CFD Simulations of Self-Pressurized Nitrous Oxide Hybrid Rocket Motors

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Abstract

Delft Aerospace Rocket Engineering has developed a 1 kN hybrid rocket motor, using Nitrous Oxide as oxidizer and a mixture of Sorbitol and Paraffin as fuel. During the campaign, different motor configurations were tested. The thesis starts with the numerical simulation of the rocket motor firing in the different tests, modelling the discharge of self-pressurized Nitrous Oxide. The simulation provides the trend over time of motor parameters such as mass flow rates, vapor quality of the oxidizer, and fuel grain thickness. Once validated through comparison with the test data, these values have been used to setup CFD simulations of the combustion chamber. An instant of the burning is simulated in steady state conditions using the eddy dissipation combustion model, gaseous injection of the fuel and no entrainment of liquefying paraffin with the oxidizer flow. The oxidizer is injected in both liquid and gas phase using the results of the numerical simulations to initialize the boundary conditions. The results are compared with the numerical data, the experimental data and the values predicted by the theory, to show the improvements that CFD simulations can provide to the designer during the development of a new hybrid rocket motor.
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Chapter 1

Introduction

1.1 Hybrid Rocket Propulsion

Chemical Rocket Motors can be categorized by the state of matter of the propellants. In a Liquid Rocket Engine both the oxidizer and the fuel are stored in liquid phase in the tanks. In a Solid Rocket Motor, on the other hand, the fuel and the oxidizer are mixed together and casted in a solid grain. The Hybrid Rocket Motor is a trade-off between the other two: one propellant is liquid and stored in a tank, the other is a solid grain [1]. In the classical Hybrid Rocket Motor, as the one in figure 1.1 and as the one studied in this thesis, the oxidizer is liquid and the fuel is solid. In the Reverse Hybrid, on the contrary, the oxidizer is solid and the fuel is liquid. The latter configuration is less common, because solid non-cryogenic oxidizers are less energetic than liquid ones, and liquid fuels have to be handled carefully to prevent explosions [2].

![Hybrid Rocket Engine Diagram](image)

Figure 1.1: Hybrid rocket Motor Configuration (Source: [3])

Even though this technology appears as a trade-off between the other two motor configurations, the operation is completely different. In a solid rocket motor the oxidizer and the fuel evaporate from
the grain surface and mix in the chamber, thus allowing to define the ideal oxidizer/fuel ratio in the design of the propellant composition. In a liquid rocket engine the two propellants are mixed together during the injection and the ratio is dependent from the mass flow rates, which can be throttled to modify the thrust of the system. In both cases the reacting mixture composition is almost uniform in all the combustion chamber [4]. In a hybrid rocket, the oxidizer is injected from one side of the chamber, usually the one opposite to the nozzle, while the fuel grain wraps the internal lateral surface. This leads to the formation of a large diffusion flame, where the O/F ratio varies along the length of the chamber, resulting in combustion inefficiencies and a low regression rate, which are the main disadvantages of hybrid rockets if compared with the other technologies. There are however numerous advantages, like more safety, simplicity, reliability, propellant versatility, environmental friendliness, throttling capabilities and low cost, thus making hybrid rockets an interesting alternative.

1.2 Computational Fluid Dynamics

Computational Fluid Dynamics is a branch of Fluid Mechanics that produces quantitative predictions of fluid phenomena based on the conservation laws governing fluid motion with the help of calculators. Since many sources of error are involved, these predictions are never completely exact and one has to interpret them with care [5]. From the beginning of the research on hybrid rocket propulsion technology, several attempts have been taken and may be find in literature to create or use numerical tools to predict rocket performances or analyze the flow field. In 2003, Serin and Gogus used CFD to study an Oxygen/HTPD hybrid rocket motor [6], while Hui and Guobiao researched a $N_2O$/HTPB in 2006 [7] [8]. In Italy, some successful attempts to use commercial software for hybrid

![Figure 1.2: CFD temperature profile of an hybrid motor combustion chamber (source: DARE)](image-url)
rocket motor CFD simulations have been conducted in the Italian Aerospace Research Centre [9] [10], but the University of Padova has been the most active in the field. The approach followed by the University Centre for Studies and Activities for Space (CISAS), under the supervision of professor D. Pavarin, has been deeply analysed in this thesis, aiming to deepen the research conducted with the implementation of new models and methods.

The research began in 2010 with the investigation of the effect on performances of diaphragms in Nitrous Oxide/Paraffin hybrid rocket motors [11]. In a similar fashion to this thesis, the analysis have been validated with the test results provided by an experimental campaign [12]. This research expanded further adding new elements as Liquid Injection [13] [14] and Vortex Injection [15] [16] [17] [18].

The baseline used for the CFD simulations conducted in this thesis is the setup finally developed by Lazzarin [19]. It will be discussed in the chapter concerning the CFD.

### 1.3 Delft Aerospace Rocket Engineering

**Delft Aerospace Rocket Engineering (DARE)** is one of the student teams of Delft University of Technology. It counts 130 student members who design, build and fly sounding rockets. They also carry out research in challenging topics such us cryogenic fuels and hybrid rockets. The team began its activities in 2001 with experiments on small solid motors. Eight years later, in 2009, DARE broke the European altitude record for amateur rocketry launching **Stratos I** to 12.3 km. From 2010 they conducted research in the hybrid propulsion field, resulting in the launch of **Stratos II+**, a Nitrous Oxide/Sorbitol-powered sounding rocket which again broke the European record, reaching an altitude of 21.5 kilometers [20].

![Figure 1.3: Stratos III Mission Patch](image)

### 1.4 The Thesis

This thesis revolves around an internship took with DARE during the **Project Phoenix** program, the first step in the realization of the 20 kN hybrid rocket motor for **Stratos III**, the next generation record breaking sounding rocket. The aim of the experience was to support the team on the design and development of a 1 kN small scale motor to train the personnel and analyze models, methodologies
CHAPTER 1. INTRODUCTION

and data useful for the creation of the biggest motor DARE ever made.

The second chapter of this work is a review of the design choices and the experimental campaign performed at TUDelft in 2016. This is an introductory part to the real thesis, that consists first in the analysis of the information gathered with the tests, then in the development of a hybrid rocket combustion chamber numerical simulator. The code aims to replicate the thermodynamical behaviour of the motor during testing. Once validated, this leads to the knowledge of the variation of quantities that couldn’t be directly measured on the field. These parameters are of fundamental importance to set the computational fluid dynamics simulation needed to reproduce the internal flow field of the combustion chamber and gain insights on the causes of performance lacks of the motor. All these results are compared with each other and validated with the test data, aiming to obtain a full understanding of the processes involved.

On a first glance, this thesis doesn’t seem to be innovative, since the methodology for the CFD simulations of hybrid rocket motors with self-pressurized Nitrous Oxide as oxidizer and a liquefying fuel has been well studied by the University of Padova. However, not only some of the weak points of those simulations will be improved and new fuel-oxidizer combination analyzed, but CFD simulations of the combustion chamber with a multiphase injection of the oxidizer have been attempted. This is performed with the actual geometry of the injector head and orifices, setting the liquid and vapor mass fractions using the results from numerical simulations of real tests. This procedure couldn’t be find in literature, proving to be an unsolved problem in the hybrid rocket motor research field.
Chapter 2

DHX-4 Phoenix Hybrid Rocket Motor

2.1 Introduction

This chapter introduces the experimental-related activities performed in this thesis with a detailed overview of the test campaign carried out from Summer to Winter 2016 at Delft University of Technology by Delft Aerospace Rocket Engineering.

2.2 Project Phoenix

Since 2006 the Hybrid Propulsion Team of DARE has been developing hybrid rocket technology. The most successful program was Project Dawn, initiated in 2010, which culminated in the manufacturing of the Morning Star and DHX200-Aurora motors. The latter powered the record-breaker Stratos II+ rocket, and its launch in 2015 marked the end of the project. To keep alive the hybrid rocket technology proficiency of DARE, Project Phoenix began for the sake of training new members of the association. The purpose of the venture is to realize a test motor to experiment new hybrid solutions, which may be used in the upcoming Stratos III. Besides serving as a test bed, the DHX-4 Phoenix motor is fully compatible with the CanSat V7 rocket\(^1\) [21].

\(^1\)The CanSat V7 is the last version of a cansat launcher commissioned to DARE in 2007 by the European Space Education Resource Office of the European Space Agency. It can carry up to 4 payloads to an apogee of 1 kilometer [22].
2.3 DHX-4 Design

To satisfy the objectives of the project, the following design requirements have been proposed:

- **Motor Type** Hybrid Propulsion;
- **Total Impulse** 4000 $Ns$;
- **Specific Impulse** 185 $s$;
- **Average Thrust** 1000 $N$;
- **Burn Time** 4 $s$;
- **Fuel** Sorbitol, Paraffin;
- **Oxidizer** Nitrous Oxide.

From the requirements the specifics of the motor have been defined during the design phase and are described in the following sections.

2.3.1 Tank and Feed System

Nitrous Oxide has been chosen as oxidizer and is considered a *green* propellant: it’s nontoxic when released to the atmosphere, it contains an adequate oxygen content for a combustion reaction and its positive heat of formation adds to combustion energy [23]. The main advantage of this choice is that Nitrous Oxide is a *Self-Pressurizing Propellant*: it exists as a saturated liquid at room temperature, and has a relatively high vapor pressure of 5.279 $MPa$ at 293.15 $K$. Therefore it can be injected into a combustion chamber without the aid of turbopumps or other pressurization systems, reducing the weight, cost and complexity of the motor [24]. The required Tank Pressure can be achieved just by heating the tank.

However, as stated by Dyer [25], “the fluid static pressure is often very close to the saturation pressure and will often drop well below it when flowing in an injector element”. This means that if the local static pressure of the flow inside the orifice descends under the vapor pressure $p_v$, the fluid will evaporate, thus becoming a two-phase flow composed of gas bubbles and liquid. From a designer perspective, it means that the injector has to be designed with care to achieve a good atomization.

The oxidizer tank, shown in figure 2.3, has been designed by Filipe Barreiro and tested and validated by Advanced Lightweight Engineering BV. It’s an aluminum$^2$ cylinder with internal radius 45 $mm$ and height 474 $mm$, with a wall thickness of 5 $mm$. The tank is sealed by two bulkheads with variable internal radius. An insulated wire is wrapped around the external surface to provide through Joule effect the heat necessary to pressurize Nitrous Oxide. The tank is then coated in stone wool to increase

$^2$EN AW-6082 T6 Aluminum Alloy
the thermal insulation from the external environment. The dry mass of the tank is about 0.5 kg. It can hold about 2 kg of oxidizer at a pressure of 60 bar.

The feed system has been developed by Kapeel Samarawickrama and improved throughout the test campaign. Its purpose is to transfer the liquid fuel from an external container to the tank of the motor, or run tank, and then transfer it from the run tank to the chamber. Sensors, hoses and connectors aside, the main features of the subsystem are:

- **Main Valve** is the main gateway connecting the run tank to the combustion chamber. During the burn phase the oxidizer flows through it.

- **Ignition Valve** connects the run tank to the combustion chamber as the MV, but lets flow only the small amount of oxidizer required to ignite the motor.

- **Bleed Valve** is attached directly to the tank and is used to discharge the gas oxidizer in excess. This process is necessary to obtain saturated vapor inside the tank.

- **Fill Valve** is attached to the external Nitrous Oxide container, and opens to transfer the oxidizer to the run tank.

- **Dump Valve**, necessary to discharge the oxidizer trapped inside the hoses while all the other valves are closed. It is also used to empty the run tank of the residual oxidizer left after the burn, if the MV is closed before the total discharge, to avoid damaging the fuel grain.

The layout of the system is depicted in figure 2.2, while the figure 2.3 is a picture of the feed system took during one of the tests. The black gas bottle is filled with Nitrogen, which is used to actuate the Fill and Dump valves.
2.3.2 Combustion Chamber

The propulsive unit of the motor is composed by three subsystems: injector plate, combustion chamber and nozzle. The envelope of the motor is an aluminum pipe with an internal diameter of 60 mm and a length of 245 mm, where the fuel grain is integrated and the nozzle and the injection assembly are inserted at the extremities. Its design was carried out by Peter van den Berg, using in house developed Matlab codes. The figure 2.4 is the plot of the predicted thrust and combustion chamber pressure curves. In order to obtain these trends, the code performs a 2D CFD analysis of the flow in the chamber. It discretizes the fuel grain and calculates for every time instant the local fuel mass flow rate. Since Matlab isn’t optimized for these applications, the grid can’t be too refined to guarantee the convergence of the calculation in a reasonable amount of time. This leads to oscillating residuals which in turn lead to oscillating results.

Injector Plate

The top part of the motor houses the Injection Head. This part is composed by a small empty gap which connects the hose coming from the feed system to the propulsive unit to a 1 mm thick aluminum plate, where holes are drilled to create the injection orifices. Several configurations were tested, changing both the relative position of the holes, the size and the inclination of the injected flow. The first configuration tested is given in figure 2.5, while the different designs are accurately described in the appendix A. The Injection Head is attached to two Pressure Sensors: one measures
the **Injector Manifold Pressure**, that is the pressure before the injection, through a hole in the gap before the drilled plate. The other one measures the **Combustion Chamber Pressure** using a hole in the fuel grain facing side of the Injection Head. From the difference between the two measurements the Pressure Drop of the injectors can be calculated.

**Fuel Grain**

The fuel grain is a hollow cylinder with an internal diameter at the beginning of the burn of 36 $mm$, and an external diameter of 58 $mm$. The grain is wrapped in a cardboard liner 1 $mm$ thick. The cylinder length is about 236 $mm$, which is less of the empty space inside the combustion chamber. It leans against the convergent part of the nozzle, thus leaving an empty space between the injector plate and the grain itself. This empty space constitutes the Pre-Combustion Chamber and is essential for the diffusion of the oxidizer inside the chamber. To build an efficient hybrid propulsion system, an high regression rate of the fuel has to be researched [26]. This can be achieved using a **Liquefying Fuel**, such as Sorbitol and Paraffin. When a liquefying fuel burns, it forms a thin liquid layer on the surface of the grain that becomes unstable under the shear force from the oxidizer flow. As a result roll waves form and liquid fuel droplets are engulfed by the gas stream. This phenomenon is known
as entrainment. The theory behind this behavior is described by Karabeyoglu [27] [28] and has been proven through testing [29]. DARE uses a blend of Sorbitol and Paraffin, in particular Shell Sarawax SX70 [30], where the first provides a high density and good structural properties, while the latter is used to increase the regression rate and specific impulse. The grain composition is of 80% Sorbitol and 20% Paraffin.

