Numerical Simulation of Scramjet Combustion

Emil Engman
Preface

This thesis is the final project for the Master of Science in Engineering Physics at Luleå University of Technology in Sweden. A substantial part of the work has been performed at the German Aerospace Center, DLR, in Germany.

I would like to thank my supervisors and colleagues at DLR, Dr. Harald Schütz and MSc. Thomas Kretschmer for their help and support during the work. I would also like to thank the teachers and personnel at the International Schools in Düsseldorf who contributed with valuable help with the German language.

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Emil Engman
Abstract

This thesis work has been carried out partly in conjunction with the Institute of Propulsion Technology of the German Aerospace Center, DLR, in Cologne, Germany. The subject is simulation of fluid flow and hydrogen combustion in a so-called scramjet engine. Scramjet is an acronym for Supersonic Combustion Ramjet, a novel type of propulsion device, interesting primarily for potential spaceflight applications. The aim is to give an indication of how fluid flow and fuel combustion proceed when both mixing and combustion are carried out at supersonic speeds, and to provide a validation of two different solver packages for fluid dynamical problems.

In this study, Reynolds-averaged Navier-Stokes models (RANS) have been used to examine supersonic flow and combustion in a model scramjet combustion chamber. The RANS-model is based on a finite volume discretization of the continuity, momentum, energy and mixture fraction equations. The configuration used is a model of a laboratory scramjet combustor at the Institute for Space Propulsion at DLR. It consists of a divergent channel with a flame-holding, wedge-shaped structure in the middle of the flow field from the base of which hydrogen is injected. Three different operational cases with varying degree of complexity have been investigated. For the purpose of validation of the simulation models the results are systematically compared with experimental data for temperature, velocity and pressure at certain cross-sections in the combustion chamber. Qualitative comparisons are also made between the simulated flow fields and experimental schlieren and shadowgraph fields.

The simulation codes used are ANSYS CFX and a solver program for fluid dynamics and combustion chemistry developed by my supervisor at DLR. Each simulation model is capable of predicting both the cold supersonic flow and the reacting flow fields reasonably well, with some quantitative inconsistencies for both models. Moreover, during the work a previously undiscovered deficiency in the non-commercial code is found, which leads to an appreciated improvement of the program.
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1 Introduction

1.1 DLR

Deutsches Zentrum für Luft- und Raumfahrt, DLR, or the German Aerospace Center as referred to in English is Germany’s national research center for Aeronautics and Space. As Germany’s space agency, the German government has given DLR the responsibility for the forward planning and implementation of the German space program, which includes Germany’s part in the European Space Agency, ESA. DLR conducts extensive research and development work in aeronautics, space, transportation and energy, which is integrated in many national and international cooperative ventures. The center operates and administers large-scale research facilities, both for its own numerous projects and as a provider of services for industry clients and partners. Its research portfolio ranges from fundamental research to cutting edge research and development of the space applications of tomorrow.

DLR has several institutes and facilities distributed over thirteen locations in Germany. This work has been conducted at the Institute of Propulsion Technology in Cologne, where also the headquarters are situated. The research work of the institute is primarily focused on the improvement of gas turbines in aviation and electricity production. One aspect of this objective is combustion research, where an important concern is the development of new combustor concepts, aimed at significantly reducing nitric oxide production in clean and efficient combustion.

The DLR facility in Cologne also hosts the European Astronaut Center, where ESA astronauts are trained and educated.
1.2 Scramjet

The name scramjet is an acronym for *Supersonic Combustion Ramjet*. A scramjet engine, hereafter where suitable only referred to as a scramjet, is a type of jet engine intended to operate in the high velocity regime usually associated with rockets. Just like its older predecessor, the ramjet engine, the scramjet belongs to a family of propulsion devices called hypersonic airbreathing vehicles. In other words it is a device that uses the surrounding atmosphere to drive different types of vehicles with velocities widely in excess of the local speed of sound. Current aerospace technology development contains several areas of application for such hypersonic vehicles, the most outstanding example being reusable launch vehicles for space applications. A reusable launch vehicle that uses the surrounding atmosphere for propulsion could possibly reduce the cost of launching payload into orbit by an order of magnitude, which is considered necessary for the commercial utilization of space and future space exploration beyond the moon. Hypersonic airbreathing vehicles could also imply a paradigm shift in commercial aviation, reducing for example the time for the long-haul flight from Stockholm to Sydney to a mere couple of hours.

1.2.1 History

Already during the later half of the nineteenth century the first ideas concerning ramjet propulsion were developed by the Swedish engineer Gustaf de Laval. Naturally, it had nothing to do with flight at that time, since the first working airplane did not fly before 1903. As soon as five years after the legendary Wright brothers flight the first concept of a ramjet engine was patented in France. Nevertheless it took until 1949 before the technology could be implemented, even this time in France. At that time the research vehicle known as the Leduc Experimental Aircraft, the world’s first aircraft with ramjet propulsion and named after its inventor René Leduc, was flown.
1 Introduction

In these days, shortly after the Second World War, large effort was put into exploring jet- and rocket-driven aircraft. Development proceeded fast and in the early 1960s many indications suggested that hypersonic velocities would be reached within the next few years. Yet the development took another path; civil aviation concentrated on reducing operational costs and designers of military aircraft focused on maneuverability and stealth. However, variations of the existing ramjets were proposed and thereby constituted the first steps toward what today is known as a scramjet engine.

1.2 Scramjet

1.2.2 Simple description

In this section a description will be given of the basic functioning and conceptual design of a scramjet engine. Since the ramjet engine constitutes a prerequisite for the development of scramjet technology, this too will be described. It is worth mentioning that a scramjet could hypothetically work both as a combined ramjet/scramjet engine at the same time. One talks about scramjet operation when the majority of the fuel is combusted supersonically. A ramjet/scramjet engine is estimated to need a speed of about Mach 4-5 to be able to demonstrate fully supersonic combustion.

Hypersonic airbreathing engines exploit the surrounding atmosphere as oxidizer for the fuel combustion. This is to be seen in contrast to most rockets that have to carry its own oxidizer in form of liquid oxygen. The surrounding air is said to be the working fluid. They also differ from conventional turbofan jet engines in the sense that the engine utilizes its own momentum for compression of the incoming air. In a simplistic sense a ramjet can be said to be an ordinary turbojet engine without a turbine or compressor. The need for these components is eliminated since enough compression takes place in the air inlet. The aft part of the engine is shaped as a convergent-divergent nozzle, or a Laval nozzle as it is often called after its Swedish inventor. Here the subsonic combustion gases are accelerated to Mach 1 at its narrowest cross-section, whereupon
they leave the engine at supersonic speeds. Figure 1.1 shows schematically the function of a ramjet engine.

![Ramjet diagram](http://commons.wikimedia.org/wiki/Image:Ramjet_operation.svg)

A ramjet has, like a scramjet, no or very few moving parts, which gives the whole construction a fundamental simplicity of design. Also in resemblance with a scramjet a ramjet uses its forward speed to compress the incoming air. The fuel is then injected and mixed with the air allowing for combustion to take place. After combustion the hot combustion gases are accelerated through a nozzle and leave the engine with a higher speed than the incoming air. Here two problems arise that more than anything sets the limitation for a ramjet engine. Collecting air from the atmosphere causes drag that increases dramatically with speed. Furthermore, at high velocities the collected air gets so hot that engine performance is affected in a negative way. Ramjets produce thrust only when the vehicle already has a forward velocity. Therefore it has to be accelerated by another propulsion system to a velocity where the ramjet engine begins to produce thrust. The performance of a ramjet engine increases with increasing vehicle velocity up to a point where aerodynamic losses become significant. As a solution of these problems the scramjet has been developed by some fundamentally simple modifications to the ramjet.
1 Introduction 1.2 Scramjet

The most significant differences are in the air inlet. While a ramjet must slow the intake air to subsonic speed a scramjet allows the air to flow with supersonic speed through the whole compression phase, reducing the pressure increase in the air intake. An effect is that the compressed air is cooler, allowing for better conditions for fuel combustion as well as a decreased risk of structural failure of the engine. Unfortunately the higher flow speed imposes the new constraint that the fuel has to mix up with the air and react within a very short period of time, one of the main engineering challenges in scramjet engine design.

All scramjet engine designs comprise an air intake that compresses incoming air, fuel injectors, a combustion chamber and a nozzle where the thrust is produced. Most concepts also involve one or more structures integrated in the combustion chamber, acting as a flameholder. Figure 1.2 shows a schematic description of a scramjet engine.

The kinetic energy of the freestream air is large compared to the total energy released by the reaction of fuel and oxidizer. At the corresponding freestream velocities for the configurations used in this study, the kinetic energy of the air and the potential heat release from fuel combustion are approximately equal. Higher velocities result in even smaller fractions of the total enthalpy of the working fluid coming from fuel combustion. Hence it is a major concern in scramjet design to make sure that as large a fraction as possible of the supplied fuel really reacts.

The design of a scramjet engine depends on two factors. Firstly, the temperature of the compressed air flowing into the combustor must be
high enough for combustion to take place, and secondly, there must be enough pressure for the complete reaction to occur before the gases are hurtled out through the back of the engine. These requirements on the incoming air are the main reason for the characteristic funnel-like design of the air inlet. The air flowing into the inlet is compressed by the forward velocity of the vehicle through the atmosphere. This means that a scramjet, just like a ramjet, requires a certain speed before it can be started at all. The minimum operating Mach number at which a scramjet can operate is therefore limited by the pressure of the incoming airflow as well as the temperature. Moreover, for the engine to be called a scramjet the compressed flow must be supersonic even after combustion.

Here are two concerns that have to be taken into consideration. Compression of a supersonic flow firstly leads to the deceleration of the flow. This implies that the freestream air speed must be high enough for the air flow not to be slowed down below Mach 1. If the flow in a scramjet engine goes below Mach 1 the engine is said to choke, transitioning to subsonic flow in the combustion chamber. Secondly, the heating of a gas causes the local speed of sound in the gas to increase, in which the Mach number decreases, despite the fact that the gas flows with the same velocity as before the heating. There is no distinct lower limit for scramjet operation, but a fair estimation is that the engine will need a speed of at least Mach 4-5 to be able to maintain fully supersonic combustion.

