$ and the mass fractions $Y_i$ of the adjacent cell are used as values on the symmetry line, which is equivalent to vanishing normal gradients.

$$\left. \frac{\partial \rho}{\partial n} \right|_{\text{wall}} = \left. \frac{\partial p}{\partial n} \right|_{\text{wall}} = \left. \frac{\partial Y_i}{\partial n} \right|_{\text{wall}} = 0$$

(3.2)

Note that $\frac{\partial}{\partial n} = \mathbf{n} \cdot \nabla$. This procedure slightly changes the total energy $E$ of the conserved variables which introduces some small error.
3.3 Viscous Wall

The viscous flow on a wall is characterized by flow velocity and pressure gradient normal to the wall to be zero.

\[
\begin{align*}
\mathbf{v}_{\text{wall}} &= 0 \\
\frac{\partial p}{\partial n} \bigg|_{\text{wall}} &= 0
\end{align*}
\] (3.3) (3.4)

This can be achieved by setting the velocity components on the boundary to zero and using the pressure value of the adjacent cell on the boundary.

From the thermodynamic point of view for viscous flows the temperature of the wall or the heat flux through the wall boundary has to be specified. The simple case of a given wall temperature requires the wall temperature to be set to the appropriate value, the case of the specified heat flux applies Fourier's law

\[ q = -\lambda \nabla T \] (3.5)

where \( q \) is the desired heat flux. For \( q = 0 \) an adiabatic wall is given. In our case we want to prescribe the heat flux normal to the wall so that the wall temperature can be calculated as

\[ q_{\text{wall}} \cdot \mathbf{n} = -\lambda \mathbf{n} \cdot \nabla T = -\lambda \mathbf{n} \left[ \frac{\partial T}{\partial z} \right] \] (3.6)

As it can be seen in the later Chapter dealing with the spatial discretization and the actual implementation of the boundary conditions, this allows us to determine the wall temperature required to achieve the prescribed heat flux. With known pressure and temperature at the wall the density can be calculated via the thermodynamic equation of state.
Chapter 4

Spatial Discretization

The starting point for the spatial discretization is the governing equations; in the case of viscous flow the Navier-Stokes equations:

$$\int_{A} \frac{\partial}{\partial t} Q \, dA + \oint_{I} \left[ \frac{G_{c} - G_{d}}{H_{c} - H_{d}} \right] \, dl = \int_{A} S \, dA$$

A cell centred finite volume scheme is being developed where the vector of conservative variables and of the source terms are replaced by cell-averaged values, while the cell geometry is assumed to be fixed. Hence, we can write

$$\frac{\partial}{\partial t} Q_{av} A = - \oint_{I} \left[ \frac{G_{c} - G_{d}}{H_{c} - H_{d}} \right] \, dl + S_{av} A = - R$$ \hspace{1cm} (4.1)

For simplicity the subscript ‘av’ for the cell averaged values will be omitted and $R$ is introduced as the ‘right hand side’ vector. The decoupling of spatial and temporal discetization allows to develop the so-called semi-discrete form. Focusing on the right hand side $R$ we replace the line integral by the appropriate summation over the cell sides. At the same time artificial dissipation is introduced by the term $D$, which has to be specified in detail later;

$$R = \sum_{k=1}^{N_{sides}} \left[ \frac{G_{c} - G_{d}}{H_{c} - H_{d}} \right]_{k} \cdot n^{0}_{k} \cdot \Delta s_{k} - A S + D \hspace{1cm} (4.2)$$

Here $n^{0}_{k}$ is the outward facing normalized vector on the side $k$ and $\Delta s_{k}$ its length.
4.1 Inviscid Fluxes

First we concentrate on the calculation of the inviscid fluxes and introduce the cell geometry in Fig. 4.1 to clarify the nomenclature: The cell $ABCD$ has four sides ($k = 1, ..., 4$) and normal vectors $\mathbf{n}^0_k$ ($|\mathbf{n}^0_k| = 1$) and side lengths $\Delta s_k$ associated with each cell side. With respect to the Cartesian $x$-$y$-coordinate system each side can be defined as vector

$$\mathbf{t}_k = \begin{bmatrix} \Delta x_k \\ \Delta y_k \end{bmatrix}$$

(4.3)

with the length

$$\Delta s_k = \sqrt{\Delta x_k^2 + \Delta y_k^2}$$

(4.4)

Subsequently, the outward directed normal vector for side $k$ becomes

$$\mathbf{n}^0_k = \frac{1}{\Delta s_k} \begin{bmatrix} \Delta y_k \\ -\Delta x_k \end{bmatrix}$$

(4.5)

For the calculation of the contributions of the inviscid fluxes we need to know the flux at the cell sides. This flux is obtained by averaging the two fluxes calculated with cell centred values of the neighbouring cells. For side $k = 2$ in the given example this yields

$$\begin{bmatrix} \mathbf{G}_c \\ \mathbf{H}_c \end{bmatrix}_{i+\frac{1}{2},j} = \frac{1}{2} \left( \begin{bmatrix} \mathbf{G}_c \\ \mathbf{H}_c \end{bmatrix}_{i,j} + \begin{bmatrix} \mathbf{G}_c \\ \mathbf{H}_c \end{bmatrix}_{i+1,j} \right)$$

(4.6)
Finally, the summation over the convective fluxes can be given as

\[
\sum_{k=1}^{N_{\text{side}}} \left[ \frac{G_c}{H_{c_k}} \right] n_k^0 \cdot \Delta s_k = \sum_{k=1}^{N_{\text{side}}} (G_{c_k} \Delta y_k - H_{c_k} \Delta x_k)
\]  

(4.7)

This discretization of the inviscid fluxes leads to second order spatial accuracy for smoothly varying cell geometries of a structured grid.

### 4.2 Viscous Fluxes

In finite volume formulations the Gauss integral identity is used to replace the integration over the cell area by an integration along the cell sides. This yields

\[
\iint_A \frac{\partial \chi}{\partial x} \, dA = \oint_i \chi (n_i^0)\, ds
\]

(4.8)

\[
\iint_A \frac{\partial \chi}{\partial y} \, dA = \oint_i \chi (n_i^0)\, ds
\]

(4.9)

where \((n_i^0)\) are the \(x\)- and \(y\)-components of the outward facing normal vector on the cell side. Hence, the cell averaged derivative of any scalar quantity can be expressed as

\[
\frac{\partial \chi}{\partial x} = \frac{1}{A} \iint_A \frac{\partial \chi}{\partial x} \, dA = \frac{1}{A} \oint_i \chi (n_i^0) \, ds
\]

(4.10)

\[
\frac{\partial \chi}{\partial y} = \frac{1}{A} \iint_A \frac{\partial \chi}{\partial y} \, dA = \frac{1}{A} \oint_i \chi (n_i^0) \, ds
\]

(4.11)

As it is demonstrated in Fig. 4.2, typically a 'virtual' cell is defined to allow the calculation of the velocity gradients on the side of the 'real' cell. This virtual cell is presented by a dashed line. The standard approach calculates values for the grid nodes using the cell centred conserved variables. In the case of the 'virtual' cell defined by A', B', C' and D' we would use \(\chi\) values from the cell centres \((i,j), (i+1,j)\) and 'reconstructed' values for nodes B and C. For the calculation of a shear tension on the side defined by nodes B and C averaged values of viscosity \(\mu = 0.5 (\mu_{i,j} + \mu_{i+1,j})\) would have to be used. The reconstruction process and the averaging of the viscosity introduce some additional error.

However, more conformal with a true finite volume approach appears the following method. The integration along the cell sides is performed for each cell. Values for
the cell side are obtained by averaging neighbouring cell centre values. The resulting gradients of the cell centres are, again, averaged to obtain the gradients on the cell sides. This is achieved by

\[
\frac{\partial X}{\partial x} \bigg|_{BC \equiv k=2} = \frac{1}{2A} \left[ \mu_{i,j} \int_{l(i,j)} \chi \left( \frac{s^0}{x} \right) ds + \mu_{i+1,j} \int_{l(i+1,j)} \chi \left( \frac{s^0}{x} \right) ds \right]
\]

\[
= + \frac{1}{2A} \left[ \mu_{i,j} \sum_{k=1,(i,j)}^{N_{\text{sides}}} \chi \Delta y^0_k \Delta s_k + \mu_{i+1,j} \sum_{k=1,(i+1,j)}^{N_{\text{sides}}} \chi \Delta y^0_k \Delta s_k \right] (4.12)
\]

\[
\frac{\partial X}{\partial y} \bigg|_{BC \equiv k=2} = \frac{1}{2A} \left[ \mu_{i,j} \int_{l(i,j)} \chi \left( \frac{s^0}{y} \right) ds + \mu_{i+1,j} \int_{l(i+1,j)} \chi \left( \frac{s^0}{y} \right) ds \right]
\]

\[
= - \frac{1}{2A} \left[ \mu_{i,j} \sum_{k=1,(i,j)}^{N_{\text{sides}}} \chi \Delta x^0_k \Delta s_k + \mu_{i+1,j} \sum_{k=1,(i+1,j)}^{N_{\text{sides}}} \chi \Delta x^0_k \Delta s_k \right] (4.13)
\]

Here $\chi$ has to be substituted with the value of interest $(u, v, ...)$ and the procedure has to be repeated for all cell sides.

For higher order derivatives this process is repeated with derivatives of one order less. At boundary sides no arithmetic averaging is needed since the exact values for the sides are known.
4.3 Implementation of Boundary Conditions

At an earlier stage the different boundary conditions were introduced. Now, within the framework of the spatial discretization, we can develop detailed methods to actually implement them. For all physical boundaries a vector of conserved variables is created, that allows the implementation of boundary conditions.

In the cases of in- and outflow boundaries, values on the boundaries are prescribed or extrapolated from the adjacent ‘real’ cells. As said earlier, the Mach number determines the number of variables to be prescribed or extrapolated.

For symmetry conditions or inviscid walls the boundary side normal vector is used to enforce tangential flow on the boundary. Recalling the earlier condition for tangential flow

\[ \mathbf{u}_\text{wall} \cdot \mathbf{n} = 0 \]

we can now give the expression used to calculate the velocity on the wall:

\[ \mathbf{u}_\text{wall} = \left( u\Delta x^0 + v\Delta y^0 \right) \cdot \begin{bmatrix} \Delta x^0 \\ \Delta y^0 \end{bmatrix} \] (4.14)

Other values except the energy \( E \) are extrapolated from within the flowfield, the energy is recalculated for the boundary.

Recalling specifications made for the viscous wall, we know that the velocity on such a wall is equal to zero. Additionally the normal gradient of the pressure is assumed to be equal to zero, which allows us to use the pressure of the adjacent cell as value for the boundary. For a specified wall temperature this temperature is used at the boundary for all relevant boundary cells. In the case of a specified heat flux through the wall, equations for the appropriate temperature at the boundary have to be solved. The heat flux normal to the wall is, as defined at an earlier stage,

\[ q_\text{wall} \cdot \mathbf{n} = -\lambda n \nabla T = -\lambda n \begin{bmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \end{bmatrix} \]

Applying the Gauss identities to calculate gradients within a cell

\[ \iint_A \frac{\partial \chi}{\partial x} \, dA = \oint_l \chi (\mathbf{n}^0)_x \, ds \] (4.15)

\[ \iint_A \frac{\partial \chi}{\partial y} \, dA = \oint_l \chi (\mathbf{n}^0)_y \, ds \] (4.16)
we can write

$$q_{\text{wall}} \cdot \hat{n} = -\frac{\lambda}{A} n \sum_{k=1}^{N_{\text{nodes}}} T_k \begin{bmatrix} \Delta y_k^0 \Delta s_k \\ -\Delta x_k^0 \Delta s_k \end{bmatrix}$$

(4.17)

where the values $\Delta y_k^0$, $\Delta x_k^0$ and $\Delta s_k$ are the geometric parameters of the cell sides, as said before. One of the cell side temperatures is the wall temperature we want to calculate. Therefore we can write

$$-\frac{\lambda}{A} T_{\text{wall}} \left( n \cdot n \right) \Delta s_{\text{wall}} = q_{\text{wall}} \cdot n + \frac{\lambda}{A} \cdot n \cdot \sum_{k=1,k \neq k(\text{wall})}^{N_{\text{nodes}}} T_k \begin{bmatrix} \Delta y_k^0 \Delta s_k \\ -\Delta x_k^0 \Delta s_k \end{bmatrix}$$

This finally yields

$$T_{\text{wall}} = -\frac{n}{\Delta s_{\text{wall}}} \left( +\frac{A}{\lambda} q_{\text{wall}} + \sum_{k=1,k \neq k(\text{wall})}^{N_{\text{nodes}}} T_k \begin{bmatrix} \Delta y_k^0 \Delta s_k \\ -\Delta x_k^0 \Delta s_k \end{bmatrix} \right)$$

(4.18)

for the wall temperature. This approach makes the approximation that the gradient in the cell centre is the same at the gradient on the wall. Note that $\hat{n}$ is the normalized normal vector on the wall side of the cell. As stated before, with known pressure and temperature at the wall the density can be calculated via the thermodynamic equation of state. This approach fully conforms with the finite volume formulation developed in this work.

### 4.4 Artificial Dissipation

The artificial dissipation used to suppress unwanted numerical instabilities is based on Roe’s flux-difference split algorithm (see [5]) and several non-linear flux limiters presented in [32]. Initially the formula developed by Roe is used to calculate the fluxes for a cell face, which can be given as

$$\begin{bmatrix} G_c \\ H_c \end{bmatrix}_{i+\frac{1}{2},j} = \frac{1}{2} \left( \begin{bmatrix} G_c \\ H_c \end{bmatrix}_{Q^L_{i+\frac{1}{2},j}} + \begin{bmatrix} G_c \\ H_c \end{bmatrix}_{Q^R_{i+\frac{1}{2},j}} \right) n^0 \cdot \Delta s$$

$$-\frac{1}{2} \hat{T}_{i+\frac{1}{2},j} \left| \hat{A}_{i+\frac{1}{2},j} \right| \hat{T}_{i+\frac{1}{2},j}^{-1} \left( Q^R_{i+\frac{1}{2},j} - Q^L_{i+\frac{1}{2},j} \right)$$

where $L$ and $R$ imply left and right states of the cell side and the hat stands for Roe-averaged values. Note that the cell side normal vector is already included in the matrices.
and its inverse. The diagonal matrix $\mathbf{A}$ has the eigenvalues $u_n, u_n, u_n+a, u_n-a, u_n, \ldots, u_n$ multiplied with the relevant cell side length as entities. The velocity normal on the cell side $u_n$ is defined by $u_n = \Delta y^0 u - \Delta x^0 v$ and the local speed of sound described by $a$.

In the approach of this work the 'basic' flux is calculated via flux averaging and the dissipation is identified as the 'rest' of the equation above. This means the full flux calculation above is separated into a basic flux calculation and the determination of the 'flux-correction', which is considered to be artificial dissipation. Before details are being discussed is has to be mentioned that the elements of an arbitrary vector $\chi$ are described as $\chi^l$.

We now define the artificial dissipation $D$ in a general form as suggested in [32]:

$$D_{i+\frac{1}{2}j} = \frac{1}{2} T_{i+\frac{1}{2}j} \Phi_{i+\frac{1}{2}j}$$

(4.19)

where $\Phi$ is computed depending on the type of flux correction selected. In addition we define a flux correction vector $\alpha$ according to

$$\alpha_{i+\frac{1}{2}j} = T^{-1}_{i+\frac{1}{2}j} \left( Q^R_{i+\frac{1}{2}j} - Q^L_{i+\frac{1}{2}j} \right)$$

(4.20)

For first order dissipation we can then write

$$\left( \Phi^l_{i+\frac{1}{2}j} \right)^{O1} = \psi \left( \lambda^l_{i+\frac{1}{2}j} \right) \alpha^l_{i+\frac{1}{2}j}$$

(4.21)

where $\lambda^l_{i+\frac{1}{2}j}$ is one of the eigenvalues on the cell side of interest and $\psi$ an entropy satisfying function, which will be defined later. The first order flux correction is the most robust, and at the same time the most inaccurate compared to higher order flux corrections. Therefore higher order formulas have to be developed which are more involved and at the same time more difficult to converge. We restrict us to second order flux correction schemes which fall into two classes, the symmetric and the upwind schemes. First we concentrate on the symmetric limiters and give a definition for the $(\Phi)^S$ associated with it:

$$\left( \Phi^l_{i+\frac{1}{2}j} \right)^S = \psi \left( \lambda^l_{i+\frac{1}{2}j} \right) \left[ \alpha^l_{i+\frac{1}{2}j} - g^l_{i+\frac{1}{2}j} \right]$$

(4.22)

The vector $g$ is introduced to add an additional flux correction which makes the scheme second order accurate in regions of smoothly varying flow variables. There is a choice of
several limiters, listed as follows:

\[ g^l_{i+\frac{1}{2},j} = \minmod\left(\alpha^l_{i-\frac{1}{2},j}, \alpha^l_{i+\frac{1}{2},j}\right) + \minmod\left(\alpha^l_{i+\frac{1}{2},j}, \alpha^l_{i+\frac{3}{2},j}\right) - \alpha^l_{i+\frac{1}{2},j} \]  
\[ g^l_{i+\frac{1}{2},j} = \minmod\left(\alpha^l_{i-\frac{1}{2},j}, \alpha^l_{i+\frac{1}{2},j}, \alpha^l_{i+\frac{3}{2},j}\right) \]  
\[ g^l_{i+\frac{1}{2},j} = \minmod\left[2\alpha^l_{i-\frac{1}{2},j}, 2\alpha^l_{i+\frac{1}{2},j}, \frac{1}{2}\left(\alpha^l_{i-\frac{1}{2},j} + \alpha^l_{i+\frac{3}{2},j}\right)\right] \]

From the equations above it is obvious that these symmetric limiters take the previous and the next cell side into account, which implies that five cell centre values are used. The minmod function returns the argument with the smallest modulus from a list of arguments whenever they are of the same sign and zero otherwise. This is equivalent to

\[ \minmod(x_{i=1..n}) = \text{sgn}(x_1) \cdot \max\{0, \min(|x_1|, \text{sgn}(x_1) \cdot x_2, ... \text{sgn}(x_1) \cdot x_n)\} \]

The second order upwind limiter \( (\Phi^U) \) can be defined as follows:

\[ \left(\Phi^U_{i+\frac{1}{2},j}\right)^U = -\frac{1}{2} \psi\left(\alpha^l_{i+\frac{1}{2},j}\right) (g^l_{i+1,j} - g^l_{i,j}) + \psi\left(\alpha^l_{i+\frac{1}{2},j} + \gamma^l_{i+\frac{1}{2},j}\right) \alpha^l_{i+\frac{1}{2},j} \]

where \( \gamma^l_{i+\frac{1}{2},j} \) is given by

\[ \gamma^l_{i+\frac{1}{2},j} = \begin{cases} \frac{1}{2} \psi\left(\alpha^l_{i+\frac{1}{2},j}\right) (g^l_{i+1,j} - g^l_{i,j}) / \alpha^l_{i+\frac{1}{2},j} & \text{for } \alpha^l_{i+\frac{1}{2},j} \neq 0 \\ 0 & \text{for } \alpha^l_{i+\frac{1}{2},j} = 0 \end{cases} \]

and \( g^l_{i,j} \) has to be calculated for the cell centre in the case of the upwind limiter,

\[ g^l_{i,j} = \minmod\left(\alpha^l_{i-\frac{1}{2},j}, \alpha^l_{i+\frac{1}{2},j}\right) \]
\[ g^l_{i,j} = \left(\alpha^l_{i+\frac{1}{2},j} + \alpha^l_{i+\frac{3}{2},j}\right) / \left(\alpha^l_{i+\frac{1}{2},j} + \alpha^l_{i+\frac{3}{2},j} + \delta\right) \]
\[ g^l_{i,j} = \frac{\alpha^l_{i-\frac{1}{2},j}\left[\left(\alpha^l_{i+\frac{1}{2},j} + \delta\right) + \alpha^l_{i+\frac{3}{2},j}\left[\left(\alpha^l_{i-\frac{1}{2},j} + \delta\right)^2 + 2\delta\right]\right]}{\left[\left(\alpha^l_{i+\frac{1}{2},j} + \delta\right)^2 + 2\delta\right]} \]
\[ g^l_{i,j} = \minmod\left[2\alpha^l_{i-\frac{1}{2},j}, 2\alpha^l_{i+\frac{1}{2},j}, \frac{1}{2}\left(\alpha^l_{i-\frac{1}{2},j} + \alpha^l_{i+\frac{3}{2},j}\right)\right] \]

where, according to [32], \( \delta \) is a small parameter between \( 10^{-7} \) and \( 10^{-5} \) to avoid division by zero.

For the time being the Roe averaged values are replaced by simply averaged values and the second symmetric limiter is used for most of the cases analyzed in this work. Furthermore an entropy fix is being applied, that solves the well-known entropy problem...
of the Roe type of flux splitting calculation. The absolute values of the eigenvalues are increased by the entropy satisfying function \( \psi \) if too small.

\[
\psi (\lambda_i) = \begin{cases} 
\frac{\lambda_i^2 + \epsilon^2}{2\epsilon} & \text{for } |\lambda_i| < \epsilon \\
|\lambda_i| & \text{otherwise}
\end{cases}
\]

(4.33)

where \( \epsilon \) is calculated according to

\[
\epsilon = \tilde{\epsilon} (|u \Delta y^0| + |v \Delta x^0| + a) \Delta s
\]

(4.34)

According to [32] the parameter \( \tilde{\epsilon} \) can be set to zero for simple unsteady shocks and has to be selected carefully especially for strong steady shocks close to stagnation points. The range for \( \tilde{\epsilon} \) varies from author to author and especially for blunt body flows higher values are needed to stabilize the numerical computation. The specific values used are given for each individual computation presented in this work at later stages.
Chapter 5

Temporal Discretization

Once the tools for the spatial discretization are developed, we can focus on the temporal discretization, which allows us to march the solution in time to reach a steady state. The two main aspects of temporal discretization are the numerical method used and the time step chosen. Within this work two families of numerical methods are presented, one explicit and another implicit. These are the explicit Runge-Kutta type of schemes and the Euler implicit, trapezoidal and Gear second order time marching methods. The latter three are all used in combination with the lower-upper symmetric Gauß-Seidel scheme, where the time accuracy of the implicit schemes mentioned is lost due to the factorization error.