Nozzle

The nozzle is a bell shaped nozzle made in graphite. Its properties are listed in table 2.1, while a picture of it is in figure 2.5.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expansion Ratio</td>
<td>7.32</td>
</tr>
<tr>
<td>Convergence Angle</td>
<td>35 degrees</td>
</tr>
<tr>
<td>Divergence Angle</td>
<td>15 degrees</td>
</tr>
<tr>
<td>Throat Radius</td>
<td>8.5 mm</td>
</tr>
<tr>
<td>Total Length</td>
<td>79.7 mm</td>
</tr>
</tbody>
</table>

Table 2.1: Nozzle Properties

Figure 2.5: Close-up of the Injector Plate and Nozzle after Test 3.
2.4 DHX-4 Test Campaign

2.4.1 Overview

The main objectives of the test campaign, as mentioned in section 2.1, were to prove that the proposed design satisfied the requirements, to train team members on the test procedures needed for hybrid rocket motor testing, and to analyse new solutions for the Stratos III motor proposal.

The test campaign lasted six months, from late June to November 2016. 8 tests have been performed, with 2 different motor configurations.

2.4.2 Experimental Setup

Test Bench Structure

The experiments have been performed on Dawn's Labscale Hybrid Engine Test Facility. This facility, built during the Spacecraft Engineering Minor 2011/2012 of TUDelft [31] [32], has been used for the development of the Morning Star motor and for the fuel characterization tests of Stratos II, in the framework of Project DAWN [24] [33]. The basic design consisted of a single vertical pole with the oxidizer tank on one side and the combustion chamber on the other. Both are mounted on plates attached to the test bench with two small thin plates to give them a vertical degree of freedom. The tank mass and thrust are then measured by a load cell attached between the top of the plate and a clamp on the pole. However, since both the tank and the motor share the same structure, the thrust created large oscillations in the tank mass measurement. To account for this source of error, Fraters improved the original setup in 2014 introducing two separate stands for the motor and the tank [34]. This version, with small modifications to account for bigger tank and combustion chamber, has been used for the test campaign.

Figure 2.6: The original test facility (left) and Fraters improved setup (right).
CHAPTER 2. DHX-4 PHOENIX HYBRID ROCKET MOTOR

Igniter

To ignite the motor some energy has to be provided to the combustion chamber. The igniter is made with two wires and gunpowder, enveloped in a small layer of steel wool. The fuse is then attached on a small balsa wood structure which is inserted in the combustion chamber before assembling and sealing the injector plate. During the ignition sequence a small quantity of nitrous oxide flows through the ignition valve inside the combustion chamber. A spark in the wires ignites the gun powder, then the steel wool burns, and the chemical reaction inside the motor begins. Once the motor is on, the only way to switch it off is to close the Main Valve. Unfortunately this igniter design can be used only once per fire, hence the motor cannot be turned on again.

Control System

The control system is located in the electronics box near the motor stand. Radu Florea realized this box, called RIO-Box, for the DHX-200 Aurora test campaign. The system is remotely controlled with a laptop by in house developed Labview programs. The computer is operated by the Command Post Operator, situated at least 50 metres away from the test bench. The features of this subsystem are:

- Control of the valves of the feed system;
- Heating of the tank;
- Ignition of the motor;

Data Acquisition System and Sensors

The aforementioned RIO-Box manages not only the control of the experiment but also the acquisition of raw data, using an internal memory storage. The data is downloaded and analysed after the test. The RIO is connected to several sensors, listed in table 2.2. The sample rate is 2000 Hz, hence for an average burn of 4 seconds 8000 samples are collected.\(^3\)

<table>
<thead>
<tr>
<th>Measured Quantity</th>
<th>Sensor Type</th>
<th>Operative Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run Tank Pressure</td>
<td>Digital Pressure Sensor</td>
<td>0 - 60 bar</td>
</tr>
<tr>
<td>Injector Manifold Pressure</td>
<td>Digital Pressure Sensor</td>
<td>0 - 50 bar</td>
</tr>
<tr>
<td>Combustion Chamber Pressure</td>
<td>Digital Pressure Sensor</td>
<td>0 - 40 bar</td>
</tr>
<tr>
<td>Motor Mass</td>
<td>S-Beam Load Cell</td>
<td>100 kg</td>
</tr>
<tr>
<td>Tank Mass Variation</td>
<td>S-Beam Load Cell</td>
<td>5 kg</td>
</tr>
</tbody>
</table>

Table 2.2: List of Sensors

\(^3\)During a single test an average of 3 to 4 millions of samples are recorded, since the data acquisition begins (ends) several minutes before (after) the actual test.
2.4. DHX-4 TEST CAMPAIGN

2.4.3 Test Location

The experiments took place on Fellowship Field of TU Delft Campus (figure 2.7). The field is located near the buildings of the Faculty of Aerospace Engineering and the Faculty of Applied Science. The test stand is placed in the center of the field to ensure a minimum distance of 50 meters from the motor to the adjacent roads. On a distance of approximately 30 meters the Command Post is located. The permission to use the field has been appointed to DARE by the University Administration for tests of small size motors and subsystems. During the test the surrounding area is cordoned off and monitored to prevent passersby from approaching. At the field a 230 V power socket is available, provided by the campus logistics center of Anthony Fokkerweg, and additional energy supply is given by a petrol generator. The power is required to run the RIO-Box and the Command Post laptop.

Figure 2.7: The Fellowship Building (source: TU Delft)

2.4.4 Test Procedure

The test procedure is a set of rules which must be followed to perform tests in an efficient and safe manner. This set of operations and roles for each operator has been refined by years of experience in rocket testing by DARE members.

The roles required for the tests are the following:

- **Test Conductor**: the director of the test, he has to read each step of the procedure to the other operators and ensure that everything is done correctly;

- **Test Operator**: the only person allowed to touch the system during the operations;

- **Safety Officer**: a trained member that supervises the execution of every step of the procedure, is the most expert person on the field;

- **Command Post**: the controller of the RIO-Box, he activates the valves, the heating of the tank and the ignition of the motor, he is also responsible for collecting the data.

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4This standard safety procedure has become stricter after a frightened horse invaded the solid motor test area.
The fundamental steps of the Test Procedure are the following:\textsuperscript{5}:

1. **Pre-Test Operations**: Casting of the fuel grain, set up of the test area, assembly of the test bench, wiring of the sensors and isolation of the field.

2. **System Check**: Verification of the assembly of all the subsystems and efficiency of the sensors.

3. **Leak Tests and Purge**: Test of the Feed Systems using pressurized Nitrogen.

4. **Engine Mounting**: Integration of the fuse and injection plate on the motor, assembly of the motor on the test bench, connection of the Nitrous Oxide bottle to the feed lines.

5. **Fire Test**: Filling and heating of the Run Tank, ignition of the system.

6. **Post-Test Operations**: Dismantling of the experimental setup, analysis of the collected data.

### 2.4.5 Test Reports

The Phoenix Test Campaign consisted of 8 tests, listed in Table 2.3. To be noticed that the high rate of misfires relates to the lack of experience of the operators, since their training was one of the main objectives of the test campaign.

<table>
<thead>
<tr>
<th>Test Number</th>
<th>Date</th>
<th>Burn Time</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test 1</td>
<td>9 July</td>
<td>-</td>
<td>Main Valve Malfunction</td>
</tr>
<tr>
<td>Test 2</td>
<td>12 July</td>
<td>-</td>
<td>Igniter Failure</td>
</tr>
<tr>
<td>Test 3</td>
<td>20 July</td>
<td>3.8 s</td>
<td>Successful, config. A</td>
</tr>
<tr>
<td>Test 4</td>
<td>24 Aug.</td>
<td>-</td>
<td>Overheating of the Tank</td>
</tr>
<tr>
<td>Test 5</td>
<td>10 Sep.</td>
<td>2.7 s</td>
<td>Successful, config. A</td>
</tr>
<tr>
<td>Test 6</td>
<td>10 Sep.</td>
<td>2 s</td>
<td>Successful, config. A</td>
</tr>
<tr>
<td>Test 7</td>
<td>14 Oct.</td>
<td>1.6 s</td>
<td>Successful, config. B</td>
</tr>
<tr>
<td>Test 8</td>
<td>25 Nov.</td>
<td>-</td>
<td>Injector Plate Failure</td>
</tr>
</tbody>
</table>

Table 2.3: Test Matrix

After these 8 tests the Phoenix Campaign ended and the project officially merged with Stratos III. Unfortunately the new test results cannot be published in these thesis, hence the thesis relies only on the four successful tests and configurations to fulfil the research objectives.

**Test 1**: Due to a failure of the Main Valve the test was aborted during the System Check. The servomotor that operates the valve malfunctioned and had to be substituted.

\textsuperscript{5}Since the Project Phoenix Procedure is property of DARE, it will not be published inside this thesis. A previous version of it can be found in the work of Fraters \[34\]
2.4. DHX-4 TEST CAMPAIGN

**Test 2:** The oxidizer flux injected in the chamber by the ignition valve ejected the fuse from the combustion chamber, thus the motor didn’t ignite. The oxidizer flowed for 4 seconds resulting in a thrust value almost null.

**Test 3:** After a redesign of the igniter and the substitution of the main valve, due to a new malfunctioning, the DHX-4 was tested with a fuel grain made of 80% Sorbitol and 20% Paraffin, and an oxidizer flow time of 6 seconds to empty the tank. The tank proved to be oversized for the motor, since the fuel grain burned completely before the end of the discharge period. The injector manifold pressure sensor malfunctioned and gave a wrong reading.

**Test 4:** Due to the really hot summer day the temperature of the tank quickly rose, increasing the tank pressure to 70 bar. Unfortunately the bleed valve didn’t work, so the dump valve was used instead. The gas flow through the dump valve was too strong and the feed system support plate failed to keep the valve in its place, which began to fly around damaging the fill valve and the hoses and shutting down the RIO.

**Test 5/6:** Two tests were successfully performed with the first injector configuration, the main valve was shut after 2.7 and 2 seconds, respectively.

**Test 7:** The second injector configuration was successfully tested for a burn time of 1.6 seconds.

**Test 8:** It was a partial success. While the motor burnt correctly, the shear thrust broke the bolt connecting the upper part of the supporting pole to the base. The test bench slid freely for a few centimeters pushed by the thrust before being arrested by the tightened ropes. This voided part of the data measured.

Figure 2.8 is a couple of high definition pictures taken during test 7. Further visual documentation of the test campaign can be found in [35] and [36]. On the bottom left part of the pictures the RIO Box can be seen.
Figure 2.8: Test 7 Ignition (left) and Burn (right).
Chapter 3

Data Analysis

3.1 Introduction

This chapter discusses the approach followed to obtain meaningful information from the raw data collected in the test campaign.

A two steps analysis has been chosen to satisfy all the queries arose by the test campaign:

- The first analysis is the elaboration of experimental data to obtain the trend over time of the motor parameters and the average performance values. From these results the adherence of the prototype to the design can be checked and countermeasures may be taken to improve both the rocket and the numerical model used to assist the design. This investigation has been carried out in Delft, promptly after the tests, with the support of Project Phoenix members.

- The second analysis is a numerical reconstruction of the rocket firing, aiming to obtain curves as close as possible to the experimental ones. With this deeper data processing the trend over time of parameters which were impossible to measure during the campaign have been evaluated, leading to an approximate but complete knowledge of the motor operation, which is fundamental for a correct setup of computational fluid dynamics simulations, the main matter of this thesis. This investigation has been carried out in Padova, with the support of the University Centre for Studies and Activities for Space (CISAS).

3.2 Experimental Data Analysis

3.2.1 Analysis Procedure

The raw data acquired from the tests are filtered using an algorithm for spike reduction, or shaving, based on the work of Backx [37] and granted by the Center of Systems and Control of TU Delft. Through this interpolation cleaner data can be obtained, thus allowing cleaner elaborations.
The second step of the analysis is the isolation of the effective burn segment from the mass of data. The identification of the portion is done using a Matlab script. After it is located, the number of isolated samples \( N \) is divided for the sampling frequency \( f_s \) to extract the **Burn Time** \( t_b \):

\[
t_b = \frac{N}{f_s}
\]

The quantities directly measured with the sensors, already listed in table 2.2, are the following:

- **Tank Mass**, \( m_T \)
- **Motor Mass**, \( m_M \)
- **Tank Pressure**, \( P_T \)
- **Injector Manifold Pressure**, \( P_{inj} \)
- **Combustion Chamber Pressure**, \( P_{CC} \)

From these quantities the following indirect measurements are extracted:

**Motor Thrust**, \( T \), multiplying the mass measured by the motor load cell during the burn by the gravitational acceleration \( g \):

\[
T = m_M g
\]

**Average Oxidizer Mass Flow**, \( \dot{m}_{ox} \), as the linear variation of the mass of the tank over the burn time:

\[
\dot{m}_{ox} = \frac{\Delta m_T}{t_b}
\]

**Average Fuel Mass Flow**, \( \dot{m}_{fuel} \), dividing the difference between the mass of the motor before and after the burn by the burn time:

\[
\dot{m}_{fuel} = \frac{\Delta m_M}{t_b}
\]

**Average Specific Impulse**, \( \bar{I}_{sp} \), using the average value of the Thrust \( \bar{T} \):

\[
\bar{I}_{sp} = \frac{\bar{T}}{g \cdot (\dot{m}_{ox} + \dot{m}_{fuel})}
\]

**Thrust Coefficient**, \( c_F \):

\[
c_F = \frac{T}{P_{CC} A_t}
\]

where \( A_t \) is the throat area of the nozzle.
3.2. EXPERIMENTAL DATA ANALYSIS

**Average Characteristic Velocity, \( \bar{c}^* \):**

\[
\bar{c}^* = \frac{P_{CC} A_t}{\bar{m}_{ox} + \bar{m}_{fuel}}
\]

where the combustion chamber pressure \( P_{CC} \) has been averaged, and the total average mass flow is obtained adding together the oxidizer and fuel average mass flows.

**Injector Pressure Drop, \( \Delta P \):**

\[
\Delta P = P_{inj} - P_{CC}
\]

An average value can be extrapolated to evaluate the injection model used in the design.