1.2.3 Prospective applications

The high costs associated with full-scale experiments with flying scramjet engines have long withheld development. However, an increasing number of actors are realizing the potentials, and there is at present a lot of research being carried out on scramjet technology at a number of companies and organizations worldwide. Since a scramjet is confined to a certain velocity interval it is often projected in combination with other propulsion systems, like rockets and/or turbojet engines. All
tested prototypes have initially been accelerated by a so-called booster rocket.

One of the potential applications of scramjet engines that raise the most attention is as a component in a prospected Single Stage to Orbit vehicle (SSTO). With this a vehicle is intended that can enter a lower earth orbit without letting go of pieces of its own structure, for example fuel tanks or burnt-out rockets. The term is almost exclusively used for reusable vehicles. A vision many people strive for is an SSTO vehicle that starts and lands horizontally like an ordinary aircraft but has the capability to bring personnel and payload to lower earth orbits. The goal of SSTO technology is to provide cheaper, faster and more secure access to space. This is to be achieved by systems that, once in operative use, require less effort on the ground than the space transportation systems of today. Many different variations of SSTO vehicles have been suggested of which several involve scramjet engines. Here two of the more promising concepts are mentioned.

TRCC stands for Turbo Rocket Combined Cycle, a propulsion concept comprising one or more turbofan engines of conventional type, one ramjet/scramjet engine and also a number of rocket engines. According to the conceptual design, the vehicle will start horizontally and accelerate to Mach 2.5 driven by turbofan engines. Additional thrust is produced by the combined ramjet/scramjet engine taken into operation when enough speed for ramjet propulsion is reached. At Mach 2.5 the turbojets are turned off and the vehicle is driven only by the ramjet/scramjet engine. Around Mach 5 the engine turns into full scramjet operation and keeps on accelerating up to Mach 14-18, where the rockets are ignited for the last kick necessary to put the vehicle in orbit. Another variation that possibly receives greater confidence goes under the collective name RBCC or Rocket Based Combined Cycle. It is operated in the same way as the TRCC but without the turbojet engines. Instead it uses rocket engines not only for the last acceleration to orbit, but also at startup, until ramjet operation can take over. In both of these concepts the vehicle returns to the earth and lands as an ordinary aircraft.
1.2.4 Technical challenges for scramjet engines

Here some of the most important pros and cons of the scramjet technology are discussed and weighed against each other. One of the greatest advantages is simplicity of design. A scramjet has no or few moving parts and the main part of its body is constituted by continuous surfaces. This admits relatively low manufacturing costs for the engine itself. A difference between hypersonic airbreathing engines and rocket engines is that the former avoids the need for carrying an oxidizer for fuel combustion. As an illustrating example NASA’s Space Shuttle can be used. The external tank of the space shuttle contains at start 616,432 kg of liquid oxygen and around 103,000 kg of liquid hydrogen. The space shuttle itself weighs about 104,000 kg. This means that approximately 75 percent of the total start weight is oxidizing liquid oxygen whose single purpose is to react with the fuel in the combustion chambers of the rocket engines. [1] If the need for carrying all this could be eliminated, the vehicle would be lighter and hopefully capable of carrying more payload. That would be a great advantage. Unfortunately, there are a number of disadvantages as well.

A scramjet cannot produce thrust if it is not first accelerated to a high velocity, around Mach 5. It could though, as earlier suggested, operate as a ramjet at lower speed. Horizontal start as outlined above would require conventional turbofan or rocket engines and fuel for those. In addition to that, various structures are needed for the suspension of these engines as well as all necessary control systems. All secondary equipment necessary to bring the vehicle to velocities suitable for scramjet operation makes the whole craft heavy. Many experts therefore advice external, preferably reusable, rockets as a first stage that simplifies design considerably.

Unlike a rocket that passes nearly vertically through the atmosphere on its way to orbit, a scramjet would take a more leveled trajectory. Because of the thrust-to-weight ratio of a scramjet engine being low compared to modern rockets the scramjet needs more time to accelerate. Such a depressed trajectory implies that the vehicle stays a long time in the atmosphere at hypersonic speeds, causing atmospheric friction to become a problem. A vehicle with scramjet propulsion consequently faces the
immense difficulties of heat insulation not only at reentry but also in its trajectory towards orbit.

One of the greatest challenges in the design of a scramjet engine concerns the combustion of the fuel. Most scramjet combustors up to date are only capable of combusting fractions of the supplied fuel and generate little heat. A significant challenge in scramjet design hence lies in the optimization of the fuel combustion. A part of the objective of this work is to gain additional understanding of the complex, reacting flow taking place in the combustion chamber. Altogether, it can be concluded that extensive development work remains before scramjets are ready for space application. But despite the costs of testing and development being high, many organizations recognize the fact that the investments would pay off if the potential of scramjet propulsion could be fully exploited.

1.2.5 Latest progress

During the latest decade scramjet technology has matured enough to be tested in flight at the higher supersonic and hypersonic regimes. Different combustor configurations have, at a few occasions, demonstrated full supersonic combustion under authentic in-flight conditions and thereby formally qualified as scramjet engines. The most distinguished project is probably the NASA Hyper-X program within which the scramjet driven research vehicle X-43 A in November 2004 reached a speed of Mach 9.6. The X-43 A was at the test occasion mounted at the tip of a modified Pegasus rocket booster. The X-43 A and the booster were released from a Boeing B-52 at an altitude of 13,000 meters, where the booster ignited and accelerated the X-43 A to its intended speed and altitude. At 29,000 m the X-43 A was separated from the booster and its scramjet engine ignited. The vehicle then independently maintained full scramjet operation at Mach 9.6 for about ten seconds. Shortly thereafter all the fuel was burnt out and the flight was terminated with a long glide and a planned crash in the Pacific Ocean. The X-43 A is thus the fastest jet driven vehicle of all times and indicates the frontline of hypersonic airbreathing propulsion. [1]
More important progress has been achieved by *HyShot* research program at the University of Queensland, Australia [2] and the CIAM/NASA Mach 6.5 Scramjet Flight Program, a Russian-American cooperation peaking at the end of the 1990s [3] [4]. Both these projects conduct research and development of scramjet engines and are intended to demonstrate supersonic combustion during flight. The latter is considered the first successful flight test of a scramjet combustor and has been subject to an additional study within this thesis project.

*Figure 1.3* The NASA X-43 A research vehicle in a protective rig before transport. Photo from [http://www.dfrc.nasa.gov/Gallery/Photo/X-43A/index.html](http://www.dfrc.nasa.gov/Gallery/Photo/X-43A/index.html)
1.3 Aim of the thesis

So far the focus has been on general scramjet technology and its physical challenges. A substantial part of the problem presentation concerns the analysis and prediction of supersonic combusting flows, and has to do with two different Computational Fluid Dynamics software packages. The first software is called BlueFlame and is a personal product of H. Schütz at DLR (contact Harald.Schuetz@dlr.de for enquiries). The source code has early roots in the US but has during the latest decade been used and developed by Schütz towards a simulation program specialized in combusting flows and with a graphical user interface comparable with commercial solver packages. BlueFlame has long been successfully used for more conventional combustion problems, such as gas turbines. Supersonic flow has not been studied, with an exception concerning atmospheric reentry. Now it is desired, however, to investigate the solver’s applicability on problems involving fluid flow and combustion at supersonic speed. The same simulations will also be performed with the commercial software package ANSYS CFX for comparison of the different simulation models.

Computational Fluid Dynamics, or CFD, as analysis and design optimization tool has only recently become powerful enough to yield reasonable results for hypersonic flows. The flow in a scramjet combustor is three-dimensional, turbulent and reactive, which make the whole process very complex. The high degree of complexity and the lack of experimental data from flight tested scramjet engines have held back development and are reasons for the knowledge in the area still being strongly limited. The aim of this thesis is thus double-sided. One part is to use CFD to strengthen the understanding of supersonic combustion in combustion chambers of scramjet type. The other part of the objective is to provide a validation of the two solvers for simulation of supersonic and chemically reacting flows.
2 Theory

2.1 Mathematical modeling of reacting flows

Combustion of gaseous fuels occurs when fuel and oxidant, for example air, are brought together, mixed at a molecular level and heated to ignition temperature, whereupon chemically bound energy is released and products are formed. When energy is released the temperature increases and the combustion gases expand, which in turn affects the flow. One usually distinguishes between pre-mixed combustion where fuel and oxidizer flow together before ignition, and diffusion combustion where fuel and oxidizer flow separately and has to be mixed before combustion can take place. Mathematical modeling of combustion, especially for aerospace application, thus has to deal with several different types of processes such as fluid mechanical processes, gas phase chemical reactions and chemical kinetics.

The foundations of fluid mechanics have been known for more than a century. The equations, originating in Newton’s equations of motion, are named Navier-Stokes equations after their discoverers. These equations are non-linear and can as such not be solved analytically, with the exception of a small number of elementary cases. Theoretical models for a given fluid-mechanical problem thus generally consist of a system of partial differential equations, which cannot be solved analytically, therefore resulting in the need for numerical methods. Numerical methods imply that the space and time are discretized in a large number of computational cells and short timesteps, over which the solution of the equations are then iterated. In most practical applications the flows are
mainly turbulent, i.e. almost random in the sense that the velocity of a flow cannot be predicted for a certain point at a certain time. The turbulent nature of a flow is basically ruled by a dimensionless number, the Reynolds number. At high Reynolds numbers there is a large gap between the large scales, where energy is supplied, and the so-called Kolmogorov scale, where energy dissipation occurs. To solve the equations “exactly” with numerical methods the computational cells have to be small enough to resolve the smallest eddies, and thereby also the energy dissipation. In addition, the solution has to be iterated over time since the solution varies, not only from one point to another, but also with time. The available computing capacity therefore limits how many computational cells and timesteps can be used to simulate a certain problem. With the computer capacity accessible today only flows at low Reynolds numbers and in simple geometries can be directly simulated. If flow at high Reynolds numbers and in complex geometries is of interest, which it usually is in most engineering and scientific applications, some form of model simplification has to be introduced. The most common way of accomplishing this so far is by utilizing what is known as Reynolds-averaged Navier-Stokes models (RANS). [5] These are based on a statistical treatment of the fluctuations of a stationary or very slowly varying flow.

Turbulence models like those described above thus provide a way of making very complex equation systems manageable. Another method of technological interest is Large Eddy Simulation (LES). In LES the large energy containing eddies are simulated and only the small scale turbulence is modeled. This method has on several occasions proved more accurate in resolving different observed phenomena. The computational cost of LES is still very high, largely owing to its requirement of a very fine computational mesh. Although expensive, the method is fast becoming feasible with massive computer clusters.

