Simulations of a Sub-scale Liquid Rocket Engine: Transient Heat Transfer in a Real Gas Environment

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Simulations of a Sub-scale Liquid Rocket Engine: 
Transient Heat Transfer in a Real Gas Environment

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# LIST OF SYMBOLS AND ABBREVIATIONS

## ACRONYMS

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<th>Description</th>
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<tr>
<td>2D_AXI</td>
<td>2D-Axisymmetric formulation.</td>
</tr>
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<td>3D_AXI_FLUX</td>
<td>3D-Axisymmetric formulation, with tangential fluxes.</td>
</tr>
<tr>
<td>3D_AXI_SRC</td>
<td>3D-Axisymmetric formulation, with source terms.</td>
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<tr>
<td>AFRL</td>
<td>Air Force Research Laboratory.</td>
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<tr>
<td>CARS</td>
<td>Coherent Anti-Stokes Raman Scattering.</td>
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<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics.</td>
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<td>CPG</td>
<td>Calorically Perfect Gas.</td>
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<tr>
<td>DLR</td>
<td>Deutches Zentrum für Luft- und Raumfahrt = German Aerospace Center.</td>
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<tr>
<td>DNS</td>
<td>Direct Numerical Simulation.</td>
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<tr>
<td>EoS</td>
<td>Equation of State.</td>
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<tr>
<td>FPL</td>
<td>Full Power Level.</td>
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<tr>
<td>GH&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Gaseous Hydrogen.</td>
</tr>
<tr>
<td>GOX</td>
<td>Gaseous Oxygen.</td>
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<tr>
<td>IWRCM</td>
<td>International Workshop on Rocket Combustion Modeling.</td>
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<td>LES</td>
<td>Large Eddy Simulation.</td>
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<td>LOX</td>
<td>Liquid Oxygen.</td>
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<tr>
<td>LRE</td>
<td>Liquid Rocket Engine.</td>
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<tr>
<td>MPI</td>
<td>Message Passing Interface.</td>
</tr>
<tr>
<td>MPL</td>
<td>Minimum Power Level.</td>
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<tr>
<td>PIV</td>
<td>Particle Image Velocimetry.</td>
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<td>PLIF</td>
<td>Planar Laser Induced Fluorescence.</td>
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<tr>
<td>PR EoS</td>
<td>Peng-Robinson Equation of State.</td>
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<td>RANS</td>
<td>Reynolds-Averaged Navier Stokes.</td>
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<td>RG</td>
<td>Real Gas.</td>
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<tr>
<td>RPL</td>
<td>Rated Power Level.</td>
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<td>SSME</td>
<td>Space Shuttle Main Engine.</td>
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<td>TML</td>
<td>Temporal Mixing Layer.</td>
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<td>TPG</td>
<td>Thermally Perfect Gas.</td>
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CONSTANTS

\( C_\varepsilon \)  
Eddy dissipation coefficient, 0.916.

\( C_\nu \)  
Eddy viscosity coefficient, 0.067.

\( k \)  
Boltzmann’s Constant, \( 1.38065 \times 10^{-23} \text{ J.K}^{-1} \).

\( R_u \)  
Universal Gas Constant, \( 8.31451 \text{ J.mol}^{-1}.\text{K}^{-1} \).

\( S \)  
Sutherland Law Constant, 111 K for air.

GREEK LETTERS

\( \eta \)  
Dipole moment, debyes.

\( \lambda \)  
Thermal conductivity, \( \text{W.(m.K)}^{-1} \).

\( \mu \)  
Dynamic viscosity, \( \text{kg.m}^{-1}.\text{s}^{-1} \).

\( \nu_t \)  
Turbulent (kinematic) viscosity, \( \text{m}^2.\text{s}^{-1} \).

\( \omega \)  
Accentric factor, dimensionless.

\( \Omega_D \)  
Collision integral for mass diffusion computation, dimensionless.

\( \dot{\omega}_k \)  
Reaction rate for species \( k \), \( \text{kg.m}^{-3}.\text{s}^{-1} \).

\( \Omega_v \)  
Collision integral for viscosity computation, dimensionless.

\( \rho \)  
Density, \( \text{kg.m}^{-3} \).

\( \varepsilon \)  
Minimum of the pair-potential energy (well depth), J.

\( \sigma \)  
Surface tension, \( \text{N.m}^{-1} \).

\( \Sigma \)  
Hard-sphere diameter, Å.

\( \tau \)  
Viscous stress, Pa.

SUBSCRIPTS

\( * \)  
Dimensionless value.

\( 0 \)  
Reference value.

\( c \)  
Critical value.

\( f \)  
Value refers to the fuel.

\( \text{ox} \)  
Value refers to the oxidizer.

\( r \)  
Reduced value, that is divided by critical value.
t Turbulent quantity.
x Axial, streamwise quantity, vector component.
y Radial quantity, vector component.

SUPERSCRIP'TS

sgs Subgrid quantity.
0 Low-pressure quantity.
− Spatially filtered quantity, see Eqn. [4]
∼ Resolved (Favre-averaged) quantity on the LES grid.

SYMBOLS

c Speed of sound, m.s$^{-1}$.
$C_v$ Specific heat at constant volume, J.mol$^{-1}$.K$^{-1}$.
Da Damkohler number, dimensionless.
$D_{AB}$ Binary diffusion coefficient between species A and B, m$^2$.s$^{-1}$.
e Massic total energy = massic internal energy + massic kinetic energy, J.kg$^{-1}$.
h Massic total enthalpy, J.kg$^{-1}$.
h$_k$ Massic enthalpy of formation of species k, J.kg$^{-1}$.
k$^{sgs}$ Subgrid kinetic energy, J.kg$^{-1}$.
M Molecular Weight, g.mol$^{-1}$.
$m$ Mass flowrate, kg.s$^{-1}$.
MR Mixture ratio = $\frac{\dot{m}_{ox}}{\dot{m}_f}$, dimensionless.
p Pressure, Pa.
Pr Prandtl number, dimensionless.
q Heat flux, W.m$^{-2}$.
$q^{sgs}$ Subgrid heat flux, W.m$^{-2}$.
We Weber number = $\frac{\rho_f(V_f-V_{ox})^2D_{ox}}{\sigma_{ox}}$, dimensionless.
Sc Schmidt number, dimensionless.
T Temperature, K.
\( u \) Velocity, m.s\(^{-1}\).

\( V \) Mean velocity, m.s\(^{-1}\).

\( v \) Molar Volume, m\(^3\).mol\(^{-1}\).

\( \mathcal{V}_{i,k} \) Diffusion velocity of species \( k \) in the direction \( i \), m.s\(^{-1}\).

\( \mathbf{VR} \) Velocity ratio = \( \frac{V_{\text{fuel}}}{V_{\text{ox}}} \), dimensionless.