5.1 Explicit Time-Marching Methods

A family of explicit multi-stage time-marching schemes is given by the Runge-Kutta schemes. Utilizing the semi-discrete form

\[ A \frac{\partial Q}{\partial t} = -R \]

and defining the 'initial intermediate' value of conserved variables as well as the intermediate change of conserved variables

\[ Q^{(1)} = Q^n \]  
\[ R^{(k)} = -A \frac{\partial Q}{\partial t}^{(k)} \]  
\[ \Delta Q^{(k)} = -\frac{\Delta t}{A} \alpha_k R^{(k-1)} \]
we can apply the following procedure to find intermediate stages

\[ Q^{(k)} = Q^n + \Delta Q^{(k)} \] (5.4)

and finally find the new values of conserved variables summarizing intermediate states according to

\[ Q^{n+1} = Q^n + \frac{\Delta t}{A} \sum_{k=1}^{N_{stages}} \beta_k R^{(k)} \] (5.5)

In the case of a point-implicit treatment of the chemical source term the modified formula

\[ \Delta Q^{(k)} = -\frac{\Delta t}{A} \alpha_k \left( \frac{R^{(k-1)}}{S} - \frac{Q^{(k)}}{S} \right) \]

\[ = - \left( I - \frac{\Delta t}{A} \alpha_k \frac{Q^{(k)}}{S} \right)^{-1} \cdot \frac{\Delta t}{A} \alpha_k R^{(k-1)} \] (5.6)

applies for the calculation of the change of the conserved variables. It is important to note that the value \( \alpha_1 \) is not used and therefore not defined. By a special selection of the coefficients \( \alpha_k \) and \( \beta_k \) well known schemes can be constructed, as indicated in the following table.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Stages</th>
<th>( \alpha_k )</th>
<th>( \beta_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euler explicit</td>
<td>1</td>
<td>-</td>
<td>( \beta_1 = 1 )</td>
</tr>
<tr>
<td>RK2 O2</td>
<td>2</td>
<td>( \alpha_2 = \frac{1}{2} )</td>
<td>( \beta_1 = 0, \beta_2 = 1 )</td>
</tr>
<tr>
<td>RK4 O4</td>
<td>4</td>
<td>( \alpha_2 = \alpha_3 = \frac{1}{2}, \alpha_4 = 1 )</td>
<td>( \beta_1 = \frac{1}{6}, \beta_2 = \beta_3 = \frac{1}{3} )</td>
</tr>
</tbody>
</table>

While explicit schemes offer simplicity with respect to coding they are limited with respect to the maximum allowed time step. Even with point implicit treatment chemically reacting flow behaves much more unstable than using a fully implicit method, presented within the next Section. While the stability range of the Euler explicit scheme is not really practical, the four stage Runge-Kutta scheme appears to be an interesting approach to time-accurate calculation. The two stage Runge-Kutta scheme is less attractive with respect to stability and accuracy but clearly superior over the four stage scheme with respect to computational expense. This computational cost appears to be a major disadvantage of the classical 'RK4' scheme, which makes the application of convergence acceleration techniques such as residual smoothing or multi-grid computation and also
parallelization attractive. However, none of these strategies have been applied in this work since the implicit time-marching schemes presented in the next Section are preferable especially for flows with non-equilibrium chemistry.

5.2 Implicit Time-Marching Methods

Starting again with the semi-discrete form

\[ A \frac{\partial Q}{\partial t} = -R \]

we can define a general multi-step time-marching method:

\[
\Delta Q^{n+1} = \frac{A}{\Delta t} (Q^{n+1} - Q^n) = -\left( \alpha - \sum_{i=1}^{N_{steps}} \beta_i \right) R^{n+1} - \left( 1 - \alpha - \sum_{i=1}^{N_{steps}} \beta_i \right) R^n + \frac{A}{\Delta t} \sum_{i=1}^{N_{steps}} \beta_i Q^{i-1}
\] (5.7)

The methods we will focus on are the implicit Euler scheme (\( \alpha = 1, \beta_i = 0 \)), the Trapezoidal scheme (\( \alpha = 0.5, \beta_i = 0 \)) and the Gear scheme (\( \alpha = 1, \beta_1 = 1/3, \beta_{\neq 1} = 0 \)). The first scheme is of first order while the latter two are of second order accuracy. This is valid even after the the term \( R^{n+1} \) is linearized in the following way:

\[
R^{n+1} = R^n + \frac{\partial R}{\partial Q}\bigg|^{n} \Delta Q^{n+1}
\] (5.8)

Assuming that there will only be one additional 'step' used, this gives

\[
\left[ \frac{A}{\Delta t} I + (\alpha - \beta) \frac{\partial R}{\partial Q}\bigg|^{n} \right] \Delta Q^{n+1} = -(1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1}
\] (5.9)

Concentrating on the 'left hand side' the equation above can be rewritten as

\[
\left[ \frac{A}{\Delta t} I + (\alpha - \beta) \left( \sum_{k=1}^{N_{sides}} \frac{\partial}{\partial Q} E_k n_k \Delta s_k - A \frac{\partial}{\partial Q} S^n \right) \right] \Delta Q^{n+1} = -(1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1}
\] (5.10)

which is equivalent to

\[
\left[ \frac{A}{\Delta t} I + (\alpha - \beta) \left( \sum_{k=1}^{N_{sides}} J^n_{F_k} \Delta s_k - A J^n_{S} \right) \right] \Delta Q^{n+1} = -(1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1}
\] (5.11)
For a structured grid the Jacobian matrices for the $k$ cell sides are calculated by averaging the cell centred Jacobian matrices, as given below:

$$J_{F_k} = \begin{cases} 0.5 \left( \frac{I}{F_{i,j}} + \frac{I}{F_{i,j-1}} \right) & \text{for } k = 1 \\ 0.5 \left( \frac{I}{F_{i,j}} + \frac{I}{F_{i+1,j}} \right) & \text{for } k = 2 \\ 0.5 \left( \frac{I}{F_{i,j}} + \frac{I}{F_{i,j+1}} \right) & \text{for } k = 3 \\ 0.5 \left( \frac{I}{F_{i,j}} + \frac{I}{F_{i-1,j}} \right) & \text{for } k = 4 \end{cases}$$  

(5.12)

The resulting system of equations is

$$\begin{bmatrix} \frac{\partial q_{i,j-1}}{\partial t} \\ \vdots \\ \frac{\partial q_{i+1,j}}{\partial t} \end{bmatrix}^{n+1} = \begin{bmatrix} \frac{\partial q_{i,j-1}}{\partial t} \\ \vdots \\ \frac{\partial q_{i+1,j}}{\partial t} \end{bmatrix}^{n} - (1 - \beta) \frac{\partial q_{i,j}}{\partial t}^{n}$$

(5.13)

with left hand side matrix entities

$$\begin{align*}
\frac{\partial q_{i,j-1}}{\partial t} &= \frac{1}{2} (\alpha - \beta) \frac{J^n}{F_{i,j-1,k=1}} \Delta s_{k=1} \\
\frac{\partial q_{i-1,j}}{\partial t} &= \frac{1}{2} (\alpha - \beta) \frac{J^n}{F_{i-1,j,k=4}} \Delta s_{k=4} \\
\frac{\partial q_{i,j}}{\partial t} &= \frac{A_{i,j}}{\Delta t} + (\alpha - \beta) \left( \sum_{k=1}^{N_{\text{inds}}} \frac{1}{2} \frac{J^n}{F_{i,j,k}} \Delta s_k - A_{i,j} \frac{J^n}{S} \right) \\
\frac{\partial q_{i+1,j}}{\partial t} &= \frac{1}{2} (\alpha - \beta) \frac{J^n}{F_{i+1,j,k=2}} \Delta s_{k=2} \\
\frac{\partial q_{i,j+1}}{\partial t} &= \frac{1}{2} (\alpha - \beta) \frac{J^n}{F_{i,j+1,k=3}} \Delta s_{k=3}
\end{align*}$$

(5.14 - 5.18)

Note that for a structured mesh the indices $k = 1, 2, 3$ and 4 are absolutely equivalent to $(i + \Delta i, j + \Delta j) = (i, j - 1), (i + 1, j), (i, j + 1)$ and $(i - 1, j)$, where $\Delta i$ and $\Delta j$ can be $-1, 0$ or 1. The system described above can be solved via approximate factorization, ADI or other methods. However, from the computational point of view, especially for
reactive flows, it makes sense to solve the problem by utilizing the LU-SGS scheme. For this, we need to split the Jacobian matrices into two parts

\[ \frac{J}{F_k} = \frac{J^+}{F_k} + \frac{J^-}{F_k} = \frac{1}{2} \left( \frac{J}{F_k} + c\Lambda_k I \right) + \frac{1}{2} \left( \frac{J}{F_k} - c\Lambda_k I \right) \]  \hspace{1cm} (5.19)

where \( \Lambda_k \) is the maximum spectral radius for cell side \( k \)

\[ \Lambda_k = |\Delta y^0 u - \Delta x^0 v| + a \]  \hspace{1cm} (5.20)

Then we apply an upwind discretization for the two matrices:

\[ \frac{J^+}{F_k} = \frac{J}{F_{i,j}} \]  \hspace{1cm} (5.21)

\[ \frac{J^-}{F_k} = \begin{cases} \frac{J}{F_{i,j-1}} & \text{for } k = 1 \\ \frac{J}{F_{i,j+1}} & \text{for } k = 2 \\ \frac{J}{F_{i,j+1}} & \text{for } k = 3 \\ \frac{J}{F_{i+1,j}} & \text{for } k = 4 \end{cases} \]  \hspace{1cm} (5.22)

For outward facing normal vectors the '+'-Jacobian matrices are always calculated using the cell information itself, while '-'-Jacobian matrices are determined via the values of the neighbour cells. This splitting combined with the constant \( c \geq 1 \) assures diagonal dominance for the resulting left hand side matrix. Our system of equations to be solved then reads

\[ \left[ \frac{A}{\Delta t} l + (\alpha - \beta) \left( \sum_{k=1}^{N_{\text{faces}}} \frac{J^+}{F_k} \Delta s_k + \sum_{k=1}^{N_{\text{faces}}} \frac{J^-}{F_k} \Delta s_k - A L^n \right) \right] \Delta Q^{n+1} = -(1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1} \]  \hspace{1cm} (5.23)

With \( \sum \frac{J}{F_{i,j}} \Delta s_k = 0 \) this can be rewritten as

\[ \left[ \left( \frac{A}{\Delta t} + (\alpha - \beta) \frac{c}{2} \sum_{k=1}^{N_{\text{faces}}} \Lambda_k \Delta s_k \right) l - A J^n \right] \Delta Q^{n+1} = -(1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1} \]  \hspace{1cm} (5.24)

and is equivalent to

\[ \left[ \{ \bar{D} \} + \{ \bar{L} \} + \{ \bar{U} \} \right] \Delta Q^{n+1} = -(1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1} \]  \hspace{1cm} (5.25)
This system of equations can be approximated by the factorization

$$ \left( \hat{D} + \hat{L} \right) \Delta Q^{n+1} = - (1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1} $$

and solved in two sweeps, a lower and an upper one

$$ \left( \hat{D} + \hat{L} \right) \Delta Q = - (1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1} $$

$$ \left( \hat{D} + \hat{U} \right) \Delta Q^{n+1} = \hat{D} \Delta Q $$

The scheme presented here is assumed to produce the lowest factorization error (see [7]). However, the need to keep left hand side matrices for all cells in memory in order to avoid very costly recalculation, another, slightly different factorization is presented. This factorization requires the calculation and inversion of the source term Jacobi matrix only once and is split in factors defined as follows:

$$ \hat{D} = \left( A \frac{\Delta t}{\Delta t} + (\alpha - \beta) \frac{\Delta t}{2} \sum_{k=1}^{N_{\text{vols}}} \Lambda_k \Delta s_k \right) I $$

$$ \hat{L} = (\alpha - \beta) \left( \frac{J^{-n}}{J_{F,i,j=k=1}^{n}} \Delta s_{k=1} + \frac{J^{-n}}{J_{F,i,j=k=4}^{n}} \Delta s_{k=4} \right) $$

$$ \hat{U} = (\alpha - \beta) \left( \frac{J^{-n}}{J_{F,i,j,k=2}^{n}} \Delta s_{k=2} + \frac{J^{-n}}{J_{F,i,j,k=3}^{n}} \Delta s_{k=3} \right) $$

The factorization in this case reads

$$ \left( \hat{D} - A \frac{\Delta t}{\Delta t} + \hat{L} \right) \hat{D}^{-1} \left( \hat{D} + \hat{U} \right) \Delta Q^{n+1} = - (1 - \beta) R^n + \frac{A}{\Delta t} \beta Q^{n-1} $$

and can be solved in two sweeps as presented above. It is important to mention that this scheme does not maintain any time accuracy, despite the fact that the trapezoidal or Gear scheme might have been used. Some authors try to regain this time accuracy by Newton-type sub-iterations (see [3]), others modify the factorization to get a first-order time accurate scheme (see [24]). However, for the solution of the point chemistry equations, where no spatial discretization and LU-SGS factorization is needed, second order accuracy in time is of great value. The parameters for the methods of interest can be found in the following:

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Steps</th>
<th>$\alpha$</th>
<th>$\beta_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euler implicit</td>
<td>0</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>Trapezoidal</td>
<td>0</td>
<td>$\alpha = \frac{1}{2}$</td>
<td>-</td>
</tr>
<tr>
<td>Gear (O2), BDF</td>
<td>1</td>
<td>$\alpha = 1$</td>
<td>$\beta_1 = \frac{1}{3}$</td>
</tr>
</tbody>
</table>
The first preference in this work is the implicit Euler scheme used in combination with the LU-SGS solution algorithm.

5.3 Time Step Calculation

Explicit time marching methods require, depending on the scheme used, a specific restriction of the time step to ensure convergence and solution accuracy. Although many implicit methods, such as the Euler implicit time marching scheme, are unconditionally stable, a limitation of the time step used is advisable here, too. One of the major reasons for this is that the factorization error introduced by the LU-SGS scheme can decrease the solution accuracy and even the stability (see [7]).

In order to determine a suitable time step, the physical information propagation is related to the numerical via the Courant-Fredrichs-Lewis, short CFL number. In the following a method for determining an estimate comparable to the physical information propagation is given, which is derived with the requirement of a structured Cartesian grid. First the maximum eigenvalue of the inviscid flux Jacobi matrix \( \lambda \) is calculated

\[
\lambda = |u \cdot n^0| \pm a
\]

\[
= |\Delta x^0 u - \Delta x^0 v| a
\]

for each cell side. Multiplying the maximum eigenvalue with the appropriate cell side yields the maximum spectral radius for the inviscid flux Jacobi matrix. These spectral radii of each cell side are then summarized to yield the convective spectral radius for the cell of interest:

\[
\Lambda_c = \left( \sum_{k=1}^{N_{side}=4} \lambda_k \cdot \Delta s_k \right) / 2A
\]

Recalling the cell nomenclature from the spatial discretization we define the metrics \( \Delta s_\xi \) and \( \Delta s_\eta \) as follows

\[
\Delta s_\xi = 0.5 (\Delta s_1 + \Delta s_3)
\]

\[
\Delta s_\eta = 0.5 (\Delta s_2 + \Delta s_4)
\]

which can be used to calculate the diffusive spectral radius for the cell examined:

\[
\Lambda_d = \frac{4\gamma \mu}{\rho Pr A^2} \cdot (\Delta s_\xi^2 + \Delta s_\eta^2) + \frac{\mu}{3 \rho A^2} \sqrt{\Delta s_\xi^2 \cdot \Delta s_\eta^2}
\]
This diffusive spectral radius is based on the eigenvalues of the Jacobian matrix for the diffusive fluxes, as shown in [15]. The equation above is obtained when the equations for the diffusive spectral radius presented in [15] are rewritten for the finite volume discretization. Finally, we can calculate the local time step of a cell for the time-marching method using the convective and diffusive spectral radii:

\[ \Delta t = CFL \cdot \frac{A}{\Lambda_t} = CFL \cdot \frac{A}{\Lambda_c + \Lambda_d} \]  

(5.39)

In the case that global instead of local time stepping is used the actual time step is the minimum of all local time steps.
Chapter 6

Grid Generation

This Chapter describes the steps that were undertaken to develop two-dimensional grids required for the numerical solution of inviscid and viscous flow problems. Step by step all necessary details are explained that finally provide the tools essential for grid generation. These steps are

- boundary definition utilizing non-uniform rational B-splines (NURBS),
- spline interpolation (interpolate given points with a spline),
- initial grid generation utilizing transfinite interpolation (TFI) and
- final grid generation utilizing elliptic equations with line and point clustering and also orthogonality at the boundaries.

It is important to mention that the notation in this Chapter is in conformance with the literature used with respect to grid generation. Therefore some variables are used in a different context, which will be explained within the Chapter.

6.1 Boundary Definition

The two aspects of boundary definitions are geometry and point distribution. In this approach non-uniform rational B-splines (NURBS) are used to define the boundary geometry. This is due to the great flexibility of the NURBS and the smoothness splines generally provide. The definition of NURBS is provided in the first Subsection. The point distribution is related to the spline length. Using the kind of blending function presented in the second Subsection it is possible to highly influence the point distribution and therefore the distance between the points. Also, an alternative method is introduced,
which allows to directly specify the distance of the first and the last two points from each other on the spline.

### 6.1.1 NURBS

The several types of splines available can be found in [30]. This book provides a very good general introduction to this topic and deals with spline-surfaces, which might be of interest in three-dimensional grid generation. However, the discussion here is limited to two-dimensional grid generation where the basic set of blending functions used for B-splines in two spatial dimensions is

\[
B_i = \frac{1}{6} u^3 \\
B_{i-1} = \frac{1}{6} (-3u^3 + 3u^2 + 3u + 1) \\
B_{i-2} = \frac{1}{6} (3u^3 - 6u^2 + 4) \\
B_{i-3} = \frac{1}{6} (1 - u)^3
\]

Note that this describes a spline of third order, which requires at least four points for its definition. The segment \( i \) of a B-spline is defined by the coordinates \( Q_{\text{spline},i} \)

\[
Q_{\text{spline},i}(u) = \sum_{k=0}^{3} P_{i-3+k} B_{i-3+k}(u)
\]

Finally, the non-uniform rational B-splines are an extension with respect to a weight associated to each point. The influence of a point defining the spline can be increased or decreased with the weight \( w \). This means, that

\[
P^{w}_i = (w_i x_i, w_i y_i, w_i)
\]

represent the \( i \) points and their weights. Now the segment \( i \) for the NURBS can be calculated using

\[
Q_{\text{spline},i}(u) = \sum_{k=0}^{3} P_{i-3+k} \cdot \frac{B_{i-3+k}(u) w_i}{\sum_{j=0}^{3} B_{i-3+j}(u) w_j}
\]

Examples for the graphs of a various number of splines can be found in [30].
6.1.2 Spline Interpolation

The spline interpolation finds a set of 'spline definition points' \( P \) for a number of given geometrical points \( Q \). Many ways to approximate given geometrical points by a spline exist and we select one, where the geometrical points \( Q \) are located at the beginning and the end of the spline and at its segment intersections. In order to make the curve produced by the spline definition points start and end at the first and last given points these points have to be repeated three times. Therefore the number of spline definition points \( N_{\text{SplineDef}} \) and the number of geometrical points \( N_{\text{GeoDef}} \) are not independent from each other since there are always four more spline definition points than geometrical points. This means that the first and last geometrical point are equivalent to the first and last three spline definition points. The remaining spline definition points have to be found by the solution of a linear system of equations. In our case we select all the weights of the NURBS to be one and get for points \( Q_{i=2,...,N_{\text{GeoDef}}-1} \)

\[
Q_i = \frac{1}{6} (P_{i+1} + 4P_{i+2} + P_{i+3})
\]

as relationship between geometrical points and spline definition points. With this the system of equations to be solved can be given as

\[
\begin{bmatrix}
4 & 1 \\
1 & 4 & 1 \\
\ddots & \ddots & \ddots \\
1 & 4 & 1 \\
1 & 4
\end{bmatrix}
\begin{bmatrix}
P_4 \\
P_5 \\
\vdots \\
P_{N_{\text{SplineDef}}-4} \\
P_{N_{\text{SplineDef}}-3}
\end{bmatrix}
= 
\begin{bmatrix}
6Q_2 - P_3 \\
6Q_3 \\
\vdots \\
6Q_{N_{\text{GeoDef}}-2} - P_{N_{\text{SplineDef}}-2}
\end{bmatrix}
\]

while

\[
P_{N_{\text{SplineDef}},-2,-1,-0} = Q_{N_{\text{GeoDef}}}
\]

The solution of the system of equations can be obtained by standard methods such as a Gauß elimination. For the four geometrical points

\[
Q_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad Q_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad Q_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad Q_4 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}
\]

the solution can be seen in Fig. 6.1. With the tools for a simple, but sufficient spline interpolation arbitrary boundaries defined with a given number of geometrical points can be approximated by splines and subsequently used for the grid generation.
6.1.3 Boundary Point Distribution

There are many possibilities to distribute the points on a boundary defined by splines as described before. The first method suggested here utilizes a family of recursively defined blending functions given by

\[ f_b(x, n) = \begin{cases} 
  x & \text{for } n = 0 \\
  f_b(x - \sin x, n - 1) & \text{for } n > 0 
\end{cases} \]

(6.12)

where \( n \) is the 'order' of the blending function. The valid range for \( x \) is from 0 to \( 2\pi \).

Once the highest order \( N \) to be used is specified, the function for distributing the points can be evaluated by

\[
f(x, N) = \sum_{i=0}^{N} g(i) f_b(x, i)
\]

(6.13)

\[
\sum_{i=0}^{N} g(i) = 1.
\]

(6.14)

The weights of each blending function of order \( i \) are given by \( g(i) \). The graphs of several combinations for \( f(x) \) are shown in Fig. 6.2. The equal spacing of points within the range of \( x \) is transformed by the function \( f(x, N) \) in order to achieve the desired point clustering on the boundary.
Assuming the length of the spline is given and normalized to 1, a range for $\xi$ from 0 to 1 can be used to identify the position of a point on the spline. Additionally, a function $f^*(\xi, N)$ is needed that gives the desired clustering within the same range. This is basically a transformation of the range from 0 to $2\pi$ to the range from 0 to 1, needed for a normalized spline. This transformation can be achieved by

$$x = 2\pi \cdot \xi \quad \longleftrightarrow \quad f^*(\xi, N) = \frac{1}{2\pi} f(x, N)$$

(6.15)

for the full range, which is equivalent to symmetric clustering. If only the first part of the graphs described by the blending functions is of interest

$$x = \pi \cdot \xi \quad \longleftrightarrow \quad f^*(\xi, N) = \frac{1}{\pi} f(x, N)$$

(6.16)

can be used, which is equivalent to a clustering of points in the beginning part of the spline; finally for a clustering of points in the ending part of the spline

$$x = \pi \cdot (\xi + 1) \quad \longleftrightarrow \quad f^*(\xi, N) = \frac{1}{\pi} [f(x, N) - \pi]$$

(6.17)

gives the desired answer. There are examples given in Fig. 6.3: the original grid, a grid with clustering towards both boundaries, one with clustering towards the upper and one with clustering towards the lower boundary. For the examples presented the order $N$
was set to 1, the coefficients $g(0)$ to 0.2 and $g(1)$ to 0.8.