In order to simulate combustion the Navier-Stokes equations must be complemented with a chemical reaction mechanism and a thermodynamic model. The chemical reaction mechanism prescribes how fuel and oxidant react, what products are formed and in what mutual relations. The thermodynamic model describes among other things how much energy is dissipated. A typical flame, in a gas turbine for example,
2 Theory

2.1 Mathematical modeling of reacting flows

...is between 0.01 and 0.1 mm thick, while the smallest (Kolmogorov) eddies are of the order 0.05 mm. Large eddies wrinkle the flame and might tear holes in it, while small eddies line up along the flame without significantly affecting it. Because of limited computing capacity a typical computational mesh in a combustion simulation has a cell size on the order of 1 mm. Thus the combustion process will occur at a sub-grid level, i.e. it cannot be resolved but has to be modeled. Models for the chemical combustion process exist in varying degrees of complexity and accuracy. The most complex models use many different reaction steps and species to describe the reaction mechanism, while the simpler models only describe the combustion as an instantaneous transition from reactants to products. Turbulence affects combustion by wrinkling the flame, whereby its surface area increases, in turn leading to increased mixing and thus to an acceleration of the reaction. In that sense turbulence is advantageous, although it should not be too strong since the reactants then would not get the time to mix on a molecular level and the flame will extinguish. [6]
2.2 Computational fluid dynamics

CFD is a computational software tool for analysis and calculation of fluid mechanical processes, such as mass, heat and momentum transfer. The numerical method most frequently used is the finite volume method. This method is used by both software tools utilized in this thesis work.

2.2.1 Governing equations

Mathematical modeling of turbulent reacting flow is a central conception since it couples fluid dynamics and chemical kinetics. This section outlines the equations governing the flow, on tensor form, as they appear when they have been complemented with models for thermodynamics and chemical reactions.

The unit vectors in x-, y- and z-directions are denoted \( \mathbf{i} \), \( \mathbf{j} \) and \( \mathbf{k} \). The position vector \( \mathbf{r} \) is written as

\[
\mathbf{r} = x \mathbf{i} + y \mathbf{j} + z \mathbf{k},
\]

and the del operator \( \nabla \) is defined as

\[
\nabla \equiv \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}.
\]

When operating on a scalar function of position \( \varphi \), it generates the gradient of \( \varphi \);

\[
\nabla \varphi = \mathbf{i} \frac{\partial \varphi}{\partial x} + \mathbf{j} \frac{\partial \varphi}{\partial y} + \mathbf{k} \frac{\partial \varphi}{\partial z},
\]

whereas the divergence of a vector field \( \mathbf{v} \) is defined as the scalar

\[
\nabla \cdot \mathbf{v} \equiv \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z}.
\]
2 Theory 2.2 Computational fluid dynamics

The velocity vector $\mathbf{u}$ is given by

$$\mathbf{u} = u(x, y, z, t) \mathbf{i} + v(x, y, z, t) \mathbf{j} + w(x, y, z, t) \mathbf{k}$$

where $u$, $v$ and $w$ are the velocity components in the x-, y- and z-directions and $t$ is time.

The mathematical models used in this work consist of the well-known Navier-Stokes equations for conservation of mass, momentum and energy, here complemented with models for thermodynamic and chemical processes. [7] [8]

A Newtonian, compressible medium is described by three partial differential equations. The continuity equation for species $m$ is

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \nabla \cdot \left[ \rho D \nabla \left( \frac{\rho_m}{\rho} \right) \right] + \rho \dot{\rho}_m \cdot \mathbf{c}, \quad \text{(2.2.1)}$$

where $\rho_m$ is the density of species $m$, $\rho$ the total density, $\mathbf{u}$ the flow velocity vector and $\dot{\rho}_m \cdot \mathbf{c}$ the chemical source term. Diffusion in accordance with Fick’s law is assumed with diffusion coefficient $D$. [7] By summing (2.2.1) over all species present in the reaction the global continuity equation describing conservation of mass is obtained. This equation states that the rate of mass-flow into a control volume per unit time equals the rate of increase of mass contained within the volume per unit time according to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \quad \text{(2.2.2)}$$

The momentum equation, describing the conservation of momentum in three dimensions, for the mixed flow is

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = - \nabla p - A_0 \nabla \left( \frac{2}{3} \rho k \right) \nabla \cdot \mathbf{\sigma} + \rho \mathbf{f}, \quad \text{(2.2.3)}$$
where \( p \) is pressure, \( k \) turbulent kinetic energy, \( A_0 \) a constant related to the turbulence model and \( f \) the total external force exerted on the volume. The viscous stress tensor \( \mathbf{\sigma} \) is defined by

\[
\mathbf{\sigma} = \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] + \lambda \nabla \cdot \mathbf{u} \mathbf{I}, \tag{2.2.4}
\]

where \( \mu \) and \( \lambda \) are the viscosities of the gas mixture and \( \mathbf{I} \) is the identity matrix. [7]

The last partial differential equation that governs the flow is the energy equation (2.2.5). This equation is derived from the first law of thermodynamics. It states that the increase in energy per unit time in a fluid element equals the net rate of heat added per unit time and the net rate of work exerted on the fluid element per unit time [7]:

\[
\frac{\partial (\rho i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} i) = -p \nabla \cdot \mathbf{u} + (1 - A_0) \mathbf{\sigma} \otimes (\nabla \mathbf{u}) - \nabla \cdot \mathbf{J} + A_0 \rho \varepsilon + \dot{Q}_c, \tag{2.2.5}
\]

where \( i \) is the internal energy, not including chemical energy and \( \varepsilon \) the turbulent energy dissipation per unit time. The heat flux vector \( \mathbf{J} \) is the sum of the contributions from heat conduction and enthalpy diffusion and \( \dot{Q}_c \) is a chemical source term.

2.2.2 Finite volume method

The Navier-Stokes equations can, as already concluded, only be solved analytically for the simplest of flows. To obtain solutions for real flows a numerical approach must be adopted, where the equations are replaced by algebraic approximations that can be solved with a numerical method.

First, the flow domain is divided into a number of small volumes, so-called control volumes or computational cells. After having divided the domain into a grid of computational cells, the governing equations are integrated over each finite volume.
Following [9], all governing equations can be said to be of the same form as the following general transport equation:

\[
\frac{\partial(\rho \phi)}{\partial t} + \nabla \cdot (\rho \phi \mathbf{u}) = \nabla \cdot \left[ D \left( \nabla \phi \right) \right] + S_\phi, \quad (2.2.6)
\]

where \( \phi \) is a fluid property, \( D \) is the diffusion coefficient and \( S_\phi \) is a source or sink of \( \phi \). When this equation is integrated over a three-dimensional control volume (CV), the general transport equation becomes

\[
\int_{CV} \frac{\partial(\rho \phi)}{\partial t} dV + \int_{CV} \nabla \cdot (\rho \phi \mathbf{u}) dV = \int_{CV} \nabla \cdot \left[ D \left( \nabla \phi \right) \right] dV + \int_{CV} S_\phi dV. \quad (2.2.7)
\]

By relating a volume integral to a surface integral, Gauss’s divergence theorem then gives

\[
\int_{A} \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA = \int_{A} \mathbf{n} \cdot \left[ D \left( \nabla \phi \right) \right] dA + \int_{CV} S_\phi dV, \quad (2.2.8)
\]

where \( \mathbf{n} \) is the outward unit normal vector. This applies to steady state flow, for transient flow the transient term must be included, i.e.

\[
\frac{\partial}{\partial t} \left( \int_{CV} \rho \phi dV \right) + \int_{A} \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA = \int_{A} \mathbf{n} \cdot \left[ D \left( \nabla \phi \right) \right] dA + \int_{CV} S_\phi dV. \quad (2.2.9)
\]

This equation is also integrated over time and the general transport equation becomes [9]

\[
\int_{A} \frac{\partial}{\partial t} \left( \int_{CV} (\rho \phi) dV \right) dt + \int_{A} \mathbf{n} \cdot (\rho \phi \mathbf{u}) dA dt = \int_{A} \mathbf{n} \cdot \left[ D \left( \nabla \phi \right) \right] dA dt + \int_{CV} S_\phi dV dt, \quad (2.2.10)
\]

This conservation equation applies to each control volume in the computational domain. Thus, by summing the equations for all control volumes global conservation automatically apply. Since the integrand is not known over the entire control volume surface, the integrals need to be approximated. This is often done in a two-level approximation, where the integral is first approximated in terms of the variable value at one or
more locations on the cell face over which the integral is evaluated. The
cell face value is in turn assumed to be the same as the value in the
computational node, which is defined as the center of the control volume.
Depending on which differencing scheme is being used, this is done in
various ways. In the upwind differencing scheme, for example, the value
of the fluid property variable is approximated as the nodal value of the
upstream control volume. This scheme is accurate to the first order and
will always be stable. A drawback is that it suffers from numerical
diffusion, which tends to smear out sharp gradients.

2.2.3 Turbulence modeling

Turbulence consists of fluctuations in the flow field in space and time. It
is a very complex and poorly understood process, mainly because it is
three-dimensional, unsteady and occurs on many scales. Turbulence
occurs when the inertial forces in a fluid becomes considerable relative to
the viscous forces, and is characterized by a high Reynolds number. [10]

As already discussed in section 2.1, a direct simulation of the turbulent
flow in a scramjet engine would require a far more detailed
computational grid than manageable with present computing power. A
way of modeling the turbulent effects of the flow is needed. The most
common turbulence modeling approach and also the one used in this
thesis is the Reynolds-averaged Navier-Stokes models. As stated before,
RANS is based on a statistical treatment of the flow. More precise, this
means that some of the variables that govern the flow are divided into a
time-averaged component of the flow and a fluctuating component that
represents the deviation from the mean flow. The governing RANS
equations are obtained as the mean of equations (2.2.2) – (2.2.5). The
resulting equations are on the same form but with a few extra terms
describing the fluctuations’ influence on the mean flow. [5]

A very successful and widely employed turbulence model is the so-called
$k-\varepsilon$ model. It is a two-equation model meaning that it includes two extra
transport equations to represent the turbulent properties of the flow. This
allows the model to account for certain historic effects, such as
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convection and diffusion of turbulent energy. The transported variables are the turbulent kinetic energy, $k$ and its dissipation per unit time, $\varepsilon$. [7] The equations for $k$ and $\varepsilon$ are

$$\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho u k) = -\frac{2}{3} \rho k \nabla \cdot u + \sigma \otimes \nabla u + \nabla \cdot \left(\frac{\mu}{P_v} \nabla k\right) - \rho \varepsilon$$

(2.2.11)

and

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho u \varepsilon) = -\left(\frac{2}{3} c_{e_1} - c_{e_3}\right) \rho \varepsilon \nabla \cdot u + \nabla \cdot \left(\frac{\mu}{P_v} \nabla \varepsilon\right) + \frac{\varepsilon}{k} \sigma \otimes \nabla u - c_{e_3} \rho \varepsilon$$

(2.2.12)

These are the standard $k$-$\varepsilon$ equations with some extra terms. [7] The quantities $c_{e_1}, c_{e_2}, c_{e_3}, P_v$ and $P_v$ are experimentally determined constants.