\( J \) Momentum (flux) ratio = \( \frac{(\rho V^2)}{(\rho V^2)_{\text{ox}}} \), dimensionless.

\( x \) Axial, streamwise coordinate, m.

\( X_k \) Mole fraction of species \( k \), dimensionless.

\( y \) Radial coordinate, m.

\( Y_k \) Mass fraction of species \( k \), dimensionless.

\( Z \) Compressibility, dimensionless.

\( R \) Specific gas constant, J.kg\(^{-1}\).K\(^{-1}\).
SUMMARY

The prediction of transient phenomena inside Liquid Rocket Engines (LREs) has not been feasible until now because of the many challenges posed by the operating conditions inside the combustion chamber. Especially, the departure from ideal gas because of the cryogenic injection in a high-pressure chamber is one of the major hurdles for such simulations. In order to begin addressing these issues, a real-gas model has been implemented in a massively parallel flow solver. This solver is capable of performing Large-Eddy Simulations (LES) in geometrical configurations ranging from an axisymmetric slice to a 3D slice up to a full 3D combustor. We present here the results from an investigation of unsteady combustion inside a small-scale, multi-injectors LRE. Both thermally perfect gas (TPG) and real gas (RG) approaches are evaluated for this LOX-GH$_2$ system. The Peng-Robinson cubic equation of state (PR EoS) is used to account for real gas effects associated with the injection of cryogenic oxygen. Realistic transport properties are computed but simplified chemistry is used in order to achieve a reasonable turnaround time. Results show the importance of the unsteady dynamics of the flow, especially the interaction between the different injectors. The role of the equation of state is assessed and the real gas model, despite a limited zone of application, seems to have a strong influence on the overall chamber behavior. Although several features in the simulated results agree well with past experimental observations, the prediction of heat flux using a simplified flux boundary condition is not completely satisfactory. This work also reviews in details the state of our knowledge on supercritical combustion in a coaxial injector configuration, stressing issues where numerical modeling could provide new insights. However, many developments and improvements are required before an LES modeling of such a flow is both feasible and valid. We finally propose a comprehensive roadmap towards the completion of this goal and the possible use of CFD as a design tool for a modern liquid rocket engine.
CHAPTER I

INTRODUCTION

1.1 Historical perspective

From the early experimentations of Goddard in the 1920’s to the latest launch vehicles designed for the Vision for Space Exploration in the new millenium, the liquid rocket engines have been used for many different applications. First, they helped to build sounding rockets that were exploring and measuring our atmosphere. Then they participated in the development of jet aircrafts around World War II and of early tactical missiles after the war. But it is really with the beginning of the Space Age that liquid rocket engines started to show their true merits. Sutton lists the following features and performance characteristics for LREs:

- High specific impulse
- Wide range of thrust
- Easy to restart, pulse and reuse
- Suitable for attitude and velocity changes
- Can be fully tested without flying
- High reliability
- High propellant mass fraction
- Environmentally friendly

Of course all these features were not available in Goddard’s early rockets but have appeared gradually with time. One of the most significant historical trend was the tremendous increase in thrust needed for space exploration, improving from the few Newtons of thrust of the early engines to the millions of Newtons (1.8 MN for the Space Shuttle Main Engine
of the latest vehicles. Along with this increase in thrust, the pressure inside the combustion chamber had also to grow dramatically, allowing engine size to remain reasonable and improving specific impulse.

With the advent of oxygen-hydrogen as the bipropellant of choice, very high densities were achieved through high pressures and very low temperatures. Thanks to these very low temperatures, usually around 100 K, the term cryogenic is often used to describe the engine and the propellants, although they do not necessarily satisfy the National Institute of Standards and Technology exact limit of 93.15 K for cryogenic regime. These high densities could mean a reduced storage volume for the propellants. Since LOX-GH₂ systems are mostly used in the Earth atmosphere, the drag reduction due to smaller tanks could have been significant. However, basic analysis of the launch vehicle design reveals that it is more beneficial to use low-pressure, lightweight but voluminous tanks for turbopump feed systems than high-pressure, heavy tanks [149]. Thus for our systems of interest, the ever increasing combustion chamber pressure is only due the advance of turbopumps technology.

However, two main drawbacks arise with this rise in operating pressure. First of all, as shown on Fig. 1, there is almost a linear growth in wall heat transfer as the pressure in the chamber increases. There we have plotted the chamber pressure and the maximum observed wall heat flux (usually at the throat) for various large liquid rocket engines that use oxygen and hydrogen as propellants. It appears that the wall peak heat flux \( Q_{w,max} \) scales as \( p_{chamber}^{0.8} \) which means cooling and material strength determine how high the chamber pressure can go. Significant progress (regenerative cooling, film cooling, ceramics, new alloys) has been achieved in these fields over the years, but they remain the limiting factors with respect to chamber pressure.

Second, operating pressures inside the combustion chamber have increased above the critical pressure of most, if not all, propellant combinations that are typically used for space propulsion. Combined with the cryogenic temperatures in the feeding system, this means that the propellants will most likely not behave like pure gases or pure liquids but rather like complex fluids. For example, the oxygen is in a compressible liquid state from the tanks to the chamber through the pumps. Then it undergoes a phase transition towards
Figure 1: Adapted from Pempie\cite{112}, throat peak heat flux trend for large liquid rocket engine with oxygen and hydrogen as propellants. Note that the x-axis represent the chamber pressure raised to the power 0.8 to clearly show the proportionality between the wall heat flux and the chamber pressure. For the \textit{SSME}, MPL means Minimum Power Level, RPL means Rated Power Level and FPL means Full Power Level. means Minimum supercritical gas as it mixes and burns with hydrogen. More details on this complex process will be given later in this work. While this does not necessarily mean that engine performance and stability has decreased with the rise in pressure, it certainly makes the physical understanding of the various processes inside the combustion chamber more difficult. For example, as covered later on, the supercritical regime seems to be beneficial to combustion stability. But the supercritical conditions inside realistic rocket engines are difficult to reproduce in laboratories and usually do not allow for extensive measurements with current technologies.

Thus, despite many early breakthroughs during the golden age of the Space Race (1957-1975), the detailed understanding needed to push further the design of rocket chambers is still somewhat lacking. But, since the early 90’s, a renewed interest has risen with nations like Europe, China and Japan also leading the way instead of just the United States or Russia. The state-of-the-art in the design of liquid rocket thrust chambers has recently been compiled in a reference volume \cite{165}, which highlights the current challenges involved with
the resolution of the detailed physiochemical processes inside a modern liquid fueled rocket engine. It has to be noted that this progress has been possible through cooperative work, either inside individual countries \[ \text{[33]} \] or internationally \[ \text{[107]} \]. An example of this important international collaboration is the International Workshop on Rocket Combustion Modeling (IWRCM) that has taken place every other year since 2000.