**Regression Rate, \( \dot{r} \).**

The value of the regression rate of the fuel is more complex to calculate and only an approximate value can be obtained. Since all the geometric parameters of the cylindrical fuel grain are known, an homogeneous regression of the web thickness can be presumed\(^1\), hence different values of the port area \( A_p \) are calculated as the base area of the cylinder increasing the values of the radius.

\[
A_p = \pi r_p^2
\]

An average value of the Oxidizer Mass Flux \( G_{ox} \) is then calculated dividing the average oxidizer mass flow by the port area. Since an average mass flow is used, a further approximation is spread in the model.

\[
G_{ox} = \frac{\dot{m}_{ox}}{A_p}
\]

From previous studies of DARE [33] the values of the Burn Rate Coefficient \( a \) and the Pressure Exponent \( n \) of the fuel grain are known, so the classical model for hybrid rocket motors regression rate calculations [40] can be applied:

\[
\dot{r} = a G_{ox}^n
\]

The value of the regression rate obtained through this rough approximation is still a valid parameter for the analysis of the design model.

### 3.2.2 Experimental Curves

This section provides a sample of the graphs resulting from the filtered measurements. The Curves are a visual tool useful to identify different system behaviours during operation.

\(^1\) The regression of the fuel grain during burning is not homogeneous over the burning surface, since is heavily influenced by the oxidizer flow. The DHX-4 injection is swirled, therefore the burning pattern is dependent both from the distance from the injector plate and the angular position on the grain.
In figures 3.1 and 3.2 different sections of the curve shall be identified. Before \( t = 0 \) it coincides with the x-axis since the motor is off. During ignition the values quickly rise up to their maximum. Then the nominal burn phase begins, the liquid oxidizer is injected in the combustion chamber and the curve slowly descends. When the liquid Nitrous in the tank depletes, the curve abruptly climbs down to a second less efficient burning phase, where the oxidizer is injected in gas phase. When the main
3.2. EXPERIMENTAL DATA ANALYSIS

valve is closed or the run tank is completely empty, the combustion stops and the curve leans on the x-axis again.

A different typology of plot is the **Spectrogram**, which is the visual representation of the spectrum of frequencies of the signal as they vary with time. It is a useful tool to locate instabilities [38]. As an example, figure 3.3 is the combustion chamber pressure spectrogram of Test 3, where stronger intensities are marked with warmer colours. Right after $t = 0$, the combustion is irregular since the motor is igniting; however, from that instant till $t \simeq 3.5$, the combustion is stable, and the vibrations arrange in regular lines at the different modal frequencies of the system. This is a further demonstration of the stability of the process, since as it may be already seen during the test, the exhaust gases tend to form *Mach Diamonds* if the combustion is stable [39]. After $t = 4$ the oxidizer is injected in the gas phase, so the combustion becomes irregular. Spikes are shown in the graph, and violent bursts have been actually observed during Test 3, probably due to the ejection of unburnt slabs of fuel. If the spectrogram is compared to the corresponding combustion chamber pressure curve of figure 3.2, the same spikes can be identified at the same time instants. Therefore the spectrogram deepens the analysis of phenomena related to instability which are not evident in the curves.

![Figure 3.3: Test 3 Combustion Chamber Pressure Spectrogram](image)

3.2.3 Experimental Results

Although the plots give a grasp on the overall behaviour of the motor, a quantitative analysis of the performances is required to prove if the requirements have been satisfied, or if changes must be made in order to choose an efficient configuration for the motor. If the curves in figures 3.1 and 3.2 are compared with the design curve of figure 2.4, it can be noticed that not only the trends aren’t linear
as expected, but also the measured values are severely lower than the required ones. To calculate the entity of the error in the prediction, the average values have been deducted and are listed in table 3.1, while the peak values are reported in table 3.2.

It is important to specify that the performance parameters, such as the combustion chamber pressure and the thrust, decrease over the increasing burn time. If the motor burns for a smaller amount of time higher average values have to be expected. Since the burn time decreases from test 3 to test 7, the average values of the thrust, the specific impulse and the combustion chamber pressure increase. On the other hand the peak values of test 7 are higher since a different injection configuration has been used, and these results demonstrate that the modification increased the overall efficiency of the system.

<table>
<thead>
<tr>
<th></th>
<th>Test 3</th>
<th>Test 5</th>
<th>Test 6</th>
<th>Test 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Burn Time [s]</td>
<td>3.8</td>
<td>2.7</td>
<td>2</td>
<td>1.6</td>
</tr>
<tr>
<td>Specific Impulse [s]</td>
<td>138</td>
<td>148</td>
<td>151</td>
<td>170</td>
</tr>
<tr>
<td>Thrust [N]</td>
<td>680</td>
<td>704</td>
<td>750</td>
<td>822</td>
</tr>
<tr>
<td>Thrust Coefficient</td>
<td>1.31</td>
<td>1.27</td>
<td>1.26</td>
<td>1.28</td>
</tr>
<tr>
<td>Characteristic Velocity [m/s]</td>
<td>1025</td>
<td>1139</td>
<td>1174</td>
<td>1303</td>
</tr>
<tr>
<td>Oxidizer Mass Flow [kg/s]</td>
<td>0.378</td>
<td>0.360</td>
<td>0.385</td>
<td>0.336</td>
</tr>
<tr>
<td>Fuel Mass Flow [kg/s]</td>
<td>0.120</td>
<td>0.113</td>
<td>0.124</td>
<td>0.157</td>
</tr>
<tr>
<td>Regression Rate [mm/s]</td>
<td>2.82</td>
<td>2.12</td>
<td>3.2</td>
<td>4</td>
</tr>
<tr>
<td>Injection Pressure Drop [bar]</td>
<td>7.9</td>
<td>9.3</td>
<td>7.87</td>
<td>17.43</td>
</tr>
<tr>
<td>Combustion Chamber Pressure [bar]</td>
<td>22.6</td>
<td>24.2</td>
<td>26.2</td>
<td>28.3</td>
</tr>
</tbody>
</table>

Table 3.1: Average Values of the Experimental Results

<table>
<thead>
<tr>
<th></th>
<th>Test 3</th>
<th>Test 5</th>
<th>Test 6</th>
<th>Test 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thrust [N]</td>
<td>877</td>
<td>877</td>
<td>884</td>
<td>1090</td>
</tr>
<tr>
<td>Characteristic Velocity [m/s]</td>
<td>1263.7</td>
<td>1318</td>
<td>1327</td>
<td>1587</td>
</tr>
<tr>
<td>Combustion Chamber Pressure [bar]</td>
<td>28.3</td>
<td>28.4</td>
<td>30.38</td>
<td>35.1</td>
</tr>
</tbody>
</table>

Table 3.2: Peak Values of the Experimental Results

These data may be promptly compared with the design predicted results to evaluate the fidelity of the model used to estimate the specifics chosen to satisfy the requirements. In tables from 3.3 to 3.5 the average values gathered for the first injector configuration are compared with the nominal values extracted from the design curve of figure 2.4.

From these tables it emerges that both the average thrust and the pressure have been overestimated in the design phase. The thrust percentual discrepancy from the nominal value is about 35 %, while
### 3.2. EXPERIMENTAL DATA ANALYSIS

<table>
<thead>
<tr>
<th>Test 3</th>
<th>Average Thrust [N]</th>
<th>Chamber Pressure [bar]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Value</td>
<td>1075</td>
<td>30.5</td>
</tr>
<tr>
<td>Experimental Result</td>
<td>680</td>
<td>22.6</td>
</tr>
<tr>
<td>% Deviation</td>
<td>36.75 %</td>
<td>25.91 %</td>
</tr>
</tbody>
</table>

Table 3.3: Deviation from the nominal design values for Test 3, $t_b = 3.8\,s$

<table>
<thead>
<tr>
<th>Test 5</th>
<th>Average Thrust [N]</th>
<th>Chamber Pressure [bar]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Value</td>
<td>1120</td>
<td>31.75</td>
</tr>
<tr>
<td>Experimental Result</td>
<td>704</td>
<td>24.2</td>
</tr>
<tr>
<td>% Deviation</td>
<td>37.15 %</td>
<td>23.78 %</td>
</tr>
</tbody>
</table>

Table 3.4: Deviation from the nominal design values for Test 5, $t_b = 2.7\,s$

<table>
<thead>
<tr>
<th>Test 6</th>
<th>Average Thrust [N]</th>
<th>Chamber Pressure [bar]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Value</td>
<td>1150</td>
<td>32.5</td>
</tr>
<tr>
<td>Experimental Result</td>
<td>750</td>
<td>26.2</td>
</tr>
<tr>
<td>% Deviation</td>
<td>34.78 %</td>
<td>19.39 %</td>
</tr>
</tbody>
</table>

Table 3.5: Deviation from the nominal design values for Test 6, $t_b = 2\,s$

The pressure gap tends towards 20 % as the burn time reduces.

The **Combustion Efficiency** of the motor is calculated as the ratio between the measured $c^*$ and the ideal value of this parameter at the measured average pressure of the combustion chamber.

$$\eta_c = \frac{c^*_{\text{meas}}}{c^*_{\text{id}}}$$

To calculate the ideal value the following equation is solved:

$$c^*_{\text{id}} = \sqrt[\frac{k}{k-1}]{\frac{R \, T}{M \, k^2}}$$

where $R$ is the *Ideal Gas Constant*, $M$ the *Molar Mass* of the gas mixture inside the combustion chamber, $k$ the *Heat Capacity Ratio* and $T$ the *Adiabatic Flame Temperature*. These last three values are calculated using the software CPROPEP [42]. Unfortunately the exact chemical composition of the paraffin used in the fuel grain is absent in the database, so the ideal characteristic velocity for the motor was set from studies of grains casted with different paraffin chemical formulae, and approximated to a value of $\approx 1420\, m/s$ for a pressure of $30\, \text{bar}$, consistent with the experimental studies of Fraters [24] and Knop [33]. This implies that the calculated efficiency is not the exact value but still a valid approximation of the actual one and is meaningful for a comparison between the tests.
The measured efficiencies are listed in table 3.6. For a higher average pressure, the efficiency increases as the average pressure of the system slightly increases. However, the efficiency is rather low, fluctuating between 70 % and 80 %.

<table>
<thead>
<tr>
<th>Test</th>
<th>$c^*$ [m/s]</th>
<th>Combustion Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test 3</td>
<td>1025</td>
<td>72.18 %</td>
</tr>
<tr>
<td>Test 5</td>
<td>1139</td>
<td>80.21 %</td>
</tr>
<tr>
<td>Test 6</td>
<td>1174</td>
<td>82.67 %</td>
</tr>
<tr>
<td>Test 7</td>
<td>1303</td>
<td>91.76 %</td>
</tr>
</tbody>
</table>

Table 3.6: Combustion Efficiency

The main issue that has been addressed to improve the low performance of the motor is the injector plate. The 7-holes configuration A was replaced in test 7 with the 13-holes configuration B. As shown in table 3.7, the performance parameters values of the system increased with the different injection assembly, thus reducing the error in the prediction. The combustion efficiency increases to $\simeq 90$ % (table 3.6), since the better atomization of the oxidizer leads to a more complete combustion, which in turn increases the overall performance.

<table>
<thead>
<tr>
<th>Test 7</th>
<th>Average Thrust [N]</th>
<th>Chamber Pressure [bar]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Value</td>
<td>1115</td>
<td>31.5</td>
</tr>
<tr>
<td>Experimental Result</td>
<td>822</td>
<td>28.3</td>
</tr>
<tr>
<td>% Deviation</td>
<td>26.28 %</td>
<td>10.16 %</td>
</tr>
</tbody>
</table>

Table 3.7: Deviation from the nominal design values for Test 7, $t_b = 1.6s$

### 3.3 Numerical Simulation

As already stated in the introductory part of the chapter, a further analysis of the data is conducted through a numerical simulation of the operation. The simulation is based on an algorithm developed at the University of Padova by Barato [41] and is described in this section.

The code neglects the transient phase of the ignition, thus only the stable burning is taken into account. The simulation is not steady state but time dependent, thus the variation of every parameter of the motor is simulated and the trends over time can be acquired hence compared with the experimental data and the design curves. The necessity of a detailed knowledge of the process which cannot be inferred from the simple analysis of the experimental curves lead to the choice of developing a code.
3.3. NUMERICAL SIMULATION

3.3.1 Ancillary Work

Before running the simulation, a model for Nitrous Oxide discharge has to be adopted, as well as the definition of the thermochemical properties of the oxidizer/fuel match.

Modeling Nitrous Oxide Discharge

The main hypothesis adopted to study the properties of the oxidizer during discharge is to consider Nitrous Oxide in the tank as a saturated liquid. With this assumption the liquid phase and the vapor phase are in equilibrium. Knowing the pressure and the temperature all the other thermodynamics properties of the fluid, such as density, vapor quality, enthalpy and entropy can be evaluated. Therefore the saturation properties of Nitrous Oxide are firstly acquired from the NIST database using the software REFPROP\(^2\) and sorted in arrays, which are interpolated by Matlab to obtain the instantaneous properties of the oxidizer.

Modeling the Chemical Reaction

To simulate the combustion inside the motor, the chemical reaction has to be taken into account. The simulation relies on a look-up table computed using the software CPROPEP [42]. A range of combustion chamber pressure is defined with a pressure step \(dP\), as well as an oxidizer/fuel ratio range with step \(d(O/F)\). A Matlab script developed by CISAS, enhanced for this thesis in order to simulate the fuel mixture of Sorbitol and Paraffin, interacts with CPROPEP to compute the table. First the lowest value of the pressure is selected, subsequently the characteristic velocity \(c^*\) and the heat capacity ratio \(k\) of the reacting mixture are calculated for the lowest \(O/F\). The ratio is then incremented of \(d(O/F)\) and the process iterates until the highest \(O/F\) ratio is reached. After that the pressure is increased of \(dP\) and the process begins again until the highest pressure is reached. The resulting matrix is used by the main script to account for the combustion. The calculation is time-consuming and can take up to several hours to end.

3.3.2 Main Script

The first step is the initialization using the motor parameters, such as the size of the nozzle, with the erosion neglected for the short burn time, the geometric and ballistic properties of the fuel grain and the initial tank pressure, measured in the experiments.

The properties of the oxidizer are subsequently taken into account. From the initial mass of the oxidizer (measured) and the tank volume, the density is acquired. Using the saturation tables, called in the script as functions, the thermodynamic properties of the saturated \(N_2O\) are calculated.