The second method presented is a one-sided clustering method where symmetric boundary point clustering in the presented form is not possible. We assume that the first and the last points are fixed to the beginning and the end of the boundary and the distance between two points is defined according to

$$
\Delta s_i = |Q_{i+1} - Q_i|
$$

(6.18)

The first and the last distances $\Delta s_{\text{first}}$ and $\Delta s_{\text{last}}$ are prescribed as well as the maximum distance increase factor $G_{\text{max}}$ for two adjacent point to point distances, defined as

$$
G_{\text{max}} \geq \frac{\Delta s_{i+1}}{\Delta s_i}
$$

(6.19)

Slowly increasing distances between points are achieved for $G$ in the range between 1.0 and 1.2. Beginning with the smallest distance between points more points are added with increasing distance. Once the actual distance between two points is equal or greater than the maximum distance between the last two points, $G$ is set to 1.0 and more points are added until the end of the boundary spline is reached or passed. With the resulting
number of points $NGeo\text{Def.}$, which is kept constant for the rest of the procedure, the
distance increase factor $G$ is iteratively changed until the last point calculated with $G$
and $NGeo\text{Def.}$ exactly matches the last point on the boundary. With known $NGeo\text{Def.}$, $G$
and $\Delta s_{\text{first}}$, the points on the boundary are uniquely defined. Obviously, for this approach
the first distance between the relevant points must be smaller than the last, and both
added must be smaller than the total length of the boundary.
The procedure suggested here is favourable for grids that are used to calculate boundary
layers in viscous flows, because the distance of the first grid line to the wall can be
exactly specified. Although turbulent flows are not considered in this work it is worth
while noting that this is of vital importance especially for these flows. To develop such
a grid we select distances of $\Delta s_{\text{first}} = 1 \cdot 10^{-4}$, $\Delta s_{\text{last}} = 1 \cdot 10^{-2}$ and $G_{\text{max}} = 1.2$
and obtain a clustering function $f(x)$ as shown in Fig. 6.4. The actual distance increase
factor used is $G = 1.19276$ (rounded) and the grid produced by this boundary point
clustering is presented in Fig. 6.5. The example grids so far have been very simple
and could be generated with boundary clustering and simple interpolation, since the
surrounding boundary was a rectangle. For a more complicated boundary geometry
more sophisticated grid generation techniques are required; this will be developed in the
next Subsections.
6.2 Transfinite Interpolation

Elliptic grid generation requires an initial grid to start the iterative solution procedure. To obtain an acceptable initial grid transfinite interpolation has become a tool widely used (see [9]), which will be described in the following. A general function $F$ can be defined as

$$F(I, J) = \begin{bmatrix} x(I, J) \\ y(I, J) \end{bmatrix},$$  \hspace{1cm} (6.20)

where $I, J$ are parameters between 0 and the maximum number of nodes in $\xi$ and $\eta$ direction, $N_\xi$ and $N_\eta$, respectively. Now the one-dimensional interpolation projectors are expressed as

$$\mathcal{P}_I[F] = \phi_0(I) F(0, J) + \phi_1(I) F(N_\xi, J)$$  \hspace{1cm} (6.21)

$$\mathcal{P}_J[F] = \psi_0(J) F(I, 0) + \psi_1(J) F(I, N_\eta)$$  \hspace{1cm} (6.22)
using the blending functions $\phi_0$, $\phi_1$, $\psi_0$ and $\psi_1$. Here linear Lagrange polynomials are used as blending functions:

\[
\phi_0 (I) = \frac{N_\xi - I}{N_\xi} \quad (6.23)
\]

\[
\phi_1 (I) = \frac{I}{N_\xi} \quad (6.24)
\]

\[
\psi_0 (J) = \frac{N_\eta - J}{N_\eta} \quad (6.25)
\]

\[
\psi_1 (J) = \frac{J}{N_\eta} \quad (6.26)
\]

Finally the boolean sum projection

\[
(P_I \oplus P_J) = P_I [F] + P_J [F] - P_I P_J [F] \quad (6.27)
\]

gives the equation used to determine grid node locations in the given domain.

\[
F(I, J) = \frac{N_\xi - I}{N_\xi} \cdot F(0, J) + \frac{I}{N_\xi} \cdot F(N_\xi, J) + \frac{N_\eta - J}{N_\eta} \cdot F(I, 0) + \frac{J}{N_\eta} \cdot F(I, N_\eta)
\]

\[
- \frac{N_\xi - I}{N_\xi} \cdot \frac{N_\eta - J}{N_\eta} \cdot F(0, 0) - \frac{N_\xi - I}{N_\xi} \cdot \frac{J}{N_\eta} \cdot F(0, N_\eta)
\]

\[
- \frac{I}{N_\xi} \cdot \frac{N_\eta - J}{N_\eta} \cdot F(N_\xi, 0) - \frac{I}{N_\xi} \cdot \frac{J}{N_\eta} \cdot F(N_\xi, N_\eta) \quad (6.28)
\]

Since the initial grid obtained with linear blending functions is acceptable for the elliptic grid generation, no further effort was made to apply higher order functions. Fig. 6.6 shows a grid generated with transfinite interpolation (clustering at the lower boundary) as example. There are many more variations of transfinite interpolation, such as using normal vectors on the boundaries or employing higher order blending functions. In this work, however, we restrict ourselves to linear blending functions and the most simple form of transfinite interpolation and recommend [28] as additional reading.
6.3 Elliptic Grid Generation

Elliptic grid generation implies the solution of the Laplace or Poisson equation to obtain grid node locations. Detailed information can be found in [26], [13] and [9]. Although transfinite interpolation already gives useful grids to some extent, smoothness can be improved further by the application of elliptic grid generation. Additionally, there is a wide variety of grid control methods to achieve point clustering or orthogonality.

6.3.1 Governing Equations

A required step for finite difference methods is to solve equations around arbitrarily shaped geometries in the computational domain, providing a rectangular and uniformly spaced grid. Therefore the original grid has to be transformed into the computational domain and the physical coordinates \( x \) and \( y \) must be expressed in terms of coordinates \( \xi \) and \( \eta \) in the computational domain.

\[
\begin{align*}
    x &= x(\xi, \eta) \quad (6.29) \\
    y &= y(\xi, \eta) \quad (6.30) \\
    \xi &= \xi(x, y) \quad (6.31) \\
    \eta &= \eta(x, y) \quad (6.32)
\end{align*}
\]

The governing equations applied for elliptic grid generation are the Poisson equations given below.

\[
\begin{align*}
    \xi_{xx} + \xi_{yy} &= P(\xi, \eta) \quad (6.33) \\
    \eta_{xx} + \eta_{yy} &= Q(\xi, \eta) \quad (6.34)
\end{align*}
\]

In the case where the sources \( P \) and \( Q \) are zero, this is reduced to the Laplace equations. However, since often grid control is required to achieve satisfactory results, the Poisson equations with appropriate source terms are used in most of the cases. The metric terms \( \xi_{xx}, \xi_{yy}, \eta_{xx} \) and \( \eta_{yy} \) are not available initially. Instead the equations are transformed to

\[
\begin{align*}
    ax_{xx} - 2bx_{x\eta} + cx_{\eta\eta} &= -\frac{1}{J^2} (P_{\xi} x_{\xi} + Q_{\eta} x_{\eta}) \quad (6.35) \\
    ay_{xx} - 2by_{x\eta} + cy_{\eta\eta} &= -\frac{1}{J^2} (P_{\xi} y_{\xi} + Q_{\eta} y_{\eta}) \quad (6.36)
\end{align*}
\]
Table 6.1: Line and point clustering parameters.

<table>
<thead>
<tr>
<th>Array Name</th>
<th>Max. Entries</th>
<th>Growth Coeff.</th>
<th>Decay Coeff.</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_{\xi}$</td>
<td>$N_{\xi}$</td>
<td>$a_{\xi}$</td>
<td>$b_{\xi}$</td>
<td>cluster $\xi = \text{const. lines}$</td>
</tr>
<tr>
<td>$I_{\eta}$</td>
<td>$N_{\eta}$</td>
<td>$a_{\eta}$</td>
<td>$b_{\eta}$</td>
<td>cluster $\eta = \text{const. lines}$</td>
</tr>
<tr>
<td>$I_P, J_P$</td>
<td>$N_P$</td>
<td>$a_P$</td>
<td>$b_P$</td>
<td>cluster around points</td>
</tr>
</tbody>
</table>

with known metrical values $x_\xi, x_{\xi\eta}, \text{etc.}$. The coefficients $a, b, c$ and the Jacobian $J$ for the metrics are given by

\[
\begin{align*}
  a &= x_\eta^2 + y_\eta^2 \\
  b &= x_\xi x_\eta + y_\xi y_\eta \\
  c &= x_\xi^2 + y_\xi^2 \\
  J &= \frac{1}{x_\xi y_\eta - y_\xi x_\eta}
\end{align*}
\]  

(6.37) 

(6.38) 

(6.39) 

(6.40) 

With the known definition of the governing equations for the grid generation methods are discussed in the next Subsections, that allow the calculation of the required source terms.

6.3.2 Line and Point Clustering

The first important note with respect to line and point clustering is, that almost everything is based on experience. The coefficients used to increase or decrease clustering around special points or lines are not unique and some sort of iterative process, in which the user changes coefficients until the desired result is achieved, is involved. Further information can be found in [13].

The approach presented here requires the specification of arrays for the points and lines that need to be clustered. Within these arrays the numbers of the lines and points, that need to be clustered, are specified. Here, $a$ and $b$ with the relevant subscript denote the coefficients that control the clustering behaviour. Tab. 6.1 summarizes the information required for line and point clustering: Once the above information is known it can be
used to calculate the source terms according to

\[
P(i, j) = - \sum_{k=1}^{N_L} a_{L \xi}(k) \tau(i - I_{L \xi}(k)) \exp[-b_{L \xi}(k) |i - I_{L \xi}(k)|] \\
- \sum_{k=1}^{N_P} a_{P}(k) \tau(i - I_{P}(k)) \exp[-b_{P}(k) ((i - I_{P}(k))^2 + (j - J_{P}(k))^2)^{0.5}] \\

Q(i, j) = - \sum_{k=1}^{N_L} a_{L \eta}(k) \tau(j - J_{L \eta}(k)) \exp[-b_{L \eta}(k) |j - J_{L \eta}(k)|] \\
- \sum_{k=1}^{N_P} a_{P}(k) \tau(j - J_{P}(k)) \exp[-b_{P}(k) ((i - I_{P}(k))^2 + (j - J_{P}(k))^2)^{0.5}] 
\]

The function \( \tau \) allows the selection of symmetric and antisymmetric clustering:

\[
\tau(\chi) = \begin{cases} 
1 & \text{antisymmetric clustering} \\
\frac{1}{|\chi|} & \text{symmetric clustering}
\end{cases}
\]

The two graphs in Fig. 6.7 show the difference in symmetric and anti-symmetric line clustering, while a similar effect of symmetry and antisymmetry can be seen for point clustering in Fig. 6.8.

### 6.3.3 Orthogonality

Orthogonality at the boundary and its vicinity can significantly improve the solution produced by a numerical method. More or less the same approach is presented by [26], [13], [9] and [25]. In this Subsection the equations for orthogonality at the \( \eta = 0 \) boundary are presented in detail, although orthogonality might be required at the \( \eta = N_\eta, \xi = 0 \) and \( \xi = N_\xi \) boundaries as well. A similar approach applies to the remaining boundaries.
The basic idea is to modify the source term in a way that yields to orthogonal grids at the boundary and, depending on a decay coefficient, within the interior parts of the grid. The proposed functions for the source terms are

\begin{align*}
P(i, j) &= P_1(i, 0) \exp[-a_0 \eta] \\
Q(i, j) &= Q_1(i, 0) \exp[-b_0 \eta]
\end{align*}

where \(a_0\) and \(b_0\) are the decay coefficients mentioned above. For the initial values of \(P_1\) and \(Q_1\) at the \(\eta = 0\) boundary the following two equations

\begin{align*}
P_1 &= J(y_\eta R_1 - x_\eta R_2)|_{\eta=0} \\
Q_1 &= J(-y_\xi R_1 + x_\xi R_2)|_{\eta=0}
\end{align*}

\begin{align*}
R_1 &= -J^2 (ax_{\xi\xi} - 2bx_{\xi\eta} + cx_{\eta\eta})|_{\eta=0} \\
R_2 &= -J^2 (ay_{\xi\xi} - 2by_{\xi\eta} + cy_{\eta\eta})|_{\eta=0}
\end{align*}

There are different approaches suggested to avoid instabilities due to the sources at the boundaries. Hoffmann and Chiang [13] suggest backward and forward differencing for the metric terms \(x_\eta, y_\eta\) and others, depending on the sign of \(P_1\) and \(Q_1\). Below it can be seen that these terms are determined by the orthogonality condition and geometrical constraints due to the point position and the boundary definition (for \(\frac{\partial}{\partial \xi}\) derivatives). It therefore is unclear how Hoffmann and Chiang intend to apply backward and forward differencing to those terms. Steger and Sorenson suggest backward and forward differencing in combination with the following limitation (underrelaxation) of the source terms.
CHAPTER 6. GRID GENERATION

$P_1$ and $Q_1$:

\[
P_1^{(n+1)} = P_1^{(n)} + \omega_p \left[ J (y_\eta R_1 - x_\eta R_2)^{(n+1)} - P_1^{(n)} \right] \tag{6.50}
\]

\[
Q_1^{(n+1)} = Q_1^{(n)} + \omega_q \left[ J (-y_\xi R_1 - x_\xi R_2)^{(n+1)} - Q_1^{(n)} \right] \tag{6.51}
\]

The iteration index is indicated by $n$ and the parameters $\omega_p$ and $\omega_q$ are to be chosen between 0.02 and 0.06. However, this approach again leaves the question open of how to backward and forward difference these terms ($x_\eta$, $y_\eta$, etc.), which are constant throughout the iteration procedure. The application of the under-relaxation formula above didn’t prevent the solution procedure from diverging in most of the cases.

An alternative approach presented by Sorenson [25] (also used by Hall [9]) favours a combination of limiting and under-relaxing the source terms within the iteration according to

\[
P_1^{(n+1)} = P_1^{(n)} + \text{SIGN} \left\{ \min \left[ \omega_p \left| P_1 - P_1^{(n)} \right| , p_{\text{lim}} \max \left( \left| P_1^{(n)} \right| , 1 \right) \right] , P_1 - P_1^{(n)} \right\} \tag{6.52}
\]

\[
Q_1^{(n+1)} = Q_1^{(n)} + \text{SIGN} \left\{ \min \left[ \omega_q \left| Q_1 - Q_1^{(n)} \right| , q_{\text{lim}} \max \left( \left| Q_1^{(n)} \right| , 1 \right) \right] , Q_1 - Q_1^{(n)} \right\} \tag{6.53}
\]

where the SIGN function returns the magnitude of the first argument with the sign of the second argument. The coefficients $\omega_p$ and $\omega_q$ should be in the range from 0 to 1 and for $p_{\text{lim}}$ and $q_{\text{lim}}$ the value 0.5 is suggested. In the paper by Sorenson [25] no comment about backward and forward differencing is made. At this stage, it looks like the means to prevent instability is given by the limiting and under-relaxation formula above, and nothing else! It is unclear, how the approaches in the other papers can be implemented in a way they work.

The way orthogonality is achieved is by a special calculation of the $\frac{\partial}{\partial \eta}$ and $\frac{\partial}{\partial \eta \eta}$ derivatives. Provided $\Delta \xi$ and $\Delta \eta$ are equal to 1, the distance to the next point on the $\xi = \text{const.}$ grid line to the boundary point is $\Delta s = s_\eta$ and the angle of the $\xi = \text{const.}$ grid lines with the $\eta = \text{const.} = 0$ grid line is $\theta = \frac{\pi}{2}$, the following expressions for $x_\eta$ and $y_\eta$ can be given

\[
x_\eta (i, 0) = \frac{s_\eta (-x_\xi \cos \theta - y_\xi \sin \theta)}{(x_\xi^2 + y_\xi^2)^{0.5}} = \frac{-s_\eta y_\xi}{(x_\xi^2 + y_\xi^2)^{0.5}} \tag{6.54}
\]

\[
y_\eta (i, 0) = \frac{s_\eta (-y_\xi \cos \theta + x_\xi \sin \theta)}{(x_\xi^2 + y_\xi^2)^{0.5}} = \frac{s_\eta x_\xi}{(x_\xi^2 + y_\xi^2)^{0.5}} \tag{6.55}
\]

At this stage it is important to realize, that all derivatives so far are kept constant within the iteration procedure. The only terms changing within the iteration applied to solve
the Poisson equations are the second derivatives $x_{\eta}$ and $y_{\eta}$:

\[
x_{\eta}(i, 0) = \frac{-7x_{i,0} + 8x_{i,1} - x_{i,2}}{2} - 3x_{\eta}(i, 0) \tag{6.56}
\]

\[
y_{\eta}(i, 0) = \frac{-7y_{i,0} + 8y_{i,1} - y_{i,2}}{2} - 3y_{\eta}(i, 0) \tag{6.57}
\]

Another problem that has to be resolved is the possible inconsistency with orthogonal gridding very close to the boundary faces for $\xi = \text{const.} = 0$ and $\xi = \text{const.} = N_\xi$ lines. The situation becomes clear in Fig. 6.9. Therefore a procedure is being developed where a smooth transition from the boundary metrics $x_{\eta}(0, 0)$, $y_{\eta}(0, 0)$ and $x_{\eta}(N_\xi, 0)$, $y_{\eta}(N_\xi, 0)$ to the interior metrics $x_{\eta}(i, 0)$, $y_{\eta}(i, 0)$, that control the orthogonality, is achieved. As before, a coefficient is controlling the decay of the influence of the boundary metrics. Specifying left and right influence functions, the equations read as:

\[
f_{\text{left}}(I) = \exp \left( -a_{\text{left}} \frac{I}{N_\xi} \right) \tag{6.58}
\]

\[
f_{\text{right}}(I) = \exp \left( -a_{\text{right}} \left[ 1 - \frac{I}{N_\xi} \right] \right) \tag{6.59}
\]

\[
x_{\eta}(I, 0)|_{\text{new}} = f_{\text{left}}(I) x_{\eta}(0, 0) + f_{\text{right}}(I) x_{\eta}(N_\xi, 0) + [1 - f_{\text{left}}(I) - f_{\text{right}}(I)] x_{\eta}(I, 0) \tag{6.60}
\]

\[
y_{\eta}(I, 0)|_{\text{new}} = f_{\text{left}}(I) y_{\eta}(0, 0) + f_{\text{right}}(I) y_{\eta}(N_\xi, 0) + [1 - f_{\text{left}}(I) - f_{\text{right}}(I)] y_{\eta}(I, 0) \tag{6.61}
\]

Obviously, a similar treatment of the other grid faces is used. The derivatives important to achieve orthogonal gridding at the four faces are given in Tab. 6.2. Additionally, the list of parameters required for orthogonality control at each face is given in Tab. 6.3. Utilizing all the information given above, a wide variety of grids with orthogonality at the boundaries can be generated. Still there are difficulties: depending on the choice of parameters the convergence of the solution procedure is often difficult to achieve. The
<table>
<thead>
<tr>
<th>Face</th>
<th>Orthogonality</th>
<th>Non-constant Derivative</th>
</tr>
</thead>
<tbody>
<tr>
<td>South</td>
<td>( x_\eta (i, 0) = \frac{-8x_i \eta}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( x_{\eta\eta} = \frac{-7x_\eta y + 8x_\eta y - x_\eta}{2} - 3x_\eta (i, 0) )</td>
</tr>
<tr>
<td></td>
<td>( y_\eta (i, 0) = \frac{x_\eta y_i}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( y_{\eta\eta} = \frac{-7y_\eta y + 8y_\eta y - y_\eta}{2} - 3y_\eta (i, 0) )</td>
</tr>
<tr>
<td>East</td>
<td>( x_\xi (N_\xi, j) = \frac{8x_i \eta}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( x_{\xi\xi} = \frac{-7y \eta + 8x \eta + x_\eta - 2x_\eta}{2} + 3x_\xi (N_\xi, j) )</td>
</tr>
<tr>
<td></td>
<td>( y_\xi (N_\xi, j) = \frac{-8y_i \eta}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( y_{\xi\xi} = \frac{-7y \eta + 8y_\eta + y_\eta - 2y_\eta}{2} + 3y_\xi (N_\xi, j) )</td>
</tr>
<tr>
<td>North</td>
<td>( x_\eta (i, N_\eta) = \frac{-8x_i \eta}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( x_{\eta\eta} = \frac{-7y \eta + 8y_\eta + x_\eta - 2x_\eta}{2} + 3x_\eta (i, N_\eta) )</td>
</tr>
<tr>
<td></td>
<td>( y_\eta (i, N_\eta) = \frac{x_\eta y_i}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( y_{\eta\eta} = \frac{-7y \eta + 8y_\eta + y_\eta - 2y_\eta}{2} + 3y_\eta (i, N_\eta) )</td>
</tr>
<tr>
<td>West</td>
<td>( x_\xi (0, j) = \frac{8x_i \eta}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( x_{\xi\xi} = \frac{-7x_\eta y + 8y_\eta y - x_\eta}{2} - 3x_\xi (0, j) )</td>
</tr>
<tr>
<td></td>
<td>( y_\xi (0, j) = \frac{-8y_i \eta}{(x_i^2 + y_i^2)^{0.5}} )</td>
<td>( y_{\xi\xi} = \frac{-7y_\eta y + 8y_\eta y - y_\eta}{2} - 3y_\xi (0, j) )</td>
</tr>
</tbody>
</table>

Table 6.2: Derivatives for orthogonality at the boundaries.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Control of</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_0, b_0 )</td>
<td>decay of boundary source influence</td>
</tr>
<tr>
<td>( \omega_p, \omega_Q )</td>
<td>under-relaxation source strength iteration</td>
</tr>
<tr>
<td>( p_{lim}, q_{lim} )</td>
<td>limiting source strength iteration</td>
</tr>
<tr>
<td>( a_{left}, a_{right} )</td>
<td>decay of boundary metric influence</td>
</tr>
<tr>
<td>( \theta )</td>
<td>boundary metric slope (non-orthogonality)</td>
</tr>
</tbody>
</table>

Table 6.3: Parameters for orthogonality control.
parameters have to be selected with care to avoid non-physical situations. Another problem becomes obvious in Fig. 6.10: the orthogonality is not propagated into the domain properly, it ends abruptly producing a grid with non-smoothness in certain regions. A significant improvement, which finally allows to generate grids with satisfactory quality especially with respect to orthogonality, can be achieved following suggestions in [20]. Instead of the source term under-relaxation (Eqs. 6.52 and 6.53) suggested by Sorenson a source term limitation according to

\[
P_{\text{limited}} = \min (\max (P, P_{\text{min}}), P_{\text{max}}) \quad (6.62)
\]
\[
Q_{\text{limited}} = \min (\max (Q, Q_{\text{min}}), Q_{\text{max}}) \quad (6.63)
\]

is suggested. The limits for the source terms \(P_{\text{min}}, P_{\text{max}}, Q_{\text{min}}\) and \(Q_{\text{max}}\) have to specified in advance and their proper selection is based upon experience. A range from \(-1 \cdot 10^{10}\) to \(1 \cdot 10^{10}\) gave decent solutions. To all source terms within the prescribed limits a smoothing procedure is applied \(n\) times with a smoothing coefficient \(\omega\) and weights \(g_i\) in order to control the smoothing in special directions. Hence, the smoothed source terms are calculated according to

\[
P_{i,j}^{n+1} = \omega P_{i,j}^n + \frac{1 - \omega}{\sum g_k} (g_1 P_{i,j-1}^n + g_2 P_{i,j+1}^n + g_3 P_{i-1,j}^n + g_4 P_{i+1,j}^n) \quad (6.64)
\]
\[
Q_{i,j}^{n+1} = \omega Q_{i,j}^n + \frac{1 - \omega}{\sum g_k} (g_1 Q_{i,j-1}^n + g_2 Q_{i,j+1}^n + g_3 Q_{i-1,j}^n + g_4 Q_{i+1,j}^n) \quad (6.65)
\]

Typical values for the parameters are \(n = 10, \omega = 0.75\) and \(g_i = 1 \ldots 4 = 1\). In Fig. 6.11 an examples for full smoothing and 'north-south' smoothing \((g_2 = g_4 = 0)\) are given. With a variety of tools for grid generation developed, the grids generated for test and thesis cases can be presented in the following Subsections.
6.4 Grids for Test Cases

In this Section the grids required for the test cases are presented in order to allow insight into why a special type of grid design was used. The meshes are presented without information on the domain size and are not always shown with a dependent scaling of the two spatial dimensions, mostly to allow a better visibility of the grid lines, especially, for very narrow domains as in the case of flat plate or diffusion flow problems. Detailed information about the domain size will be given in the Chapter discussing the results of the test cases.