\subsection*{1.2 Overview of a typical liquid rocket engine}

A typical modern liquid rocket engine designed for space launch consists of tens of components, from the tanks to the feeding lines, from the turbopumps to the exhaust and pressurization systems, from the regenerative cooling system to the gas turbines, from the exhaust nozzle to the combustion chamber. From a system point of view, the interactions between these different components is modeled considering each entity as a black box. For the combustion chamber, basic thermodynamics coupled with some assumptions on the quality of the combustion yields relatively accurate estimates of quantities such as the specific impulse, the thrust or the amount of heat that needs to be extracted by the cooling system. The modest objective of this work is to establish the guidelines for the use of numerical simulations as a future design tool for liquid rocket engines and will focus almost exclusively on the understanding and the modeling of the physical processes in the combustion chamber. As already known by system designers and as we will show, it is difficult to isolate the combustion chamber from the regenerative cooling system as they are closely coupled. So, keeping in mind the importance of the cooling components, we will take a closer look at the combustion chamber of a liquid rocket engine using the bipropellant oxygen-hydrogen.

In the case of a staged-combustion cycle, the propellants first go through a gas generator where the fuel-to-oxidizer ratio is far from stoichiometry. This usually leads to the injection of supercritical gaseous propellants in the chamber with very different mixing and combustion characteristics compared to the other four main rocket cycles (gas generator, combustion tap-off, expander, coolant bleed). Although not our main interest in this work, gaseous
oxygen-gaseous hydrogen (GOX-GH$_2$) injection in rocket engines has been extensively investigated experimentally (see the work done at Pennsylvania State University [82, 109, 132]) and its modeling should also be studied in parallel with our solver. For the other engine cycles, the likeliest scenario is that the hydrogen enters the chamber in a supercritical gaseous state after having cooled the chamber walls while the oxygen is injected straight from the turbopump in a compressible liquid state. The most common solution to mix the two propellants is the shear coaxial injector because of its technological simplicity. A typical large liquid rocket engine will have an injector plate made of hundreds of single elements and thus the simplicity and reliability of each component is crucial. Also, shear coaxial injectors are naturally characterized by a good chamber compatibility and a good combustion stability. However, as the dynamics of the swirl coaxial injectors are better understood, such technology is gaining in popularity because of its potential higher performance[151]. In fact, they combine the benefits of two families of injectors, the pressure swirl atomizers and the airblast atomizers. Thus, they are especially effective for liquid-liquid injection. For example, they are part of the original design of the Japanese engines H2-A and H2-B but are also in use in the current version of the RL-10 engine by Pratt & Whitney Rocketdyne as well as in several Russian engines.

After injection, the combustion chamber remains cylindrical for as long as it is necessary to get complete combustion and thus convert the maximum chemical energy of the reactants. Once this is achieved, a convergent-divergent nozzle accelerates the flow to achieve the best combination of specific impulse and thrust. The main constraints for the design of the nozzle are:

- Generate a uniform axial flow at the nozzle exit to prevent divergence losses
- Prevent boundary layer separations
- Remain as short as possible to reduce weight

These constraints are critical for the engine performance and represent unique fields of research. However, the impact of nozzle design on the combustion processes inside the chamber are limited and an accurate nozzle geometry is not critical when modeling the
Thus, although we will take a look at the heat transfer through a typical nozzle walls, the main focus of this work will be on the combustion of cryogenic propellants injected through a shear coaxial injector in a high pressure cylindrical combustion chamber.

### 1.3 Previous work

Since the focus of this work is on modeling modern liquid rocket engines, we will limit our literature review to experimental and numerical investigations of coaxial, reacting injection systems under large pressure conditions. We could have chosen to include swirl coaxial injectors in our study, as both technologies appear relevant in today’s engines (see previous section), but we choose not to add another level of complexity and to focus on shear coaxial injectors. This choice all but eliminates several fields of investigation.

First, although of great importance for the validation of our flow solver, the very large literature on single jet injection into a subcritical or supercritical environment will be almost entirely avoided. For additional details, we point the reader to the recent work of Chehroudi et al. [17, 18, 19] for experimental studies and Gokalp et al. [44] for numerical studies. Even the recent work of Davis et al. [30, 29, 28] or the review of the joint effort by the DLR and the AFRL [107] on supercritical coaxial injection will not be considered at this time. We also will not an in-depth review of the numerous publications on temporal mixing layers under supercritical conditions. We will only consider their formulations and models when needed, but we will not detail the findings of their simulations [7]. We do acknowledge the need to review these works as they constitute a large database of validation data. The validation and optimization of our flow solver for supercritical mixing will be a necessary milestone to meet our objective to model modern liquid rocket engine. Additional details and guidelines will be given in the concluding chapter. Because we focus on modern liquid rocket engines, we are not really interested in the study of the atomization process because of the large pressures cited in the previous sections. Until the middle of last decade, most of the experimental investigations on liquid rocket engine injection focused on cold flow atomization, with fluids such as liquid water or liquid nitrogen. This field of research raises
many interesting and challenging issues but the physical processes at stake are significantly different from supercritical mixing. A review of earlier work has been compiled by Ferraro et al. 

More recently, focus has shifted towards an accurate determination of the boundary between the two-phase and the single-phase regime. To this end, not only liquid water and liquid nitrogen are being investigated, but also actual propellants such as the couple LOX/\text{GH}_2. While the flows with water or nitrogen are useful at low pressures with proper scaling (in order to achieve realistic Reynolds and Weber numbers), the use of actual propellants becomes necessary as we approach the critical conditions and each fluid behaves differently from the others. Finally, as stated earlier, we focus on gas-liquid injection and will only list works on gas-gas injection for further reference and possible comparison.

For reacting, coaxial flows at high pressures, characteristic of actual rocket engines conditions, the bulk of the experimental effort started about ten years ago. The principal leaders of these investigations were:

- The group led by Santoro at Pennsylvania State University. They have concurrently directed investigations on GOX/\text{GH}_2 combustion and LOX/\text{GH}_2 combustion, although most studies were not under supercritical conditions.

- The group led by Mayer at the DLR. Their initial effort, on collaboration with the Japanese Space Agency, pioneered the visualization of supercritical mixing and combustion. The latest studies focus on the acquisition of more quantitative data for both mixing and burning under supercritical conditions.

- The group led by Candel at "Ecole Centrale de Paris" focuses mostly on the supercritical combustion and especially the stabilization of the flame: how it is anchored, the influence of the injector geometry and the understanding and control of combustion instabilities.