An advantage with RANS is that it is fast and readily available in most commercial CFD tools. The predominant disadvantage is that all turbulent flows are unstable, and it is practically impossible to extract any detailed information about such a flow from its mean flow. However, since it has proven to be stable and numerically robust, the $k$-$\varepsilon$ model offers a good compromise between accuracy and robustness for simulation of supersonic flow.

In most CFD applications handling the near-wall flow is a major issue. Many CFD tools use a logarithmic law of the wall to model such flows. In the log-law region, the tangential velocity of the flow near the wall is related to the wall shear stress $\tau_w$ by a logarithmic relation. Turbulent flows near a no-slip wall do not depend on the speed of the freestream flow, only the wall distance $y$, the density of the fluid $\rho$, the viscosity $\mu$ and the wall shear stress $\tau_w$ are important. The relation for the near-wall tangential velocity is given by

$$u^* = \frac{U_\infty}{u_c} \frac{1}{\kappa} \ln(y^*) + C,$$

(2.2.13)
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where

\[ y^+ = \frac{\mu \Delta y u_\tau}{\mu} \]  \hspace{1cm} (2.2.14)

and

\[ u_\tau = \left( \frac{\tau_{\text{w}}}{\rho} \right)^{\frac{1}{2}}. \] \hspace{1cm} (2.2.15)

Here \( y^+ \) is the near-wall velocity, \( u_\tau \) is the friction velocity, \( U_t \) is the known velocity tangent to the wall at a distance of \( \Delta y \) from the wall, \( \kappa \) is the von Karman constant and \( C \) is a log-layer constant related to the wall roughness. [10]

2.2.4 Errors in CFD

When modeling a flow with CFD it is important to know the limitations. There are several potential sources of errors and uncertainties, which can be divided into certain categories.

**Model uncertainties**
Models are often incorporated to avoid the need for resolving all physical scales, which would result in excessive computing requirements. Applying a model implies uncertainties due to assumptions and simplifications of the real flow. Once a model has been selected the accuracy of the solution cannot be extended beyond the capability of the model. This is the largest factor of uncertainty in CFD methods. Examples are turbulence models, combustion models and multi-phase models. [11]

**Numerical errors**
Solution errors are the difference between the exact solution of the model equation and the numerical solution. The errors can be reduced if a higher-order differencing scheme is employed instead of a first-order scheme. [11]
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Application uncertainties
Insufficient information of boundary conditions or of the details of the geometry can also cause uncertainties in a simulation. [11]

Software errors
Software errors are defined as any inconsistency in the software package. This can be caused by coding errors or errors in the graphical user interface. [11]

User errors
User error is another source of error that can result from inadequate use of the resources available for a simulation. Examples are oversimplification of a given problem, poor geometry or grid generation, or use of incorrect boundary conditions. [11]
2.3 Combustion modeling

As suggested earlier combustion, like turbulence, comes about on such small length scales that limited computer capacity makes direct simulation impossible. Here too, a model has to be introduced. Chemical reactions are in general not an instantaneous transition from reactants to products, but rather a long sequence of elementary reactions. A reaction mechanism lists these elementary reactions and describes in detail what happens in every step of a chemical reaction. It describes what bonds are broken and what are formed and in what order, and it describes the rate with which every reaction takes place. Mechanisms for different reactions are used in a number of appearances, where the most detailed consist of hundreds of reaction steps. But there are shorter reaction mechanisms consisting only of one or two steps that are a sort of contraction of longer, more detailed mechanisms. These are common and frequently used since they are less computationally demanding. The drawback is that they are less accurate.

2.3.1 Finite rate chemistry

The finite rate chemistry model assumes that the rate of progress of an elementary reaction $n$ can be reversible only if a backward reaction is defined. [10]

Every reaction $n$ therefore proceeds with a rate $\omega_n$ given by

$$\dot{\omega}_n = k_{m} \prod_m [I_m]^{a_{nr}} - k_{bn} \prod_m [I_m]^{b_{nr}},$$  \hspace{1cm} (2.3.1)

where $I_m$ is the molar concentration for species $m$, $a_{nr}$ and $b_{nr}$ are experimentally determined numbers for the reaction orders, and $k_{m}$ and $k_{bn}$ are the reaction rate coefficients in the forward and backward directions respectively. These are normally given on Arrhenius form:

$$k = AT^\theta e^{-E/kt},$$  \hspace{1cm} (2.3.2)
2.3 Combustion modeling

where \( A \) is the pre-exponential Arrhenius coefficient, \( T \) is the temperature in Kelvin, \( B \) the temperature dependency exponent, \( E \) is the activation energy for the reaction and \( R \) is the gas constant. [7] The constants \( A, B \) and \( E \) are listed in the reaction mechanism.

### 2.3.2 The eddy dissipation model

The eddy dissipation model is based on the assumption that chemical reactions are fast relative to the transport processes of the flow. When the reactants mix at a molecular level they instantaneously form products. The model assumes that the reaction rate may be directly related to the time required to mix the reactants at the molecular level. In turbulent flows this time is determined mainly by the eddy properties. Therefore, the reaction rate is proportional to a mixing time defined by the turbulent kinetic energy, \( k \), and its dissipation, \( \varepsilon \) according to

\[
\text{rate} \propto \frac{\varepsilon}{k}.
\]  

(2.3.3)

This concept of reaction control is applicable to a wide range of industrial combustion problems. [10] However, the eddy dissipation model is best applied to flows when the chemical reaction rate is fast relative to the transport processes of the flow. This is not always the case in a supersonic flow and the eddy dissipation model on its own is therefore not preferable for scramjet combustion.

On the other hand, both of these models can be used in conjunction in what is known as the combined finite rate chemistry/eddy dissipation model. Here, the reaction rates are first computed for each model separately, and then the minimum of the two is used. In particular, this combined model is valid for reactions that have a whole range of Damköhler numbers, \( Da \), i.e. the ratio of flow time scale to chemical time scale:

\[
Da = \frac{t_{\text{flow}}}{t_{\text{chem}}}.
\]  

(2.3.4)
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2.3 Combustion modeling

Use of this model is particularly suitable when reaction rates are limited by turbulent mixing in one area of the domain and limited by kinetics elsewhere. In the simulations performed with ANSYS CFX the combined finite rate chemistry/eddy dissipation model has been employed along with a shorter, single-step reaction mechanism.

2.3.3 Reaction mechanisms

With BlueFlame, one of the CFD-softwares used for this work, finite rate chemistry was used. Because of its high capacity for chemistry calculation, a fairly detailed reaction mechanism was desired for the BlueFlame calculations. At DLR no suitable mechanism was available for the type of diffusion combustion present in this case, where hydrogen, H₂, reacts with the oxygen in the air at very high flow velocities. Consequently, an appropriate mechanism had to be acquired before any combustion simulation could be performed. My choice finally fell on a reaction mechanism developed by NASA comprising 33 reactions and 13 species. [13] The mechanism is comprehensively presented on the following page.
2 Theory

### 2.3 Combustion modeling

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( A )</th>
<th>( B )</th>
<th>( E )</th>
</tr>
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<tr>
<td>(1) ( \text{H}_2 + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{H} )</td>
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<td>3430</td>
</tr>
<tr>
<td>(5) ( \text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O} )</td>
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<td>0</td>
</tr>
<tr>
<td>(6) ( \text{H} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M} )</td>
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<tr>
<td>(7) ( \text{H} + \text{N} + \text{M} \rightarrow \text{H}_2 + \text{M} )</td>
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<tr>
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<td>(20) ( \text{N} + \text{N} + \text{M} \rightarrow \text{N}_2 + \text{M} )</td>
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<td>6300</td>
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<tr>
<td>(23) ( \text{N} + \text{OH} \rightarrow \text{NO} + \text{H} )</td>
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<td>(25) ( \text{H} + \text{HNO} \rightarrow \text{NO} + \text{H}_2 )</td>
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<td>(26) ( \text{O} + \text{HNO} \rightarrow \text{NO} + \text{OH} )</td>
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<td>(27) ( \text{OH} + \text{HNO} \rightarrow \text{NO} + \text{H}_2\text{O} )</td>
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<td>0</td>
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<td>( 1.16 \times 10^{16} )</td>
<td>0</td>
<td>66000</td>
</tr>
</tbody>
</table>

**Table 2.1** The reaction mechanism used with BlueFlame. The pre-exponential constant \( A \) has units of \([\text{s}^{-1}]\) whereas the temperature dependency exponent, \( B \), is dimensionless. The activation energy, \( E \), is here given in \([\text{cal/mole}]\). [13]

The coefficients \( A \), \( B \) and \( E \) are defined in section 2.3.1. The entries in the table are reaction-specific values, used in equation (2.3.2) to calculate the forward and backward reaction rate coefficients for each elementary reaction step, which together constitute the global reaction.
3 Method and results