6.4.1 Free Stream Flow

The reactive free stream flow uses the most simple grid possible. a rectangular domain with equally spaced grid lines. In the streamwise direction 150 cells, and normal to it 10 cells are used, which adds up to a total of 1500 cells, as it can be seen in Fig. 6.12.

![Figure 6.12: Grid for reactive free stream flow.](image)

The second free stream flow problem, examining the diffusion of a species in the top half of the domain into another in the bottom half of the domain, is similar to a flat plate problem. Therefore the grid is generated clustering grid lines close to the inflow
boundary on the left and also along the contact region in the middle of the domain. To ease the initialization and inflow situation with two different mass fractions on the same domain boundary, a two block grid system is created, which can be seen in Fig. 6.13. Each block has 25 cells in the streamwise and 25 cells in the other direction, adding up to 1250 cells.

![Grid for diffusion problem](image)

Figure 6.13: Grid for diffusion problem (aspect ratio not maintained).

### 6.4.2 Flat Plate Flow

The grid used to calculate the flow over a flat plate is similar to the grid blocks used for the diffusion problem, but this time 100 cells are used in horizontal and 50 cells in vertical direction. This gives 5000 cells in total and the grid presented in Fig. 6.14.

### 6.4.3 Wedge Flow

The three test cases simulating wedge flow have to simulate certain physical features and therefore the grids used are generated accordingly. Firstly, a shock angle for inviscid, nonreactive flow is examined and compared with theoretical results. Since this type of flow does not pose too much of a problem a relatively coarse grid with 80 cells horizontally and 50 cells vertically, adding up to 4000 cells in total, is used. The resulting grid is given in Fig. 6.15. Secondly, a viscous nonreactive corner flow is calculated. Therefore grid lines close to the wall need to be clustered sufficiently in order to provide a satisfactory boundary layer.
resolution. Also regions of flow separation and reattachment need to be resolved properly in the case of their appearance. For this, two blocks with 75 cells in streamwise and 100 cells normal to it are generated for each block with clustering close to the wall, at the inflow and at the intersection of the two blocks. Fig. 6.16 shows the resulting grid system with 15000 cells in total.

Thirdly, an inviscid, reactive wedge flow is solved to obtain information about the location and angle of the detonation wave generated. This implies that the grid should be relatively fine, but without clustering at inflow or the wall. We use 300 by 100 cells, adding up to 30000 cells in total, as presented in Fig. 6.17.
6.4.4 Channel Flow

The three block grid system for the channel flow must be able to resolve boundary layers and separation regions close to the wall properly. For this grid lines close to the walls are clustered, resulting in 30 by 100 cells for the first two blocks and 90 by 100 cells for the last block. In total this gives 15000 cells for the grid system presented in Fig. 6.18.

6.4.5 Blunt Body Flow

For the blunt body flow a grid is developed around a circle segment with 0.01m diameter. The minimal grid spacing on the cylinder wall has a spacing of $1 \cdot 10^{-6}m$ with 125 cells in angular and 150 in radial direction. The resulting grid with 1875 cells is shown in Fig. 6.19.
Figure 6.18: Grid for viscous channel flow.

Figure 6.19: Grid for viscous blunt body flow.
6.5 Grids for Thesis Cases

Although the details of the geometrical specifications for the thesis cases will be explained in a later Chapter, the basic concepts for the generation of the multi-block grid system for the thesis cases are introduced here. A ten block multi-block grid system is developed where certain blocks are interchangeable to allow changes with respect to geometry or boundary grid line clustering. The difficulty created by the geometrical shape of the flow domain is that a circular body has to be fitted into a rectangular channel. In order to solve this problem the arrangement shown in Fig. 6.20 is suggested.

The physical block numbers and the numbering required for the sweeps in the LU-SGS scheme in brackets are given within each block. Blocks 3, 7 and 9 at the top boundary are exchangeable and can consist of grids generated for inviscid or viscous flows. This is required in the case where the symmetry line is replaced by a solid wall, which is of great importance for future investigations of this problem. However, in this work a solid boundary is only present in the form of a cylinder. Before the inner grid ring consisting of blocks 0 and 4 is presented for the different blunt body diameters 0.010m, 0.015m and 0.020m, we have a closer look at the whole gridding for the thesis case with a blunt body diameter of 0.010m shown in Fig. 6.21. The computational domain is mirrored around the streamwise axis cutting the cylinder in to two halves and both the computational domain and its image are displayed. The domain height (image included) is 0.060m, its length 0.1m and the centre of the blunt body located 0.024m downstream from the leading edge of the domain.

An adjustment of this grid system to different diameters or different flow types around the cylinder, inviscid or viscous, is possible by generating appropriate ‘inner circle’ grid
Figure 6.21: Thesis case grid and its image.
blocks. Hence, grid block 0 and 4 are generated with respect to the needs yielding to a selection of six different block types. In Figs. 6.22, 6.23 and 6.24 the results for the three diameters 0.010m, 0.015m and 0.020m are given, with the grids for inviscid flow in the top and those for viscous flow on the bottom half. Finally, the grid details for all grids generated to spatially discretize the flow domain of the thesis cases are summarized in Tab. 6.4. For all blocks applicable the blunt body diameter is given in column ‘$\sigma$’, while the number of cells in $\xi$-direction is denoted with $N_{\xi}$, that in $\eta$-direction with $N_{\eta}$ and the total number of cells is $N_{\text{total}}$. The following abbreviations are used for the grid generation methods: $TFI$ stands for transfinite interpolation, $LI$ for linear interpolation between the boundaries, $RI$ for radial interpolation between boundaries using radius and angle and $PE$ for Poisson equation with the appropriate selection of source terms to ensure orthogonality. Furthermore, the minimum grid line spacing for inner grid ring circles is given by $\Delta s_{\text{min}}$ and the last grid line spacing by $\Delta s_{\text{max}}$. In the case of grids used for viscous flow the maximum grid line spacing for blocks 0 and 4 is adjusted to the spacing of the adjacent grid blocks 1 and 5, which ensures a very smooth transition from the inner block ring to the neighbouring grid blocks.

Finally, the total number of cells for each thesis case summarizes to the values in column

Figure 6.22: Inner grid ring (10mm diameter).
Figure 6.24: Inner grid ring (20mm diameter).

Figure 6.23: Inner grid ring (15mm diameter).
<table>
<thead>
<tr>
<th>Block</th>
<th>( \delta )</th>
<th>( N_\xi )</th>
<th>( N_\eta )</th>
<th>( N_{\text{total}} )</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>0. inv.</td>
<td>0.010m</td>
<td>35</td>
<td>50</td>
<td>1750</td>
<td>( TFI )</td>
</tr>
<tr>
<td>0. vis.</td>
<td>0.010m</td>
<td>60</td>
<td>50</td>
<td>3000</td>
<td>( RI, \Delta s_{\text{min}} = 1.0 \cdot 10^{-6}, \Delta s_{\text{max}} = 2.3 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>0. inv.</td>
<td>0.015m</td>
<td>21</td>
<td>50</td>
<td>1050</td>
<td>( TFI )</td>
</tr>
<tr>
<td>0. vis.</td>
<td>0.015m</td>
<td>45</td>
<td>50</td>
<td>2250</td>
<td>( RI, \Delta s_{\text{min}} = 1.5 \cdot 10^{-6}, \Delta s_{\text{max}} = 2.3 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>0. inv.</td>
<td>0.020m</td>
<td>10</td>
<td>50</td>
<td>500</td>
<td>( TFI )</td>
</tr>
<tr>
<td>0. vis.</td>
<td>0.020m</td>
<td>31</td>
<td>50</td>
<td>1550</td>
<td>( RI, \Delta s_{\text{min}} = 2.0 \cdot 10^{-6}, \Delta s_{\text{max}} = 2.3 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>1</td>
<td>-</td>
<td>40</td>
<td>50</td>
<td>2000</td>
<td>( PE, 2 \times ) orthogonal boundary</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>40</td>
<td>50</td>
<td>2000</td>
<td>( PE, 2 \times ) orthogonal boundary</td>
</tr>
<tr>
<td>3, inv.</td>
<td>-</td>
<td>10</td>
<td>50</td>
<td>500</td>
<td>( LI )</td>
</tr>
<tr>
<td>4, inv.</td>
<td>0.010m</td>
<td>35</td>
<td>50</td>
<td>1750</td>
<td>( TFI )</td>
</tr>
<tr>
<td>4, vis.</td>
<td>0.010m</td>
<td>60</td>
<td>50</td>
<td>3000</td>
<td>( RI, \Delta s_{\text{min}} = 1.0 \cdot 10^{-6}, \Delta s_{\text{max}} = 2.3 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>4, inv.</td>
<td>0.015m</td>
<td>21</td>
<td>50</td>
<td>1050</td>
<td>( TFI )</td>
</tr>
<tr>
<td>4, vis.</td>
<td>0.015m</td>
<td>45</td>
<td>50</td>
<td>2250</td>
<td>( RI, \Delta s_{\text{min}} = 1.5 \cdot 10^{-6}, \Delta s_{\text{max}} = 2.3 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>4, inv.</td>
<td>0.020m</td>
<td>10</td>
<td>50</td>
<td>500</td>
<td>( TFI )</td>
</tr>
<tr>
<td>4, vis.</td>
<td>0.020m</td>
<td>31</td>
<td>50</td>
<td>1550</td>
<td>( RI, \Delta s_{\text{min}} = 2.0 \cdot 10^{-6}, \Delta s_{\text{max}} = 2.3 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>40</td>
<td>50</td>
<td>2000</td>
<td>( PE, 2 \times ) orthogonal boundary</td>
</tr>
<tr>
<td>6</td>
<td>-</td>
<td>40</td>
<td>50</td>
<td>2000</td>
<td>( PE, 3 \times ) orthogonal boundary</td>
</tr>
<tr>
<td>7, inv.</td>
<td>-</td>
<td>10</td>
<td>50</td>
<td>500</td>
<td>( LI )</td>
</tr>
<tr>
<td>8</td>
<td>-</td>
<td>40</td>
<td>100</td>
<td>4000</td>
<td>( LI )</td>
</tr>
<tr>
<td>9, inv.</td>
<td>-</td>
<td>10</td>
<td>100</td>
<td>1000</td>
<td>( LI )</td>
</tr>
</tbody>
</table>

Table 6.4: Individual grid blocks for thesis cases.
### Table 6.5: Total number of grid cells for thesis cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\phi$</th>
<th>$N_{\text{total}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, inv.</td>
<td>0.010$m$</td>
<td>17500</td>
</tr>
<tr>
<td>1, vis.</td>
<td>0.010$m$</td>
<td>20000</td>
</tr>
<tr>
<td>2, inv.</td>
<td>0.015$m$</td>
<td>16100</td>
</tr>
<tr>
<td>2, vis.</td>
<td>0.015$m$</td>
<td>18500</td>
</tr>
<tr>
<td>3, inv.</td>
<td>0.020$m$</td>
<td>15000</td>
</tr>
<tr>
<td>3, vis.</td>
<td>0.020$m$</td>
<td>17100</td>
</tr>
</tbody>
</table>

$N_{\text{total}}$ given in Tab. 6.5.
Chapter 7

Test Cases

In this Chapter a selection of test cases is presented that is used to validate the flow solver. The test cases are suitable to verify proper physical behaviour for a wide range of aspects, from chemical models to boundary layers in blunt body flows. This will ensure that the thesis cases, the actual problems to be solved, will give meaningful answers. Most of the test cases are qualitatively or quantitatively compared with experimental, analytical or numerical results obtained by other researchers.

7.1 Point Chemistry

Although the direct comparison with experimental results is not presented here, the point chemistry test cases allow insight into the chemical behaviour of the different reaction schemes and the appropriate species properties. The analysis is carried out in a constant volume environment, which implies that the density of the mixture will remain constant. Obviously all velocity components and the heat transfer to the imaginary cell are zero, so that an adiabatic, constant density control volume is used to examine chemical behaviour depending on a wide range of initial conditions. The chemical schemes of interest are presented in Tab. 7.1. The air-hydrogen scheme with 13 species and 33 reactions is widely used for high speed combustion problems of air and hydrogen, especially in the field of ramjets and scramjets. It does treat nitrogen as reactive component, while the similar scheme with 9 species and 19 reactions assumes nitrogen to be inert. Similar behaviour for most cases can be expected for both air-hydrogen schemes, however, apart from the missing nitrogen reaction equations two equations from the 33 reactions scheme are combined to form one equation in the 19 reactions scheme. The oxygen-hydrogen
scheme containing 8 species and 17 reactions, is computationally cheaper to solve and a useful addition to the air-hydrogen schemes, which allows the solution of pure rocket propulsion problems.

Of particular interest is a first estimate of ignition delay times within the unperturbed freestream and under ‘idealized’ flow conditions directly after the first shock generated by the blunt body. The flow conditions after the shock are called ‘idealized’ because we use air with constant specific heat ratio for the calculation of pressure and temperature after the shock and additionally neglect the fact that instant combustion after the shock might transform the shock wave to a detonation wave. This simplification may be allowable here, however, for the solution of the real thesis cases problems a more realistic modelling must be used. To conclude, three types of initial conditions are used, where the first two address changes of inflow conditions and the last conditions after the first shock. Firstly, the temperature is varied at constant pressure, secondly the pressure is varied at constant temperature and thirdly the pressure and temperature are both varied according to the relevant shock relations.

7.1.1 Initial Conditions

The initial conditions for the point chemistry test cases are based upon those relevant for the thesis cases, whereby inflow conditions for the latter will be outlined in a later Chapter. In detail, the inflow Mach number is 5, the static pressure $10000 Pa$ and the static temperature $700 K$, while the gas is premixed stoichiometrically. Hence, the mass fractions for the oxygen-hydrogen mixture are $Y_{O_2} = 0.888$ and $Y_{H_2} = 0.112$ and those for the air-hydrogen mixture $Y_{N_2} = 0.743$, $Y_{O_2} = 0.228$ and $Y_{H_2} = 0.029$. In order to cover a range most relevant to the thesis cases we assume that the lower limit of parameters is roughly prescribed by the inflow conditions and the upper limit by the gas mixture passing through a normal shock in front of the blunt body. Assuming the specific heat
ratio of air as $\gamma = 1.4$ we calculate an approximation for the maximum temperature and pressure behind the normal shock according to

$$\frac{T_2}{T_1} = \frac{[2\gamma Ma^2 - (\gamma - 1)] \cdot [2 + (\gamma - 1) Ma^2]}{(\gamma + 1)^2 Ma^2} \quad (7.1)$$

$$\frac{p_2}{p_1} = \frac{2\gamma Ma^2 - (\gamma - 1)}{\gamma + 1} \quad (7.2)$$

where the index 1 stands for values before the shock and 2 for those after the shock. We can also directly relate the pressure ratios $p_{21} = \frac{p_2}{p_1}$ to the temperature ratios $T_{21} = \frac{T_2}{T_1}$ following

$$T_{21} = p_{21} \frac{\frac{\gamma - 1}{\gamma + 1} p_{21} + 1}{p_{21} + \frac{\gamma - 1}{\gamma + 1}} \quad (7.3)$$

Certainly this is a strong simplification since the specific heat ratio for a multi-species gas is not constant, but for a very rough first guess it is satisfactory. For the inflow Mach number of 5 we obtain $T_{21} = 5.8$ and $p_{21} = 26$ which can easily be verified by shock tables (see [33]). Fig. 7.1 shows the graphs for the equations relating pressure and temperature ratios of a normal shock to the inflow Mach number. However, for real gas flows the resulting temperatures after a shock cannot be above the adiabatic flame temperature. Therefore, within this analysis, the upper temperature examined is limited to 2500K for all schemes.

It is important to realize that the shock generated by a circular blunt body is a bow shock that becomes approximately normal for the streamline ending in the stagnation point. Despite the constant inflow Mach number the Mach number normal to the bow shock is, depending on the location, significantly lower and we therefore need to analyse a Mach number range. This range is defined beginning with a Mach number of zero and ending at a Mach number of five, combined with the initial temperature of 700K and the pressure of 10000Pa. Hence, for the point chemistry analysis we vary the shock strength directly via the pressure ratio $p_{21}$ and indirectly via the temperature ratio $T_{21}$. Subsequently we cover most of the conditions shortly after the bow shock with our selection of initial conditions for the point chemistry, consisting of $T_2$ and $p_2$.

The total time for the time accurate calculations is 0.01s at a prescribed time step varying from $1 \cdot 10^{-10}$ to $1 \cdot 10^{-7}s$, depending on the initial conditions. Although the stability of the numerical computation with the implicit treatment of the source term allows a larger time step, a relatively small one is used for accuracy reasons. Using a
Temperature and Pressure Ratios for Normal Shock

(a) $\frac{T_2}{T_1}$ and $\frac{p_2}{p_1}$ as function of $Ma$ number

(b) $T_{21} = T_{21}(p_{21})$

Figure 7.1: Temperature and pressure ratios for normal shock.
Table 7.2: Initial conditions for point chemistry

second order accurate implicit trapezoidal time marching method this therefore provides accurate answers for all chemical schemes examined. At the given inflow conditions the total time allows a particle to travel a distance of about 26m, which is 260 times the thesis cases channel length. Consequently, a resulting ignition delay of more than 0.01s is by far too long for the examined problems and would be considered as initial conditions that do not lead to an ignition of the gas mixture.
7.1.2 Oxygen-Hydrogen, 8 Species and 17 Reactions

For the oxygen-hydrogen system the results with the same initial pressure and varying temperature are presented in Fig. 7.2 and those with varying initial pressure and temperature in Fig. 7.3. In none of the cases with varying initial pressure and the same initial temperature of 700K ignition could be observed.

7.1.3 Air-Hydrogen, 9 Species and 19 Reactions

The air-hydrogen system with inert nitrogen yields the results presented in Fig. 7.4 for the same initial pressure and varying initial temperature and in Fig. 7.5 for varying initial pressure and temperature. Again, none of the cases with the same initial temperature of 700K and varying initial pressure leads to ignition.

7.1.4 Air-Hydrogen, 13 Species and 33 Reactions

The results for the 'full' air-hydrogen scheme are very similar to those of the scheme presented in the previous Subsection, apart from the fact that the ignition delay times
Figure 7.3: Temperature graphs for oxygen-hydrogen system at varying pressure.

Figure 7.4: Temperature graphs for air-hydrogen system \((N_2\text{ inert})\) at constant pressure.
are slightly reduced especially for the lower initial temperatures. This can be observed in Figs. 7.6 and 7.7. With a fixed initial temperature of 700\textdegree K no ignition is observed for all initial pressures observed, as it was the case with the schemes presented previously.
Figure 7.6: Temperature graphs for air-hydrogen system at constant pressure.

Figure 7.7: Temperature graphs for air-hydrogen system at varying pressure.
7.1.5 Ignition Delay Times

The ignition delay times for all schemes and all initial conditions examined are presented in Fig. 7.8. As one can expect, the ignition delay times for both the initial pressure and temperature increased according to the shock relations are significantly shorter than those with only the initial temperature increased at constant initial pressure of 10000Pa. Also, the ignition delay times of the oxygen-hydrogen scheme are lower than those of the air-hydrogen schemes. The full air-hydrogen scheme yields slightly shorter ignition delay times than the air-hydrogen scheme with inert nitrogen. In contrast to an often used definition of the ignition delay as a 10% increase in temperature here a slightly different limit is used to accommodate the fact that for high initial temperatures the temperature rise in total is much less than for low initial temperatures. Therefore the limit used for the determination of the ignition delay times is a 1% increase of the initial temperature. One vital result of this analysis is that the blunt body within the flowfield can shorten the ignition delay time by about three orders of magnitude, for all schemes examined. The oblique shock due to a wedge at certain angle of attack does not
produce an increase of pressure and temperature as high as the blunt body does. Hence, it can be expected that a scramjet combustor utilizing a wedge generated ignition for the same initial conditions yields a much longer combustor length than the combustor with embedded blunt bodies. At similar geometrical dimensions the blunt body generated combustion should work for lower combustor inflow temperatures and consequently lower flight Mach numbers as the wedge generated does. It should be noted that the inflow Mach number influences the combustor inflow temperature since more kinetic energy can be utilized for the compression.
7.2 Freestream

Non-reactive free-stream flow is only of interest to validate a flow solver for the very first time. If the flow solver does not maintain free-stream most likely something with the spatial discretization is not working properly. For the flow solver used within this work it is ensured that freestream is maintained for single- and multi-block configurations. Due to the simplicity of the results they are not presented here.

Two more interesting cases are presented instead. The first is a transfer of the point chemistry problem to a two dimensional flow domain - the first step to validate the functionality of the source term calculation and its Jacobian matrix within a real flow solver context. Furthermore, the flux Jacobian matrices and the corresponding eigenvector matrices are needed in addition. Still, the flow problem itself does not additionally complicate the task that has to be solved. No recirculation or strong shocks due to a directional change of the flow are imposed. Also, only inviscid flow with symmetry boundary conditions at the lower and upper boundary is considered here.

The second case is important to compare the diffusion rates with solutions derived analytically. For this, two jets with different species are entering a 'free-stream domain' at the same velocity and pressure. For Navier-Stokes flow with diffusion included in the physical model the exact boundary between the two species increasingly smears out and the region with a gas mixture spreads normal to the flow direction. It is important to note that this is a non-reactive multi-species flow. In order to focus attention on the diffusion the chemical species production and destruction is switched off.

7.2.1 Supersonic Combustion

The supersonic combustion problem has been solved in [24] already and its setup is given in Fig. 7.9. It is stressed again, that inviscid multi-species flow with initial conditions as given in Tab. 7.3 is solved. The results from the numerical computation are in excellent agreement with those in [24]. This is not surprising, because the same numerical methods are used to solve the problem. The residual of the computation is shown in Fig. 7.10 and the resulting Mach number contours and temperature and pressure in streamwise direction in Figs. 7.11 and 7.12. The mass fractions in the streamwise direction are given in Figs. 7.13 and 7.14. The streamwise location for a 10% increase in temperature, defined as ignition of the gas flow, is located at \( x = 0.319m \) and the maximum resulting temperature of \( 2938K \) agree well with results previously obtained (see [24]). This ensures
Supersonic Combustion Problem

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Inflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>pressure $p$</td>
<td>$1 \cdot 10^8 Pa$</td>
</tr>
<tr>
<td>temperature $T$</td>
<td>$1100K$</td>
</tr>
<tr>
<td>Mach number $Ma$</td>
<td>8</td>
</tr>
<tr>
<td>mass fractions $Y_i$</td>
<td>$Y_{N_2} = 0.743, Y_{O_2} = 0.228, Y_{H_2} = 0.029$</td>
</tr>
<tr>
<td>chemical model</td>
<td>air-hydrogen: 13 species, 33 reactions</td>
</tr>
</tbody>
</table>

Table 7.3: Initial conditions for supersonic combustion problem.

that the species properties, the reaction scheme and the Jacobian matrices for both source term and inviscid fluxes are working well.
Figure 7.10: Residual for supersonic combustion problem.