The instant \(t = 0\) is completely modeled through analytical relationships and the initial values acquired from the experimental data. The combustion chamber pressure and the injector pressure

\(^2\)NIST Reference Fluid Thermodynamics and Transport Properties Database
The oxidizer mass flow is calculated from the experiments as the difference between the tank mass before and after the test, divided by the burn time. This is an average value, however the mass flow rate magnitude changes over time. At the beginning of the burn is higher than the average, at the end is lower. To develop a reliable simulation this variation had to be taken into account. Since the mass flow depends on the tank pressure a correlation exists between the ratio of the instantaneous tank pressure to the initial tank pressure and the instantaneous mass flow to the initial mass flow. The correlation derives from the laws of gasdynamics for the maximum mass flow rate in a duct [43]. The equation is valid since the injectors are choked, therefore the flow does not depend on the combustion chamber pressure but only on the pressure drop between the tank and the chamber. The equation at the $i$-th instant is the following:

$$\dot{m}_{ox,i} = A\dot{m}_{ox}\sqrt{\frac{P_{t,i}}{P_{t,0}}}$$

(3.1)

where the initial tank pressure is $P_{t,0}$ and the initial mass flow rate is calculated as the average mass flow rate multiplied by an amplification coefficient $A$. The value of $A$ is determined applying the law of mass conservation to the system. The total oxidizer mass discharged has to equal the sum of the mass discharge in every time instant with the mass flow rate of equation 3.1:

$$\dot{m}_{ox,t_b} = \sum_{i=1}^{n} (\dot{m}_{ox,i}\Delta t)$$

(3.2)

From the oxidizer mass flow and the port area, the regression rate, fuel mass flow and O/F ratio are finally estimated.

The thermochemistry look-up table for the liquid phase injection is then loaded: from the combustion chamber pressure and the oxidizer/fuel ratio it returns the characteristic velocity, which is used in the subsequent iteration to calculate the new combustion chamber pressure.

For every time instant $dt$ the mass in the tank decreases of a quantity calculated with the instantaneous mass flow rate. A new tank pressure is then estimated and the iterative cycle updates every property of the motor following a procedure analogous to the initialization of the code: a new oxidizer mass flow is determined, then the regression rate, fuel mass flow rate, combustion chamber pressure. At the end of the recursive process the trend over time of every parameter of the motor is acquired.

### 3.3.3 Setup

While some parameters, like the length or the composition of the grain, remained constant through the tests, more values changed from one test to the other, hence the initialization of the simulations is different. The quantities are listed in tables 3.8 and 3.9.
3.3. Numerical Simulation

<table>
<thead>
<tr>
<th>Grain Length [m]</th>
<th>0.236</th>
<th>Fuel Density [kg/m³]</th>
<th>1260</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burn Rate Coefficient [m/s]</td>
<td>0.004</td>
<td>Pressure Exponent</td>
<td>0.31</td>
</tr>
<tr>
<td>Port Diameter [m]</td>
<td>0.036</td>
<td>Throat Diameter [m]</td>
<td>0.017</td>
</tr>
<tr>
<td>Tank Volume [m³]</td>
<td>0.003</td>
<td>Pressure Line Losses [bar]</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 3.8: Constant Inputs

<table>
<thead>
<tr>
<th>Burn Time [s]</th>
<th>Test 3</th>
<th>Test 5</th>
<th>Test 6</th>
<th>Test 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.8</td>
<td>2.7</td>
<td>2</td>
<td>1.6</td>
<td></td>
</tr>
<tr>
<td>Initial Tank Pressure [bar]</td>
<td>57.4</td>
<td>58</td>
<td>58.5</td>
<td>57</td>
</tr>
<tr>
<td>Initial $N_2O$ Mass [kg]</td>
<td>2</td>
<td>1.55</td>
<td>1.57</td>
<td>1.45</td>
</tr>
<tr>
<td>Average $N_2O$ Mass Flow Rate</td>
<td>0.321</td>
<td>0.360</td>
<td>0.385</td>
<td>0.336</td>
</tr>
<tr>
<td>$N_2O$ Flow Rate Constant</td>
<td>1.0932</td>
<td>1.0728</td>
<td>1.0559</td>
<td>1.0740</td>
</tr>
<tr>
<td>Combustion Efficiency %</td>
<td>72.18</td>
<td>80.21</td>
<td>82.67</td>
<td>91.76</td>
</tr>
<tr>
<td>Pressure Drop %</td>
<td>35</td>
<td>30</td>
<td>30</td>
<td>40</td>
</tr>
</tbody>
</table>

Table 3.9: Variable Inputs

3.3.4 Simulation Results

The simulations have been performed for liquid discharge only, since the CFD simulations are performed with multiphase injection and the simulation of the gas-only oxidizer injection is not necessary for the setup of the boundary conditions. The trend over time of every thermodynamic property of the system was extracted. In particular, the mass flow rate of the oxidizer, the fuel and the vapor quality in the tank are necessary to define the inlet boundaries in the CFD simulation. This analysis will be described in the next chapter.

Figure 3.4 is the plot of the tank pressure. The slope of Test 3 discharge is less steep since the oxidizer mass flow rate is lower. This plot agrees with the experimental data, therefore the reason for this oddity has been investigated. The behaviour could be related to thermal stratification, since the tank stayed in the field for a longer time, to the design of the feed system, which was improved for the consecutive tests, and to the inexperience of the operator.

The oxidizer mass flow rate and the combustion efficiencies influence the combustion chamber pressure: in figure 3.5 test 3 has the lowest efficiency and the lowest mass flow rate, hence it has the lowest pressure. Tests 5 and 6 resemble each other while test 7 compensates a lower mass flow with an higher efficiency due to the improved injector plate. A systematic error made during testing is also a different initial tank pressure. This fault should be eliminated performing more tests with the same initial pressure.

Figure 3.6 is the comparison between the resulting Characteristic Velocities $c^*$. The value predicted
CHAPTER 3. DATA ANALYSIS

Figure 3.4: Simulated Tank Pressure

Figure 3.5: Simulated Combustion Chamber Pressure

reflects the value measured. Test 3 has a $c^*$ of $\simeq 1000$, Test 5 and 6 have a higher value, $\simeq 1200$, while Test 7 is the most efficient with $c^* > 1300$. As already pointed out, the last test is characterized by a different injection plate. This plate allowed for a better atomization of the liquid oxidizer, thus increasing the efficiency of the system of about 10 to 15 points percentage from the motor of the first tests.

The regression rate, plotted in figure 3.7, varies from 2.6 to 2 mm/s for all the simulations, reflecting the mass flow rate imposed as input. Test 7, which has a lower oxidizer mass flow rate value, has a lower regression rate, but the difference is negligible.

A lower regression rate leads to a lower fuel mass flow rate, hence to a lower Oxidizer/fuel Ratio. This ratio, figure 3.8, follows the same pattern of $\dot{r}$. The ideal oxidizer fuel ratio for the mixture is $\simeq 3.7$. The simulation is oxidizer rich. Impurities in the grain, external disturbances and transitory effects
3.3. NUMERICAL SIMULATION

Figure 3.6: Simulated Characteristic Velocity

Figure 3.7: Simulated Regression Rate

Figure 3.8: Simulated Oxidizer/Fuel Ratio
related to the ignition of the motor are not accounted, and this could be a cause for the underestimation of the fuel mass flow rate, since the model used to predict the regression rate using the properties of the fuel and the oxidizer mass flux is valid only in steady state conditions [40].

3.4 Validation of the Simulations

The proof of dependability of the simulations can only be achieved through comparison with the experimental results. This comparison is made both graphically, through superimposition of the experimental and numerical values, and analysis of statistical parameters such as the standard deviation to quantify the effectiveness of the code. The investigation is conducted on the curves of the Tank Pressure and Combustion Chamber Pressure, and the comparison between predicted and experimental parameters such as the Combustion Efficiency.

The experimental curve is plotted in red in the figure, while the Matlab simulation in blue.

3.4.1 Test 3

In the figures 3.9 and 3.10 the experimental results for the Tank and Combustion Chamber Pressure are compared with the curves obtained from the simulation for the liquid phase injection. The simulated tank discharge is well simulated. Only the initial part, which is transitory, is different. When the discharge begins the liquid Nitrous flows from the tank into the feed lines. To remain in equilibrium, since the pressure decreases, more fluid has to evaporate. The process has a latency which is depicted in the plots and has been explained by Waxman: “As the liquid front of nitrous oxide expands rapidly into the pre-injector volume, much of it flashes to vapor, resulting in rapid cooling and low temperatures for a short duration in the beginning of a test. However, once the ensuing liquid fills in the volume upstream of the injector, the temperature returns to the bulk liquid temperature and stabilizes” [44].

The combustion chamber pressure is underestimated at the beginning of the burn, while the end is overestimated. The average value remains the same. This was expected from the simulation, which is ideal and does not take into account the transitory variations.

To quantify the anomaly of the simulated results from the measured data the Standard Deviation has been calculated. For this test the deviation of the simulated combustion pressure curve from the measured data is of $\sim 1.7$ bar, which is 7.5 % of the average combustion chamber pressure.
3.4. VALIDATION OF THE SIMULATIONS

Figure 3.9: Test 3 Tank Pressure

Figure 3.10: Test 3 Combustion Chamber Pressure
### 3.4.2 Test 5

Compared with the results for Test 3, this time both the simulated tank discharge and the combustion chamber pressure are closer with the experimental curve. The transitory phase at the beginning of the burn is still underestimated, but the rest of the stable burn phase is well simulated. The standard deviation of the simulated combustion pressure from the measured one is of $\approx 1.55 \text{ bar}$, 6% of the average combustion chamber pressure.

![Figure 3.11: Test 5 Tank Pressure](image1)

![Figure 3.12: Test 5 Combustion Chamber Pressure](image2)
3.4. VALIDATION OF THE SIMULATIONS

3.4.3 Test 6

The simulation of Test 6 is close to the experimental data. The combustion chamber pressure is almost coincident with the experimental results, while the Tank Pressure during discharge is well simulated. The standard deviation of the simulated combustion pressure from the measured one is of 1.24 bar, which is 5% of the average combustion chamber pressure.

Figure 3.13: Test 6 Tank Pressure

Figure 3.14: Test 6 Combustion Chamber Pressure
3.4.4 Test 7

The very small burn time of the last test heavily influences the accuracy of the simulation, since the transitory effects are no longer negligible. The combustion chamber pressure trend is poorly predicted, and a justification may be found observing the tank discharge of figure 3.15. The oxidizer injected is modeled as a saturated liquid, and the hypothesis proved to be reliable in the other three simulations. However Test 7 is too short and the latency of the liquid boiling is not overcome during the burn time.

![Figure 3.15: Test 7 Tank Pressure](image1)

![Figure 3.16: Test 7 Combustion Chamber Pressure](image2)
Chapter 4

CFD Simulations Setup

The CFD simulations have been carried out using the commercial software Ansys CFX, version 16. The license used is the Academic Research License, which allows for a number of mesh elements higher than 512000 and multiprocessing, which are the main limitations of the student version. There is a gain in the quality of the results as well as a saving in time required for the simulations to reach convergence. The computers used featured a 8-core CPU Intel Xeon E3-1245 v5 with 3.5 GHz clock and 16 gigabytes of RAM.

4.1 Test Cases

The Simulations have been performed using the results of Tests 5 and 6. Unfortunately the injector manifold pressure sensor of Test 3 malfunctioned, thus voiding the calculation of the expansion from the tank to the injection plate, since the pressure drop at the injectors is unknown. Moreover, Test 3 performed different from the other tests even though the motor was exactly the same, so the results could be unreliable. On the other hand, Test 7 has been overlooked due to its really short burn time. Since the transient ignition phase barely had ended while the switching off began, the absence of a quasi-steady state phase may make a steady state CFD analysis not only lacking, but also misleading.

4.2 Geometry

As discussed in the introductory chapter, the setup for the CFD is similar to the one developed at CISAS, therefore the geometry chosen as the fluid flow domain is nevertheless the inside boundary of the combustion chamber, from the injector plate to the exit section of the nozzle, including the fuel grain internal border. While the other geometrical characteristics are invariant during the fire, the fuel grain thickness reduces over time, therefore the port area increases. Section 4.6 discusses how this feature has been reproduced. The geometries have been realized with the 3D CAD software Solidworks 2016. Figure 4.1 is a representation of a model used for the simulations, in particular for
Test 6 at burn time 1.5 seconds. The frontal part of the rocket is the precombustion chamber, where the injector orifices are located. The middle part is the burning area of the fuel grain while the rear part is the convergent-divergent nozzle. Figure 4.2 is the dimensioned section of the model of Test 6. The construction is axisymmetric so the sketch is simply rotated of 360° degrees to obtain the 3D figure.

![Figure 4.1: CFD Geometry Model](image)

4.3 Mesh

The fluid volume has been discretized with tetrahedron cells. Both gas-only and multiphase injection conditions have been simulated, involving two different meshes. The choice of the element size is related to the time for convergence and the quality of the results. A 4.5 millions elements grid has been adopted, refined in the volume sector corresponding to the fuel grain, where the chemical reaction takes place. The combustion is highly sensitive to the solidity of the mesh. Simulations run on a coarse mesh may never reach convergence, and the pressure and temperature are often underestimated. Figure 4.3 is an image of the meshed model.
4.4 Turbulence

In Bellomo et al. work [11], different turbulence models were applied to the CFD simulation of the Nitrous Oxide/Paraffin hybrid rocket motor of Grosse [12]. In table 4.1 the values of the error between the measured and predicted pressure in the combustion chamber and between the measured and predicted combustion efficiency are reported.

<table>
<thead>
<tr>
<th>Turbulence Model</th>
<th>Pressure Error</th>
<th>Efficiency Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard K-Epsilon</td>
<td>-2.0 %</td>
<td>+3.91 %</td>
</tr>
<tr>
<td>K-Epsilon RNG</td>
<td>+0.4 %</td>
<td>+6.58 %</td>
</tr>
<tr>
<td>Standard K-Omega</td>
<td>-6.2 %</td>
<td>-0.36 %</td>
</tr>
<tr>
<td>K-Omega SST</td>
<td>-6.5 %</td>
<td>-0.61 %</td>
</tr>
</tbody>
</table>

Table 4.1: Comparison of different Turbulence Models (Source: [11])

Bellomo inferred from the results that $k-$ and $k-$ RNG gave comparable results, whereas $k-$ gave a different outcome. Again, $k-$ and $k-$ SST gave similar results. The turbulent mixing is lower predicted with $k-$, so the flame temperature is lower than with $k-$-$\epsilon$. However, this agrees with the experimental results on flame temperature investigations [45]. The combustion efficiency obtained with $k-$-$\omega$ is also very close to the experimental value. The authors of [11] suggest that the approximations of the models probably tend to compensate each other. So they used $k-$-$\epsilon$ in most of their works, preferring a simple and robust model to avoid nontrivial errors in the solution [19]. In [15], a CFD investigation on the influence of swirling flow field inside the combustion chamber is carried out, and the model used is $k-$-$\epsilon$ again. However, in Paccagnella’s work [18] a similar analysis is carried out with the $k-$-$\omega$ SST model instead. This model adopts a blending function to combine the
advantages of both k-\( \varepsilon \) and k-\( \omega \) models: while k-\( \varepsilon \) is more accurate in the free-stream zone, k-\( \omega \) is more accurate in the near-wall region [46] [47] [48].