The Institute of Space Propulsion at DLR has, as one out of only a few organizations in the world, built a scale model of a scramjet combustor. With this experimental facility supersonic flow fields, temperature and chemical composition have been measured with sufficient precision for the data to be used for analysis. A schematic of the scramjet experimental rig is presented in figure 3.1. Preheated air is expanded through a Laval nozzle and enters the combustion chamber at Mach 2. The combustor has a rectangular cross section with a width of 40 mm and a height of 50 mm at the inflow and a divergence angle of the upper combustor wall to compensate for the expanding boundary layer. A flame-holding, wedge shaped structure is placed in the center of the channel downstream the nozzle. Hydrogen (H\textsubscript{2}) is injected sonically through a row of 15 holes in the base of the wedge. The holes have a diameter of 1 mm and a distance between adjacent holes of 2.4 mm. Combustion is initiated by pre-burning a small amount of O\textsubscript{2} in a tube in the H\textsubscript{2} fuel pipe by a spark. Numerous measurements have been performed in the rig, including LDV and PIV measurements of the velocity, CARS measurements of the temperature, OH-LIF for mapping of the combustion along with more conventional schlieren and shadowgraph imagery for the purpose of characterizing the dynamics of the flow. [12]

![Figure 3.1](image)

Figure 3.1 A schematic overview of the entire scramjet combustor including the Laval nozzle at the left end and the wedge shaped flameholder in the middle of the channel. The diverging upper combustor wall and the outlet are also represented. Total size of the combustor is about one meter. [12]
3 Method and results  

3.1 Outline of work

The work in this thesis has been outlined as follows:

- Set up a three-dimensional model of the scramjet combustor
- Discretize the domain in a computational grid
- Perform CFD and combustion simulation using BlueFlame
- Perform CFD and combustion simulation using ANSYS CFX
- Compare the results with experimental data
- Evaluate both simulation models respectively

The software used in the work is:

- Rhinoceros 4.0 for CAD modeling of the geometry
- ICEM CFD 11.0 for grid generation
- ANSYS CFX 11.0 and BlueFlame for fluid analysis and combustion analysis
- ANSYS CFX Post, Tecplot 10.0 and Matlab 7.0 for visualization of the computational results

From now on ANSYS CFX is sometimes referred to as CFX only.

The simulations have been carried out alternatingly in both Unix and Windows environment, but other operative systems can be used as well.
3.2 Modeling the flow

The general procedure when solving a problem in CFX is as follows:

- Define the geometry of the problem
- Divide the domain into a mesh of finite volumes
- Define the run in ANSYS CFX Pre
- Solve the problem with the CFX Solver
- View and visualize the results in ANSYS CFX Post

The procedure is similar for problem solving with BlueFlame.

Geometry design
In this section, the geometry design and mesh generation are presented. For the CAD geometry of the scramjet combustor configuration making up the computational domain, the 3D modeling tool Rhinoceros 4.0 Beta has been used. Rhinoceros is relatively easy to use and offers all tools necessary for creation of complex geometries. Low cost, user friendliness and capability of exporting geometry in a variety of formats makes it a good alternative for creation of CFD geometry.

Figure 3.2 Schematic of the part of the DLR scramjet experimental facility constituting the computational domain. The figure shows the dimensions of the domain (in millimeters) and the position of the flameholder. The backward-facing arrow at the base of the wedge represents the location and direction of the hydrogen injection. [12]
Prior to the simulations, two different geometries have been produced. The first is a two-dimensional model, simplified in the sense that it is invariant in the $z$-, or depth-direction. The simplification is made by modeling only one millimeter instead of the full 40 mm of the channel’s width. In addition, the fuel injector holes are modeled with a rectangular slit with an injector hole-to-wedge base area ratio equal to that of the real configuration. The slit extends through the full depth of the model. This is a great simplification of the real configuration designed in order to obtain a first, preliminary solution providing a characterization of the flow and combustion fields.

The second is fully three-dimensional and is the geometry used for the main simulations in this thesis. Here too, the configuration is simplified, although in a much less intrusive way. Instead of modeling the entire combustor with all 15 injector holes and the side walls, a smaller domain comprising one injector hole with periodic (symmetry) boundary conditions in the $z$-direction is chosen as the computational domain. The domain is limited in the $z$-direction halfway between two adjacent injector holes. The motivation for this simplification is to reduce the computational costs to a manageable level, while still retaining as much of the relevant physics of the scramjet combustor as possible. The CAD model is presented in figure 3.3.

Figure 3.3 A perspective view from the rear of the three-dimensional CAD model.
Mesh generation

Next, the CAD geometries are imported to the mesh generator ANSYS ICEM CFD and three different meshes are fabricated.

The computational mesh created for the 2D configuration is a coarse mesh consisting of approximately 18,100 hexahedral control volumes. The mesh is presented in figure 3.4. The rectangular slit representing the fuel injector holes is highlighted in red, which clearly reveals the two-dimensional character of the model.

![Figure 3.4 A perspective view of the computational mesh for the 2D configuration.](image)

For the 3D configuration two different computational grids have been fabricated, with 537,000 and 1.2 million control volumes respectively. The grids are block structured using hexahedral elements only. The finer grid has its first nodes located at a normalized wall distance of $y^+ \approx 60$ in order to make optimal use of the sub-grid wall model, based on the logarithmic law-of-the-wall. This model is used to handle the near-wall resolution problem. The mesh is presented in figure 3.5 on the following page.
Figure 3.5 Perspective view of the computational grid for the 3D configuration (a) and a closer view of the grid in the vicinity of the flameholder. (b) The location of the fuel injection hole on the wedge base is clearly visible.
When the meshes have been imported to the solver software the boundary conditions are specified.

- The inflowing air is given the velocity 730 m/s, corresponding to Ma = 2.0, the pressure 1 atm and the temperature 340 K
- The mass flow rate is set to 0.1 g/s, corresponding to a total flow rate of 1.5 g/s in the experiments
- On all walls a no-slip condition is applied at which the wall function models the flow using the logarithmic law-of-the-wall
- The bounding planes in the span wise (or z) direction are modeled as symmetry surfaces
- At the outlet an average static pressure is used

As initial conditions, the state of the inflowing air is used in the whole domain.
3.3 BlueFlame simulations

This section presents the results from the calculations carried out with the BlueFlame solver. The simulations are divided into three different cases; i) supersonic flow without hydrogen injection (2D), (ii) supersonic flow with hydrogen injection and combustion (2D) and (iii) supersonic flow with hydrogen injection and combustion (3D).

3.3.1 2D simulation of the cold flow case

This case only models the flow, i.e. the fuel injection and subsequent combustion are turned off. This first two-dimensional simulation serves the main purpose of characterizing the flow prior to the later, more detailed simulations. Since experimental data are available, the simulations will also contribute to the validation of BlueFlame as a solver of supersonic problems.

The measurements carried out for the cold flow case consist largely of schlieren photographs and time-averaged pressure data from the bottom wall [12]. Schlieren photography measures the deflections in the optical path length when a light wave is transmitted through an inhomogeneous medium with varying refractive index. In the experiments a horizontal knife-edge has been used in order to accentuate the effect. The knife-edge is placed in front of the camera so that it blocks about half of the incident light. In a uniform flow this would simply make the image half as bright. In a turbulent flow on the other hand, the optical path is deflected by variations in the refractive index of the medium caused by density gradients. In this case, light that would otherwise hit the camera will hit the knife-edge and some of the light that would otherwise be blocked will become visible. The result is a shadow pattern of lighter and darker fields. This is a light intensity representation of the expansions (regions with low density) and compressions (regions with high density) that characterizes the flow.
The flow in figure 3.6 is from left to right and the wedge shaped flameholder, from the base of which hydrogen will be injected, can be seen in the center of the channel. The dashed box just downstream the wedge indicate the region where the experimental schlieren photographs have been taken. The flow field bears a clear pattern and the resemblance with the experimental schlieren image (Figure 4 in [12]) is very good. At the tip of the wedge an oblique shock is created that reflects off the channel walls behind the wedge. This forms a very characteristic shock pattern in the rear regions of the combustor that is essentially stationary. The boundary layer at the wedge walls separates as expected at the base of the wedge because of the rapid expansion, whereupon a shear layer emerges. In the flow field there are indications that the shocks reflecting off the walls are also reflected in these shear layers. Strong expansion fans quickly deflect the flow towards the centerline of the combustor. Moreover, a small triangular recirculation region is formed just behind the wedge caused by low back pressure.

Figure 3.6 Results from the cold flow case involving supersonic flow, but without fuel injection. The figure presents a velocity profile of the simulated flow. The leading edge shock and the downstream shock wave pattern are clearly visible, as are the triangular recirculation region and the slower wake flow further down behind the wedge. The dashed box indicates the location of the experimental schlieren image, although not shown here [12].
3.3.2 2D simulation of the reacting case

In order to conduct a preliminary investigation of the reacting case, where hydrogen is injected parallel to the supersonic flow and combustion initiated, the 2D configuration has also been subject to a simulation of the combusting case. This simulation is restarted from the previous run, with the solution from the cold flow case as an initial guess, in order to save time and computational effort.

The finite rate chemistry model used here requires that some measure be taken in order to initialize combustion. In this case ignition has been simulated by giving a point within the combustion region in the computational domain a temperature corresponding to the self-ignition temperature of hydrogen. This leads to the initiation of the reaction process constituting the combustion of the fuel. Figure 3.7 (b) and (c) visualize the combustion of the fuel-air mixture in terms of heat release, the energy liberated in the combustion process, and temperature distribution in the combustor.

The fraction of the injected fuel that reacts before exiting the combustor is high, almost 98%. Almost all of the heat release seems to originate in the shear layers between the hydrogen-rich wake and the fast main flow. This is explained by the flow in these areas being highly turbulent, which makes up good conditions for convective mixing of air and hydrogen, which in turn is a prerequisite for combustion to occur. The recirculation region directly behind the wedge is longer and wider than in the non-reacting case, serving as a flameholder for the hydrogen diffusion flame.

The simulated flow field reproduces some features of the experimental flow field, but with deviations in, for example, shock angles. Figure 3.7 shows a comparison between the simulated flow and an experimental shadowgraph image [12]. Shadowgraph photography works essentially like schlieren photography. The difference is that in shadowgraph photography no knife-edge is used and the radius of curvature of the optical path length, or the second derivative of the refractive index field of the medium, is measured rather than the first derivative being measured in schlieren photography. It is noted how the reflected shock
waves are gradually weakened by the interaction with the shear layers and the somewhat increased recirculation region in the wake downstream the flameholder.