Figure 7.11: Mach number contours for supersonic combustion problem.
Figure 7.12: Pressure and temperature for supersonic combustion problem.

Figure 7.13: Mass fractions without nitrogen for supersonic combustion problem.
Figure 7.14: Mass fractions with for supersonic combustion problem.
7.2.2 Diffusive Mixing

The mixing problem analysed here is given in Fig. 7.15 and its inflow conditions are summarized in Tab. 7.4. Firstly, an analytical procedure of determining the mole fraction in the mixing layer is presented, and secondly, the results of the numerical method are given and compared to the analytical ones.

The type of mixing problem with the same velocity for both the nitrogen and oxygen gas jet is referred to as 'zero-shear mixing layer' (see [10]). Thus, the local rate of molecular diffusion is given by Fick's law, which states that the time rate of molecular transport of two species into each other is proportional to the product of the interfacial

![Diagram of mixing of parallel streams of nitrogen and oxygen.](image)

**Figure 7.15: Mixing of parallel streams of nitrogen and oxygen.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Jet 1</th>
<th>Jet 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>velocity ( u )</td>
<td>( 1000 \text{m/s} )</td>
<td></td>
</tr>
<tr>
<td>pressure ( p )</td>
<td>( 1 \cdot 10^5 \text{Pa} )</td>
<td></td>
</tr>
<tr>
<td>temperature ( T )</td>
<td>( 273.2 \text{K} )</td>
<td></td>
</tr>
<tr>
<td>mass fractions ( Y_i )</td>
<td>( Y_{N_2} = 1, Y_{O_2} = 0 )</td>
<td>( Y_{N_2} = 0, Y_{O_2} = 1 )</td>
</tr>
<tr>
<td>chemical model</td>
<td>nitrogen-oxygen: 2 species, 0 reactions</td>
<td></td>
</tr>
</tbody>
</table>

**Table 7.4: Initial conditions diffusive mixing.**
area and the local concentration gradient. The proportionality constant is the diffusion coefficient $D_{12}$ already introduced in an earlier Chapter. In [10] the interesting statement is made that the product of density and diffusion coefficient $\rho D_{12}$ is approximately equal to the dynamic viscosity $\mu_{12}$ for most gases, and therefore varies approximately with the square root of the temperature as the dynamic viscosity does. However, for our initial conditions we find the diffusion coefficient for a $N_2 - O_2$ system to be $D_{N_2-O_2} = 1.75 \cdot 10^{-5} m^2/s$ according to kinetic gas theory and $D_{N_2-O_2} = 1.81 \cdot 10^{-5} m^2/s$ according to experiments (see p. 579 in [12]). We use the value obtained by means of kinetic gas theory for our analytical calculation since we want to validate the details of the numerical method dealing with diffusion, which uses a calculated coefficient as well. It would be counterproductive to use different values for the diffusion coefficient because an assessment of the accuracy of this coefficient calculated by means of the kinetic gas theory with respect to experimental values is not in the scope of this research. Following [10] (p. 283) we find for the thickness $\delta_m$ of the mixing layer the approximation

$$\delta_m \approx 8 \sqrt{\frac{D_{N_2-O_2} \cdot x}{u}}$$

(7.4)

where $x$ is the position downstream in the computational domain as outlined in Fig. 7.15 and $u$ the inflow velocity of the two jets. Further, we can calculate the mole fraction of nitrogen according to

$$X_{N_2} = 0.5 \left[ 1 + \text{erf} \left( \frac{4y}{\delta_m} \right) \right]$$

(7.5)

with the error function defined as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

(7.6)

The last step is to calculate the resulting mass fraction via the well known equation (see earlier Chapter)

$$Y_{N_2} = \frac{X_{N_2} M_{N_2}}{M}$$

where $M$ is the molecular weight of the gas mixture. The mass fraction for oxygen can then be calculated by subtracting the mass fraction of hydrogen from one.

Results obtained by the numerical method developed vary significantly, depending on the magnitude of entropy correction ($\bar{e}$) used. Three cases are computed with $\bar{e} = 0.2, 0.5$
and 1.5, where the latter value is typically chosen for blunt body flows. A look at the residual in Fig. 7.16 shows that for this problem the entropy correction $\varepsilon$ significantly influences the convergence, the higher $\varepsilon$ the better the convergence. The resulting Mach number contours for $\varepsilon = 0.5$ are presented in Fig. 7.17. The solution is being smeared out significantly with increasing entropy correction, especially for the highest value examined. The nitrogen mass fractions at the outflow boundary of the domain shown in Fig. 7.18 clearly proof the overestimation on diffusion that will occur for blunt body flows as they are examined in this paper. In conclusion, we can state that the proper calculation of the physical diffusion process with the flow solver developed here is difficult and, to some extend, unsatisfactory. The accurate calculation of the diffusion is a problem worth while looking at in future research.

![Figure 7.16: Residual diffusion problem.](image)
Figure 7.17: Nitrogen mass fraction contours for the diffusion problem.

Figure 7.18: Nitrogen mass fraction at the outflow boundary of the diffusion problem.
7.3 Flat Plate Flow

As in the case of the freestream flow, calculations of flow over a flat plate are used to verify a component of the flow solver, this time the viscous terms. Before the results are presented and compared with those found in [16], we have a look at the problem described in Fig. 7.19 and the relevant inflow conditions in Tab. 7.5. The residual for

![Diagram of Viscous Flow on Flat Plate]

Figure 7.19: Viscous flow on flat plate with fixed wall temperature.

<table>
<thead>
<tr>
<th>Flat Plate Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
</tr>
<tr>
<td>pressure $p$</td>
</tr>
<tr>
<td>temperature $T$</td>
</tr>
<tr>
<td>wall temperature $T_w$</td>
</tr>
<tr>
<td>Mach number $Ma$</td>
</tr>
</tbody>
</table>

Table 7.5: Initial conditions for viscous flow on flat plate.

the calculation of the flat plate flow is shown in Fig. 7.20 and the contours of the velocity $u$ in the $x$-coordinate direction in Fig. 7.21. More important, however, are the $u$ velocity and temperature profiles in direction normal to the flat plate, taken at a streamwise position of $x = 0.915m$ and the skin friction and heat transfer coefficients along the flat
Figure 7.20: Residual for viscous flow on flat plate.

plate. They are given in Figs. 7.22 to 7.24 and, apart from the highest temperature (Fig. 7.22 b)), which is not quite reached in the computation with the numerical method developed here, the agreement is good and confirms the accurate calculation of viscous terms.
Figure 7.21: $u$ velocity contours for viscous flow on flat plate.

Figure 7.22: Velocity (a) and temperature (b) profile for viscous flow on flat plate.
Figure 7.23: Skin friction coefficient for viscous flow on flat plate.

Figure 7.24: Heat transfer coefficient for viscous flow on flat plate.
7.4 Wedge

The wedge cases examine the redirection of flow due to a solid boundary. First, a comparison with theoretical results is made by analyzing inviscid non-reactive flow over a wedge.

The second case, often referred to as ‘corner flow’, is posing a difficult problem involving viscous flow with boundary layer and wedge generated shocks that interact with each other.

The selection of wedge cases is completed by a comparison with an inviscid reactive wedge flow containing a shock and detonation wave.

7.4.1 Oblique Shock

The setup for the oblique shock due to a wedge is given in Fig. 7.25 and the initial conditions for the case in Tab. 7.6. Following the theory for inviscid compressible flows the resulting shock wave has an angle of 13.77 degrees for the given inflow conditions. This result is also obtained by the numerical computation done here (14.0 degrees shock angle). Its residual is given in Fig. 7.26 and the resulting Mach number contours in Fig. 7.27. It can therefore be stated that the code developed here is capable of calculating basic shock waves for inviscid flows.

Figure 7.25: Oblique shock flow problem.
Table 7.6: Initial conditions for oblique shock flow problem.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Inflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>pressure ( p )</td>
<td>475 Pa</td>
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<tr>
<td>temperature ( T )</td>
<td>240.28 K</td>
</tr>
<tr>
<td>Mach number ( Ma )</td>
<td>12</td>
</tr>
</tbody>
</table>

Figure 7.26: Residual for oblique shock flow.

Figure 7.27: Mach number contours for oblique shock flow.
7.4.2 Corner Flow

The next step is to validate the interaction of shocks with boundary layers. This is done with the test case presented in Fig. 7.28 with the initial conditions given in Tab. 7.7.

<table>
<thead>
<tr>
<th>Corner Flow</th>
<th>Inflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>parameter</td>
<td>Inflow</td>
</tr>
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<td>pressure ( p )</td>
<td>15.7 Pa</td>
</tr>
<tr>
<td>temperature ( T )</td>
<td>88.89 K</td>
</tr>
<tr>
<td>wall temperature ( T_w )</td>
<td>297 K</td>
</tr>
<tr>
<td>Mach number ( Ma )</td>
<td>14.1</td>
</tr>
</tbody>
</table>

Table 7.7: Initial conditions for corner flow problem.

Special characteristics of this test case are the very low inflow pressure and temperature combined with a high Mach number. The residual of the computation performed is shown in Fig. 7.29 and the resulting Mach number and pressure contours in Figs. 7.30 and 7.31. A strong shock-boundary layer interaction can be found for both of the contour plots.

The pressure coefficient is compared with results presented in [16]. Fig. 7.32 shows the comparison between the result from the code developed here and that obtained by Lawrence, Tannehill and Chaussee. The calculation of the pressure coefficient presented
in the paper was applied to the result of the code used for this work. Acceptable agreement is achieved for this cases although some grid refinement might be of interest to improve the pressure coefficient in the beginning of the second half of the wall. Overall, the prediction of flows involving shock-boundary layer interaction is validated with this case.

Figure 7.29: Residual for corner flow.
Figure 7.30: Mach number contours for corner flow.

Figure 7.31: Pressure contours for corner flow.

Figure 7.32: Pressure coefficient for corner flow.
7.4.3 Reactive Wedge Flow

Although this case is only an inviscid one it involves a premixed air-hydrogen gas flow in order to further validate the proper simulation of reactive flows. The geometrical setup is similar to that of the wedge flow examined in a previous Subsection. However, dimensions are changed as it can be seen in Fig. 7.33. The initial conditions are presented in Tab. 7.8. including the mass fractions of the stoichiometrically premixed gas. The residual,

![Diagram of reactive wedge flow]

Figure 7.33: Reactive wedge flow.

<table>
<thead>
<tr>
<th>Reactive Wedge Flow</th>
<th>Inflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
<td></td>
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<tr>
<td>pressure $p$</td>
<td>23000 Pa</td>
</tr>
<tr>
<td>temperature $T$</td>
<td>900K</td>
</tr>
<tr>
<td>Mach number $Ma$</td>
<td>7</td>
</tr>
<tr>
<td>mass fractions $Y_i$</td>
<td>$Y_{N_2} = 0.743$, $Y_{O_2} = 0.228$, $Y_{H_2} = 0.029$</td>
</tr>
<tr>
<td>chemical model</td>
<td>air-hydrogen: 13 species, 33 reactions</td>
</tr>
</tbody>
</table>

Table 7.8: Initial conditions for reactive wedge flow.

Mach number and Temperature contours of the calculation are presented in Figs. 7.34 to 7.36. They are in good agreement with the results given in [24], where the detonation
wave angle was 22 degrees and the location of its origin, the flame front, at a streamwise position of 0.48m. Due to the great similarity of the numerical methods used this
good agreement is not surprising, and at the same time gives confidence in the numerical modelling of reactive flows.

Figure 7.34: Residual for reactive wedge flow.
Figure 7.35: Mach number contours for reactive wedge flow.

Figure 7.36: Temperature contours for reactive wedge flow.
7.5 Viscous Flow in Channel

The viscous flow channel test case should not pose too much of a problem once the wedge cases are completed satisfactory. Still, for the given thesis cases a close look at internal flows will be taken. For this, a test case is posed which involves viscous internal flow with separation, shock, reflected shock and rarefaction waves. The problem setup is presented in Fig. 7.37 and the relevant initial conditions in Tab. 7.9. With the given setup and initial conditions we obtain a residual as given in Fig. 7.38 from the computation with the code developed. The resulting Mach number and pressure contours are presented in Figs. 7.39 and 7.40. Detailed pressure contours for the shocks due to the boundary layer at the inflow and at the upper wall where the wedge generated shock is reflected are given in Fig. 7.41. At the location where the shock is reflected at the upper wall a significant influence of the flow separation can be observed. This becomes

![Viscous flow in a channel](image)

**Figure 7.37:** Viscous flow in a channel.

<table>
<thead>
<tr>
<th>Channel Flow</th>
<th>Inflow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
<td></td>
</tr>
<tr>
<td>pressure $p$</td>
<td>101300 Pa</td>
</tr>
<tr>
<td>temperature $T$</td>
<td>293K</td>
</tr>
<tr>
<td>Mach number $Ma$</td>
<td>5</td>
</tr>
</tbody>
</table>

**Table 7.9:** Initial conditions for channel flow problem.
Figure 7.38: Residual for viscous channel flow.

more clear looking at the velocity vectors close to the wall shown in Fig. 7.42. A sufficient number of cells must lie within this region and is essential for the proper detection of the recirculation region. It must be stressed that with coarser grids the boundary layer at the walls is still resolved acceptably. However, with a grid too coarse no recirculation region will be detected and the convergence of the solution can be achieved with much greater ease. It can be found in [8] that the size of the recirculation zone highly depends on the resolution of the spatial discretization in the relevant region. Recalling results from [8] and comparing them with results found with the present code in Figs. 7.43 and 7.44, a good agreement can be observed for the pressure on the upper and lower wall. In the case of the upper wall the sensitivity of the recirculation zone to the grid used becomes evident. For the fine mesh used by Gnoffo ([8]) the recirculation zone has about twice the length as it has for the results obtained with the code developed in this work. Also the shock strength obtained is slightly lower than that in [8], but the overall agreement of shock position and the magnitude of the pressure along the wall is very good. In the case of the lower wall very good agreement can be observed for the shock position,
strength and the magnitude of the pressure along the wall. This case dealing with an internal flow problem including a recirculation zone is now presented and ensures that even phenomena such as recirculation zones are computed satisfactory. However, the fact has to be kept in mind that a sufficiently dense spatial discretization is essential. Here a grid convergence study usually allows to actually find when a spatial discretization is 'fine' enough. In this work such a study is not approached, but left for future research.
Figure 7.41: Pressure contour details for viscous channel flow.

Figure 7.42: Recirculation region for viscous channel flow.
Figure 7.43: Relative pressure on top wall for viscous channel flow.

Figure 7.44: Relative pressure on bottom wall for viscous channel flow.
7.6 Blunt Body Flow

The thesis cases consist of blunt bodies with different diameters embedded in a flow domain. Hence, blunt body flows are of vital interest in this study and examined thoroughly.

Significant work has been done on blunt body flows, mostly for axis-symmetric cases and in front of the blunt body. For steady inflow conditions close to the Chapman-Jouguet state the flow in front of the blunt body can become unstable, eg. the shock position is not stable and oscillates. These effects created by an interaction of shock and detonation waves have been studied in [31] and [17]. Despite their implication on the thesis cases, in this work unsteady effects are not dealt with. However, in future research these have to be taken into account, with more focus on at least second order accurate time marching methods.

At this stage we refer to [23] and concentrate on steady state solutions for two-dimensional blunt bodies. According to Billig [2] Ambrosio and Wortman [1] developed an approximation for the standoff distance $\Delta$ with respect to the inflow Mach number:

$$\frac{\Delta}{d/2} = 0.386 \cdot e^{4.67/M_a^2} \quad (7.7)$$

where $d$ is the blunt body diameter. For the calculation we apply symmetry conditions and obtain a computational domain as shown in Fig. 7.45. In order to verify the flow solver we compute the flowfield around a blunt body of 0.01m diameter, determine the
stand-off distance and compare the result with the analytical approximation proposed by Billig. This is done for the initial conditions and inflow Mach numbers given in Tab. 7.10, whereby the heat flux of zero through the wall implies an adiabatic wall. In

| Blunt Body Flow |
|-----------------|-----------------|
| Parameter       | Inflow          |
| pressure $p$    | $1.013 \cdot 10^5 Pa$ |
| temperature $T$ | $600K$          |
| wall heat flux $q_{wall}$ | $0 W/m^2$ |
| Mach number $Ma$ | 5 | 6 | 7 |
| mass fractions  | ideal gas -     |
|                 | $O_2 - H_2$ $Y_{O_2} = 0.888$ and $Y_{H_2} = 0.112$ |
|                 | $air - H_2$ $Y_{N_2} = 0.743$, $Y_{O_2} = 0.228$ and $Y_{H_2} = 0.029$ |

Table 7.10: Initial conditions for blunt body flow.

addition reactive flow around the blunt body is calculated for the Mach number of 5 in order to allow a qualitative comparison. Both the oxygen-hydrogen and the air-hydrogen schemes with 8 species for 17 reactions and with 9 species for 19 reactions, respectively, are used. The residuals for the inert and reactive calculations are presented in Fig. 7.46. The technique of 'Mach number sequencing' is used extensively for blunt body flows, whereby the Mach number at the beginning of the calculation in the flow domain and at the boundaries is significantly lower than that of the free stream. In combination with blunt body flows, for both test and thesis cases, the initial Mach number is 1.2, which is increased step by step every specified iteration interval to finally reach the desired inflow Mach number. This procedure ensures stability for the sensitive blunt body flows and yields good results once the solution is converged. The Mach number contours obtained for the oxygen-hydrogen gas mixture are presented in Fig. 7.46. The other results are similar in principle, but with different standoff distance. This standoff distance can be observed in detail in Figs. 7.48 and 7.49. Defining the shock position at about the middle of the Mach number increase through the shock we can locate the shock position. Interesting from the physical point of view is the temperature increase for nonreactive cases with constant specific heat and that for reactive air-hydrogen and oxygen-hydrogen gas mixtures. As it can be seen in 7.49 the real gas flows yield a higher standoff distance.
For the Mach number of 5 the maximum temperature of the real gas flow is higher, too. This might change, however, when the maximum temperature due to the shock for the inert gas flow with constant specific heat ratio exceeds the adiabatic flame temperature of the reactive gas mixture. Finally, the results for the blunt body flow standoff distances are compared to those obtained by the analytical approximation given at the beginning of the Subsection. A slight over-prediction of the standoff distance can be observed in Fig. 7.50 for the inert flows with constant specific heat ratio. This over-prediction in comparison with Billig's correlation was found by [23] as well, although a bit less pronounced. The standoff distances for the reactive flows are increased in comparison to the inert gas flow at the same Mach number. For the examined cases at a Mach number of 5 the oxygen-hydrogen inflow yields a greater standoff distance than the air-hydrogen gas mixture. Shuen examined pure air schemes in his work (see [23]) and found a reduced standoff distance for the reactive flows. This is not surprising since for the air scheme energy is consumed by the endothermic reaction and in the case of our schemes energy is released by the exothermic reactions.
Figure 7.47: Mach number contours for oxygen-hydrogen blunt body flow.

Figure 7.48: Standoff distances for blunt body flows.
Figure 7.49: Temperature on stagnation streamline for blunt body flows.

Figure 7.50: Comparison of standoff distances for examined blunt body cases.
### Table 7.11: Overview of all test cases presented.

<table>
<thead>
<tr>
<th>Case/Subcase</th>
<th>Mode</th>
<th>Species</th>
<th>Reactions</th>
<th>Grid Cells</th>
<th>Entropy Corr.</th>
<th>Reference(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PChem (1)</td>
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<td>8</td>
<td>17</td>
<td>-</td>
<td>-</td>
<td>[22]</td>
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<td>2</td>
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<td>[24]</td>
</tr>
<tr>
<td>FStream (2)</td>
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<td>13</td>
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<td>[24]</td>
</tr>
<tr>
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<td>2</td>
<td>6</td>
<td>2</td>
<td>-</td>
<td>$\bar{\varepsilon} = 0.2 - 1.5$</td>
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</tr>
<tr>
<td>FPlate (3)</td>
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<td>-</td>
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<tr>
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<td>-</td>
<td>-</td>
<td>$\bar{\varepsilon} = 0.25$</td>
<td>[24, 33]</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>5</td>
<td>-</td>
<td>-</td>
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<td>[16, 5]</td>
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<td>4</td>
<td>13</td>
<td>33</td>
<td>$\bar{\varepsilon} = 1.5$</td>
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<tr>
<td>Channel (5)</td>
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<td>-</td>
<td>-</td>
<td>$\bar{\varepsilon} = 0.25$</td>
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<td>BBody (6)</td>
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<td>13</td>
<td>33</td>
<td>$\bar{\varepsilon} = 1.5$</td>
<td></td>
</tr>
</tbody>
</table>

#### 7.7 Test Cases Overview

To conclude this Chapter an overview of all test cases discussed is given in Tab. 7.11. The information about the relevant 'program modes', which refers to the option for the flow solver, that selects the level of 'physical modelling' required, is shown in Tab. 7.12. With the selection of test cases solved here the necessary confidence in the results produced by the numerical method is gained. Hence, we can expect physically meaningful answers for the thesis cases, which will be presented in the next Chapter.
Table 7.12: Program modes.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Physical Modelling</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>point chemistry</td>
</tr>
<tr>
<td>2</td>
<td>inviscid single species flow</td>
</tr>
<tr>
<td>3</td>
<td>inviscid inert multi-species flow</td>
</tr>
<tr>
<td>4</td>
<td>inviscid reactive multi-species flow</td>
</tr>
<tr>
<td>5</td>
<td>viscous single species flow</td>
</tr>
<tr>
<td>6</td>
<td>viscous inert multi-species flow</td>
</tr>
<tr>
<td>7</td>
<td>viscous reactive multi-species flow</td>
</tr>
</tbody>
</table>
Chapter 8

Thesis Cases

The thesis cases are providing the results required for an analysis of the given problem. Based on the validations of the numerical method in the previous Chapter, it can be expected, that these results are accurate enough with respect to all relevant physical features needed for a thorough analysis. Before detailed results are presented, geometrical aspects and inflow conditions for this study are being developed in the following Subsection. Afterwards, the results for the three different blunt body diameters and the comparative wedge flow calculation are given in the consecutive Subsections.

8.1 Geometrical and Physical Setup

Within the framework of the given problem the selection of thesis cases is made in order to cover a certain range of physical and geometrical boundary conditions. The main parameters for such an analysis are

- the blunt body diameter (at a given constant channel height)
- the inflow Mach number
- the thermodynamic inflow variables (density, pressure and temperature)

The main concern in this work is the blunt body diameter, while the other parameters are chosen and then fixed for the remaining studies. Obviously, it is an important step in future research to also examine the effects of different inflow Mach numbers and thermodynamic inflow variables on this type of scramjet concept. However, the test cases solved in this work include the blunt body diameters of 10\text{mm}, 15\text{mm} and 20\text{mm} at a given flow domain height of 60\text{mm}, referred to as 'channel segment'.