We have compiled important data about these studies in Tables 1.3 and 1.3. These tables present an overview of the range of conditions investigated until today and the amount of
measurement and visualization available. In fact, we can see that mostly qualitative data have been obtained so far. The experimental community has recognized the need for better hot-fire data for CFD validation and several programs are currently underway. However, this is a long process as the working environment for simulating realistic liquid rocket engines conditions is difficult to setup in a typical university laboratory. The difficulty of combining in the chamber high pressures and large heat release often means that only one of these two features is experimentally simulated at one time. Kenny et al. [71] have started an exhaustive investigation on scaling and throttling of full-scale engines by focusing only on cold flow experiments while operating their chamber at about 83 bar (1200 psi). On the other hand, Schumaker et al. [136] are focusing their study on gaseous coaxial combustion at moderate pressures (10 bar), with additional measurements at higher pressures planned for the future. Currently, velocity and concentration profiles are only available for moderate pressure configurations such as early studies from Pennsylvania State University [39] and atmospheric pressure setups, e.g. Takahashi et al. [150]. Recently, we have observed a diversification of the experimental (and numerical) investigations towards propellants other than the oxygen/hydrogen combination. While some studies have revisited the work done decades ago on kerosene-fueled rocket engine, the main effort now is turned towards the use of methane with liquid oxygen. With several programs underway because of the future evolution of the main launch vehicles in the United States (Crew Exploration Vehicle for NASA’s Constellation Project) and in Europe (collaboration Russia-EU on the Volga project), the number of investigations on this topic is significant. Some of these studies (gas-gas low-pressure combustion and methane combustion) are also listed in Tables 1.3 and 1.3. Additionally, there has been a recent focus on the heat flux measurements in typical LRE configurations. We can cite two main reasons for this effort. First is the importance of the heat transfer for the design of the cooling system and for the life cycle of the combustion chamber. Second is the need for experimental data to validate the increasing number of attempts at modeling the combustion inside a rocket chamber, the wall heat flux being an easily obtainable, easily comparable physical quantity. However, most (if not all) experimental data currently available suffer from at least one of the following shortcomings:
• Non-realistic configuration, especially the ratio $\frac{D_{\text{chamber}}}{D_{\text{injector}}}$, which defines the size of the combustion chamber with respect to the size of the injector.

• Lack of accurate and easy to implement boundary conditions for CFD.

• Failure to measure additional quantitative flowfield data needed to validate heat transfer results. Because of the very challenging conditions inside the rocket chamber, it is difficult to make direct measurements and so far the best information available are the length of the liquid core or the location of the onset of jet instabilities[27].

To quote Smith et al.[142] in 2004, ”validation of numerical models with high pressure, reacting LOx/H2 experimental data with well defined boundary conditions are yet to be realized”. We believe this statement still holds today.

Improvement in measurements methods such as Coherent Anti-Stokes Raman Scattering (CARS) [143 48], Planar Laser Induced Fluorescence (PLIF) [154 141], Planar Laser Induced Exciplex Fluorescence[116] for scalars or Particle Image Velocimetry (PIV) [41] will probably provide useful data for the validation of numerical models in the near-future. However, currently, the reliability and variability of the measurements in such a difficult environment prevent definitive analysis. An example of what is possible when these techniques are used in conjunction is given by Gicquel et al.[43]: the cross-correlations between velocity components, temperature and species concentrations are critical for the validation of numerical simulations. In general, the ability to use two visualization techniques at the same time is very useful[129]: comparison of chemiluminescence and OH-PLIF gives more insight on the heat release regions while superposition of laser-light-scattering and shadowgraph imaging allows to distinguish the liquid phase in the flow.

Before we take a closer look at supercritical combustion inside a liquid rocket engine, we should characterize precisely our coaxial injector. Figure 2 is a schematic of a recessed, tapered coaxial injector and defines the main variables of our problem. The geometry is set by the three diameters $D_1$, $D_2$ and $D_3$, which correspond respectively to the inner diameter of the inner pipe, the outer diameter of the inner pipe and the inner diameter of the outer annulus. Also, the injector sometimes includes a recess, which means the exit planes for the
inner pipe and the outer annulus are different. Finally, the inner pipe is sometimes tapered by an angle \( \alpha \), which introduces another characteristic diameter \( D_{10} \) for the inner pipe. Along the centerline of the injector, we find the oxidizer, referred to with the subscript \( \text{ox} \). Coming from the annular pipe around the oxygen pipe is the hydrogen which acts as fuel and thus its related variables will be labeled with the subscript \( \text{f} \). The physical quantities of interest are the flowrate \( \dot{m} \), the mean injection velocity \( V \), the injection density \( \rho \), the dynamic viscosity \( \mu \), the surface tension \( \sigma \), the injection temperature \( T \) and the chamber pressure \( p_{\text{chamber}} \). Five dimensionless numbers are widely considered\[37, 80, 157\] as the main parameters for characterizing the injection conditions in a typical liquid rocket engine:

- **Mixture ratio**: \( \text{MR} = \frac{\dot{m}_{\text{ox}}}{\dot{m}_{\text{f}}} \)
- **Velocity ratio**: \( \text{VR} = \frac{V_{\text{fuel}}}{V_{\text{ox}}} \)
- **Momentum (flux) ratio**: \( J = \frac{(\rho V^2)_{\text{f}}}{(\rho V^2)_{\text{ox}}} \)
- **Reynolds number for the oxidizer**: \( \text{Re}_{\text{ox}} = \frac{\rho_{\text{ox}} V_{\text{ox}} D_{1}}{\mu_{\text{ox}}} \)
- **Weber number between the two flows**: \( \text{We} = \frac{\rho_{\text{f}} (V_{\text{f}} - V_{\text{ox}})^2 D_{1}}{\Sigma_{\text{ox}}} \)

Other quantities such as the Ohnesorge number\[71\], the viscosity ratio\[36\], the density ratio\[121\] can also be considered for more details about the atomization regime. Of course, in a typical liquid rocket engine, the Reynolds number is very large \((Re > 1 \times 10^5)\) and...
the flow is turbulent. Thus, when looking at the combustion in a typical liquid rocket engine, we also need to consider the Damköhler $\text{Da}$ number as an influential dimensionless parameter:

$$\text{Da} = \frac{\text{Turbulent time scale}}{\text{Chemical time scale}}$$

(1)