In this thesis the k-\( \omega \) SST model is used. The DHX-4 motor is a lab-scale motor, with a free-stream zone inside the combustion chamber fairly limited, so an accurate modeling of the near-wall flow field is extremely important to obtain a realistic flame structure. Furthermore, since a light swirl motion is given to the liquid injection, the analogy with the work of [18] was exploited using the same turbulence model. Some simulations have been carried out using the k-\( \varepsilon \) model as well, however divergence in the solver eventually appeared.

Since the model is already implemented inside the software, and its mathematical description lies outside the aim of this thesis, the equations are not listed here but can be found in reference [49].

4.5 Oxidizer Injection

From the Matlab simulations of the previous chapter emerged that the oxidizer reaches the combustion chamber with a vapor quality \( x \) different than zero. This implies that the injection is multiphase, since \( N_2O \) is injected as a mixture of gas and liquid. In particular, on the actual atomizer plate geometry, two overlapping inlet boundaries have been identified. One is a gas phase inlet, the other a liquid droplets source. This section discusses the models chosen and the parameters needed for the initialization.

4.5.1 Mass Flow Rate

The Matlab simulations discussed in the previous chapter highlighted that the liquid oxidizer drew from the tank does not reach the chamber as a single-phase fluid, but partially evaporates in the feed system. Presenting a vapor quality \( x \) not negligible, the propellant is not injected as a single-phase fluid but as a multiphase mixture. The development of a tool to predict more accurately the fluid discharge from the tank to upstream the injectors, and the choice of the injection model, have been critical for the \( N_2O \) injection simulation.

To account for this physical condition an expansion model had to be investigated. Figure 4.4 is the Pressure-Time experimental plot of Test 6. It represents the measured values of the Tank Pressure, Injector Manifold Pressure (measured upstream of the injection plate) and the Combustion Chamber Pressure (measured downstream of the injection plate). The pressure difference between the lower curves (green and red) is the pressure drop inside the injector, whereas the the gap between the tank and the upstream pressures is correlated to the expansion process inside the feed system. To model the flow in the orifices, an estimate of the properties change during discharge is required.

In the Matlab simulations of the motor carried out for each test the mass flow rate follows the
4.5. **OXIDIZER INJECTION**

At the i-th time instant, the oxidizer mass flow rate is proportional to the square root of the ratio between the i-th tank pressure and the initial tank pressure. \( \dot{m}_{ox,i} \) is the average oxidizer mass flow acquired from the test data and A a constant required to satisfy the law of mass conservation during the discharge. This model has been chosen since the injectors are choked therefore there is a proportionality between the ratio of the oxidizer mass flow rates (which is the maximum possible) in two different time instants and the square root of the ratio of the corresponding tank pressures. Even though the modeling of the discharge deduced from the injectors choking hypothesis fitted well the mass and pressure variations in the tank, it did not account for the actual expansion process inside the injectors, so it couldn’t be used for the initialization of the CFD and a different model had to be researched.

**Injection Models**

One method used to predict the mass flow rate of a two-phase flow through an injector is the **Homogeneous Equilibrium Model** (HEM) [50]. This model assumes that the depressurization in the injector is isoentropic, that the liquid and vapor phases are in thermodynamic equilibrium and that there is no velocity difference between the two phases (no-slip condition).
\[ \dot{m}_{HEM} = C_d A \rho_2 \sqrt{2 (h_1 - h_2)} \]

In this model, the mass flow rate \( \dot{m}_{HEM} \) is a function of the discharge coefficient \( C_d \), the cross sectional area of the orifice \( A \), the downstream density of the fluid \( \rho_2 \) and the upstream and downstream fluid specific enthalpies, respectively \( h_1 \) and \( h_2 \). The procedure to calculate the enthalpies is described by Leung [51]:

- Known the downstream pressure \( p_2 \), the specific entropies \( s^L \) and \( s^V \) are calculated, where the superscript \( L \) denote the liquid phase and \( V \) the vapor phase.

- Once the upstream stagnation condition is defined and so the total entropy \( s_0 \), the vapor quality \( x \) of the flow is determined by the isoentropic expansion assumption. The upstream stagnation conditions are the properties of the liquid phase Nitrous Oxide inside the tank.

\[
x = \frac{s_0 - s^L}{s^V - s^L}
\]

- From the vapor quality and the values of \( h^L \) and \( h^V \) upstream and downstream the injector nozzle, the value of the enthalpy \( h \) is calculated as:

\[
h = x h^V + (1 - x) h^L
\]

Unfortunately the mass flow predicted using the HEM model tends to be much lower than the one measured during experimental tests, since the non-equilibrium effects are not negligible in the injectors [52]. Dyer proposed that these effects are predominantly caused by the superheating of the liquid during expansion and by a finite vapor bubble growth rate.

In this specific case, however, HEM overestimates the mass flow rate. This happens because the flow in the feed system is far from isoentropic, due to the long line and the numerous valves involved. For a total pressure drop of about 30 bar the difference of the tank and combustion chamber enthalpies is large enough to overpredict the mass flow rate. The losses therefore can’t be neglected.

The flow inside the feed system floods through numerous valves required to control the injection process. This is similar to the flow inside a refrigeration cycle, which is forced to pass through thermal expansion valves, decreasing the temperature as well as the pressure, but increasing the entropy of the system. This process is the expansion from point 4 to 5 in figure 4.5.

The non-equilibrium expansion process has been simulated in the feed system between the tank pressure and the injector manifold pressure. To calculate the properties after the expansion a procedure analogous to the enthalpy calculation for the HEM model is applied, however this time is the enthalpy of the liquid nitrous in the tank that remains constant, whereas the entropy varies:

- Known the downstream pressure \( p_2 \), the specific enthalpies \( h^L \) and \( h^V \) are calculated, where the superscript \( L \) denote the liquid phase and \( V \) the vapor phase.
Once the upstream stagnation condition is defined and so the total enthalpy $h_0$, the vapor quality $x$ of the flow is determined by the isenthalpic expansion assumption. The upstream stagnation conditions are the properties of the liquid phase Nitrous Oxide inside the tank.

$$x = \frac{h_0 - h^L}{h^V - h^L}$$

- From the vapor quality and the values of $s^L$ and $s^V$ upstream and downstream the injector nozzle, the value of the entropy $s$ is calculated as:

$$s = xs^V + (1-x)s^L$$

The isenthalpic expansion is more appropriate to model the losses in the lines, which were not taken into account by the isentropic. Even though the flow condition upstream the injector is known, the injection still remains unsolved. From the upstream pressure to the combustion chamber pressure two models have been applied, HEM and Bernoulli.

With the HEM model an isentropic expansion is applied to the entropy calculated with the isenthalpic discharge from the tank to the pressure upstream of the injectors. This resulted in an underestimation of the injected mass flow rate, adhering to the experiments of Darby [52].

On the contrary, Bernoulli’s model was closer to the physical conditions. The equation is the following [1]:

$$\dot{m} = C_dA\sqrt{2\rho\Delta p}$$

Where the density $\rho$ used for the calculation is the density averaged by the vapor quality with the following law:

$$\frac{1}{\rho} = \frac{x}{\rho^V} + \frac{1-x}{\rho^L}$$
the vapor quality and the liquid and vapor densities are calculated upstream of the injector, since in Benroulli’s law the fluid is incompressible, hence the density remains unchanged during the injection. The mass flow rate estimated is multiphase, and the separation between the two components is described later in the chapter.

In figure 4.6 the measured mass flow approximated with Matlab is compared with the mass flow rates predicted with the aforementioned models. The rate predicted with the isoenthalpic expansion in the feed system and the Bernoulli law in the injector orifice almost coincides with the simulated one. Since the Bernoulli prediction is the closest to the experimental results, represented by the Matlab simulation curve in the plot, it can be used to setup the CFD.

![Test 6 Mass Flow Rate](image)

**Figure 4.6: Mass Flow Rates of Test 6**

**Discharge Coefficient**

The liquid injection is implemented in CFX defining as many droplets sources as the injectors. This model implies that the liquid jet is subjected to a Primary Break-up: the flow injected in the combustion chamber is not a continuous phase but a discrete Lagrangian phase [13]. A Lagrangian Flow consists of spherical particles, namely the droplets, dispersed in a continuous gas phase. This model is less memory intensive than the multiphase model, and fits perfectly this problem, since designed for flows in which particle streams are injected into a continuous phase flow with well defined entrance and exit conditions, and the assumption that the second phase is sufficiently diluted that the effects of the particle volume fraction on the gas is negligible. [53]. The spray characteristics predicted
are strongly dependent on the regime of the flow inside the orifice. The Plain-Orifice Atomizer Model of CFX suits the injectors used in the Phoenix motor [54]. According to this model the atomizers may operate in three different regimes [55]:

- **Single-Phase**: the liquid completely fills the orifice;
- **Cavitating**: vapor pockets form inside the injector nozzle;
- **Flipped**: downstream gas surrounds the liquid jet inside the injector nozzle.

The procedure described here to calculate the discharge coefficient is given by [55]. The parameters needed by the model are given in Table 4.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle Diameter</td>
<td>$d$</td>
</tr>
<tr>
<td>Nozzle Length</td>
<td>$L$</td>
</tr>
<tr>
<td>Radius of Curvature of the Inlet Corner</td>
<td>$r$</td>
</tr>
<tr>
<td>Upstream Pressure</td>
<td>$p_1$</td>
</tr>
<tr>
<td>Downstream Pressure</td>
<td>$p_2$</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>$\mu$</td>
</tr>
<tr>
<td>Liquid Density</td>
<td>$\rho_l$</td>
</tr>
<tr>
<td>Vapor Pressure</td>
<td>$p_v$</td>
</tr>
</tbody>
</table>

**Table 4.2: List of the governing parameters for an injector flow**

With these values two non-dimensional numbers, the *Reynolds number* $Re$ and the *Cavitation Parameter* $K$ can be defined:

$$ Re = \frac{d \rho_l}{\mu} \sqrt{\frac{2 (p_1 - p_2)}{\rho_l}} $$

(4.1)

$$ K = \frac{p_1 - p_v}{p_1 - p_2} $$

(4.2)

The information about the internal flow state is provided by the *Discharge Coefficient* $C_d$, defined as the ratio between the measured mass flow rate in the injector nozzle, $\dot{m}$, and the theoretical maximum mass flow rate obtained with an ideal nozzle which expands the same fluid with the same pressure drop $\Delta p$. Mathematically:

$$ C_d = \frac{\dot{m}}{A \sqrt{2 \rho_l \Delta p}} $$

(4.3)

where $A$ is the cross-sectional area of the orifice (assumed constant) and $\Delta p$ is the difference between the upstream pressure $p_1$ and downstream pressure $p_2$. 
The discharge coefficient takes into account the losses the resistance of the nozzle imposes on the flow. A higher resistance corresponds to a lower mass flow and therefore to a lower value of the coefficient. For an ideal nozzle, \( C_d = 1 \).

If pressure drop, liquid density and mass flow rate are known, \( C_d \) can be experimentally determined for a particular nozzle configuration. Otherwise the injector state may be identified comparing the Cavitation Parameter \( K \) with \( K_{\text{incep}} \) and \( K_{\text{crit}} \), two numbers defined by the following empirical relationships:

\[
K_{\text{incep}} = 1.9 \left( 1 - \frac{r}{d} \right)^2 - \frac{1000}{Re} \tag{4.4}
\]

\[
K_{\text{crit}} = 1 + \frac{1}{\left( 1 + \frac{L}{4d} \right) \left( 1 + \frac{2000}{Re} \right) e^{70r/d}} \tag{4.5}
\]

where \( Re \) is given by equation 4.1 and \( e \) is Euler’s number. \( K_{\text{incep}} \) is related to the inception of cavitation, whereas \( K_{\text{crit}} \) is related to the flipped regime. However, if \( r/d > 0.05 \), flip is impossible and \( K_{\text{crit}} = 1 \). Through comparison, the following cases can be identified:

If \( K > K_{\text{incep}} \) and \( K \geq K_{\text{crit}} \), then the nozzle is in single-phase state and \( C_d \) is given by the relationship:

\[
C_d = \frac{1}{C_{du} + 20 \left( 1 + 2.25 \frac{L}{d} \right) \frac{L}{Re_h}} \tag{4.6}
\]

\( C_{du} \) is the **Ultimate Discharge Coefficient**, defined as:

\[
C_{du} = 0.827 - 0.00085 \frac{L}{d}
\]

If \( K_{\text{crit}} \leq K \leq K_{\text{incep}} \), then the nozzle flow is cavitating, and \( C_d \) is defined as:

\[
C_d = 0.611 \sqrt{K} \tag{4.7}
\]

If \( K < K_{\text{crit}} \) the nozzle is flipped, hence \( C_d \) is constant:

\[
C_d = 0.611 \tag{4.8}
\]

Unfortunately, if \( K < 1 \), these relations are not strictly valid, which is the case of the motor in this thesis. If this happens, an arbitrary value of \( C_d \) must be assumed for calculations. The discharge coefficient of the atomizers therefore should be assumed to be 0.611, as suggested by Barato in his PhD thesis [69]. However, he also pointed out that the use of \( C_d \) becomes questionable when not strictly related to the incompressible model. Since the isenthalpic expansion used to model the tank discharge in the feed system overestimates the losses, as already discussed, an higher value of the \( C_d \) has been used to compensate more complex phenomena which are not taken into account by the classical model of the discharge coefficient and are present in the feed system of the motor. The value has been set to 0.72.
Matlab Algorithm

To calculate the variation of the injected flow parameters values over time, the Matlab simulations described in the previous chapter have been combined with a new algorithm. In particular, it implements the procedures illustrated for the calculation of the isoentropic and isoenthalpic expansions.

The script initializes with the tank pressure of the i-th time instant of the simulation. Using the entropy and enthalpy of the liquid fraction of the fluid, which is discharged through the feed lines, an isoenthalpic expansion is applied from the tank pressure to the pressure upstream of the injectors.