119
It is important to note that this is not the total combustor height! The combustor is divided into several channel segments which are examined individually. Furthermore the channel segment, or flow domain, is reduced to the computational domain by the application of a symmetry line through the centre of the blunt body, as outlined already in the Introduction. The detailed geometrical dimensions are given in Fig. 8.1.

The inflow Mach number for a shock induced combustion ramjet (SHCRAMJET) is from about 10 to 25. This yields a combustor Mach number from 5 to 12.5. Due to the polynomials describing the fuel and air species components for heat transfer coefficients at constant pressure ($C_p$), which limit the allowed temperature to $6000K$, only the lower limit of this combustor Mach number range is being examined here. Later on, with polynomials accurate up to a higher temperature, the analysis should be extended to the whole Mach number range. Hence, at this stage the inflow Mach number examined is 5. Obviously, even for this Mach number, the normal shock in front of the blunt body, the chemical reaction after the shock and the deceleration of the fluid limit the maximum possible inflow temperature. The inflow conditions for all thesis cases are summarized in Tab. 8.1. Since the study is a basic one the parameters reflect an estimate of the inflow conditions to the combustor, not exact values for a given prototype analysis. Also different flight conditions are imposing different inflow parameters. Note that the
dynamic pressure is about 1400psf which roughly corresponds to 65000Pa. Via the relation

\[ q_{\text{dyn}} = \frac{1}{2} \gamma_{\infty} p_{\infty} M^2_{\infty} \]  

(8.1)

this gives 1000Pa as shock induced combustion ramjet inflow pressure. Due to two oblique shocks the gas is being compressed up to 10000Pa. Details of the shock induced combustion ramjet design can be found in a report by Sislian et. al. [24].

With combustor inflow conditions fixed the only parameter left for optimization is the ratio between channel segment height and blunt body diameter.

In the following Subsections solutions for the different thesis cases are presented, ordered with respect to the channel blockage ratio. This ratio is defined by

\[ CBR = \frac{\text{blunt body diameter}}{\text{channel segment height}} \]  

(8.2)

In our case this gives ratios of \( \frac{1}{6}, \frac{1}{4} \) and \( \frac{1}{3} \). For the particular discussions of flow phenomena within the next three Subsections regions of interest are addressed as given in Fig. 8.2. Finally, in the last Subsections of the Chapter a comparative wedge flow and an overview of the results obtained will be given.
8.1.1 Channel Blockage Ratio 16%

The smallest blunt body diameter used yields a channel blockage ratio of $\frac{1}{6}$ and, compared to the other two cases, has the smallest influence on the incoming flow.

The Mach number contours in Fig. 8.3 show that the bow shock generated by the blunt body (region a to b) has some change in slope close to region b due to the expansion fan generated in the front upper part of the blunt body (region c). For the viscous flow the region with strong vortices and recirculation behind the blunt body (region e) becomes significantly larger and the point of flow separation (region d) moves upwards on the back side of the blunt body.

The temperature distribution in Fig. 8.4 clearly demonstrates the cooling effect of the blunt body in the case of the viscous flow. The wall temperature of 700K strongly influences the temperature distribution in region d. Again, the reflected shock area in region f is more developed as in the case of the inviscid flow.

The water ($H_2O$) production given in Fig. 8.5 is important to determine the extent to which the premixed gas has reacted. Clearly the highest production of water takes place in combination with the temperature increase due to the bow shock (regions a to b). However, the highest temperatures do not yield the highest water concentrations. Slightly lower temperatures (about 3000K instead of 3500K) do obviously favour the
highest water concentrations, as can be seen in the area above region f) and also directly behind the blunt body, where the water concentration in region d) becomes surprisingly high in a relatively cold region. The latter is true for the viscous flow only, where further research of the influence of the wall temperature is worth while being studied. It can be expected that the blunt body influence here becomes even stronger for blunt bodies with greater diameter.

Another interesting indicator from the chemistry point of view is the hydroxyl (OH) mass fraction within the flowfield. Again, around the blunt body the wall temperature strongly influences the results in comparison to the inviscid flow. Here, the hydroxyl mass fraction is greatly reduced due to the low temperature. The highest levels of hydroxyl can be found in region f).
Figure 8.3: Mach number contours for the thesis case with $CBR = 1/6$ (viscous at the top, inviscid at the bottom).
Figure 8.4: Temperature contours for the thesis case with $CBR = 1/6$ (viscous at the top, inviscid at the bottom).
Figure 8.5: $H_2O$ contours for the thesis case with $CBR = 1/6$. (viscous at the top, inviscid at the bottom)
Figure 8.6: $OH$ contours for the thesis case with $CBR = 1/6$ (viscous at the top, inviscid at the bottom).
8.1.2 Channel Blockage Ratio 25%

The increased blunt body diameter leads to stronger influences on the flow field as can be seen in Fig. 8.7. The vortex/recirculation zone behind the blunt body (region d) and f) is greatly increased in comparison to the case with the channel blockage ratio of 16%. The region of significantly lower Mach number stretches downstream even past region f). Again, the separation for the viscous flow (region d) happens slightly before it does for the inviscid flow.

Fig. 8.8 demonstrates the increased cooling effect of the blunt body in the case of viscous flow. The average temperature within the flowfield appears to be higher than in the case with the smaller channel blockage. Also, the hot region due to the shock directly in front of the blunt body almost interacts with the reflected shock originating from region b).

For the water mass fraction within the flow field the same as in the previous case can be said. Fig. 8.9 demonstrates that highest temperatures do not coincide with the highest water mass fractions. Also, in the case of viscous flow the cool wall of the blunt body increases the water mass fraction in the relevant region. This becomes very obvious in region d).

The hydroxyl mass fractions in Fig. 8.10 show the increased influence of the larger blunt body diameter. Especially after the blunt body the level of hydroxyl is increased in comparison with the previous case. For the viscous flow the cooling due to the blunt body reduces the hydroxyl mass fractions compared to the inviscid case, where the higher temperature in the ‘wake’ produces more hydroxyl.
Figure 8.7: Mach number contours for the thesis case with $CBR = 1/4$ (viscous at the top, inviscid at the bottom).
Figure 8.8: Temperature contours for the thesis case with $CBR = 1/4$ (viscous at the top, inviscid at the bottom).
Figure 8.9: $H_2O$ contours for the thesis case with $CBR = 1/4$ (viscous at the top, inviscid at the bottom).
Figure 8.10: \( OH \) contours for the thesis case with \( CBR = 1/4 \) (viscous at the top, inviscid at the bottom).
8.1.3 Channel Blockage Ratio 33%

As it can be seen in Fig. 8.11 for the highest channel blockage ratio examined the region with strongly reduced Mach number (region e)) is larger than for the previous cases. Here the reflected shock (regions b) to f)) strongly interacts with the wake behind the blunt body. Also in region b) the Mach number is greatly reduced behind the shock that becomes normal due to the chemical reaction, as it can be observed in Fig. 8.12.

In Fig. 8.12 we can see that the hot gas created behind the shock directly in front of the blunt body now interacts with the reflected shock originating in region b). Additionally, at this reflection point the shock becomes almost normal creating a very hot zone behind it. As in the previous cases for the viscous flow a strong cooling effect can be recognized around the blunt body and especially in region d). This leads to slightly reduced temperatures behind the blunt body as well. The point where the shock reflected in region b) and the low Mach number field behind the blunt body interact (region f)) is moved upstream towards the blunt body. This creates a region with very hot gas behind the blunt body which is expanding downstream in a direction normal to the inflow.

The water production is started right behind the bow shock, as shown in Fig. 8.13. The water mass fraction distribution is another good example that the highest temperatures do not yield the highest water mass fractions. Instead, around the blunt body (for the viscous case) and above the increasing zone of very hot gas behind the blunt body the highest water mass fractions can be found. At the same time in the 'hot gas' region behind region f) and the region b), where the bow shock is being reflected, the water mass fractions do not reach their highest values.

Similarly, in the case of viscous flow the cooling due to the blunt body significantly reduces the hydroxyl mass fraction behind the blunt body. In contrast to water, the high temperature favours hydroxyl production. Hence, as Fig. 8.14 proves, the highest mass fractions can be found in front of the blunt body in region a) and in region b), where the bow shock is being reflected. After the chemical reaction has been started the lowest hydroxyl mass fractions for the viscous case can be found around the blunt body.
Figure 8.11: Mach number contours for the thesis case with $CBR = 1/3$ (viscous at the top, inviscid at the bottom).
Figure 8.12: Temperature contours for the thesis case with $CBR = 1/3$ (viscous at the top, inviscid at the bottom).
Figure 8.13: $H_2O$ contours for the thesis case with $CBR = 1/3$ (viscous at the top, inviscid at the bottom).
Figure 8.14: $OH$ contours for the thesis case with $CBR = 1/3$ (viscous at the top, inviscid at the bottom).
8.1.4 Comparative Wedge Flow

The study of the comparative wedge flow includes three subcases; one case with a large domain of 1.5\,m length and 0.6\,m height and an inflow angle of 10°, a small domain with the same dimensions as the blunt body thesis cases and the same inflow angle and finally another small domain with an inflow angle of 25°.

Utilizing these three subcases we can demonstrate one strength of the blunt body generated combustion. While for the selected inflow conditions the combustion easily occurs within the domain in the case of a blunt body, for an inflow angle of 10° no ignition occurs unless the physical domain is very long. It has been shown (see [24]) that such an angle is very efficient and produces low entropy increases and total pressure losses. If an ignition is desired in a physical domain comparable to that examined for the blunt body cases, the inflow angle has to be increased. In our last case 25° has been selected.

The residual for all three wedge cases can be found in Fig. 8.15. There has not been any difficulty in obtaining the solutions for these cases, in contrast to the blunt body cases where care has to be taken to ensure solution convergence. In order to further illustrate
the differences in geometry of the two domains examined the large and small domains are compared in Fig. 8.16. With the focus on the large domain Fig. 8.17 shows some slight ignition at the very end of the domain. Since the domain size directly influences the weight of the flight vehicle this situation is clearly undesirable! Not too much of a combustion happens here and most of the gas mixture remains unignited. After the results obtained for the large domain it is obvious that a smaller domain with the same angle of incidence does not produce an ignition. This can be found in Fig. 8.18 which is a confirmation of the results obtained before. However, in the case of an increased angle of incidence (25°) we can create a detonation wave covering half the domain, as shown in Fig. 8.19. Compared to the blunt body flows this is still poor since the blunt body can easily ignite the whole incoming gas flow within a domain of the same size.

As conclusion for the comparative wedge flows we can state, that it is difficult to produce
Figure 8.18: Temperature contours for small ($10^\circ$) comparative wedge case ($T$ in [K]).

Figure 8.19: Temperature contours for small ($25^\circ$) comparative wedge case ($T$ in [K]).
data of use, since the selected inflow conditions are not suitable for a satisfactory ignition of the incoming gas flow for a comparable domain size. Increasing the angle of attack improves the situation, but increases the entropy production at the same time. If there is a comparison possible, then only at somewhat worse conditions with respect to the wedge flow.

This points out one clear advantage of the blunt body generated combustion, where the scramjet can be operated at lower flight Mach numbers and the wedge generated combustion would require non-acceptable combustor dimensions.
8.1.5 Overview

The results for the different thesis cases were presented in the previous Subsections and will be compared in the following, focusing on the results for the viscous cases. Fig. 8.20 shows the residuals for the cases. Generally the inviscid cases converged more easily than the viscous ones. Furthermore, the cases with the increased channel blockage ratio pose more of a problem than those with the small channel blockage ratio. This can be expected since the perturbation of the flow in the channel is less strong for smaller blunt bodies. The velocities in the x-coordinate direction given for the different cases in Fig. 8.21 imply for the top boundary, that an increased channel blockage yields to stronger reduction of the inflow velocity at the reflection point (region b)) and also a reflection point that is moving more and more upstream. The latter can be related to the fact that the bow shock position is moved upstream due to the increased blunt body diameter. This is confirmed by the graphs of the velocities at the bottom of the domain, where the initial shock position is moved upstream. The velocity becomes zero around the solid wall of the blunt body and negative in the recirculation zone behind the blunt
Figure 8.21: Velocity profiles for thesis cases (top and bottom of domain).

body. With increasing blunt body diameter this negative velocity increases in magnitude. While the smallest blunt body produces a relatively small recirculation zone the length is increased for larger diameters. Interestingly the length of the zone with negative velocity in the x-coordinate direction is the highest for the case with the intermediate channel blockage. In the case of the smallest channel blockage the fluid greatly reaccelerates after the recirculation zone and then goes through another shock in region f). Similar information about shock positions can be gained from pressure and temperature graphs in Figs. 8.22 to 8.25. In Fig. 8.25 the cooling effect of the blunt body is shown once more.
Figure 8.22: Pressure for thesis cases (top of domain).

Figure 8.23: Pressure for thesis cases (bottom of domain).
Figure 8.24: Temperature for thesis cases (top of domain).

Figure 8.25: Temperature for thesis cases (bottom of domain).
As it can be found in Fig. 8.26 the subsonic regions increase with increasing blunt body diameter. Also, in the case of the channel blockage ratio of $\frac{1}{3}$ there is a small subsonic region created at the top boundary of the domain. It has been discussed in a previous Subsection that this is due to the nearly normal shock in region b) created by the combustion in that particular area. The subsonic region for the intermediate channel blockage is stretched more than that of the largest channel blockage, where at the same time the subsonic region in the case of the largest channel blockage extends most normal to the incoming flow direction. The recirculation zones presented in Fig. 8.27 are increasing in thickness (dimension normal to that of the incoming flow) with increasing channel blockage ratio and are stretched the most for the intermediate blunt
Figure 8.27: Recirculation zone for the different thesis cases.

body diameter examined.
Chapter 9

Propulsive Performance Analysis

In this Chapter the results for global parameters of the three analysed channel blockage ratios will be presented, focusing on viscous flow only. The parameters presented in the following are the drag force, and changes of entropy, enthalpy and total pressure. Afterwards a preferable channel blockage ratio will be identified by evaluating changes of the relevant quantities.

Firstly, a look at the drag forces (in x-coordinate direction) for the three channel blockage ratios (CBR) in Fig. 9.1 reveals almost linear behaviour with a small decrease in slope towards the higher channel blockage ratio. The key fact is that, not unexpectedly, the drag increases with increasing blunt body diameter.

As it can be seen in Fig. 9.2 the specific entropy increases in the same, geometrically similar, pattern as the drag force. Higher channel blockage ratio yields an increase in entropy. Again, this is not surprising since the increased blunt body size leads to a higher fraction of a normal or almost normal shock wave in front of the blunt body and also an increased recirculation zone behind the blunt body.

The total enthalpy increases with increasing channel blockage ratio, while the 'reaction' enthalpy and the enthalpy of formation are being reduced. At the same time the kinetic energy decreases, as shown in Fig. 9.3. As shown in a previous Chapter, the enthalpy is calculated by an integration along the boundaries using the actual temperatures, while the heat of 'reaction' $\Delta h_r$ and the heat of formation $\Delta h_f$ are taken at fixed values of the inflow temperature (700K) and standard temperature (298.15K), respectively, for both inflow and outflow. Consequently the heat of reaction and heat of formation released into the fluid due to the combustion are almost the same, just differing slightly due to
Figure 9.1: Drag for thesis cases.

Figure 9.2: Entropy increase for thesis cases.
the change of enthalpy for these two temperatures. It is important to mention that pure elements, eg. \( H_2, O_2 \) and \( N_2 \), have an enthalpy of zero in their stable state at standard conditions. The standard heat of formation of a species is the energy required for its formation from the elements at standard conditions. In the case of an exothermic reaction, eg. the formation of water out of hydrogen and oxygen, the resulting reaction yields a negative heat of formation, \(-241.81kJ/mol\) in this example. For a premixed combustible gas therefore a negative heat of formation can be expected, as it actually is the case for the thesis cases. That means that energy is released to the fluid and the amount of 'more stable' species, such as water, increases. An interesting result shown in Fig. 9.3 is the reduction of the absolute value of the heat of formation, which is equivalent to the fact that slightly less energy out of the combustion is being added to the flow for increasing blunt body diameter. Hence, we can expect that the combustion for the increased blunt body diameter is slightly less complete. Furthermore, Tab. 9.1 gives information about the hydrogen and oxygen consumption and water production, which confirms the less complete combustion for the higher channel blockage ratio.

The blunt body and the shock waves created reduce the kinetic energy significantly. Here a modification of the geometrical shape of the blunt body might allow a reduction of this loss by the application of a droplet type of shape. This particular shape forms a nozzle like shape and should allow an efficient reacceleration of the fluid. The shock in front of the blunt body and the boundary layer on its surface due to viscosity, however, remain even for the modified shape.

Mass and area averaged total pressure losses are very similar for the three thesis cases. Fig. 9.4 confirms that the losses increase with increasing channel blockage, while the slope slightly decreases at the same time. The slope of the loss of total pressure from a channel blockage of 16% to 25% is higher for the area averaged value than for the mass averaged one.

At this stage the changes for all global variables of interest are presented. We now want to identify the changes of these quantities in proportion of the related inflow values to get an idea of a preferred channel blockage ratio that allows to gain the most energy at acceptable cost. For this Tab. 9.1 gives the absolute values at the inflow for all quantities examined and relates them with a change in percent for each channel blockage ratio. Additionally the change in mass fractions for hydrogen and oxygen are given as well as the emission index for water \((EI_{H_2O} = \dot{m}_{H_2O}[g]/\dot{m}_{H_2}[kg])\).

The momentum loss (drag force) for the highest blunt body diameter examined is almost
Figure 9.3: Enthalpy changes for thesis cases.

Figure 9.4: Total pressure losses for thesis cases.
Chapter 9. Propulsive Performance Analysis

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Inflow Value</th>
<th>CBR = 16%</th>
<th>CBR = 25%</th>
<th>CBR = 33%</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass flux</td>
<td>3.3232 kg/s</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>force (drag, x-coord.)</td>
<td>10592.4 N</td>
<td>11.0%</td>
<td>14.5%</td>
<td>17.5%</td>
</tr>
<tr>
<td>entropy</td>
<td>10492.6 J/(kg·K)</td>
<td>13.5%</td>
<td>14.8%</td>
<td>15.8%</td>
</tr>
<tr>
<td>enthalpy</td>
<td>579348.9 J/kg</td>
<td>303.5%</td>
<td>355.1%</td>
<td>393.5%</td>
</tr>
<tr>
<td>heat of reaction</td>
<td>579348.9 J/kg</td>
<td>-279.2%</td>
<td>-269.0%</td>
<td>-256.5%</td>
</tr>
<tr>
<td>heat of formation</td>
<td>0.0 J/kg</td>
<td>∞</td>
<td>∞</td>
<td>∞</td>
</tr>
<tr>
<td>kinetic energy</td>
<td>4796024.2 J/kg</td>
<td>-39.2%</td>
<td>-47.4%</td>
<td>-53.9%</td>
</tr>
<tr>
<td>total pressure (mass av.)</td>
<td>5930421.7 Pa</td>
<td>-90.1%</td>
<td>-92.7%</td>
<td>-94.2%</td>
</tr>
<tr>
<td>total pressure (area av.)</td>
<td>5930421.7 Pa</td>
<td>-90.0%</td>
<td>-93.0%</td>
<td>-94.4%</td>
</tr>
<tr>
<td>oxygen consumption (Y_{O_2})</td>
<td>0.228</td>
<td>-85.1%</td>
<td>-85.1%</td>
<td>-85.1%</td>
</tr>
<tr>
<td>hydrogen consumption (Y_{H_2})</td>
<td>0.029</td>
<td>-79.3%</td>
<td>-78.6%</td>
<td>-77.6%</td>
</tr>
<tr>
<td>water production (EIH_{2O})</td>
<td>-</td>
<td>5828</td>
<td>5690</td>
<td>5510</td>
</tr>
</tbody>
</table>

Table 9.1: Changes of global variables.

double that of the smallest, while the entropy increase in and the loss of kinetic energy of the fluid do not vary that significantly. Also, the total pressure for all cases is reduced about an order of magnitude, both for mass and area averaged calculations the loss of the total pressure at the inflow is 90% to 95%. This feature of the blunt body generated combustion can be considered a disadvantage that, however, is in contradiction with the extended usability for lower Mach numbers in comparison to the wedge generated combustion. The smallest blunt body diameter yields the highest reduction of hydrogen and therefore the most complete combustion, where the most heat is released. With about the same level of heat released for all channel blockage ratios the smallest blunt body appears favourable since it causes the least losses.
Chapter 10

Outlook

In the presented work blunt body generated detonation wave ramjet flowfields have been numerically simulated. An implicit method with TVD characteristics has been developed for a steady state solution on structured multi-block grids. Before the code was applied to the thesis cases it has been validated thoroughly with several test cases addressing different physical features needed for a satisfactory simulation of the problem approached. At the moment the study can only be seen as a preliminary one. Initial insight could be gained still leaving many questions unanswered.

One main result obtained from this study is the applicability of the blunt body generated combustion for lower inflow Mach numbers as for the wedge generated combustion. This is mostly due to the normal shock wave in front of the blunt body that ignites the fuel at much lower inflow Mach numbers than the wedge with its oblique shock wave would. An exact quantitative comparison with the wedge generated combustion is not easily possible since at the selected inflow conditions the wedge can only ignite the fuel over half the channel segment height at even 25 degrees wedge angle. Thus, the blunt body generated combustion is by far more suitable to ignite fuel within a domain of great height. Furthermore the loss of momentum, kinetic energy and total pressure as well as the increase of entropy and enthalpy are almost linear with increasing channel blockage ratio. However, the most complete reduction of hydrogen ($H_2$) is found for the smallest blunt body diameter, where the most heat is released at the least losses of total pressure.

The results so far are encouraging and a good basis for further research needed in order to gain a full understanding of the capabilities of the blunt body generated combustion.
From the chemistry point of view methane-air and Kerosene-air schemes would be of great value in addition to the oxygen-hydrogen and hydrogen-air schemes already implemented. Since it is widely used for conventional jet engine propulsion especially Kerosene is of interest here. Not only the theoretical feasibility of a scramjet utilizing blunt bodies for the ignition of the gas mixture is important but the price of the operation of such an engine. Therefore the capability of assessing the most widely used types of fuel for this application would be a significant addition to the present work.

The implication of the used grid systems on the solution accuracy has to be studied in more detail. Consequently grid convergence studies are a must in further research efforts to ensure the proper resolution of interactions between boundary layers, shock waves and detonation waves. Especially in the case of the unsteady flow phenomena (see [31, 17]) this becomes important. The multi-block grid system used so far can be seen as a compromise that allows the spatial discretization of relatively complex geometries without the application of fully unstructured grids. How satisfactory this approach will be in the future has to be found. An interesting approach would be the implementation of first unstructured grids and subsequently that of hybrid grids to regain the high quality of boundary layer solutions achieved with structured meshes. Whether the extra effort of hybrid grids is justified by an improvement of solution quality has to be studied.