As well as having high Reynolds numbers, flows in typical liquid rocket engine usually have high Weber numbers, and thus the breakup of the oxygen jet belongs to the atomization regime\[71\]. This has been confirmed by numerous studies of cold flow atomization but with combustion and high pressure, the exact picture is known to be different. Over the last decade, it has been reliably established\[164 88\] that the different physical processes that control combustion in a typical liquid rocket engine, namely atomization, mixing, vaporization and ignition, have a very different behavior depending on the value of the chamber pressure with respect to the critical pressure of the propellants. However, the actual details and the influence of other parameters such as momentum or velocity ratio have yet to be assessed. We will now present an overview of what we know about a supercritical, coaxial flame before discussing some issues that will be critical for our modeling effort.
<table>
<thead>
<tr>
<th>Reference</th>
<th>Injector dimensions (mm)</th>
<th>Recess (mm)</th>
<th>Taper</th>
<th>Chamber size (Dch/D3)</th>
<th>Chamber Shape</th>
<th>Propellants</th>
<th>Film cooling</th>
<th>Measurements and Visualization</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSME preburner [147]</td>
<td>2.26–2.90–4.98</td>
<td>2.54</td>
<td>Yes</td>
<td>N/A</td>
<td>N/A</td>
<td>LOX-GH2</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Ferraro et al. [37, 38]</td>
<td>2.26–3.76–5.03</td>
<td>2.54</td>
<td>Both</td>
<td>4.13</td>
<td>Round sq.</td>
<td>LOX-GH2</td>
<td>No</td>
<td>PDPA</td>
</tr>
<tr>
<td>Schumaker et al. [136]</td>
<td>3.00–4.78–7.52</td>
<td>No</td>
<td>No</td>
<td>6.75</td>
<td>Round</td>
<td>LOX-GH2</td>
<td>No</td>
<td>HSP, OH* Ch</td>
</tr>
<tr>
<td>Lux et al. [80]</td>
<td>4.00–4.60–6.96</td>
<td>No</td>
<td>No</td>
<td>7.19</td>
<td>Round</td>
<td>LOX-GCH4</td>
<td>GH2</td>
<td>HSP, OH* Ch, Sh</td>
</tr>
<tr>
<td>Woodward et al. [161]</td>
<td>4.39–5.16–6.52</td>
<td>No</td>
<td>No</td>
<td>8.07</td>
<td>Round sq.</td>
<td>LOX-GH2</td>
<td>No</td>
<td>HSP, BL, Sh</td>
</tr>
<tr>
<td>Boniface et al. [8]</td>
<td>3.43–4.19–7.11</td>
<td>No</td>
<td>No</td>
<td>7.17</td>
<td>Round sq.</td>
<td>LOX-GH2</td>
<td>No</td>
<td>Co-flow</td>
</tr>
<tr>
<td>Smith et al. [143]</td>
<td>4.00–4.32–6.5</td>
<td>No</td>
<td>No</td>
<td>7.69</td>
<td>Round</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>CARS, OH, Sh</td>
</tr>
<tr>
<td>Smith et al. [142]</td>
<td>4.00–4.32–5.8</td>
<td>No</td>
<td>No</td>
<td>8.62</td>
<td>Round</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>CARS, OH, Sh</td>
</tr>
<tr>
<td>Candel et al. [12]</td>
<td>5.00–5.60–12.2</td>
<td>No</td>
<td>Yes</td>
<td>4.1</td>
<td>Square</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>BL, LLS, CARS, PLIF, OH* Ch</td>
</tr>
<tr>
<td>Case RCM-2 [64]</td>
<td>5.00–5.60–10.0</td>
<td>No</td>
<td>Yes (8°)</td>
<td>5</td>
<td>Square</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>Sp, OH* Ch, BL</td>
</tr>
<tr>
<td>Juniper et al. [67]</td>
<td>5.00–5.60–10.0</td>
<td>No</td>
<td>Yes (8°)</td>
<td>5</td>
<td>Square</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>Sp, OH* Ch, OH PLIF</td>
</tr>
<tr>
<td>Singla et al. [141]</td>
<td>5.00–5.60–10.0</td>
<td>No</td>
<td>Yes (8°)</td>
<td>5</td>
<td>Square</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>HSP, BL, CARS, PDA</td>
</tr>
<tr>
<td>Salguès et al. [120]</td>
<td>3.43–4.19–5.18</td>
<td>No</td>
<td>No</td>
<td>9.8</td>
<td>Square</td>
<td>LOX-GCH4</td>
<td>GN2</td>
<td>Sh, LLS, PLIF, OH* Ch</td>
</tr>
<tr>
<td>Habiballah et al. [50]</td>
<td>5.00–5.60–10.0</td>
<td>No</td>
<td>Yes (8°)</td>
<td>5</td>
<td>Square</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>HSP, BL, CARS, PDA</td>
</tr>
<tr>
<td>Shipton et al. [159]</td>
<td>7.75–9.53–12.7</td>
<td>No</td>
<td>No</td>
<td>4</td>
<td>Square</td>
<td>GOX-GH2</td>
<td>GN2</td>
<td>LDV, Sp</td>
</tr>
<tr>
<td>Smith et al. [135]</td>
<td>7.75–9.53–10.74</td>
<td>No</td>
<td>No</td>
<td>4.73</td>
<td>Square</td>
<td>GOX-GH2</td>
<td>GN2</td>
<td>OH PLIF</td>
</tr>
<tr>
<td>Conley et al. [27]</td>
<td>1.20–2.20–2.687</td>
<td>No</td>
<td>No</td>
<td>9.30</td>
<td>Round sq.</td>
<td>GOX-GH2</td>
<td>No</td>
<td>HF, BE</td>
</tr>
<tr>
<td>Ivancic et al. [62, 85]</td>
<td>4.00–4.60–6.50</td>
<td>No</td>
<td>No</td>
<td>7.69</td>
<td>Round</td>
<td>LOX-GH2</td>
<td>GH2</td>
<td>Sh, OH, H2O Ch</td>
</tr>
<tr>
<td>Pal et al. [109, 63]</td>
<td>5.26–6.30–7.49</td>
<td>0.43</td>
<td>No</td>
<td>5.07</td>
<td>Round</td>
<td>GOX-GH2</td>
<td>No</td>
<td>HT</td>
</tr>
</tbody>
</table>

Table 1. Review of coaxial injector hot-fire investigations under typical liquid rocket engine conditions. For the last column, the following acronyms are used: BL = Backlighting, Sp = Raman Spectroscopy, PLIF = Planar Laser Induced Fluorescence, Sh = Shadowgraph Imaging, LLS = Laser Light-Scattering, CARS = Coherent Anti-Stokes Raman Scattering, PDPA = Phase Doppler Particle Anemometry, LDV = Laser Doppler Velocimetry, HF = Heat Flux, BE = Broadband Emission.
### Table 2: Review of LOX-GH2 coaxial injector hot-fire investigations under typical liquid rocket engine conditions. Flow conditions. Note that for Ref. [142], there is some uncertainty on the operating conditions.