The mass flow rate using Bernoulli’s Law is then calculated, using the discharge coefficient specified in the previous section, the density upstream the orifice and the pressure drop in the i-th instant, which is provided by the Matlab simulation:

\[ \dot{m}_B = C_d A_{inj} \sqrt{2 \rho \Delta P} \]

Later, an isoentropic expansion is implemented from the upstream injector pressure to the downstream injector pressure. The enthalpy downstream is calculated and the HEM model applied. The Saint Venant - Wantzel equation used to estimate the mass flow in an isentropic expansion does not take into account the choking phenomena [43]. Since the flow is choked in the injectors, the mass flow rate is evaluated for a discrete number of pressure drops \( \Delta P \) from zero to the actual drop from the upstream pressure to the combustion chamber pressure. In particular, for a given expansion the enthalpy \( h \) is calculated. From the enthalpy the velocity of the fluid in the injector is:

\[ v = \sqrt{2(h_0 - h)} \]

with \( h_0 \) the enthalpy of the liquid \( N_2O \) in the tank. Using the velocity and the density of the fluid after the expansion, the mass flux is estimated:

\[ G_{ox} = \rho v \]

The process is iterated for an increasing \( \Delta P \). Since the atomizer nozzle is choked, the maximum value of the mass flux is selected and used to calculate the HEM mass flow at the i-th instant:

\[ \dot{m}_{HEM} = C_d A_{inj} \max(G_{ox}) \]

The cycle ends and the process iterates for every time step, returning the mass flow rate over time estimated with the two different models.

Initialization Parameters

Once a time instant has been chosen, the properties of the injected Nitrous Oxide can be extracted from the simulations. The actual injection plate geometry is reproduced in the CFD model, and the multiphase injection is simulated dividing the boundary in two different inlets:
- The gas phase is injected through the surface of the injector;

- The liquid phase is injected as a Lagrangian phase from sources overlapping to the orifices.

The properties of the two flows are defined by the gas phase and liquid phase conditions gathered from the Matlab simulation, using, as already stated, the isoenthalpic expansion from the tank to the upstream injector surface, and a Bernoulli expansion through the atomizer.

The steps taken to initialize the injection are the following:

- A time instant is chosen, preferably after the ignition transitory, in the quasi-steady combustion phase.

- For that time instant, the vapor quality $x$, the densities of liquid phase $\rho_l$ and vapor phase $\rho_v$, the total oxidizer mass flow rate and the temperature are given by the simulation.

- From the vapor quality and the total oxidizer mass flow rate, the vapor and liquid phase mass flow rates are calculated with the following equations:

$$\dot{m}_v = x\dot{m}_{tot}$$

$$\dot{m}_l = \dot{m}_{tot} - \dot{m}_v$$

The parameters calculated are listed in table 4.3.

<table>
<thead>
<tr>
<th></th>
<th>Test 5</th>
<th>Test 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time instant [s]</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>Total Mass Flow Rate [g/s]</td>
<td>377.2021</td>
<td>380.6381</td>
</tr>
<tr>
<td>Vapor Quality [-]</td>
<td>0.1866</td>
<td>0.1864</td>
</tr>
<tr>
<td>Liquid Mass Flow Rate [g/s]</td>
<td>306.8162</td>
<td>309.6872</td>
</tr>
<tr>
<td>Liquid Mass Flow Rate per Injector [g/s]</td>
<td>43.8309</td>
<td>44.2410</td>
</tr>
<tr>
<td>Vapor Mass Flow Rate [g/s]</td>
<td>70.3859</td>
<td>70.9509</td>
</tr>
<tr>
<td>Vapor Mass Flow Rate per Injector [g/s]</td>
<td>10.0551</td>
<td>10.1358</td>
</tr>
<tr>
<td>Density [kg/m$^3$]</td>
<td>336.0419</td>
<td>346.5202</td>
</tr>
<tr>
<td>Liquid Density [kg/m$^3$]</td>
<td>897.1387</td>
<td>888.6412</td>
</tr>
<tr>
<td>Vapor Density [kg/m$^3$]</td>
<td>90.1821</td>
<td>94.6012</td>
</tr>
<tr>
<td>Temperature [K]</td>
<td>275.0763</td>
<td>276.6827</td>
</tr>
<tr>
<td>Port Radius [mm]</td>
<td>21.5</td>
<td>21</td>
</tr>
</tbody>
</table>

Table 4.3: Injection Parameters
4.5. OXIDIZER INJECTION

4.5.2 Injection Direction

The DHX-4 Phoenix motor injectors are not perpendicular to the plate, in order to imprint a swirling motion to the oxidizer flow. Therefore the velocity vector has been thoroughly defined in order to reproduce the actual fluid pattern inside the combustion chamber.

In the simulation, the coordinates of the orifices are required, which can be calculated if the number of holes and their distance from the center of the plate are known.

The coordinate system is defined while creating the geometry in the 3D CAD software, and this convention is adopted: the axis of symmetry of the motor is the $x$ axis, while $y$ and $z$ are the normal directions. The origin of the coordinate system can be anywhere in the motor, even though it is desirable to put it on the injection plate with the incrementing value of the $x$ axis coincident with the length of the combustion chamber. If the coordinate system is defined in this way, the injection plate is parallel to the plane $yz$, while $x$ is the normal direction to the plate, positive inside the combustion chamber.

The $n$ holes on the plate are assumed to be lined up on the same circle of radius $r$.

The central angle $\alpha$, which is defined as the angle between two consecutive holes on the circle, is calculated as:

$$\alpha = \frac{360^\circ}{n}$$

The angular distance $\alpha_i$ of the $i$-th orifice is defined as the angle between the orifice centre and the reference point on the circle. The reference axis is chosen as the positive half of the $y$-axis, and the reference point is the intersection between the circle and the reference axis. The orifice on the center of the plate is marked as number 1, while the other points are enumerated counterclockwise from 2 to $n$. The value of $\alpha$ increases for a counterclockwise rotation.

From the central angle and radius the coordinates of every point are calculated as follow, where the $x$ coordinate is assumed to be zero at the injection plate:

\[
\begin{align*}
(x_1, y_1, z_1) &= (0, r, 0) \\
(x_2, y_2, z_2) &= (0, r\cos(\alpha_2), r\sin(\alpha_2)) \\
(x_3, y_3, z_3) &= (0, r\cos(\alpha_3), r\sin(\alpha_3)) \\
&\vdots
\end{align*}
\]

If the swirl angle $\varphi$ is zero, and the injection is fully axial, then the injection versor is the same for every nozzle:

$$(\hat{x}, \hat{y}, \hat{z}) = (1, 0, 0)$$

Since the swirl angle $\varphi$ is different from zero, a change of coordinates has to be implemented in order to obtain the actual velocity versor. The swirl angle is positive for a counterclockwise rotation in a direction perpendicular to $x$. For the $i$-th injector:
\[
\begin{align*}
\hat{x}_i &= \cos(\varphi) \\
\hat{y}_i &= \sin(\varphi)\sin(\alpha_i) \\
\hat{z}_i &= -\sin(\varphi)\cos(\alpha_i)
\end{align*}
\]

The vector found using this coordinate transformation is still a versor:

\[
\cos^2(\varphi) + \sin^2(\varphi)\sin^2(\alpha_i) + \sin^2(\varphi)\cos^2(\alpha_i) = 1
\]

The motor studied in this thesis has a swirl angle of 15 degrees, while the angle \( \alpha \) is of 60 degrees.

Figure 4.7 is a screenshot of Ansys CFX depicting the pre-combustion chamber with the inlet boundaries highlighted.

![Figure 4.7: Oxidizer Inlet Boundaries. Gas phase on the left, liquid on the right.](image)

### 4.5.3 Gas Phase Inlet

An inlet boundary is identified in the surfaces corresponding to the seven holes of the injectors. The mass flow rate condition is selected, with the temperature and vapor mass flow identified from the simulations.

### 4.5.4 Liquid Phase Inlet

Liquid Nitrous Oxide is absent from the Ansys Database, so it was necessary to create a new material table. The properties of the substance have been inferred from the Matlab simulations and are listed in tables 4.4 and 4.5. The specific heat capacity has been calculated with Refprop for the specified reference state, while the latent heat of vaporization and the surface tension had to be acquired for the saturated liquid condition. These two properties can be defined only during a phase change, thus only for a saturated liquid.
4.5. OXIDIZER INJECTION

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar Mass</td>
<td>44.013 kg/kmol</td>
</tr>
<tr>
<td>Density</td>
<td>897.1387 kg/m³</td>
</tr>
<tr>
<td>Specific Heat Capacity</td>
<td>2317.0 J/kgK, at constant pressure</td>
</tr>
<tr>
<td>Reference State (p,T)</td>
<td>32.791 bar, 275.0763 K</td>
</tr>
<tr>
<td>Reference Specific Enthalpy</td>
<td>169.85 kJ/kg</td>
</tr>
<tr>
<td>Reference Specific Entropy</td>
<td>0.7299 kJ/kgK</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>85.615 µPas</td>
</tr>
<tr>
<td>Latent Heat of Vaporization</td>
<td>227.71 kJ/kg</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>5.0385 mN/m</td>
</tr>
</tbody>
</table>

Table 4.4: Properties of Liquid Nitrous Oxide for Test 5

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar Mass</td>
<td>44.013 kg/kmol</td>
</tr>
<tr>
<td>Density</td>
<td>888.6385 kg/m³</td>
</tr>
<tr>
<td>Specific Heat Capacity</td>
<td>2583.3 J/kgK, at constant pressure</td>
</tr>
<tr>
<td>Reference State (p,T)</td>
<td>34.145 bar, 276.6827 K</td>
</tr>
<tr>
<td>Reference Specific Enthalpy</td>
<td>173.48 kJ/kg</td>
</tr>
<tr>
<td>Reference Specific Entropy</td>
<td>0.7425 kJ/kgK</td>
</tr>
<tr>
<td>Dynamic Viscosity</td>
<td>83.702 µPas</td>
</tr>
<tr>
<td>Latent Heat of Vaporization</td>
<td>223.46 kJ/kg</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>4.7575 mN/m</td>
</tr>
</tbody>
</table>

Table 4.5: Properties of Liquid Nitrous Oxide for Test 6

To define the injection also the velocity of the flow, the aperture of the liquid jet cone and the number and diameter of droplets are required.

**Exit Velocity**

The velocity \( u \) of the droplets is calculated using the mass flow rate and density acquired from the Matlab simulation of the tank discharge. Since the Bernoulli injection model is adopted, which presumes that the properties remain unchanged during the expansion in the orifice, the density is the one determined after the isoenthalpic expansion. The exit velocity for each atomizer is calculated using the law of mass conservation:

\[
  u = \frac{\dot{m}}{\rho A}
\]

where \( \dot{m} \) is the liquid oxidizer mass flow rate per atomizer, \( A \) the cross sectional area of the injector and \( \rho \) the \( \text{N}_2\text{O} \) density. The average density of the oxidizer biphasic mixture is used instead of \( \rho_l \) since the no-slip condition at the inlet is adopted.
For Test 5 the exit velocity is 41.52 m/s, for Test 6 is 34 m/s.

**Spray Angle**

The spray angle $\theta$ can be determined with the *Ranz Correlation* [56], and both for a single-phase and cavitating nozzle depends on the ratio of the gas and liquid densities:

$$\frac{\theta}{2} = \tan^{-1} \left[ \frac{4\pi}{C_A} \sqrt[3]{\frac{\rho_{gc} \sqrt{3}}{\rho_l \frac{1}{6}}} \right]$$

(4.9)

$C_A$ is a geometric constant, and is determined using the Reitz formula [57] as a function of nozzle length and diameter:

$$C_A = 3 + \frac{L}{3.6d}$$

(4.10)

In the DHX-4 Phoenix the ratio $L/d$ is 0.5. For both the test cases the aperture of the jet cone is approximately 40 degrees, so the angle between the axis and the generatrix, which is the input for CFX, is 20 degrees.

### 4.5.5 Droplet Diameter and Distribution

To characterize the droplet behaviour, its diameter needs to be determined. A simple way to calculate it is given by the *Blob Method*, developed by Reitz and Diwakar [58]. In this model, the parcels of liquid are injected as “blobs”, large droplets with a characteristic size equal to the nozzle hole diameter. This model is well suited for dense sprays, but, as stated in the previous sections, Nitrous Oxide is injected as a mixture of liquid droplets and gas, and the blob method overestimates the initial diameter of the particles. The *Rosin-Rammler Distribution* has proven to be more in agreement with experimental measurements of spray injections [59].

The Rosin-Rammler Distribution is characterized by the *Most Probable Droplet Size*, which is the initial diameter of the injected liquid droplet, $d_0$, and the *Spread Parameter* $s$ [60].

The Spread Parameter is chosen from modeling experience and experimental observations, and its possible values are listed in table 4.6. The larger its value, the narrower the droplet distribution.

<table>
<thead>
<tr>
<th>State</th>
<th>Spread Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single Phase</td>
<td>3.5</td>
</tr>
<tr>
<td>Cavitating</td>
<td>1.5</td>
</tr>
<tr>
<td>Flipped</td>
<td>$\infty$</td>
</tr>
</tbody>
</table>

Table 4.6: Spread Parameter

The value of $d_0$ is calculated as follows:
- The problem is initialized with the parameters in table 4.7, where $\lambda = d/8$, with $d$ the nozzle diameter [61].

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas Phase Density</td>
<td>$\rho_g$</td>
</tr>
<tr>
<td>Exit Velocity</td>
<td>$u$</td>
</tr>
<tr>
<td>Droplet Surface Tension</td>
<td>$\sigma$</td>
</tr>
<tr>
<td>Length Scale</td>
<td>$\lambda$</td>
</tr>
<tr>
<td>Spread Parameter</td>
<td>$s$</td>
</tr>
</tbody>
</table>

Table 4.7: Droplet Size Calculation: Initialization

- The Weber Number $We$ of the droplet is calculated:

\[
We = \frac{\rho u^2 \lambda}{\sigma}
\]  

(4.11)

- A parameter called Sauter Mean Diameter, $d_{32}$, is then calculated using the following equation:

\[
d_{32} = 133\lambda We^{-0.74}
\]  

(4.12)

- With $d_{32}$ and $s$ the value of $d_0$ is then calculated.

\[
d_0 = 1,2726d_{32} \left(1 - \frac{1}{s}\right)^{1/s}
\]  

(4.13)

The Weber Number, required to initialize the droplet size, is used also to identify the break-up mechanism of the droplet, as shown in the following sections. In the simulations the diameter of the droplets is in the order of magnitude of a tenth of millimeter.

4.5.6 Number of Particles

The last input required by the atomization model is the number of injected particles per injector nozzle per iteration. This parameter should not be confused with the number of particles injected per second, that can be calculated with the continuity equations, since the mass flow rate, the droplet diameter and the density are known. The number of particles $n$ is therefore a numerical parameter and has to be chosen with a convergence study:

- The simulation is set-up with $n$ particles;
- Another simulation is set-up with an increased value of $n$;
- The results are compared, if the solutions are different iterate the process increasing the number of particles;
- When the difference between the two solutions is negligible, the lower value of $n$ should be chosen.