![Velocity field from the simulations of the reacting case (a) along with a visualization of the simulated combustion in terms of heat release (b) and temperature distribution (c), all accompanied by an experimental shadowgraph (d).](image)

**Figure 3.7** Velocity field from the simulations of the reacting case (a) along with a visualization of the simulated combustion in terms of heat release (b) and temperature distribution (c), all accompanied by an experimental shadowgraph (d). [12]
Even though these preliminary calculations render some reasonable results, there are still large inconsistencies with the experiments. The simulations both overrate the velocity and underrate the temperature along the centerline of the combustor and predict a faster reacceleration to supersonic speed than observed in the experiments. And although continuous ignition is expected to occur in the shear layers directly behind the wedge, the main part of the reaction does not occur there. Also, there is a faster temperature drop along the centerline of the combustion chamber and it can be concluded that the simulated flame is shorter than its experimental counterpart.

These differences between the simulated flow and the experiments are all caused by a strong overrating of the static combustor pressure. The unphysical character of the predicted pressure established the need for an examination of the source code of the simulation tool. It became evident that the last cell columns before the outlet did not manage to adjust the combustor pressure to ambient pressure with the consequence that the pressure increased for each iteration. This obvious shortcoming of the solver would later lead to a revision of concerned sections of the code. The most important outcome of these changes is that BlueFlame now provides the option to constrain the pressure in the first cells at an inlet via the graphical user interface and thus keep the pressure at a reasonable level.

3.3.3 3D simulation of the reacting case

These simulations are performed in a sequential manner similar to the earlier 2D simulations and with the revised version of the simulation tool. The computation of this particular case is performed by H. Schütz at DLR in Cologne using a configuration comprising one half injector hole, bounded by a symmetry plane cutting through the hole, and another one halfway to the adjacent injector hole.

Not surprisingly, the modified code and the three-dimensional configuration yields results in much better agreement with experimental measurements. The flame is depicted in figure 3.8 by means of a
temperature plot, a heat release plot and a molar fraction plot for the combustion product $\text{H}_2\text{O}$. These plots give the impression of good qualitative agreement concerning the flame front when compared to the experimental shadowgraph in figure 3.8 (d).

![Temperature plot](image1.png)

![Heat release plot](image2.png)

![Molar fraction plot](image3.png)

![Shadowgraph image](image4.png)

**Figure 3.8** Temperature (a), heat release (b) and $\text{H}_2\text{O}$ molar fraction fields (c) from the 3D simulations of the reacting case compared to a shadowgraph image from the experiments (d) [12].
However, the simulated wake temperature appears to peak just a short distance behind the wedge, a prediction not consistent with experiments. A quantitative comparison of the temperature along three cross-sections at three different axial positions in the combustion chamber reveals a significant inconsistency with the experimental temperatures measured at one of the corresponding locations. Figure 3.9 shows temperature profiles at these locations along with experimental data.

Figure 3.9 Results from the reacting case in terms of temperature $\gamma$-profiles downstream of the wedge. (a) Temperature at $x = 120$ mm, (b) Temperature at $x = 167$ mm and (c) Temperature at $x = 275$ mm. Legend: Computational results are presented with solid lines and experimental measurements are presented with symbols (+). [14]

It is clear from the first profile above that the temperature in the center of the wake directly behind the wedge is strongly overpredicted at this particular location. The simulation also fails to reproduce the high temperatures in the reacting mixing layers between the fast main flow and the slower, hydrogen-rich wake flow observed in the experiments. The second profile at $x = 167$ mm is in the region of maximum exothermicity and here reasonable agreement is found, with a slightly lower peak temperature. The shape and location of the third profile are well predicted, whereas the peak temperature is lower than the peak
temperature of the experiments. Altogether, the simulated flame resembles the experimental one in size and location, but with the hot shear layers missing and with lower peak temperature at the last cross-section, making the flame look a bit shorter than in the experiments. The inconsistency found in the profile shape directly behind the wedge might indicate that the solver, with the present reaction mechanism, might calculate too high reaction rates and/or overestimate the mixing rate for the mixed hydrogen/air flow.

Two similar graphs are presented in the figure 3.10; a velocity profile along the geometric centerline of the combustor, originating at the fuel injector hole, and a pressure trace along the lower wall of the combustion chamber.

![Figure 3.10](image)

**Figure 3.10** (a) Simulated velocity profile along the geometrical centerline of the combustor downstream the wedge, plotted together with experimental data. (b) Static pressure profile along the lower combustor wall. Legend: Computational results are presented with solid lines and experimental measurements are presented with symbols (+). [14][12]

The calculated velocity profile shows a sharp dip just behind the wedge, where the fast hydrogen jet has been slowed down, which is not present in the experimental trace, as well as a somewhat faster reacceleration of the wake flow. Beside that, the agreement with experimental data is reasonable. Once the steepest velocity increase is over, the simulated velocity profile coincides neatly with the experimental profile.

For the pressure trace in figure 3.10 (b), only fair agreement is found. The experimental pressure trace corresponds to the leading edge shock and the shape of the flame front. Evidently, the simulations are not really
capable of reproducing the expected pressure increase following from exothermicity. A possible source of error in this comparison is that the pressures measured in the experiments showed indications of considerable unsteadiness and might therefore be less typical than other measurements.
3.4 ANSYS CFX simulations

Here the results from the CFX simulations are presented. All simulation carried out with CFX are fully three-dimensional with the computational domain comprising one injector hole as described in section 3.2. The calculations can be divided into three cases as follows: (i) supersonic flow without hydrogen injection and combustion, (ii) supersonic flow with hydrogen injection but no combustion and (iii) supersonic flow with hydrogen injection and combustion. These different cases will in the following be referred to as Case I, Case II and Case III.

3.4.1 Case I

As outlined earlier the first test case only involves the flow; fuel injection and subsequent combustion are thus turned off. The experimental documentation of this case consists mainly of schlieren photography of the flow fields [12]. The simulations of Case I also serve the purpose of characterizing the flow and to provide an initial guess for the following simulations of Case II. I will here focus on the results from the finer grid, consisting of about 1.2 million cells. This simulation is performed in steady state mode and the computations are carried on until the numerical solutions have converged. As convergence criteria a maximum value of the root-mean-square (RMS) residuals is often used. In this simulation, RMS residuals as small as $3 \cdot 10^{-6}$ are reached, which is very tight convergence, approaching machine round-off. [10]

Figure 3.11 on the next page shows a perspective view of the simulated flow in terms of velocity and pressure contours. The lower figure is a numerically emulated schlieren image essentially representing large density gradients with darker color, and the resemblance with the experimental schlieren image (Figure 4 in [12]) is very good. All the main characteristics of the flow from the two-dimensional BlueFlame simulation of the same case are present here too, although in much greater detail. Since the spatial resolution is imperative for capturing
certain characteristics of the flow field, such as shocks and expansion fans, I wanted to use as fine a mesh as computationally possible. For this reason, the first nodes of the grid are located at a normalized wall distance of $y^+ \approx 60$ in order to make maximal use of the turbulence model and better resolve the boundary layers along the walls of the combustor.

![Figure 3.11 Results from Case I. In (a) a perspective view of the simulated flow in terms of velocity (in m/s) and pressure contours and in (b) a numerical schlieren image.](image)

The slanted shock coming off the wedge tip is clearly visible and in good qualitative agreement with the experiments. Because of the diverging angle, the shock reflected off the upper wall hits the wake a bit further...
down the channel than the one coming off the lower wall, giving the wake a slightly asymmetrical shape. In the figure above it can also be seen how the shock interacts with, and is deflected by, the reaccelerating wake behind the wedge, a feature also recognized in the experiments. After some distance downstream the wedge, the wake flow is accelerated back to supersonic speed, although decelerated again when passing through the remaining shock waves.

The boundary layer on the wedge separates and forms a shear layer between the wake and the fast main flow that persists almost through the whole computational domain. Originating at the base of the wedge, strong Prandtl-Meyer expansion fans can be observed that result in partially curved recompression shocks, which are reflected off the combustor wall and start to interact with the rest of the flow field. An expansion fan is basically a collection of Mach lines with the Mach number increasing when following a streamline through the fan. Figure 3.11 (a) clearly reveals how the flow behind the wedge is rapidly accelerated towards the centerline of the combustor. Another notable effect is that the shocks reflecting off the channel walls strongly affect the boundary layers at certain locations along the wall. These distortions include considerable thickening of the boundary layer and raised wall temperatures. It is also interesting to note that the flow is duly deflected (toward the shock) when passing through the shock waves, in good qualitative agreement with the theory of compressible flow. This is depicted by the streamlines in figure 3.12.

![Figure 3.12](image.png)

**Figure 3.12** Pressure distribution with streamlines in the scramjet combustion chamber.
3.4.2 Case II

In order to investigate how the injection of inert hydrogen affects the flow, the next test case is simulated in which hydrogen is injected and mixed, but no combustion initiated. This simulation is restarted from the results obtained in Case I in order to save additional computer time and will also provide a starting guess for the simulation of the reacting case.

The results from the simulation are visualized in figure 3.13. It shows a perspective view from the rear including the hydrogen jet and numerical as well as experimental schlieren photographs. The flow is similar to that in Case I with a few differences imposed by the hydrogen injection: (i) the by now hydrogen-filled recirculation zone is longer and wider than in Case I, (ii) the expansion fans coming off the corners of the wedge are not as strong as in Case I due to the presence of hydrogen and (iii) the following recompression shocks are now weaker and affected by the hydrogen-rich wake, giving them a straighter shape than observed in Case I.

The mixing of hydrogen with the mainstream air has not been studied in greater detail due to lack of time. The presence of the lighter hydrogen is clearly visible though, in particular in the now more pronounced shear layers between the wake and the main flow caused by large density gradients. It is also observed how the angle of the reflected shocks is increased when passing through the wake flow. The strength of the shear layers is also found to decrease with increasing distance from the wedge, due to the effects of mixing.