<table>
<thead>
<tr>
<th>Reference</th>
<th>$p_{chamber}$ (bar)</th>
<th>Subcritical Injection Temperature</th>
<th>$\dot{m}_{oxidizer}$ (kg/s)</th>
<th>$We$</th>
<th>$Re_{oxidizer}$</th>
<th>$p$</th>
<th>$Re$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSME preburner [147]</td>
<td>332</td>
<td>Yes</td>
<td>3.45</td>
<td>10</td>
<td>$3.8 \times 10^5$</td>
<td>Supercritical</td>
<td>0.108 for MR = 0.931</td>
</tr>
<tr>
<td>Ferraro et al. [37, 38]</td>
<td>22–55</td>
<td>N/A</td>
<td>2.54</td>
<td>10.4–30.1</td>
<td>$8 \times 10^5$</td>
<td>1–10$^6$–1$\times 10^6$</td>
<td>0.113 for MR = 4.25</td>
</tr>
<tr>
<td>Schumaker et al. [136]</td>
<td>7.5</td>
<td>No (294 K)</td>
<td>N/A</td>
<td>1.5–2.5</td>
<td>N/A</td>
<td>N/A</td>
<td>0.00282 for MR = 2.52</td>
</tr>
<tr>
<td>Woodward et al. [161]</td>
<td>51.7</td>
<td>N/A</td>
<td>22</td>
<td>70</td>
<td>N/A</td>
<td>N/A</td>
<td>0.218 for MR = 4.67</td>
</tr>
<tr>
<td>Woodward et al. [161]</td>
<td>51.7</td>
<td>N/A</td>
<td>50</td>
<td>107</td>
<td>N/A</td>
<td>N/A</td>
<td>0.139 for MR = 3.065</td>
</tr>
<tr>
<td>Woodward et al. [161]</td>
<td>65.5</td>
<td>N/A</td>
<td>50</td>
<td>95</td>
<td>N/A</td>
<td>N/A</td>
<td>0.139 for MR = 2.744</td>
</tr>
<tr>
<td>Boniface et al. [8]</td>
<td>12.2</td>
<td>Yes (122 K)</td>
<td>4.85</td>
<td>68.07</td>
<td>$6.66 \times 10^4$</td>
<td>4.94$\times 10^5$</td>
<td>0.17 for MR = 5.0</td>
</tr>
<tr>
<td>Boniface et al. [8]</td>
<td>12.7</td>
<td>Yes (122 K)</td>
<td>8</td>
<td>70.9</td>
<td>$6.66 \times 10^4$</td>
<td>8.13$\times 10^5$</td>
<td>0.17 for MR = 3.2</td>
</tr>
<tr>
<td>Boniface et al. [8]</td>
<td>29.9</td>
<td>Yes (122 K)</td>
<td>2.01</td>
<td>18.88</td>
<td>$6.42 \times 10^4$</td>
<td>1.94$\times 10^5$</td>
<td>0.17 for MR = 5.0</td>
</tr>
<tr>
<td>Boniface et al. [8]</td>
<td>17.7</td>
<td>Yes (122 K)</td>
<td>3.37</td>
<td>19.01</td>
<td>$6.58 \times 10^4$</td>
<td>3.38$\times 10^5$</td>
<td>0.17 for MR = 5.0</td>
</tr>
<tr>
<td>Smith et al. [143]</td>
<td>59.4</td>
<td>Yes (115.5 K)</td>
<td>3.8 ?</td>
<td>12.1 ?</td>
<td>N/A</td>
<td>Supercritical</td>
<td>0.29 for MR = 4.83</td>
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<tr>
<td>Smith et al. [143]</td>
<td>63.1</td>
<td>Yes (95.7 K)</td>
<td>1.73 ?</td>
<td>11.5 ?</td>
<td>N/A</td>
<td>Supercritical</td>
<td>0.30 for MR = 3.75</td>
</tr>
<tr>
<td>Smith et al. [142]</td>
<td>52–60</td>
<td>Yes (110–130 K)</td>
<td>0.2–20</td>
<td>6–70</td>
<td>N/A</td>
<td>Supercritical</td>
<td>N/A</td>
</tr>
<tr>
<td>Smith et al. [142]</td>
<td>49–51</td>
<td>Yes (110–130 K)</td>
<td>0.09–12</td>
<td>3–40</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Smith et al. [142]</td>
<td>39–41</td>
<td>Yes (110–130 K)</td>
<td>0.08–12</td>
<td>3–35</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Candel et al. [12]</td>
<td>10</td>
<td>Yes (89 K)</td>
<td>14.5</td>
<td>138</td>
<td>N/A</td>
<td>$2.82 \times 10^4$</td>
<td>0.05 for MR = 2.11</td>
</tr>
<tr>
<td>Candel et al. [12]</td>
<td>10</td>
<td>Yes (89 K)</td>
<td>6.55</td>
<td>92.8</td>
<td>N/A</td>
<td>$1.26 \times 10^4$</td>
<td>0.05 for MR = 3.16</td>
</tr>
<tr>
<td>Candel et al. [12]</td>
<td>10</td>
<td>Yes (89 K)</td>
<td>4.48</td>
<td>30.7</td>
<td>$1.04 \times 10^4$</td>
<td>Supercritical</td>
<td>0.105 for MR = 2.5</td>
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<tr>
<td>Juniper et al. [67]</td>
<td>70</td>
<td>Yes (80 K)</td>
<td>11</td>
<td>47.5</td>
<td>$1.34 \times 10^4$</td>
<td>Supercritical</td>
<td>0.10 for MR = 1.6</td>
</tr>
<tr>
<td>Juniper et al. [67]</td>
<td>70</td>
<td>Yes (80 K)</td>
<td>6</td>
<td>37.5</td>
<td>$1.34 \times 10^4$</td>
<td>Supercritical</td>
<td>0.10 for MR = 2.2</td>
</tr>
<tr>
<td>Singla et al. [141]</td>
<td>36</td>
<td>Yes (80 K)</td>
<td>0.645</td>
<td>15.3</td>
<td>N/A</td>
<td>N/A</td>
<td>0.065 for MR = 8.66</td>
</tr>
<tr>
<td>Singla et al. [141]</td>
<td>63</td>
<td>Yes (80 K)</td>
<td>8.91</td>
<td>45</td>
<td>N/A</td>
<td>Supercritical</td>
<td>0.092 for MR = 1.84</td>
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<tr>
<td>Habiballah et al. [50]</td>
<td>60</td>
<td>Yes (83 K)</td>
<td>16.1</td>
<td>58.9</td>
<td>N/A</td>
<td>Supercritical</td>
<td>0.100 for MR = 1.33</td>
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<tr>
<td>Conley et al. [27]</td>
<td>62.1</td>
<td>No (300 K)</td>
<td>0.358</td>
<td>2.44</td>
<td>N/A</td>
<td>Supercritical</td>
<td>0.00158 for MR = 4</td>
</tr>
<tr>
<td>Ivancic et al. [62, 85]</td>
<td>60.0</td>
<td>Yes (127 K)</td>
<td>1.88</td>
<td>12.4</td>
<td>N/A</td>
<td>Supercritical</td>
<td>0.30 for MR = 5</td>
</tr>
</tbody>
</table>
Table 3: Review of other, non-LOX-GH2 coaxial injector hot-fire investigations under typical liquid rocket engine conditions. Flow conditions.