Since the number of particles the solver has to track is proportional to the time required by the solver to perform an iteration, the lowest value of $n$ possible should be taken for the injection model, to avoid an increase of the time required for the solution. In this thesis, the number of liquid parcels chosen per injector was 150.

4.5.7 Atomizer Model - Summary

The parameters needed to characterize the liquid injection with the Plain-Orifice Atomizer Model, and how they were calculated, are summarized in table 4.8.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate</td>
<td>$\dot{m}$</td>
</tr>
<tr>
<td>Isoenthalpic Expansion + Bernoulli</td>
<td></td>
</tr>
<tr>
<td>Exit Velocity</td>
<td>$u$</td>
</tr>
<tr>
<td>Conservation of Mass</td>
<td></td>
</tr>
<tr>
<td>Spray Angle</td>
<td>$\theta$</td>
</tr>
<tr>
<td>Ranz Correlation</td>
<td></td>
</tr>
<tr>
<td>Droplet Diameter</td>
<td>$d_0$</td>
</tr>
<tr>
<td>Rosin-Rammler Distrib</td>
<td></td>
</tr>
<tr>
<td>Particles Number</td>
<td>$n$</td>
</tr>
<tr>
<td>Convergence Study</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.8: Liquid Injection: Parameters and Models

4.5.8 Secondary Break-up

After droplets are injected in the combustion chamber, the secondary break-up process takes place. It causes the fragmentation and atomization of droplets into smaller particles, which in the end evaporate and fill the combustion chamber. This break-up is induced both by internal forces, such as turbulence and instabilities within the droplet core, and by external aerodynamics forces acting on the surface. Another possible cause is the implosion of eventual cavitation bubbles trapped in the liquid parcels.

Quoting Schmehl, “Although Computational Fluid Dynamics has established a position as an effective analysis tool for many engineering flow applications, two phase flows in a combustor still represent one of the most challenging objectives for numerical simulation” [59]. The model chosen is critical to achieve a realistic simulation of the flow inside the motor, since the droplet can break-up in several ways which influence the behaviour of the liquid spray and the combustion.

To choose the correct break-up model, the influence of forces acting on the droplet must be identified. Two dimensionless parameters can be used. One is the *Weber Number*, $We$, defined as the ratio between the external aerodynamic forces acting on the droplet and the surface tension of the droplet itself. In other words, it’s the ratio between the disruptive forces which tend to break the droplet, and the internal forces which act against deformation in order to maintain the equilibrium, hence the spherical shape [62]. The other dimensionless parameter is the *Ohnesorge Number*, $Oh$, which is the
ratio between viscous forces and inertial and surface tension forces.

\[ We = \frac{\rho_g u_{rel}^2 d}{\sigma} \]

\[ Oh = \frac{\mu}{\sqrt{\rho_l d\sigma}} \]

The velocity term \( u_{rel} \) is the relative velocity between the droplet velocity and the gas phase flow velocity, \( d \) is the diameter of the droplet and \( \rho_l \) is the liquid density. The deformation of the droplet begins if \( We > 1 \).

Depending on the intensity of the aerodynamic forces, three mechanisms can be observed [63], and are described in the work of Schmehl [59]:

- From \( We = 1 \) to \( We \approx 10 \) the droplet warps without breaking.

- From \( We \approx 10 \) to \( We \approx 20 \) Bag break-up takes place. This mechanism is characterized by the formation of a bag-like fluid film which expands from a toroidal rim.

- From \( We \approx 20 \) to \( We \approx 30 \) Multimode break-up takes place. In this mechanism a fluid column remains in the center of an umbrella-like film structure.

- From \( We \approx 30 \) to \( We \approx 50 \) There is a Transition phase between the Multimode break-up and the Shear break-up.

- Above \( We \approx 50 \) the Shear break-up takes place, where a liquid film is stripped off the rim of a disc shaped droplet.

After the break-up regime is identified, a suitable model for secondary break-up should be chosen. Lazzarin used the Schmehl Model on Ansys CFX, which proved to be reliable. It was also used in later work at Padova and in this thesis as well. In the work of Bartz [65] a comparison is made between the Schmehl Model and two other models used in CFD analysis, the Taylor Analogy Break-up Model (TAB) and the Wave Break-up Model. The TAB Model relies on the analogy between an oscillating distorted drop and a mass - spring - damper system. The main limitation of this model is its linearity. Schmehl improved it by adding the non-linear effects present in a droplet break-up process: his model in fact is also known as NLTAB, Non Linear Taylor Analogy Break-up Model. The Wave Model, on the other hand, is used to model the break-up induced by Kelvin - Helmholtz instabilities, which are not relevant in the spray break-up of the motor studied in this thesis.
4.5.9 Liquid Evaporation

When liquid Nitrous droplets enter the fluid domain they are outright surrounded by hot gases. A heat exchange and mass transfer process begins, and the droplets evaporate. When the vapor pressure of the liquid is greater than the ambient gas pressure, the particle starts to boil. The mass transport follows this equation [66]:

\[
\frac{dm_d}{dt} = -\frac{Q_C}{L_V}
\] (4.14)

The left side of the equation is the time derivative of the mass of the droplet \( m_d \), while on the right side there is the ratio of the convective heat transfer \( Q_C \) and the latent heat of evaporation of the droplet \( L_V \).

To enable the liquid evaporation model, the saturated vapor pressure curve as a function of temperature needs to be identified. This curve can be fitted with the Antoine Equation, which describes the relationship between vapor pressure and temperature for pure components [67]:

\[
\log_{10} p_v = A - B \frac{C}{C + T}
\] (4.15)

where \( p_v \) is the vapor pressure in millimeters of mercury \((760 \text{ mmHg} = 101.325 \text{ kPa})\), \( T \) is the temperature in °C, \( A \) is the Reference Constant, \( B \) the Enthalpy Coefficient and \( C \) the Temperature Offset. The three coefficients in equation 4.15 have to be calculated to fit the relevant temperature interval, since this equation is not strong enough to fit the whole curve but only local trends.

In engineering problems, a more convenient form of the equation 4.15 can be used:

\[
\ln p_v = A - B \frac{T}{C + T}
\] (4.16)

In this form, the base 10 logarithm is replaced by the natural logarithm and the denominator of the right part of the equation is different because SI Units are used: the vapor pressure is expressed in \( kPa \) and the temperature in \( K \).
In [13] these coefficients were calculated assuming that the expansion from the reservoir to the injector is isoentropic, so the temperature assigned to the liquid is the saturation temperature corresponding to the combustion chamber pressure. The values obtained in the intervals \([-5^\circ C ; 25^\circ C]\) and \([10^\circ C ; 30^\circ C]\) using equation 4.16 are listed in table 4.9. The first results are given by [13], the latter have been calculated as shown. Also, the difference of values obtained using 4.15 and 4.16 is underlined. The \textit{Pressure Scale} parameter is an input requested by the CFD code.

\[
\begin{align*}
\log_{10} 44159.12 &= A - \frac{B}{C+26.85} \\
\log_{10} 35261.89 &= A - \frac{B}{C+16.85} \\
\log_{10} 27803.28 &= A - \frac{B}{C+6.85}
\end{align*}
\Rightarrow
\begin{align*}
A &= 8.5846 \\
B &= 1623.1152 \\
C &= 385.15
\end{align*}
\]

\[
\begin{align*}
\ln 5887.40 &= A - \frac{B}{300-C} \\
\ln 4701.20 &= A - \frac{B}{290-C} \\
\ln 3706.80 &= A - \frac{B}{280-C}
\end{align*}
\Rightarrow
\begin{align*}
A &= 16.9079 \\
B &= 3090.73 \\
C &= -75.6656
\end{align*}
\]

<table>
<thead>
<tr>
<th>Temperature Range</th>
<th>([-5^\circ C ; 25^\circ C])</th>
<th>([10^\circ C ; 30^\circ C])</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{Reference Constant} \text{ } A</td>
<td>9.67086</td>
<td>16.9079</td>
</tr>
<tr>
<td>\text{Enthalpy Coefficient} \text{ } B</td>
<td>1429.91 \text{ } K</td>
<td>3090.73 \text{ } K</td>
</tr>
<tr>
<td>\text{Temperature Offset} \text{ } C</td>
<td>-44 \text{ } K</td>
<td>-75.6656 \text{ } K</td>
</tr>
<tr>
<td>\text{Pressure Scale}</td>
<td>1 \text{ } \text{bar}</td>
<td>1 \text{ } \text{bar}</td>
</tr>
</tbody>
</table>

Table 4.9: Antoine Coefficients

Ansys CFX manages the saturation curve calculating the Antoine Equation, hence the coefficients have to be determined with eq. 4.16 and inserted as input.

### 4.6 Fuel Injection

The oxidizer flows in the cylindrical cavity of the combustion chamber, feeding the flame at the interface between the gas flow and the solid fuel. This chemical process erodes the internal surface of the grain, enlarging the cavity therefore the burning area. The amount of reduction is directly proportional to the regression rate: a faster \(\dot{r}\) means a faster consumption, hence an increasing burning area and mass flow rate.

In this thesis, the fuel is injected as gas phase from an inlet boundary, identified as the internal surface of the hollow cylindrical grain. The setup parameters are the mass flow rate, which is inferred from the Matlab simulation, and the Temperature of the flow, which was set to \(\approx 700 \text{ } K\) which is the boiling point of paraffin wax [68]. The two bases are not considered burning surfaces, because they
are protected by a liner. By sectioning the combustion chamber after the tests it should be possible to infer a regression model for the whole cylindrical grain. However it would be valid only for that specific configuration of the motor. This is actually a limitation since it could introduce a source of error impossible to measure and deprives the thesis of scientific generality, because the study of the effect on the system of variations of some parameters would become no longer quantifiable.

The grain thickness at the simulated instant, hence the Port Area required for the geometrical model in CFX, is an output of the Matlab simulations.

4.6.1 Fuel Decomposition

After the ignition a diffusion flame develops above the fuel grain. The heat of the flame decomposes and vaporizes the solid fuel, which mixes with the oxidizer sustaining the combustion [69].

Near the fuel grain, in the boundary layer, this phenomenon take place. In particular, due to the high heat transfer, the surface of the vaporizing fuel is subjected to pyrolysis [40]. The fuel polymeric-chain breaks-up into smaller molecules, that enter the combustion chamber in gas phase. The reagents of the combustion chemical reaction are not the original fuel molecules but a mixture of smaller elements. Karabeyoglu proposed a theory to model the pyrolysis chemistry of homologous series of normal alkanes, like paraffin waxes, in hybrid rocket motors. The regression rate predicted by his theory matched test data with reasonable accuracy [70]. In particular, a normal alkane decomposition abides by the following rule:

\[ C_nH_{2n+2} = H_2 + \frac{n}{2} C_2H_4 \]

The alkane is decomposed into a mixture of Hydrogen and Ethylene. The paraffin wax used for the experiments is the Shell Sarawax SX70. From the data sheet given by the supplier, the properties of the fuel are approximately the same of Hentriacontane, \( C_{31}H_{64} \), so the following decomposition is adopted:

\[ C_{31}H_{64} = H_2 + 15.5C_2H_4 \]

As suggested by Karabeyoglu, this methodology could be applied to normal alcohols or normal acids.

Using this theory as a baseline, a similar approach is used for Sorbitol, \( C_6H_{14}O_6 \), which is a sugar alcohol. Pyrolysis decomposes sorbitol into Hexane, Carbon Dioxide and Water [71]. Unfortunately an exact stoichiometric rule couldn’t be find in literature, and an arbitrary choice had to be made to fit the theory of Karabeyoglu. Different chemical equivalences have been tried and simulated. The combination closest to the results for the actual Sorbitol - Nitrous Oxide reaction has been adopted:

\[ 19C_6H_{14}O_6 = 13C_6H_{14} + 36CO_2 + 42H_2O \]

The species obtained from the decomposition are then injected in the combustion chamber as a gas mixture. The mass fractions of the components are listed in table 4.10.
4.7. Combustion

4.7.1 Chemical Reaction

The influence of the chemical reaction on the results is related to the number of species used: the higher the number, the closer to reality is the simulation [11]. Using the software Rocket Propulsion Analysis, that uses the minimization of Gibbs Free Energy to obtain the equilibrium composition, the reaction products and the adiabatic flame temperature can be calculated [72] [73].

From the mass fraction of the products, the stoichiometric coefficients of the reaction have been calculated, while the coefficients of the products are set to the stoichiometric O/F ratio. A trade-off has to be made between the number of species and the memory requirements, so the products with a mass fraction magnitude lower than $10^{-3}$ have been neglected.

The resulting balanced equations are:

- **Paraffin**:
  \[
  193N_2O + 32C_2H_4 + H_2 = 189N_2 + 51H_2O + 35CO + \\
  +29CO_2 + 13O_2 + 13OH + 8NO + 6H_2 + 3H + 2O
  \]

- **Sorbitol**:
  \[
  160N_2O + 10C_6H_{14} = 158N_2 + 56H_2O + 26CO_2 + \\
  +34CO + 2.5O_2 + 9OH + 9.5H_2 + 4NO
  \]

If the number of chemical species used is too low, the flame temperature of the reaction would become higher than the real flame adiabatic temperature, thus creating an error in the simulation. A similar reaction was used for paraffin wax by Lazzarin [19], even though the paraffin used in her research is Pentacosane, $C_{50}H_{102}$.

The chemical reactions have to be calculated and balanced, since these are inputs required by the CFD solver to simulate the combustion process inside the chamber. For simplicity’s sake the combustion is single-phase, therefore the elements react only in gas phase: liquid Nitrous Oxide has to evaporate before it can react with the gaseous fuel injected from the walls. The evaporation greatly

<table>
<thead>
<tr>
<th></th>
<th>Sorbitol 100%</th>
<th>Paraffin 100%</th>
<th>S. 80% P. 20%</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_6H_{14}$</td>
<td>0.32331</td>
<td>-</td>
<td>0.25865</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>0.45807</td>
<td>-</td>
<td>0.36645</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>0.21862</td>
<td>-</td>
<td>0.17490</td>
</tr>
<tr>
<td>$C_2H_4$</td>
<td>-</td>
<td>0.977</td>
<td>0.19940</td>
</tr>
<tr>
<td>$H_2$</td>
<td>-</td>
<td>0.003</td>
<td>0.0006</td>
</tr>
</tbody>
</table>

Table 4.10: Fuel Mass Fractions
influences the structure of the flame inside the combustion chamber, highlighting again why accurate secondary break-up and evaporation models have to be chosen.