Another key element in our numerical studies is the proper calculation of the fluxes on the cell sides. So far, a simple averaging has been used to calculate values on the cell sides that yields second order spatial accuracy for smooth, structured meshes. The aspect of how approximate or exact Riemann solvers can improve the results has to be examined. Obviously the additional computational cost of an exact Riemann solver has to be weighted against the gain in solution quality. This could help solving the problems related to the accurate modelling of the diffusion already mentioned before. Closely related is the question of the flux difference splitting scheme applied. For the blunt body cases examined the Roe type of flux difference splitting requires a reasonable amount of entropy correction which at the same time leads to an over-prediction of the diffusion. Alternative methods should be examined and used in case they can improve this deficiency at no other drawback. Interestingly enough, the Roe type of flux difference splitting is commonly used for blunt body flows by other researchers (see [5, 23]) and can therefore be seen as an acceptable method.

To confirm results obtained at this stage more channel blockage ratios must be examined, extending the range below a channel blockage ratio of 16% and above 33% as well as in-
between the examined ratios. With furtherly improved numerical methods the influence of different inflow Mach numbers and blunt body wall temperatures should be studied in detail. The upper boundary of the domain has been modelled as an axis of symmetry which can be replaced by a wall in order to analyse the interaction between the boundary layer on that wall and the incoming bow shock due to the blunt body. This is essential in order to study the flowfield between the first rod embedded in the combustor and its wall.

Finally, the capturing of the unsteady effects of the given flow problem has to be seen as the most important task to complete this research. With increasing blunt body diameter a point will be reached where the flow channel is choked, resulting in a shock or detonation wave moving upstream. A more detailed analysis of different blunt body diameters, essential for the finding of the optimum channel blockage ratio, only makes sense when a time accurate computation can precisely capture this effect. In addition interactions between boundary layers, shock waves and detonation waves might have unsteady effects inherent, that need to be captured for an accurate estimation of required cooling and resulting forces.

In conclusion it can be noted that the research carried out has not reached an end yet and opens many more interesting and challenging aspects for future studies.
Appendix A

Source Term Jacobi Matrix

The source term Jacobi matrix is defined by

\[ \mathbf{J}_S = \frac{\partial \mathbf{S}}{\partial \mathbf{Q}} = \begin{bmatrix} \frac{\partial S_1}{\partial Q_1} & \frac{\partial S_1}{\partial Q_2} & \cdots & \frac{\partial S_1}{\partial Q_m} \\ \frac{\partial S_2}{\partial Q_1} & \frac{\partial S_2}{\partial Q_2} & \cdots & \frac{\partial S_2}{\partial Q_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial S_m}{\partial Q_1} & \frac{\partial S_m}{\partial Q_2} & \cdots & \frac{\partial S_m}{\partial Q_m} \end{bmatrix} \]  

(A.1)

where \( \mathbf{S} \) is the chemical source vector and \( \mathbf{Q} \) the vector of conserved variables. Depending on the number of species used for the chemical model the calculation of the source term Jacobian can be quite time consuming. There are two different ways to evaluate \( \mathbf{J}_S \), numerically or analytically. Both ways are described in the following Sections.

A.1 Numerical Source Term Jacobi Matrix

The numerical calculation of the source term Jacobian simply follows the pattern of numerical differencing. For each source term vector component the change with respect to each component of the conserved variable vector has to be evaluated:

\[ \frac{\partial S_i}{\partial Q_j} = \frac{S_i (Q_1, Q_2, ..., Q_j + \frac{1}{2} \Delta Q_j, ..., Q_m) - S_i (Q_1, Q_2, ..., Q_j - \frac{1}{2} \Delta Q_j, ..., Q_m)}{\Delta Q_j} \]  

(A.2)

where often \( \Delta Q_j \approx 0.01 Q_j \) is used. Special care has to be taken in case \( Q_j \) equals zero, where a suitable \( \Delta Q_j \) has to be found by other means. Also one-sided differencing might be preferable over the central differencing presented here, since for initial mass fractions of zero the central differencing leads to negative and therefore unphysical values.
Unfortunately the one-sided differencing is only of first order accuracy compared to the central differencing, which makes the analytical calculation the superior one. Still, a numerical Jacobi matrix with one-sided differencing is a valuable tool to validate the results of the analytical calculation.

A.2 Analytical Source Term Jacobi Matrix

The source term $S_i$ is given as a function of $\rho, T$ and $\rho Y_k$, where $Y_k$ stands for $Y_1, Y_2, \ldots$ to $Y_{N_s-1}$. Since derivatives with respect to the conserved variables $\rho, \rho u, \rho v, \rho E$ and $\rho Y_k$ are required, differentiation via the chain rule has to be used. It is convenient to express the total differential of the source term in terms of both sets of independent variables. In the general case a function $\chi$ can be expressed in terms of sets of independent variables such as $\mathbf{Q} = [q_1, q_2, \ldots, q_N]$ and $\mathbf{P} = [p_1, p_2, \ldots, p_N]$. Then the total differential can be expressed by (\(Q \backslash q_i\) means, that $q_i$ is not constant)

$$d\chi = \sum_{i=1}^{N} \frac{\partial \chi}{\partial q_i} \, dq_i = \sum_{i=1}^{N} \frac{\partial \chi}{\partial p_i} \, dp_i \quad (A.3)$$

Hence, for the conserved variables and those used to describe the source term the following equation can be written

$$dS_i = \frac{\partial S_i}{\partial \rho} \bigg|_{\rho u, \rho v, \rho E, \rho Y_k} \, d\rho + \frac{\partial S_i}{\partial \rho u} \bigg|_{\rho u, \rho \rho E, \rho \rho Y_k} \, d\rho u + \frac{\partial S_i}{\partial \rho v} \bigg|_{\rho u, \rho \rho E, \rho \rho Y_k} \, d\rho v +$$

$$+ \frac{\partial S_i}{\partial \rho E} \bigg|_{\rho u, \rho v, \rho \rho Y_k} \, d\rho E + \sum_{j=1}^{N_s-1} \frac{\partial S_i}{\partial \rho Y_j} \bigg|_{\rho u, \rho v, \rho \rho E, \rho \rho Y_k} \, d\rho Y_j =$$

$$= \frac{\partial S_i}{\partial \rho} \bigg|_{T, \rho Y_k} \, d\rho + \frac{\partial S_i}{\partial T} \bigg|_{\rho, \rho Y_k} \, dT + \sum_{j=1}^{N_s-1} \frac{\partial S_i}{\partial \rho Y_j} \bigg|_{T, \rho Y_k} \, d\rho Y_j \quad (A.4)$$

Now it is easy to identify the terms that have to be summarized to obtain the required partial differentials of the source term with respect to the conserved variables. The temperature $T$, which can be implicitly defined as a function of $\rho$, $e$ and $\rho Y_k$, is given by:

$$T(\rho, e, \rho Y_k) \rightarrow e = \frac{1}{\rho} \sum_{k=1}^{N_s} \rho Y_k \left( h_k(T) - \frac{R M T}{M_k} \right) = \frac{1}{\rho} \sum_{k=1}^{N_s} \rho Y_k e_k(T) \quad (A.5)$$

The internal energy $e$ in terms of conserved variables is defined with the well known equation

$$e(\rho, \rho u, \rho v, \rho E, \rho Y_k) = \frac{1}{\rho} \left( \rho E - \frac{1}{2\rho} \left[ (\rho u)^2 + (\rho v)^2 \right] \right) = E - \frac{1}{2} (u^2 + v^2) \quad (A.6)$$
where the $\rho Y_k$'s are not really required. Summations and products have to be evaluated in a way where the functions only contain conserved variables. This means

$$Y_{N_\star} = 1 - \sum_{k=1}^{N_\star - 1} Y_k$$  \hspace{1cm} (A.7)

has to be used everywhere. This is especially important for calculating the derivatives properly. In the following the derivatives of the source term with respect to the conserved variables are expressed via ‘known’ derivatives:

$$\frac{\partial S_i}{\partial \rho} \bigg|_{\rho, Y_k} = \frac{\partial S_i}{\partial \rho} \bigg|_{T, \rho Y_k} + \frac{\partial S_i}{\partial T} \bigg|_{\rho, \rho Y_k} \cdot \left( \frac{\partial T}{\partial \rho} \bigg|_{e, \rho Y_k} + \frac{\partial T}{\partial e} \bigg|_{\rho, \rho Y_k} \right) \frac{\partial e}{\partial \rho} \bigg|_{\rho, \rho Y_k, \rho E, \rho Y_k}$$  \hspace{1cm} (A.8)

$$\frac{\partial S_i}{\partial \rho u} \bigg|_{\rho, \rho v, \rho Y_k} = \frac{\partial S_i}{\partial \rho T} \bigg|_{\rho, \rho Y_k} \cdot \frac{\partial T}{\partial e} \bigg|_{\rho, \rho Y_k} \frac{\partial e}{\partial \rho u} \bigg|_{\rho, \rho v, \rho E, \rho Y_k}$$  \hspace{1cm} (A.9)

$$\frac{\partial S_i}{\partial \rho v} \bigg|_{\rho, \rho v, \rho Y_k} = \frac{\partial S_i}{\partial \rho T} \bigg|_{\rho, \rho Y_k} \cdot \frac{\partial T}{\partial e} \bigg|_{\rho, \rho Y_k} \frac{\partial e}{\partial \rho v} \bigg|_{\rho, \rho v, \rho E, \rho Y_k}$$  \hspace{1cm} (A.10)

$$\frac{\partial S_i}{\partial \rho E} \bigg|_{\rho, \rho v, \rho Y_k} = \frac{\partial S_i}{\partial \rho T} \bigg|_{\rho, \rho Y_k} \cdot \frac{\partial T}{\partial e} \bigg|_{\rho, \rho Y_k} \frac{\partial e}{\partial \rho E} \bigg|_{\rho, \rho v, \rho Y_k}$$  \hspace{1cm} (A.11)

$$\frac{\partial S_i}{\partial \rho Y_j} \bigg|_{\rho, \rho u, \rho v, \rho E, \rho Y_k, \rho \neq j} = \frac{\partial S_i}{\partial \rho T} \bigg|_{\rho, \rho Y_k} \cdot \frac{\partial T}{\partial \rho Y_j} \bigg|_{\rho, \rho T, \rho Y_{\neq j}} + \frac{\partial S_i}{\partial \rho Y_j} \bigg|_{\rho, \rho T, \rho Y_{\neq j}}$$  \hspace{1cm} (A.12)

Finally, the ‘known’ derivatives are presented, first for the source term, for the temperature and last for the energy. The derivatives of the source term are:

$$\frac{\partial S_i}{\partial \rho} \bigg|_{T, \rho Y_k} = M_i \sum_{j=1}^{N} \left[ \left( \nu_{j} - \nu_{ij} \right) \frac{\alpha_{1,n}}{M_{n}} \sum_{j=1}^{N} \left[ M_{j} \nu_{j} - k_{1, j} \prod_{j=1}^{N} \right] + \right. \frac{[M_i]}{(\nu_{j} - \nu_{ij})} \left( k_{f, l} \nu_{j, l} \prod_{j=1}^{N} [M_j] - k_{b, l} \prod_{j=1}^{N} \right) \right]$$  \hspace{1cm} (A.13)

$$\frac{\partial S_i}{\partial T} \bigg|_{\rho, \rho Y_k} = M_i \sum_{j=1}^{N} \left[ \frac{[M_i]}{(\nu_{j} - \nu_{ij})} \frac{E_{A,i}}{R_{m T}} \prod_{j=1}^{N} [M_j] \right]$$  \hspace{1cm} (A.14)

$$\frac{\partial S_i}{\partial \rho Y_j} \bigg|_{\rho, \rho T, \rho Y_{\neq j}} = M_i \sum_{j=1}^{N} \left[ \left( \nu_{j} - \nu_{ij} \right) \left( \alpha_{1,n} \frac{M_{n}}{M_{n}} \prod_{j=1}^{N} \left[ M_{m} \nu_{m} \right] - k_{b, l} \prod_{j=1}^{N} \right) \right] + \frac{[M_i]}{(\nu_{j} - \nu_{ij})} \left( k_{f, l} \left( \frac{\nu_{j, l}}{\rho Y_{j}} \prod_{j=1}^{N} [M_j] \right) - k_{b, l} \prod_{j=1}^{N} \right) -$$  \hspace{1cm} (A.15)
The derivatives of the temperature are given by

$$\frac{\partial T}{\partial \rho}|_{\rho, \rho Y_j} = \frac{e - e_{N_j}}{\rho c_v} \quad \text{(A.16)}$$

$$\frac{\partial T}{\partial e}|_{\rho, \rho Y_j} = \frac{1}{c_v} \quad \text{(A.17)}$$

$$\frac{\partial T}{\partial p Y_j}|_{\rho, \rho, \rho Y_k, \rho, \rho Y_m} = \frac{e_{N_j} - e_j}{\rho c_v} \quad \text{(A.18)}$$

Furthermore the derivatives of the energy are defined as

$$\frac{\partial e}{\partial \rho}|_{\rho, \rho Y_j} = \frac{1}{\rho} (u^2 + v^2 - E) \quad \text{(A.19)}$$

$$\frac{\partial e}{\partial \rho u}|_{\rho, \rho Y_j} = -\frac{u}{\rho} \quad \text{(A.20)}$$

$$\frac{\partial e}{\partial \rho v}|_{\rho, \rho Y_j} = -\frac{v}{\rho} \quad \text{(A.21)}$$

$$\frac{\partial e}{\partial p E}|_{\rho, \rho Y_j} = \frac{1}{\rho} \quad \text{(A.22)}$$

$$\frac{\partial e}{\partial p Y_j}|_{\rho, \rho, \rho Y_j} = 0 \quad \text{(A.23)}$$

This finally allows the analytical calculation of the source term Jacobian. The equation $c_p - c_v = R$, where $c_p$ and $c_v$ are the specific heat coefficients and $R$ the gas constant, can be used to calculate $c_v$ for multi-species gas mixtures.

$$c_p = \sum_{i=1}^{N_s} Y_i c_{p_i}$$

$$R = \sum_{i=1}^{N_s} \frac{Y_i}{M_i} \cdot R_m$$

This can be applied to find

$$c_v = R_m \left( \sum_{i=1}^{N_s} \frac{Y_i}{M_i} \left( \frac{c^*_{p_i}}{R_m} - 1 \right) \right) \quad \text{(A.24)}$$

Although its derivation is straightforward, the calculation of the first derivative of the equilibrium constant $K_{\theta, l}$ with respect to the temperature $T$ for reaction $l$ is given below. The definition of $K_{\theta, l}$ utilizes molar enthalpy and entropy, as stated before:

$$K_{\theta, l} (p_0, T) = \exp \left( -\sum_{k=1}^{N_s} \nu_{k, r} \left( \frac{h_k^*}{R_m T} - \frac{s_k^*}{R_m} \right) \right)$$
where

\[
\frac{h_i^*}{R_m T} = \frac{a_{h,i}}{T} + \sum_{k=1}^{N_{cp}} \frac{a_{k,i}}{k} T^{k-1}
\]

\[
\frac{s_i^*}{R_m} = a_{s,i} + a_{1,i} \ln T + \sum_{k=2}^{N_{cp}} \frac{a_{k,i}}{k-1} T^{k-1}
\]

This gives

\[
\frac{\partial}{\partial T} \left( \frac{h_i^*}{R_m T} \right) = -\frac{a_{h,i}}{T^2} + \frac{1}{2} a_{2,i} + \ldots + a_{k,i} \frac{T^{k-1}}{k} \tag{A.25}
\]

\[
\frac{\partial}{\partial T} \left( \frac{s_i^*}{R_m} \right) = \frac{a_{s,i}}{T} + a_{2,i} + \ldots + a_{k,i} T^{k-2} \tag{A.26}
\]

which finally yields to

\[
\frac{\partial}{\partial T} K_{\theta,r} (p_0, T) = K_{\theta,r} (p_0, T) \cdot \left( \sum_{k=1}^{N_x} \nu_{k,r} \left( \frac{a_{h,r}}{T^2} + \sum_{l=1}^{N_{cp}} a_{l,k} \frac{T^{l-1}}{l} \right) \right) \tag{A.27}
\]

Also the derivatives of the concentration products with respect to one specific species concentration have to be explained in detail. The given forms for species \( j \) and reaction \( l \)

\[
\frac{\nu_{j,l}}{\rho Y_j} \cdot \prod_{m=1}^{N_{x}} [M_m]^{\nu_{m,l}} \tag{A.28}
\]

\[
\frac{\nu_{j,l}}{\rho Y_j} \cdot \prod_{m=1}^{N_{x}} [M_m]^{\nu_{m,l}} \tag{A.29}
\]

are valid results for \( Y_j \neq 0 \), otherwise the result depends on \( \nu_{j,l} \) as well. Below all the possibilities are given (for products of the reaction products the same is valid):

\[
\frac{\nu_{j,l}}{\rho Y_j} \cdot \prod_{m=1}^{N_{x}} [M_m]^{\nu_{m,l}} = \begin{cases} 
0 & \text{for } \nu_{j,l} = 0 \text{ and all } Y_j \\
\frac{1}{M_j} \cdot \prod_{m=1,m \neq j}^{N_{x}} [M_m]^{\nu_{m,l}} & \text{for } \nu_{j,l} = 1 \text{ and all } Y_j \\
0 & \text{for } \nu_{j,l} > 1 \text{ and } Y_j = 0 \\
\frac{\nu_{j,l}'}{\rho Y_j} \cdot \prod_{m=1}^{N_{x}} [M_m]^{\nu_{m,l}} & \text{for } \nu_{j,l} > 1 \text{ and } Y_j \neq 0
\end{cases} \tag{A.30}
\]
Appendix B

Inviscid Flux Jacobi Matrix

The inviscid flux Jacobi matrices are defined as

\[
\begin{align*}
J_{G_e} &= \frac{\partial G_e}{\partial Q} \\
J_{H_e} &= \frac{\partial H_e}{\partial Q}
\end{align*}
\]  

(B.1)  
(B.2)

where \(G_e\) and \(H_e\) are the inviscid fluxes in \(x\) and \(y\) direction. As for the source term Jacobi matrix the calculation of the inviscid flux Jacobi matrices can be done numerically or analytically. The numerical evaluation follows exactly the pattern presented for the source term Jacobi matrix and the analytical evaluation will be derived in the following. The derivation of the flux Jacobi matrices is straightforward apart from that of the pressure term. Here we have to differentiate between multispecies and single species flow. Hence, the derivatives of the pressure with respect to the conserved variables will be derived within the next two Subsections. Before, the general form of the inviscid flux Jacobi matrices is given for the inviscid flux vector in \(x\) direction \(G_e\) and in \(y\) direction for \(H_e\).
Inviscid Multispecies Flux Jacobi Matrix: Pressure Derivatives

In addition to partial derivatives of the temperature $T$ with respect to the variables $\rho, e$ and $\rho Y_i$ and of the internal energy $e$ with respect to the conserved variables $\rho, pu, \rho v, \rho E$ and $\rho Y_i$ given in the Appendix for the source term Jacobi matrix, we need to derive partial derivatives of the temperature $T$ with respect to $\rho, pu, \rho v, \rho E$ and $\rho Y_i$ and those of the pressure $p$ with respect to $\rho, T$ and $\rho Y_i$. Firstly, the temperature derivatives ($T = T(\rho, e, \rho Y_i)$) are given. Note that

$$
\frac{\partial T}{\partial \chi} \bigg|_{Q_\rho} \, d\chi = \frac{\partial T}{\partial \rho} \bigg|_{e, \rho Y_i} \, dp + \frac{\partial T}{\partial e} \bigg|_{\rho, \rho Y_i} \, de + \sum_{j=1}^{N_i-1} \frac{\partial T}{\partial \rho Y_j} \bigg|_{\rho, e, \rho Y_i, \rho Y_j} \, dpY_j
$$
which leads to

\[
\frac{\partial T}{\partial \rho} \bigg|_{Q,\rho} = \frac{1}{\rho c_v} \left[ u^2 + v^2 - E + \sum_{i=1}^{N_s-1} Y_i (e_i - e_{N_s}) \right]
\]

(B.6)

\[
\frac{\partial T}{\partial \rho u} \bigg|_{Q,\rho u} = -\frac{u}{\rho c_v}
\]

(B.7)

\[
\frac{\partial T}{\partial \rho v} \bigg|_{Q,\rho v} = -\frac{v}{\rho c_v}
\]

(B.8)

\[
\frac{\partial T}{\partial \rho E} \bigg|_{Q,\rho E} = -\frac{1}{\rho c_v}
\]

(B.9)

\[
\frac{\partial T}{\partial \rho Y_j} \bigg|_{Q,\rho Y_j} = \frac{e_{N_s} - e_j}{\rho c_v}
\]

(B.10)

Secondly, the pressure derivatives for \( p = p(\rho, T, \rho Y_i) \) are presented:

\[
\frac{\partial p}{\partial \rho} \bigg|_{T, \rho Y_i} = \frac{R_m T}{M N_s}
\]

(B.11)

\[
\frac{\partial p}{\partial T} \bigg|_{\rho, \rho Y_i} = R_m \left[ \frac{\rho}{M N_s} + \sum_{i=1}^{N_s-1} \rho Y_i \left( \frac{1}{M_i} - \frac{1}{M_{N_s}} \right) \right] = \frac{\rho R_m}{M}
\]

(B.12)

\[
\frac{\partial p}{\partial \rho Y_j} \bigg|_{\rho, T, \rho Y_i, \rho Y_j} = R_m T \left[ \frac{1}{M_j} - \frac{1}{M_{N_s}} \right]
\]

(B.13)

This can be used to finally compose the pressure derivatives for \( p = p(\rho, \rho u, \rho v, \rho E, \rho Y_i) \):

\[
\frac{\partial p}{\partial \rho} \bigg|_{Q,\rho} = R_m \left\{ \frac{T}{M N_s} + \frac{1}{M c_v} \left[ u^2 + v^2 - E + \sum_{i=1}^{N_s-1} Y_i (e_i - e_{N_s}) \right] \right\}
\]

\[
= R_m \left\{ \frac{T}{M N_s} + \frac{1}{M c_v} \left[ \frac{1}{2} (u^2 + v^2) - e_{N_s} \right] \right\}
\]

(B.14)

\[
\frac{\partial p}{\partial \rho u} \bigg|_{Q,\rho u} = -\frac{u R_m}{c_v M}
\]

(B.15)

\[
\frac{\partial p}{\partial \rho v} \bigg|_{Q,\rho v} = -\frac{v R_m}{c_v M}
\]

(B.16)

\[
\frac{\partial p}{\partial \rho E} \bigg|_{Q,\rho E} = \frac{R_m}{c_v M}
\]

(B.17)

\[
\frac{\partial p}{\partial \rho Y_j} \bigg|_{Q,\rho Y_i,\rho Y_j} = \frac{R_m}{c_v M} (e_{N_s} - e_j) + R_m T \left( \frac{1}{M_j} - \frac{1}{M_{N_s}} \right)
\]

(B.18)
In the case of single species flow the pressure can be expressed in terms of conserved variables as:

\[ p = (\gamma - 1) \left\{ \rho E - \frac{1}{2\rho} [ (\rho u)^2 + (\rho v)^2] \right\} \]  

(B.19)

Then the derivatives with respect to the conserved variables become

\[
\left. \frac{\partial p}{\partial \rho} \right|_{Q,\rho} = \frac{\gamma - 1}{2} (u^2 + v^2) \]  