<table>
<thead>
<tr>
<th>Reference</th>
<th>$P_{chamber}$ (bar)</th>
<th>Subcritical Injection Temperature</th>
<th>Momentum ratio</th>
<th>Velocity Ratio</th>
<th>$Re_{oxidizer}$</th>
<th>$We$</th>
<th>$\dot{m}_{oxidizer}$ (kg.s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lux et al.[80]</td>
<td>67.9</td>
<td>Yes (115.9 K)</td>
<td>2.62</td>
<td>6.84</td>
<td>$9.73 \times 10^4$</td>
<td>Supercritical</td>
<td>0.358 for MR = 3.4</td>
</tr>
<tr>
<td>Lux et al.[80]</td>
<td>50.8</td>
<td>Yes (117.8 K)</td>
<td>3.42</td>
<td>9.02</td>
<td>$5.99 \times 10^5$</td>
<td>Supercritical</td>
<td>0.206 for MR = 3.4</td>
</tr>
<tr>
<td>Lux et al.[80]</td>
<td>41.4</td>
<td>Yes (120.7 K)</td>
<td>4.09</td>
<td>10.89</td>
<td>$4.50 \times 10^6$</td>
<td>Supercritical</td>
<td>0.143 for MR = 3.4</td>
</tr>
<tr>
<td>Salgues et al.[129]</td>
<td>39.3</td>
<td>Yes (122 K)</td>
<td>5.84</td>
<td>13.94</td>
<td>N/A</td>
<td>$4.38 \times 10^5$</td>
<td>0.118 for MR = 3</td>
</tr>
<tr>
<td>Foust et al.[39]</td>
<td>12.9</td>
<td>No (297 K)</td>
<td>0.725</td>
<td>3.47</td>
<td>N/A</td>
<td>N/A</td>
<td>0.042 for MR = 4.08</td>
</tr>
<tr>
<td>Santoro et al.[131]</td>
<td>13.1</td>
<td>No (297 K)</td>
<td>5.94</td>
<td>9.92</td>
<td>N/A</td>
<td>N/A</td>
<td>0.045 for MR = 4.09</td>
</tr>
<tr>
<td>Takahashi et al.[150]</td>
<td>1</td>
<td>No (297 K)</td>
<td>1.78</td>
<td>5.0</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Conley et al.[27]</td>
<td>62.1</td>
<td>No (300 K)</td>
<td>0.358</td>
<td>2.44</td>
<td>N/A</td>
<td>N/A</td>
<td>0.001584 for MR = 4</td>
</tr>
<tr>
<td>Pal et al.[109, 63]</td>
<td>54.2</td>
<td>No</td>
<td>3.15</td>
<td>5.10</td>
<td>N/A</td>
<td>N/A</td>
<td>2.86 for MR = 2.73</td>
</tr>
</tbody>
</table>
1.3.1 Coaxial flame structure under supercritical conditions

We consider here a typical single-element coaxial injector in a sub-scale combustion chamber. Figure 3, modified from Candel et al. [14], shows a composite visualization of supercritical combustion downstream of a shear-coaxial injection. The color scale corresponds to a slice of OH* emission and the grayscale to the average backlighting image. The operating conditions correspond to the MASCOTTE case C-60 used as a baseline case for CFD validation at the recent 3rd International Workshop of Rocket Combustion Modeling (Case RCM-2). Numerical values are listed in Tables 1.3 and 1.3. We enumerate the most important regions of the flow and describe the most important physical phenomena in each
region. For more details about some physical processes or for additional information where there is disagreement between theories, the reader will refer to the next section:

1. At the entrance of the combustion chamber, in **region 1**, the oxygen enters as a liquid jet with a finite surface tension since the chamber pressure is above the critical pressure of oxygen and the oxygen injection temperature is below the critical temperature of oxygen.

2. **Region 2** corresponds to the close-up view of the tip of the injector. For the past 10 years, it has been shown that, in supercritical regimes, the flame was anchoring in the small but intense recirculation region downstream of the tip separating the two flows. This does not seem to depend on the geometry of the injector for LOX-GH2 injectors. Whether the injector is recessed, whether the oxygen post is tapered or whether the oxygen post tip is thin or thick, there is no experimental evidence that the flame does not start here. However, it has been recently discovered[114] that the anchor point actually moves around downstream of the tip. The next section provides additional details about this phenomenon. For LOX-GCH4, although current investigations show the same anchoring mechanism, the flame structure appears to slightly vary with the geometry[129]. Thus, there might be regimes where this anchoring does not exist steadily.

3. In **region 3** the flame is the thinnest and also the least intense. The oxygen and the hydrogen that had mixed in the wake of the tip have been burned and the shear layer is too thin to mix more reactants. Burning here occurs as a pure diffusion flame.

4. **Region 4** shows a rather smooth surface of the oxygen jet. In contrast with the picture at subcritical pressures, we cannot see any droplets or ligaments being shed from the jet. However, this does not necessarily mean they cannot exist locally (see the discussion on the mixture supercriticality in the next section), just that they are too small (less than 10 microns in this particular example) to be observed by current visualization techniques[50][87]. Also we can start to distinguish some density gradients inside the oxygen jet. Two phenomena are probably responsible for these
Most likely, it is caused by the diffusion of hydrogen into the oxygen. At such high pressures, the power of dilution of the two species is very strong, even with the oxygen possibly still a liquid\[107\]. Also, the oxygen jet can be heated up by the flame and thus becoming supercritical at the edge of the jet.

5. **Region 5** shows the broadening shell flame around the oxygen jet. However, this broadening is limited at supercritical pressures compared to subcritical pressures. It does not usually exceed half the oxygen jet diameter. For subcritical combustion, this is where the atomization would take place, with burning groups of droplets extending the combustion region further away from the jet. But for supercritical chamber pressures, the oxygen jet only displays small scale wrinkles and disturbances. Close-up, one can see ”stringy or thread-like structures”\[88\] growing at the surface and mixing with the hydrogen flow before they could detach from the jet surface.

6. Further downstream, in **region 6**, it appears that every kind of flame\[140\] or combustion regime\[62\] can occur depending on the flow conditions. Palle et al.\[110\] show that the mass diffusion, thanks to the Soret effect, plays a very important role and some have suggested the presence of partially premixed flames at least for LOX-GCH\(_4\)\[140\]. Supercritical fluids are known powerful solvents and there could be some intense premixing at the edge of the oxygen jet. Ivancic et al.\[62\] show that the turbulent time scales and the chemical time scales cover the whole range of the Borghi’s turbulent combustion diagram\[9\]. Depending on the flow conditions, the shell flame can totally embrace an oxygen jet that remains relatively stable or long wavelength helical instabilities\[88\], especially with recessed injectors\[14\], can grow and force the breakup of the oxygen jet core. The resulting pockets of unburned oxygen react further downstream.