4.7.2 Combustion Model

To model the combustion process the Eddy Dissipation Model has been used in the thesis. It was developed by Magnussen and Hjertager [74]. It uses the Arrhenius chemistry equations with their local averaged values. In this way the turbulence-chemistry interaction is neglected. Furthermore, a one-step equation has been used since the multi-step mechanism produces incorrect results if applied to this model [13].

The Eddy Dissipation is a Mixed is Burnt model, which means that the real complex kinetic of the chemical reaction is not taken into account. This model is semi-empirical and is valid with the hypothesis of fast chemistry, which can be quantified by the Damköhler Number, $Da$, defined as:

$$Da = \frac{\tau_f}{\tau_c}$$

where $\tau_f$ is the flow time scale, related to the turbulent mass transfer inside the flow, and $\tau_c$ is the chemical time scale, related to the reaction rate of the chemical reaction. For fast chemistry, $Da \rightarrow \infty$.

The flame structure inside a conventional hybrid rocket motor is a Laminar Diffusion Flame, shown in figure 4.9. For this kind of flame the chemistry effects are important only in the zone where the reaction takes place, in particular in the boundary layer near the fuel grain, on the walls of the combustion chamber. Outside of this thin layer $Da$ is infinite, so the hypothesis of fast chemistry is valid to describe the general behaviour of the combustion chamber. Therefore the Eddy Dissipation Model can be applied [75]. On the other hand, several authors used the two-step Finite Rate Chemistry Model to simulate the combustion process inside hybrid rocket motors, such as Antoniou [76], Guobiao [77] and Kuo [78]. This model is more complex than the Eddy Dissipation Model, because it takes into account
the turbulence-chemistry interaction and the chemical kinetics inside the boundary layer. However, those researches focused on describing accurately what happens inside the burning layer of the motor. Since this thesis aim is investigating the global performance behaviour of the hybrid motor and not in accurately modelling the complex kinetics inside the combustion chamber, the results given by the Eddy Dissipation Model are reliable enough [13]. Moreover, this model is more efficient for the designer approach, since is less time consuming, more robust, and the complex chemical kinetics can be neglected.

4.8 Outlet

The nozzle constitutes the outlet of the motor. Its function is to accelerate and eject the hot gases from the combustion chamber, creating thrust. In the CFD simulation the boundary condition is an outlet with an average external pressure of around 0 Pa. In this way the flow is always choked in the nozzle throat and the low pressure suppresses the possibility of insurgency of shockwaves that would provoke numerical instabilities. Figure 4.10 represents the nozzle modeled in CFX.

Figure 4.10: DHX-4 Phoenix Nozzle
Chapter 5

CFD Results

This chapter discusses the CFD outcomes. The flow field is accurately analysed to identify the causes of combustion inefficiency, and the results are compared with the Matlab interpolations and the experimental measurements to infer the reliability of the model.

5.1 Gas Phase Simulations

The first simulations have been carried out in order to validate the chemical reaction and turbulence model adopted. The liquid injection has been initially avoided to reduce the complexity of the calculation, hence reducing the time required by the solver to converge. The numerical experiments already feature oxidizer swirled injection. Only a portion of total Nitrous mass flow is injected, thus the fuel mass flow rate had to be set proportionally, to avoid an unrealistic fuel rich simulation. Since the mass flow is lower, the chamber pressure is lower as well. However some peculiarities can be identified in the flow field, like the effect on the flow of the swirling motion of the oxidizer. These characteristics will be discussed in the next section, however it is already clear that the reactants don’t mix well enough inside the chamber, since a large amount of Nitrous Oxide leaves the motor undisturbed, as shown in figure 5.1. The reaction is concentrated near the walls, as shown by the contour of the $OH$ mass fraction of figure 5.2. The combustion is incomplete and the efficiency of the system decreases.
5.2 Test 5

Set with the parameters inferred in the previous chapter, the simulation of Test 5 is described in this section. The chamber pressure predicted by Matlab at $t_b = 1.5$ s is 24.5 bar, while the experimental measure is $\approx 24$ bar. Figure 5.3 is a mapping of the combustion chamber pressure calculated with CFX. The software overestimates the pressure providing an average measure of 26 bar, which is the 108.3% of the measured combustion chamber pressure. This error is probably due to the combustion and turbulence models chosen, and different solutions will be implemented in a future research.

While the absolute values predicted with the CFD often prove to be unreliable, they can be used for a comparison between design solutions and to investigate why the performance of the DHX-4 Phoenix dissatisfied the requirements. As shown in this section, in fact, the predicted flow field resembles the experimental observations.

The temperature contour of figure 5.4 illustrates the flame structure inside the chamber. As expected, the flame is a diffusion flame attached to the fuel-blowing walls.

The plot highlights two relevant features of the flow field. Near the injection plate, due to the step connecting the fuel grain to the precombustion chamber, the hot gas recirculates. This vorticity acts as...
flameholder. The gas envelopes the liquid oxidizer and the high temperature fosters the evaporation. However, this phenomenon is harmful for the motor, since it erodes the liner, as shown in the picture of the precombustion chamber taken after Test 3 (figure 5.5). If the burn time is long enough, the temperature rise could provoke the fusion of the motor case, as already happened for the DHX-200 Aurora, as shown in figure 5.6, which featured an analogous configuration on a larger scale [79]. The absolute value of the temperature is overestimated, and this is one of the main flaws of the Eddy Dissipation Model which simulates the combustion reaction.

Between the end of the fuel grain and the beginning of the convergent part of the nozzle there is another step. In this point the fuel accumulates enhancing the combustion. The quick deceleration of the flow combined with the turbulence creates another flameholder and promotes the mixing of the reactants. The inner part of the motor is colder since there is an excess of oxidizer. The absence of a mixing device like a diaphragm or a mixer makes a complete combustion impossible to achieve [12]. This trend is highlighted by the plots of the \( N_2O \) and \( N_2 \) mass fractions of figures 5.7 and 5.8.

The liquid oxidizer strikes the frontal part of the grain while evaporating and expanding. The flame is closer to the chamber walls but the flow is faster so the fuel is stripped away from the grain. The temperature in this region is slightly lower than on the rest of the burning surface. However this is true only for the surface hit by the injectors. If the contour is taken on a plane perpendicular to the one if figure 5.7, the mass fraction profile near the wall is slightly different, as shown in figure 5.9. Since the oxidizer stream is swirling it doesn’t impact homogeneously with the grain, thus resulting in a different combustion behaviour, dependent on the angular position with respect to the plate. This was experimentally confirmed, as shown in figure 5.10, which is a photograph of the inside of the combustion chamber, seen from the injectors, after a burn shorter than 2 seconds.

The excess of oxidizer in the internal part of the combustion chamber is also highlighted by the streamlines of the flow. If they are plotted from an external injector to the nozzle (figure 5.11), it can be seen that the rotation given by the swirl pushes the oxidizer closer to the walls feeding the reaction. The streamline from the internal injector (figure 5.12), on the other hand, never deviates from a straight trajectory and the flow exits the motor almost undisturbed. The actual benefit provided by the central orifice to the combustion should therefore be investigated to improve the design of the system.

The accumulation of Nitrous is also underlined by a plot of the life time of the droplets before evaporation, figure 5.13. The internal liquid parcels are more likely to evaporate after a longer residence in the chamber, because the core of the flow is colder and more oxidizer-rich. The figure gives also a glance on the swirling motion of the fluid.
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Figure 5.3: Test 5 Pressure

Figure 5.4: Test 5 Temperature

Figure 5.5: Damaged liner after Test 3
5.2. TEST 5

Figure 5.6: Burning DHX-200 Aurora motor

Figure 5.7: Test 5 $N_2O$ Mass Fraction

Figure 5.8: Test 5 $N_2$ Mass Fraction
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Figure 5.9: Test 5 $N_2O$ Mass Fraction on the orthogonal plane

Figure 5.10: Fuel Grain burn pattern
5.2. TEST 5

Figure 5.11: External injector velocity streamline

Figure 5.12: Central injector velocity streamline

Figure 5.13: External injector velocity streamline
5.3 Test 6

The results for Test 6 resemble the previous CFD simulation. The chamber pressure predicted by Matlab at $t_b = 1.5 \, s$ is 25.8 bar, while the experimental measure is $\simeq 25.5 \, \text{bar}$. Ansys CFX estimates a pressure of 26 bar, which is 101.96 % of the real value. Unlike Test 5, in this scenario the mass flow rate is higher and the volume is smaller, but since the Matlab plot of this test resembles closely the experimental data, the initial values for the simulation are also more accurate. This result underlines the importance of a correct tuning of the mathematical models to fit the experimental measurements.

Figure 5.14 is the temperature contour inside the combustion chamber. It is almost identical to the plot of the previous test, only the values slightly change. This is a demonstration of the solidity of the models adopted and the reproducibility of the numerical experiments if the boundary conditions are coherently changed.

The fuel is injected from the wall already decomposed. Figure 5.15 is the contour of the Ethylene mass fraction. The oxidizer mass pushes the fuel towards the nozzle, that suctions the flow. As already stated, this plot shows that the reactants accumulate at the beginning of the convergent part of the nozzle. Only a small amount of fuel flows in the precombustion chamber, but nevertheless the temperature increases. This phenomenon is explained by the recirculation of the hot gases induced by the turbulence. The products accumulate and get warmer; the wall is also modeled as adiabatic so there is no cooling of the flow by heat dissipation. The adiabatic hypothesis is valid for a burn time as short as 1.5 seconds. A closer look on the vorticity in the precombustion chamber is given in figure 5.16, where the plot of the velocity vectors in the plane highlights the hot eddies.
5.3. TEST 6

Figure 5.15: Test 6 $C_2H_4$ Mass Fraction

Figure 5.16: Flow recirculation in the precombustion chamber
5.4 Axial Injection

What if the oxidizer stream wasn’t swirled but axial? Simulations with a null angle of injection have been performed, leading to interesting results. Some plots are provided in figures from 5.17 to 5.20. The axial flow distributes the oxidizer more uniformly in the chamber, however Nitrous still accumulates in the core of the motor. The heat still rises in the precombustion chamber, this time to an higher value since the turbulence provided by the liquid stream is less accentuated, so the hot gas will more likely remain in the region.

If these results are compared with the tests results it emerges that the introduction of a swirl angle of 15 degrees doesn’t drastically increase the performances. It should be questioned whether the use of a plate harder to manufacture is actually essential for the performance of the system. Another solution could be increasing the swirl angle, which would increase the turbulence in the precombustion chamber, hence the evaporation of Nitrous Oxide, and could reduce the phenomenon of recirculation that reduces the resistency of the motor case. All these statements, as well as the effect of the introduction of a mixer in the system, will be discussed in a future work through more CFD simulations and experimental tests.

Figure 5.17: Axial injection $N_2O$ Mass Fraction
5.4. AXIAL INJECTION

Figure 5.18: Axial injection $N_2$ Mass Fraction

Figure 5.19: Axial injection Temperature contour

Figure 5.20: Axial injection particles trajectory
Chapter 6

Conclusions

6.1 Research Overview

The thesis consisted in the investigation of the causes of performance lack in the hybrid rocket motor DHX-4 Phoenix.

After gathering the test data, a Matlab simulator has been developed to characterize the variation of the thermodynamical properties of the system during the burn. The program provided a reliable interpolation of the measured experimental curves and served as a baseline for the setup of the CFD.

Every aspect of the flow inside the motor has been examined in depth to find the most reliable models for the numerical analysis. Some hypothesis and approximations had to be made, but every choice had physical sense.

6.2 CFD Results Analysis

The CFD shed some light on the flow field inside the combustion chamber, underlining some weak points of the design:

- The swirl injection isn’t pronounced enough to actually increase the mixing of the reactants. The results obtained with the axial injection simulations almost coincide with the swirled ones.

- The step between the precombustion chamber and the fuel grain induces a recirculation of the flow which increases the temperature of the gas at the beginning of the motor. This vorticity envelops the Nitrous Oxide flow going against the diffusion of the oxidizer and the break-up of the droplets.

- The absence of a recirculation zone at the end of the fuel grain and before the nozzle doesn’t allow for the mixing of the reactants, decreasing the efficiency of the system.

- Nitrous Oxide flowing through the central orifice doesn’t leave the core of the motor and is ejected almost undisturbed from the combustion chamber.
6.3 Design Improvements

From the CFD results some consideration can be made on the design of the system, to increase the performances:

- The precombustion chamber should be longer or with a cross section narrower than the port area, creating a recirculation of the flow on the opposite direction which could allow for a better diffusion of the oxidizer. This should also decrease the accumulation of hot gas in the area, increasing the life of the liner and the motor case.

- The swirl angle should be either increased, otherwise an axial injection could be adopted, since the vorticity proved to be insufficient to increase the oxidizer diffusion.

- A mixing device should be adopted to increase the reactants blending in the combustion chamber, using either a diaphragm or a mixer at the end of the fuel grain. This would change the flame pattern in the convergent part of the nozzle leading to a complete combustion.

- The central orifice could be removed, since the oxidizer accumulates in the core of the chamber. Different injection plate configurations should be tested. In particular a better atomization may be achieved changing the L/d ratio of the orifices.

- The feed system should be improved to reduce the losses hence the effective oxidizer mass flow rate injected in the chamber.

6.4 Research Improvements

More experiments would refine the knowledge of the ballistic properties of the motor. In particular, the coefficients $a$ and $n$ required to calculate the regression rates used in the Matlab simulations should be determined with more precision. More experiments would also decrease the disturbances to the model caused by errors and imprecisions in the measurements and setup of the tests.

With more accurate data, a more accurate CFD model could be developed, leading to a better simulation not only of the internal flow field but also to a better prediction of thermodynamical quantities like pressure and temperature.

Finally, the design improvements suggested in this thesis in order to increase the performance of the motor will be analyzed both with numerical CFD simulations and through more experimental tests. These design modifications concern the injector plate, the precombustion chamber dimensions and the introduction of mixers or diaphragms to increase the turbulence in the flow and the mixing of the reactants.
Appendix A - Injection Configurations

Configuration A

The first version of the injector plate is made with 7 orifices of 2 mm diameter. One of them is in the center of the plate, the other six are equispaced on a circle of radius 6 mm. The external holes are inclined of 15° to swirl of the oxidizer flow.

Figure 6.1: Injector Configuration A

Configuration B

The second version of the injector plate features 13 holes of 1.5 mm diameter. One of them is in the center of the plate, while the other are equispaced in series of six on two circles of different diameters. The smaller one has a radius of 4 mm, the biggest of 7 mm. Again, the external holes are inclined of 15° to swirl the oxidizer flow.

Figure 6.2: Injector Configuration A
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