An experimental feature not captured by the averaging RANS model is the Kelvin–Helmholtz instability of the shear layers, caused by the destabilizing effect of shear, which overcomes the stabilizing effect of stratification. The characteristic flow pattern between the wake and the main flow in the experimental schlieren images are basically rolled-up layers of vorticity. This results in shredded vortex sheets where hydrogen and air are mixed by advection, a process far more efficient than diffusion. The energy needed for generating the Kelvin–Helmholtz instability is derived from the kinetic energy of the shear flow.
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3.4 ANSYS CFX simulations

**Figure 3.13** Results from Case II. (a) A perspective view of the flow in terms of velocity and pressure contours. The hydrogen jet is visualized by streamlines originating in the fuel injection hole. (b) Numerical schlieren image, the location of the experimental image (c) is superimposed in (b). (c) Experimental schlieren image. [12]
3.4.3 Case III

The third test case involves the full operation of the scramjet test rig including hydrogen injection and combustion. Detailed documentation from the experiments at DLR is available for this case. The experimental data consist, among other things, of schlieren and shadowgraph photography, Particle Image Displacement Velocimetry (PIV) measurements, Laser Doppler Velocimetry (LDV) measurements for the velocity, Coherent Anti-Stokes Raman Spectroscopy (CARS) measurements of the temperature at three different cross sections in the combustion chamber, as well as side wall pressure measurements. Schlieren and shadowgraph photography gives qualitative information only, whereas LDV and CARS measurements gives quantitative information about the average velocity and temperature at several discrete lines along the combustor. CARS employs multiple photons (a laser beam) to address the quantum mechanical vibrations of the molecules in the medium of interest and produce a signal that can be detected. The strength of the CARS signal scales with differences in the ground state and vibrational state populations. Since the populations of these quantum states follow the temperature dependent Boltzmann distribution, the CARS method carries an intrinsic temperature dependence. This is frequently taken advantage of in monitoring flames and combustion.

The simulations serve a double-sided purpose; one part is to gain additional understanding of scramjet combustion and the other part is to validate CFX’s capabilities in predicting supersonic reacting flows. Since the combusting flow is very complex and, as such, very computationally demanding, the simulations had to be performed with the coarser mesh, consisting of about 537,000 cells. Furthermore, the simulations of the reacting flow are carried out in transient mode, in contrast to Cases I and II, which were steady state. This is because the flame is naturally unstable and exhibits an undulating behavior, i.e. varying with time. This simulation is also restarted from the results obtained in Case II with obvious advantages.
When the injected fuel mixes with the air as described in the previous section, it forms a combustible mixture, which is ignited, leading in turn to the combustion of the fuel. The exothermicity resulting from the chemical reactions will likely alter the flow field due to density and temperature changes.

Figure 3.14 shows a perspective view from the rear, which aims to visualize the combustion by means of a temperature isovolume (the flame), blue streamlines representing the hydrogen injection and pressure gradients for the shocks.

Figure 3.14 Results from Case III. Perspective view from the rear, visualizing the simulated supersonic flow and hydrogen combustion in the DLR scramjet engine model.

With combustion present, the recirculation region behind the wedge becomes larger as compared to Case II and acts as a flameholder for the hydrogen diffusion flame. It is also evident from the above image that the combustion affects the flow field significantly. The leading edge shock reflected off the upper and lower combustor walls facilitates the onseting of combustion when it hits the wake in a region where large portions of the injected fuel have been mixed up with the air. After its first encounter
with the flame the leading edge shock is drastically weakened and the characteristic shock wave pattern of the cold flow cases is almost gone. Moreover, the distinguished Prandtl-Meyer expansion fans of the earlier cases vanish and the recompression shocks originating at the upper and lower wedge corners become much weaker than in Case II. The shear layers originating at the base of the wedge becomes more pronounced with combustion due to the fact that continuous ignition occurs within these shear layers. Ignition in turn, is made possible by the rapid advection mixing of fuel and air in the shear layers between the wake and the freestream air. Figure 3.15 shows a qualitative comparison between numerical schlieren and experimental shadowgraph images, where especially the shear layers are clearly visible.

Figure 3.15 (a) Numerical schlieren image from the simulations, the location of the experimental image (b) is superimposed in (a). (b) Shadowgraph photograph from the experiments [14].

Concerning the qualitative comparison between the numerical and experimental images above I find good agreement. It appears that the computations here are capable of accurately predicting the growth of the wake and the shear layers resulting from volumetric dilation caused by the temperature rise; a flow detail that previous (LES) calculations performed by other authors fail to reproduce. Also the leading edge shock is predicted well by the simulations, both in position and magnitude. Magnitude agreement for the shock is supported by lower wall pressure data. The reflected leading edge shock is reflected as an
expansion when interacting with the shear layers, an observation also made by the authors of the experimental documentation [12].

Another way of visualizing combustion is by plotting the rate with which hydrogen and oxygen react. Figure 3.16 (a) shows such a plot.

![Figure 3.16 (a) The molar reaction rate of the simulated combustion process and (b) temperature distribution in the combustion chamber.](image)

This figure shows clearly how the combustion is concentrated to the thickened shear layers between the hydrogen-rich wake and the main air flow. The lower figure shows a temperature distribution where also the leading edge shock is vaguely visible. An interesting effect is that at the intersection of the shock and the reacting shear layer the wake temperature rises quickly, suggesting an intensification of the combustion. This intensification due to shock interaction was also observed in the experiments and is important in terms of flame stabilization and combustion control [12] [17]. Today, shock-induced combustion control is being exploited and further investigated in current
research projects. Another effect is that the turbulent near-wall boundary flow increases the temperature with about 200 K due to viscous heating, an effect that influences the thermal load.

![Velocity field](image)

**Figure 3.17** Simulated velocity field along a plane in the middle of the computational domain. Velocity in m/s.

The velocity field in figure 3.17 is principally used for comparison with the PIV images from the experiments (figure 10 in [12]) and the resemblance is good for the part of the combustor that was recorded. For the PIV experiments the air and hydrogen flow was seeded with particles. The exposures then recorded the light scattered from particles moving inside the light sheet in the middle of the combustor [15]. The PIV images identify the leading edge shock by the decrease in speed across the shock, which can also be seen as lighter regions in the numerical image above. After being reflected off the upper and lower combustor walls the shock is reflected again in the shear layers between the supersonic outer and subsonic inner flow, this time as an expansion. At the points where the shock meets the flame boundary there is a bend in the flame front where the flame front becomes convergent, clearly visible also in the numerical schlieren image and the experimental shadowgraph in figure 3.15 earlier in this section. The cross-section for the supersonic airflow is therefore increased. The acceleration of the flow at the expansion fan (shock reflected in the shear layer) is clearly visible both in the PIV images and in the simulated flow in figure 3.17. The reacceleration of the wake back to supersonic speed is more moderate here and in better agreement with experimental data than observed in the preliminary investigations of section 3.3.2. [12]
In figure 3.18 I show profiles of the temperature along three different axial positions downstream of the wedge along with experimental data to give a quantitative comparison between simulation and experiments.

![Figure 3.18 Results from Case III in terms of temperature y-profiles along three different cross-sections across the combustion region. (a) Temperature at x = 120 mm, (b) Temperature at x = 167 mm and (c) Temperature at x = 275 mm. Legend: Computational results are presented with solid lines and experimental measurements are presented with symbols (+). [14]](image)

The experimental data points are obtained from CARS measurements. The mean temperatures were calculated from temperature probability density functions gained with 180 single laser shots at each position along the profiles [12]. Concerning the simulated temperatures I find reasonable agreement with experimental data for the cross-sections at x = 120 mm and x = 167 mm, whereas the simulations overpredict the peak temperature at the last of the three cross-sections at x = 275 mm. It is interesting to observe how the temperature field develops when moving downstream the combustor. The first plot in figure 3.18 (a) corresponds to the shear layers just downstream the wedge, the profile in 3.18 (b) is in the region with maximum exothermicity and the last profile is in the faster flowing combustion region far downstream the combustor where the wake has been reaccelerated to the speed of the undisturbed
flow. The temperature profile at \( x = 275 \) mm has a higher peak temperature than the profile obtained in the experiments for the same hydrogen mass flow rate. It looks rather like the profile obtained for an \( \text{H}_2 \) mass flow rate about twice as high as the one used in the simulations (figure 7 (c) in [14]). A possible cause of this inconsistency could be that the one-step combined eddy dissipation/finite rate chemistry combustion model is too simple and calculates too high reaction rates.

Figure 3.19 (a) presents a velocity profile along the centerline of the combustor, in reasonable agreement with the experimental measurement data shown in the same plot. Figure 3.19 (b) shows a profile of the static wall pressure along the lower combustion chamber wall. Here I find fair agreement and although the simulations do not succeed completely in reproducing the experimental measurements, the trend is apparent.

![Figure 3.19](image)

**Figure 3.19** (a) Simulated velocity profile along the geometrical centerline of the combustor downstream the wedge, plotted together with experimental data. (b) Static pressure profile along the lower combustor wall. Legend: Computational results are presented with solid lines and experimental measurements are presented with symbols (+). [14] [12]

It is clear that the simulations manage to predict the reacceleration of the wake with good accuracy. The sharp dip in the simulated velocity profile just behind the wedge could be due to the transient nature of the simulations and the fact that the simulated velocities are not averaged over time. A time-averaged curve would most likely have a smoother appearance without the sharpest dips and peaks of figure 3.19 (a). The pressure trace corresponds to the location of the leading edge shock and the shape of the flame front in figure 3.15. The simulations do not
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entirely succeed in predicting the expected pressure rise due to combustion as can be seen in figure 3.19 (b). The inconsistencies found between the simulated and experimental pressure traces appear somewhat odd, considering the otherwise well predicted flow field, but can be due to several reasons: (i) The simulations are carried out in transient mode - meaning that the solution varies with time - and the numerical curve is not time-averaged. (ii) The high resolution advection scheme employed in the computations is a blend of first- and second-order advection schemes to calculate the advection terms in the discrete finite volume equations. The blend factor varies throughout the domain based on the local solution field. In flow regions with low variable gradients a blend with more second-order advection terms is used for accuracy. In areas with steep gradients (such as shocks) the blend will contain a larger fraction of first-order terms, mainly to maintain robustness. In regions where a blend consisting of large fractions of second-order terms is used, overshoots and undershoots can appear in the solution. This may be a source of error concerning the discrepancies discussed above. (iii) The static pressure at the upper and lower walls in the combustor showed indications of considerable unsteadiness during the experiments due to the complex shock and expansion structures. [12] [16]
4 Concluding remarks

In Computational Fluid Dynamics several approximations are made. This section outlines the approximations that have been made in this work and attempts to account for the effects. The computational results are also discussed for the BlueFlame and ANSYS CFX simulations respectively.

The first approximation in CFD is the spatial discretization of the geometry. Creating a good computational grid may sometimes be difficult and demands years of experience from the analyst to decide whether it is good or bad. Especially for complicated geometries achieving a good grid can be very difficult and the analyst is likely to find herself in a situation where she must weigh grid quality requirements against working hours and computational cost.