(B.20)

\[
\left. \frac{\partial p}{\partial \rho u} \right|_{Q,\rho u} = -(\gamma - 1) u \]  

(B.21)

\[
\left. \frac{\partial p}{\partial \rho v} \right|_{Q,\rho v} = -(\gamma - 1) v \]  

(B.22)

\[
\left. \frac{\partial p}{\partial \rho E} \right|_{Q,\rho E} = \gamma - 1 \]  

(B.23)
Appendix C

Inviscid Flux Eigenvector Matrices

Recalling the convective flux $F_c$ for a cell side

$$F_c = \frac{\Delta y G_c - \Delta x H_c}{\Delta s} = \Delta y^0 G_c - \Delta x^0 H_c$$

and the Jacobi matrix for this flux

$$\frac{\partial F_c}{\partial \Omega} = \frac{\Delta y \frac{\partial}{\partial x} G_c - \Delta x \frac{\partial}{\partial x} H_c}{\Delta s} = \Delta y^0 \frac{\partial}{\partial x} G_c - \Delta x^0 \frac{\partial}{\partial x} H_c$$

with $\frac{\partial}{\partial x} G_c$ and $\frac{\partial}{\partial x} H_c$ being the Jacobi matrices for the inviscid fluxes in $x$ and $y$ directions, we can express the Jacobi matrix for the convective flux via its eigenvalues and the appropriate eigenvector matrices:

$$\frac{\partial F_c}{\partial \Omega} = T \cdot \Lambda_c \cdot T^{-1}$$  \hspace{1cm} (C.1)

The diagonal matrix $\Lambda_c$ has the eigenvalues $u_n, u_n, u_n + a, u_n - a, u_n, ...,$ $u_n$ as entities on the diagonal where $u_n = \Delta y^0 u - \Delta x^0 v$. The left and right eigenvector matrices $T$ and $T^{-1}$ can be found in Shuen's paper [23] and are given in the following.
\[ H = \frac{p}{\rho} \left( k_2 u - k_1 v \right) \]

\[
T = \begin{bmatrix}
1 & 0 & \frac{\rho}{\sqrt{2a}} & \frac{u}{\sqrt{2a}} & \frac{v}{\sqrt{2a}} & 0 & 0 & \ldots & 0 \\
u & k_2 \rho & \frac{p(u+k_1 u)}{\sqrt{2a}} & \frac{p(u-k_1 u)}{\sqrt{2a}} & 0 & 0 & \ldots & 0 \\
v & -k_1 \rho & \frac{p(u+k_1 u)}{\sqrt{2a}} & \frac{p(u-k_1 u)}{\sqrt{2a}} & 0 & 0 & \ldots & 0 \\
H - \frac{p}{\rho} \left( k_2 u - k_1 v \right) & \frac{p(H + \Theta)}{\sqrt{2a}} & \frac{p(H - \Theta)}{\sqrt{2a}} & \frac{-p^2 \rho Y_1}{\rho} & \frac{-p^2 \rho Y_2}{\rho} & \ldots & \frac{-p^2 \rho Y_{N_s-1}}{\rho} \\
Y_1 & 0 & \frac{\rho Y_1}{\sqrt{2a}} & \frac{\rho Y_1}{\sqrt{2a}} & \rho & 0 & \ldots & 0 \\
Y_2 & 0 & \frac{\rho Y_2}{\sqrt{2a}} & \frac{\rho Y_2}{\sqrt{2a}} & 0 & \rho & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
Y_{N_s-1} & 0 & \frac{\rho Y_{N_s-1}}{\sqrt{2a}} & \frac{\rho Y_{N_s-1}}{\sqrt{2a}} & 0 & 0 & \ldots & \rho
\end{bmatrix}
\]

\[ (C.2) \]

and

\[
T^{-1} = \begin{bmatrix}
1 - \frac{\Phi}{\rho} & \frac{\Phi}{\sqrt{2a}} & \frac{\Phi}{\sqrt{2a}} & \frac{-p_e}{\rho} & \frac{-p_e}{\sqrt{2a}} & \frac{-p_e}{\sqrt{2a}} & \ldots & \frac{-p_e Y_{N_s-1}}{\sqrt{2a}} \\
k_2 - k_1 \rho & \frac{k_2 \rho}{\sqrt{2a}} & \frac{k_2 \rho}{\sqrt{2a}} & 0 & 0 & 0 & \ldots & 0 \\
k_2 - k_1 \rho & \frac{k_2 \rho}{\sqrt{2a}} & \frac{k_2 \rho}{\sqrt{2a}} & 0 & 0 & 0 & \ldots & 0 \\
-\frac{\Phi - \Theta}{\sqrt{2pa}} & \frac{k_2 - k_1 \rho}{\sqrt{2pa}} & \frac{k_2 - k_1 \rho}{\sqrt{2pa}} & \frac{p_e}{\sqrt{2pa}} & \frac{p_e}{\sqrt{2pa}} & \frac{p_e}{\sqrt{2pa}} & \ldots & \frac{p_e Y_{N_s-1}}{\sqrt{2pa}} \\
-\frac{\Theta}{\sqrt{2pa}} & \frac{k_2 + k_1 \rho}{\sqrt{2pa}} & \frac{k_2 + k_1 \rho}{\sqrt{2pa}} & \frac{p_e}{\sqrt{2pa}} & \frac{p_e}{\sqrt{2pa}} & \frac{p_e}{\sqrt{2pa}} & \ldots & \frac{p_e Y_{N_s-1}}{\sqrt{2pa}} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-\frac{Y_{N_s-1}}{\sqrt{2pa}} & 0 & 0 & 0 & 0 & 0 & \ldots & \frac{1}{\rho}
\end{bmatrix}
\]

\[ (C.3) \]

where

\[ \Theta = a \left( k_1 u + k_2 v \right) \]

\[ \Phi = p_\rho + \frac{p p_e}{\rho^2} - \frac{p_e}{\rho} \left( H - u^2 - v^2 \right) \]

\[ k_1 = \frac{\Delta y}{\Delta s} = \Delta y^0 \]

\[ k_2 = -\frac{\Delta x}{\Delta s} = -\Delta x^0 \]

Here \( H \) is the specific total enthalpy and \( p_\rho, p_e \) and \( p_\rho Y_i \) are the pressure derivatives with respect to density, internal energy and the species density. The frozen speed of sound is described by \( a \).

The calculation of the relevant pressure derivatives and the frozen speed of sound are outlined for multi-species and single species gases in the next Subsections, which leads to the analysis of the pressure derivatives with respect to the variables \( \rho, e, \rho Y_1, \ldots, \rho Y_{N_s-1} \).
Appendix C. Inviscid Flux Eigenvector Matrices

C.1 Inviscid Multispecies Flux Eigenvector Matrices: Pressure Derivatives

The pressure derivatives used for the calculation of the frozen speed of sound for a multi-species gas mixture are

\[
\frac{\partial p}{\partial \rho}_{|_{e, Y_i}} = R_m \left( \frac{T}{M_{N_s}} + \frac{e - e_{N_s}}{M_{c_v}} \right) \tag{C.8}
\]

\[
\frac{\partial p}{\partial e}_{|_{\rho, Y_i}} = \frac{\rho R_m}{M_{c_v}} \tag{C.9}
\]

\[
\frac{\partial p}{\partial Y_j}_{|_{\rho, e, Y_i \neq j}} = \frac{R_m}{M_{c_v}} (e_{N_s} - e_j) + R_m T \left( \frac{1}{M_j} - \frac{1}{M_{N_s}} \right) \tag{C.10}
\]

They can easily be derived from pressure derivatives given in previous Appendices.

C.2 Inviscid Single Species Flux Eigenvector Matrices: Pressure Derivatives

Using the relation \( e = \frac{p}{\rho (\gamma - 1)} \), the single species pressure derivatives can be calculated in a straightforward manner:

\[
\frac{\partial p}{\partial \rho}_{|_e} = \frac{p}{\rho} \tag{C.11}
\]

\[
\frac{\partial p}{\partial e}_{|_\rho} = \rho (\gamma - 1) \tag{C.12}
\]

Mass fraction derivatives obviously do not play any role for gases with only one species.

C.3 Frozen Speed of Sound

The ‘frozen’ speed of sound for multi-species and single species gases is defined according to

\[
a^2 = \left( \frac{\partial p}{\partial \rho} \right)_s = \frac{\partial p}{\partial \rho}_{|_{e, Y_i}} + \frac{p}{\rho^2} \frac{\partial p}{\partial e}_{|_{\rho, Y_i}} + \sum_{j=1}^{N_s-1} Y_j \frac{\partial p}{\partial \rho Y_j}_{|_{e, Y_i \neq j}} \tag{C.14}
\]

and it does not take into account the possible variation of chemical composition in a sound wave. The appropriate pressure derivatives must be used and for single species gas flow this simplifies to the well-known expression \( a = \sqrt{\gamma p / \rho} \).
Appendix D

Physical Data

In this Chapter all data used for the calculation of molecular, species and transport properties is presented as well as the different reaction schemes used. All coefficients and constants are given in SI units.

D.1 Molecular Species Properties

The molecular weights for the different species are obtained from [19] in order to be consistent with the coefficients used for the polynomials to calculate the specific heats at constant pressure. The collision diameters and Lennard-Jones potentials given in [6] and [12] are used for the calculation of viscous transport properties. These molecular properties needed for the relevant species are listed in Tab. D.1

D.2 Thermodynamic Species Properties

The temperature intervals for the coefficients used within the polynomials to calculate specific heat at constant pressure, enthalpy and entropy are given in Tab. D.2, the coefficients itself in D.3. For the data used here reference [19] is consulted.
<table>
<thead>
<tr>
<th>Species</th>
<th>Molecular Weight $[M] = \frac{kg}{kmol}$</th>
<th>Collision Diameter $[\sigma] = m$</th>
<th>Lennard-Jones Potential $[\epsilon] = K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>1.00794</td>
<td>$0.2070 \cdot 10^{-9}$</td>
<td>37.00</td>
</tr>
<tr>
<td>$N$</td>
<td>14.00674</td>
<td>$0.3298 \cdot 10^{-9}$</td>
<td>71.40</td>
</tr>
<tr>
<td>$O$</td>
<td>15.99940</td>
<td>$0.3050 \cdot 10^{-9}$</td>
<td>106.70</td>
</tr>
<tr>
<td>$H_2$</td>
<td>2.01528</td>
<td>$0.2827 \cdot 10^{-9}$</td>
<td>59.70</td>
</tr>
<tr>
<td>$OH$</td>
<td>17.00734</td>
<td>$0.3147 \cdot 10^{-9}$</td>
<td>79.80</td>
</tr>
<tr>
<td>$NO$</td>
<td>30.00614</td>
<td>$0.3621 \cdot 10^{-9}$</td>
<td>97.53</td>
</tr>
<tr>
<td>$O_2$</td>
<td>31.99880</td>
<td>$0.3467 \cdot 10^{-9}$</td>
<td>106.70</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>18.01528</td>
<td>$0.2800 \cdot 10^{-9}$</td>
<td>260.00</td>
</tr>
<tr>
<td>$HNO$</td>
<td>31.01408</td>
<td>$0.3798 \cdot 10^{-9}$</td>
<td>71.40</td>
</tr>
<tr>
<td>$HO_2$</td>
<td>33.00674</td>
<td>$0.3068 \cdot 10^{-9}$</td>
<td>168.00</td>
</tr>
<tr>
<td>$NO_2$</td>
<td>46.00554</td>
<td>$0.3500 \cdot 10^{-9}$</td>
<td>200.00</td>
</tr>
<tr>
<td>$H_2O_2$</td>
<td>34.01468</td>
<td>$0.4196 \cdot 10^{-9}$</td>
<td>289.30</td>
</tr>
<tr>
<td>$N_2$</td>
<td>28.01348</td>
<td>$0.3798 \cdot 10^{-9}$</td>
<td>71.40</td>
</tr>
</tbody>
</table>

Table D.1: Molecular Properties.

<table>
<thead>
<tr>
<th>Interval</th>
<th>$T_{min}$</th>
<th>$T_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>200</td>
<td>1000</td>
</tr>
<tr>
<td>2</td>
<td>1000</td>
<td>6000</td>
</tr>
</tbody>
</table>

Table D.2: Temperature intervals for species property polynomials.
D.3 Transport Properties

For the calculation of the transport properties by means of the kinetic gas theory we need to calculate collision integrals. According to [6] there are different intervals with respect to the reduced temperature, given in Tab. D.4, in order to improve the accuracy of the collision integrals. They are calculated via polynomials with coefficients shown in Tab. D.5.

D.4 Chemical Reaction Schemes

All values in the tables below are expressed in SI-units (s, m³, kmol, J and K) leading to the following dimensions for collision frequency factor $A_{0,i}$, temperature exponent $\alpha_i$ and activation energy $E_{A,i}$:

$$[A_{0,i}] = \left( \frac{kmol}{m^3} \right)^{1-\frac{\sum \nu_i}{s \cdot K^{\alpha_i}}} \cdot \frac{1}{s \cdot K^{\alpha_i}}$$

$$[\alpha_i] = 1$$

$$[E_{A,i}] = \frac{J}{kmol}$$

D.4.1 The 8 Species and 17 Reactions Oxygen-Hydrogen System

The 8 species involved in this oxygen-hydrogen system are $H$, $O$, $H_2$, $OH$, $O_2$, $H_2O$, $HO_2$ and $H_2O_2$ and the system of reaction equations can be found in Tab. D.6. The scheme was obtained from [22] and was proposed by Westbrook.

D.4.2 The 9 Species and 19 Reactions Air-Hydrogen System

The 9 species involved in this air-hydrogen system are $H$, $N$, $O$, $H_2$, $OH$, $NO$, $O_2$, $H_2O$, $HNO$, $HO_2$, $NO_2$, $H_2O_2$ and $N_2$ and the system of reaction equations can be found in Tab. D.7. The scheme was obtained from [3] and was proposed by Jachimowski. This is a reduced version of the scheme presented in the next Subsection with nitrogen $N_2$ treated as an inert component of the gas mixture.
<table>
<thead>
<tr>
<th>Spec.</th>
<th>H</th>
<th>N</th>
<th>O</th>
<th>H₂</th>
<th>O₂</th>
<th>HNO</th>
<th>HO₂</th>
<th>NO₂</th>
<th>N₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>iTemp.</td>
<td>2.54736509 E + 04</td>
<td>5.61046378 E + 04</td>
<td>2.61222509 E + 04</td>
<td>1.97095173 E + 03</td>
<td>1.31032767 E + 04</td>
<td>1.03988005 E + 04</td>
<td>2.08090804 E + 04</td>
<td>1.27752989 E + 04</td>
<td>1.28047685 E + 04</td>
</tr>
<tr>
<td>a₁</td>
<td>-4.46683535 E - 01</td>
<td>4.19390032 E + 00</td>
<td>2.05162346 E + 00</td>
<td>8.63010938 E - 03</td>
<td>6.49035208 E - 01</td>
<td>6.86830065 E - 03</td>
<td>6.86830065 E - 03</td>
<td>-8.17035173 E - 02</td>
<td>-8.13085570 E - 02</td>
</tr>
<tr>
<td>a₂</td>
<td>2.50000000 E + 00</td>
<td>2.50000000 E + 00</td>
<td>2.50000000 E + 00</td>
<td>2.34331123 E + 00</td>
<td>2.34331123 E + 00</td>
<td>2.34331123 E + 00</td>
<td>2.34331123 E + 00</td>
<td>2.34331123 E + 00</td>
<td>2.34331123 E + 00</td>
</tr>
<tr>
<td>a₂p,1</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
</tr>
<tr>
<td>a₂p,2</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
</tr>
<tr>
<td>a₂p,3</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
</tr>
<tr>
<td>a₂p,4</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
</tr>
<tr>
<td>a₂p,5</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
<td>0.00000000 E + 00</td>
</tr>
</tbody>
</table>

Table D.3. Coefficients for polynomials of species properties.
### Table D.4: Reduced temperature intervals.

<table>
<thead>
<tr>
<th>Interval</th>
<th>$T_{\text{min}}^*$</th>
<th>$T_{\text{max}}^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>$\infty$</td>
</tr>
</tbody>
</table>

Table D.4: Reduced temperature intervals.

### Table D.5: Parameters for the calculation of the collision integrals.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$a_{\lambda, 1}$</th>
<th>$a_{\lambda, 2}$</th>
<th>$a_{\lambda, 3}$</th>
<th>$a_{\lambda, 4}$</th>
<th>$a_{\lambda, 5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H + O_2$</td>
<td>0.23527333E + 01</td>
<td>-0.13589968E + 01</td>
<td>0.52202460E + 00</td>
<td>-0.94282843E - 01</td>
<td>0.64334629E - 02</td>
</tr>
<tr>
<td>$H_2 + O$</td>
<td>0.12660389E + 01</td>
<td>-0.10441443E + 00</td>
<td>0.22945932E + 00</td>
<td>-0.16321468E - 01</td>
<td>0.45833572E - 04</td>
</tr>
<tr>
<td>$H_2O + O$</td>
<td>0.85583333E + 00</td>
<td>-0.13552911E + 00</td>
<td>0.26162804E - 03</td>
<td>-0.24647854E - 05</td>
<td>0.86533866E - 08</td>
</tr>
<tr>
<td>$H + O_2 + M$</td>
<td>0.11077773E + 01</td>
<td>-0.94402344E - 02</td>
<td>0.16918277E - 02</td>
<td>-0.89285589E - 04</td>
<td>0.86533866E - 08</td>
</tr>
<tr>
<td>$H + O_2 + H$</td>
<td>0.10814232E + 01</td>
<td>0.31954282E - 02</td>
<td>-0.69285589E - 04</td>
<td>0.86533866E - 08</td>
<td>0.86533866E - 08</td>
</tr>
<tr>
<td>$H_2 + O + M$</td>
<td>0.11059000E + 01</td>
<td>0.64135654E - 03</td>
<td>-0.3400910E - 05</td>
<td>0.86533866E - 08</td>
<td>0.86533866E - 08</td>
</tr>
</tbody>
</table>

Table D.5: Parameters for the calculation of the collision integrals.

### Table D.6: 8 Species and 17 reactions oxygen-hydrogen reaction scheme.

<table>
<thead>
<tr>
<th>#</th>
<th>Reaction</th>
<th>$a_{\lambda}$</th>
<th>$b$</th>
<th>$E_{\Delta}$</th>
<th>Third Body Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H + O_2$</td>
<td>1.86 $\cdot 10^{11}$</td>
<td>0</td>
<td>70396.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 1}$ = 1, $b_{\lambda, 1}$ = 1</td>
</tr>
<tr>
<td>2</td>
<td>$H_2 + O$</td>
<td>1.82 $\cdot 10^{10}$</td>
<td>1</td>
<td>37263.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 2}$ = 1, $b_{\lambda, 2}$ = 1</td>
</tr>
<tr>
<td>3</td>
<td>$H_2O + O$</td>
<td>3.39 $\cdot 10^{10}$</td>
<td>0</td>
<td>76828.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 3}$ = 1, $b_{\lambda, 3}$ = 1</td>
</tr>
<tr>
<td>4</td>
<td>$H_2O + H$</td>
<td>9.55 $\cdot 10^{10}$</td>
<td>0</td>
<td>84992.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 4}$ = 1, $b_{\lambda, 4}$ = 1</td>
</tr>
<tr>
<td>5</td>
<td>$H_2O_2 + O$</td>
<td>1.58 $\cdot 10^{10}$</td>
<td>0</td>
<td>51363.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 5}$ = 1, $b_{\lambda, 5}$ = 1</td>
</tr>
<tr>
<td>6</td>
<td>$H_2O + H$</td>
<td>5.01 $\cdot 10^{10}$</td>
<td>0</td>
<td>4187.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 6}$ = 1, $b_{\lambda, 6}$ = 1</td>
</tr>
<tr>
<td>7</td>
<td>$H_2 + O + H$</td>
<td>2.51 $\cdot 10^{11}$</td>
<td>0</td>
<td>7055.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 7}$ = 1, $b_{\lambda, 7}$ = 1</td>
</tr>
<tr>
<td>8</td>
<td>$H_2O_2 + H$</td>
<td>2.51 $\cdot 10^{10}$</td>
<td>0</td>
<td>2931.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 8}$ = 1, $b_{\lambda, 8}$ = 1</td>
</tr>
<tr>
<td>9</td>
<td>$H_2O + O + H$</td>
<td>5.02 $\cdot 10^{10}$</td>
<td>0</td>
<td>4187.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 9}$ = 1, $b_{\lambda, 9}$ = 1</td>
</tr>
<tr>
<td>10</td>
<td>$H_2O + O$</td>
<td>3.08 $\cdot 10^{10}$</td>
<td>0</td>
<td>17852.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 10}$ = 1, $b_{\lambda, 10}$ = 1</td>
</tr>
<tr>
<td>11</td>
<td>$H_2O_2 + O$</td>
<td>3.98 $\cdot 10^{10}$</td>
<td>0</td>
<td>80850.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 11}$ = 1, $b_{\lambda, 11}$ = 1</td>
</tr>
<tr>
<td>12</td>
<td>$H_2O_2 + O$</td>
<td>1.20 $\cdot 10^{10}$</td>
<td>0</td>
<td>80850.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 12}$ = 1, $b_{\lambda, 12}$ = 1</td>
</tr>
<tr>
<td>13</td>
<td>$H_2O + H$</td>
<td>5.16 $\cdot 10^{10}$</td>
<td>0</td>
<td>80850.000 $\cdot 10^3$</td>
<td>$a_{\lambda, 13}$ = 1, $b_{\lambda, 13}$ = 1</td>
</tr>
<tr>
<td>14</td>
<td>$O + H + M$</td>
<td>1.10 $\cdot 10^{10}$</td>
<td>0</td>
<td>0</td>
<td>$a_{\lambda, 14}$ = 1, $b_{\lambda, 14}$ = 1</td>
</tr>
<tr>
<td>15</td>
<td>$H_2 + O_2$</td>
<td>2.19 $\cdot 10^{10}$</td>
<td>0</td>
<td>0</td>
<td>$a_{\lambda, 15}$ = 1, $b_{\lambda, 15}$ = 1</td>
</tr>
<tr>
<td>16</td>
<td>$H_2O + H + M$</td>
<td>5.13 $\cdot 10^{12}$</td>
<td>0</td>
<td>0</td>
<td>$a_{\lambda, 16}$ = 1, $b_{\lambda, 16}$ = 1</td>
</tr>
</tbody>
</table>

Table D.6: 8 Species and 17 reactions oxygen-hydrogen reaction scheme.
D.4.3 The 13 Species and 33 Reactions Air-Hydrogen System

The 13 species involved in this air-hydrogen system are $H$, $N$, $O$, $H_2$, $OH$, $NO$, $O_2$, $H_2O$, $HNO$, $HO_2$, $NO_2$, $H_3O_2$ and $N_2$ and the system of reaction equations can be found in Tab. D.8. The scheme was proposed by Jachimowski (see [14]) especially for the calculation of scramjet combustion. Nitrogen is not considered as an inert species to increase the accuracy at higher temperatures.
Table D.8: 13 Species and 33 reactions air-hydrogen reaction scheme.
Bibliography