In order to correctly predict the near-wall flow, a resolved boundary layer is needed in the CFX calculations. For the k-ε turbulence model a resolved boundary layer has a $y^+$ value of less than 100. However, CFX simulations of Cases I and II have been performed with two different computational grids and there were no significant differences in the boundary layer flows for the two grids, even though the coarser mesh had a $y^+$ value of about 260.

Approximations are also made, to a varying extent, in the boundary conditions. A rough approximation was made in the 2D simulations with BlueFlame, where the fuel injection holes were modeled as a uniform slit across the base of the wedge. Along with a coarser mesh the simulation results too were a crude approximation. The subsequent (3D) simulations were, along with finer computational grids, a much better approximation of the real configuration. Here periodic (symmetry) boundary conditions were used in the z-direction, and one of a total 15 injector holes was explicitly modeled. Although this can appear a rough approximation, it can quite safely be utilized when the geometry is as symmetric as in this case.
Modeling complex processes like combustion is a difficult undertaking and there are many parameters to consider. The models used in this work are a finite rate chemistry model and a combined eddy dissipation/finite rate chemistry model, with varying number of elementary reaction steps. Both models produce reasonable results, but they could, of course, be optimized. The single-step reaction mechanism used in CFX, for example, is a strong simplification from reality and seems to overpredict the temperature in the downstream regions of the combustor. A more appropriate model would include a more detailed reaction mechanism involving more elementary reactions and more species. The reason that such a reaction mechanism has not been used here is the excessive simulation time such a model would yield on the computer systems available in the present work.

The time also has to be discretized. For supersonic combusting flows the physical time scales are very small due to turbulence and chemistry. When using a finite rate chemistry model, using a timestep that is too large at the beginning may cause the solver to fail due to reaction rates not converging. Under such circumstances the timestep has to be reduced. The timestep in the CFX simulations were of the order of 1 µs. [16]
4.1 ANSYS CFX vs. BlueFlame

For Case I involving supersonic flow but no hydrogen injection the simulations performed with CFX show very good agreement with experimental schlieren images. The shocks, boundary layers and shear layers present in the flow are well reproduced and the obtained solution field provided a good starting point for subsequent simulations. Case II was restarted from the solution of Case I with the addition of hydrogen being injected through the injector hole at the base of the wedge. Some minor changes were noticed in the flow field, in good qualitative agreement with the experiments. Case III involves supersonic flow with hydrogen injection and combustion and is the case being most extensively analyzed. This simulation was restarted from the results obtained in the previous case. The simulated combustion showed good qualitative agreement with experimental schlieren images and shadowgraphs concerning shear layers, shocks and flame front. Quantitative comparison showed reasonable agreement with LDV measurements of the axial flow velocity and CARS temperature profiles at two out of three cross-sections downstream the wedge. Discrepancies are found in the last temperature profile at \( x = 275 \) mm and in the static pressure profile acquired along the lower combustor wall.

Preliminary two-dimensional BlueFlame simulations of the cold flow case without hydrogen injection and the fully operative reacting case gave a fair hint of the flow field properties and served as a foundation for the more detailed, three-dimensional investigations performed later. The 3D simulations of the combusting flow show reasonable qualitative agreement with experimental schlieren images and shadowgraphs, most noticeably concerning the leading edge shocks and the flame front. Also BlueFlame manages to predict the growth of the wake and the shear layers that other studies on this particular case fail to reproduce.

Regarding the quantitative comparison, BlueFlame is capable of predicting the temperature reasonably well in the region where the exothermicity derived from combustion is at its maximum. Fair agreement with the experimental temperature profile is found in the
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downstream region whereas there seems to be a major temperature overshoot in the wake flow just downstream the flameholder.

LDV measurements for velocity along the combustor centerline are reasonably well reproduced by the BlueFlame calculations. There is a dip in the simulated temperature profile just behind the wedge that is not present in the experimental curve, probably originating in the recirculating nature of the wake flow in the area directly behind the wedge. Reacceleration of the wake flow is set off a little earlier in the simulations as compared to experiments but otherwise the numerical and experimental velocity profiles coincide neatly.

The lower wall pressure trace calculated by BlueFlame is very similar to the pressure trace from the CFX calculations with the same deviations from the experimental profile. Even when these particular measurements reportedly are among the most unstable data recorded for the scramjet experimental rig, the inconsistencies with the experiments are still quite large.

Comparing the two solver programs is difficult, even if comparisons of the resemblance of individual flow field extractions are easily made. The final result depends to a great extent on the model and the computational setup. However, the CFX simulations of the reacting case capture the shape of the experimental temperature profile corresponding to the reacting mixing layers at x = 120 mm. This is not captured in the BlueFlame simulations, where the simulated temperature profile deviates significantly from the experimental CARS measurements at this particular cross-section. Considering the further data, BlueFlame simulations in some aspects agree with experiments where CFX simulations deviate and vice versa.
4.2 Limitations and problems

There are several limitations to the methods used and described in this thesis and many problems have occurred during the work. The largest and most obvious problem is the long simulation times, particularly for the combusting cases. Although the simulations might be worth the time, there is a large risk that the run is aborted during a computation. When the length of a complicated simulation amounts to days it is very annoying if a run crashes due to computer problems, lack of disk space or diverging computations. Available computational capacity has in this work restricted the CFX simulations of the reacting case to a coarser mesh and a simple reaction mechanism, two factors that could have a large impact on the results.

The demand for disk space is also a concern when performing large and complex simulations, due to the immense amounts of data produced. The results files become very large, especially with a fine computational grid, since the value of every variable is stored in every computational node in the domain. Large results files also impose high system requirements on the computer being used for post-processing the data, which can make the visualization of the results very time consuming as well. Computing power is therefore of central importance and should be regarded a key element when attempting to simulate large and complex cases.

Another obstacle has been the cooperative nature of the work, since all the BlueFlame simulations have been performed at DLR in Germany. This influences, among other things, the work concerning the comparison between the two solvers ANSYS CFX and BlueFlame. The BlueFlame and CFX simulations of the 3D configuration, for instance, have used slightly different computational configurations and different meshes for the spatial discretization. This might not have influenced the results at all, but in order to provide a careful comparison between the two solvers one should ideally use the same mesh for all simulations.
4.3 Conclusions

In this thesis Reynolds-averaged Navier-Stokes models has been used in conjunction with two different solver packages to investigate supersonic airflow and hydrogen combustion in a realistic scramjet model. Both solvers are capable of predicting the most important properties of the flow with reasonable accuracy, although with quantitative discrepancies between the simulations and the experimental measurements for both software packages.

Some additional understanding in the field of supersonic hydrogen combustion has been gained during the work. An illustrative example is the interaction of a flame front and a shock wave, in this case the leading edge shock being reflected off the upper and lower combustion chamber walls. There are indications, in this thesis as well as in other research documentation, that this sort of interaction could have an enhancing influence on the combustion in a scramjet engine. Here the impact of the leading edge shock on the reacting mixing layers has a temperature rising effect on the combusting wake flow, suggesting a local intensification of the combustion in this region. This type of combustion intensification due to shock interaction offers a potential tool for flame stabilization and combustion control [12]. The technique is currently being exploited and is likely to be an important component in future scramjet configurations.

The simulations performed with ANSYS CFX have systematically been subject to qualitative and quantitative comparison with experimental data for temperature, velocity and pressure. These comparisons are supplemented with comparisons with schlieren images, shadowgraph photographs and PIV velocity fields obtained in the experiments. In summary, I find that the simulations are capable of predicting the experimental data reasonably well for both the non-reacting and the reacting cases. The qualitative comparisons in particular show very good agreement with the experiments, whereas the quantitative comparisons reveal some inconsistencies with the experimental data, primarily in the static combustor pressure.
The BlueFlame computations demonstrate reasonable qualitative and quantitative agreement with the experimental flow fields, most clearly evident in the shock wave pattern, the shape of the flame front and the temperature and velocity in the region of most intense combustion. The judgment is therefore that the solver is well capable of predicting supersonic combusting flows, at least to a reasonable extent.
4.4 Future work

An interesting continuation of this work could be to investigate other scramjet configurations with different types of flameholders, such as ramps or steps that are associated with smaller aerodynamic losses than the wedge configuration studied here. Preferably, this work would further develop the concept of shock-induced combustion intensification for flame anchoring and combustion control.

For this particular case, a recommended measure is to apply a more detailed reaction mechanism if working with ANSYS CFX. Available computing capacity is in many situations likely to prohibit this act. A possible compromise could in such a case be to further simplify the computational domain by cutting the geometry in two and use a symmetry boundary condition on the plane that divides the injector hole in two equal parts. This would probably enable the analyst to use a more detailed combustion model while still using the same grid size, at the possible expense of reduced physical accuracy.

If working with BlueFlame a recommendable measure could be to analyze whether the applied combustion model and reaction mechanism overpredict the reaction rates, since the simulated combustion appear a bit too concentrated to the region directly downstream the flameholder.

If the goal is to perform an even more detailed comparison between CFX and BlueFlame (or any other simulation software) it is recommended that the same mesh be used and preferably also the same reaction mechanism.

Finally, if provided sufficient computing resources, performing a Large Eddy Simulation (LES) might yield a more accurate prediction of the large-scale turbulent structures, possibly resulting in better agreement with available experimental data.
References


References


Appendix

The interested reader will here find a plot of the temperature at different monitor points positioned in the vicinity of the compared cross-sections in the combustor. The plots are not an important result themselves, but represent the development of the simulation run. The curves show the temperature development at the monitor points as timesteps accumulate. The plot is from the CFX simulation of Case III.

![Figure A.1](image-url)  
**Figure A.1** Temperature development at three monitor points versus timestep number. The blue curve corresponds to a point in the shear layer directly behind the wedge, red curve is in the middle of the flame and green curve is in the downstream regions of the combustor.
Here is a convergence history plot for the same run in terms of the RMS residuals for the momentum and mass transport equations. The dip in the blue temperature curve in figure A.1 corresponds to the transition from oscillatory to smoothly converging solution in the residual plot on this page. This transition was accomplished by changing the solver timestep parameter.

**Figure A.2** Convergence history plot. Each curve represents the numerical convergence of a certain equation. Red is the mass transport equation, whereas green, blue and yellow are the momentum equations in x-, y- and z-directions.