7. **Region 7** shows the recirculation of hot gases because of the large relative size of the chamber with respect to the injector. While intuitively, this configuration with a rapid hydrogen flow expansion seems quite different from the situation in a multi-element injector, these recirculating gases do mimic in a limited way the co-flow that would be
present otherwise. Indeed, some single-element hot-fire testing have been conducted with a real surrounding co-flow, with only limited changes from the freely expanding single-element\cite{8}.

\subsection{1.3.2 Experimental}

The purpose of this section is to give additional details on the physics of supercritical combustion and also to pinpoint some features and issues that are especially critical for the numerical modeling of liquid rocket engines.

The supercritical nature of the mixture of reactants is an interesting issue. This is a point often mentioned when looking at the atomization processes under high-pressure\cite{161}. Even though both reactants can individually enter the chamber in a supercritical state and thus in a single phase whose behavior would be very analog to the one of a gas, the situation is much more complex once they start mixing. Due to the non-linearity of the physical phenomena around the critical point, the resulting multi-component mixture can, for example, display a critical pressure much larger than the critical pressure of any of the individual reactants. This translates into the persistence of surface tension at the interface between the reactants and the possibility of the formation of a multi-phase flow\cite{161}. But even more bizarre situations can arise, with the appearance of multiple critical points or even critical points with a negative pressure\cite{146}. Recently, new theoretical, numerical\cite{146} and experimental\cite{68} methods have been developed to determine more easily and with more accuracy the boundaries of the supercritical state of multi-component mixtures. Although the cost of such computation is still too high to implement it in our simulations, it could be used during post-processing for verifying the validity of our modeling of real gas mixtures.

Woodward et al.\cite{161}, as well as other investigations from Pennsylvania State University, report rather longer LOX cores than what the classical spray processes predict. In particular, these results seem a little bit at odd with other studies such as the ones lead by Candel\cite{12}. According to Boniface et al.\cite{8}, the influence of the large recirculation region created in sub-scale chamber that are too large compared to the size of the injector is very limited. Results from experiments with and without co-flow surrounding the injector seem
to display similar dense LOX core lengths (at least 40 LOX diameter in length). Also, the jet spreading is indeed reduced by the co-flow while the atomization process, in the range of pressure studied (10-20 bar), seems to be dampened. The mixing between the hydrogen and the liquid oxygen appears more efficient with the co-flow (higher Weber number) and leads to a rapid vaporization of the liquid oxygen once the critical temperature is reached. According to Woodward et al. [161], this suggests that the break-up/atomization process would be better modeled by a core fragmentation model [3], even for chamber pressures slightly above the critical pressures of the propellants. An important consequence of these contradicting experiments is that for the classic aerodynamic stripping of the liquid jet, the flow remains axisymmetric over a rather large length whereas the core break-up seems to be driven by helical waves where the axisymmetric assumption is no longer valid. It is difficult to compare all these experiments because of the wide range of operating conditions they cover as seen in Tables 1.3 and 1.3. But we can observe that the various experimental studies conducted in Germany by Mayer and his successors seem to agree with the theory suggested by Woodward et al. [161]. But the question of the real behavior of the flow in a multi-injector configuration remains open, although maybe not for long. In fact, several new facilities have been built to allow the study of such configurations [83, 73, 126].

Another consequence of these chambers with a high contraction ratio is the higher computational cost that they require to be modeled. For RANS simulations, the main issue is that the large recirculation region unnecessarily increases the convergence time needed for the simulation. This is also a problem for LES simulations but the high contraction ratio also implies a very compact grid at the throat if the solver cannot handle multiple grids with hanging nodes.

It seems rather odd that, to our knowledge, no other experimental work has been done for single element coaxial injection with co-flow since the work of Boniface et al. [8]. It would be very interesting to have these same experiments extended to the supercritical regime to see if similar mechanisms still control the mixing and the break-up of the oxygen jet.

While quantitative data such as velocity profiles or turbulence intensities are still missing in order to characterize the flowfield for subcritical injection into supercritical environment,
the investigation of the combustion instabilities in subscale rocket engines have provided more results. For example, Smith et al.\cite{142} show very stable combustion around the critical pressure of oxygen, rather stable combustion at supercritical pressures and unstable combustion for a liquid, i.e. subcritical, oxygen jet. This means that near-critical and supercritical combustions are subject to only limited high frequency instabilities with limited amplitude. These high frequency instabilities correspond to the longitudinal modes of the chamber. Subcritical combustion display also a low frequency (about 40 Hz) instability that is probably linked to the specific injection system. This low frequency instability is mostly axial, and the authors make no mention of any helical instability. However, under similar conditions and in what appears to be the same experimental setup (although the authors are not clear about it), Smith et al.\cite{143} had previously reported the "occurrence of strong LOX jet core oscillations" under supercritical conditions. They specifically mention the LOX core helical instabilities and their influence on the shear layer and combustion zone thickness. It is possible that the onset of these instabilities is sensitive to very small changes in various injection parameters and thus hard to reproduce with consistency. More investigation is definitely needed but the range of parameters to explore is very large and maybe numerical modeling might be able to narrow the scope of such investigation.

While the momentum and velocity ratios have a positive influence on the stability and the quality of the combustion, the chamber pressure has a much larger influence. Also, supercritical jets appear less sensitive to pressure fluctuations than liquid jets and this could play a role in the feedback loop for combustion instabilities. This would explain the fact that Smith et al.\cite{142} observe that the combustion instabilities in supercritical regime never reach large amplitudes. Also, as we already mentioned earlier, the combustion instabilities in multi-element injectors are also under renewed investigations\cite{83, 73, 126}. Finally, Ghosh et al.\cite{42} have reported recently on a possibly new mechanism for the flame-acoustic interaction in LOX-GH2 coaxial injector. However, further investigation under more realistic conditions is needed to confirm the role of what appears to be baroclinic vortex generation.

The characterization of the mixing of the reactants for single injector configurations is
another interesting issue with respect to the modeling of the combustion chamber. For example, Smith et al.\cite{143} are unable to find near-stoichiometric flame temperature in the near-injector region. They argue that although the shear layer between the two flows is a region where mixing is high and combustion is intense, this region is so thin that the measured temperature is quite diluted. They expect much higher temperature further downstream once the mixing is more widespread. These kind of observations could have a huge impact on the choice of the combustion modeling for a numerical simulation. On a related topic, Juniper et al.\cite{66} report that extinction in the injector near-field is highly unlikely because of the very reactive chemistry at work. Since the LOX/GH2 flames appear very resistant to strain rate, the modeling of the extinction phenomena for the study of the steady-state combustion of a single coaxial injector is not a priority. On the other hand, some unsteadiness of the flame anchor point is reported by Singla et al.\cite{141} and this would probably require some detailed chemistry so that an unsteady numerical simulation could capture it. Candel et al.\cite{14} suggest that this unsteadiness is linked to the non-dimensional step height $\Psi$ of the injector lip:

$$\Psi = \frac{\text{Step height}}{\text{Flame thickness}} \quad (2)$$

When the step is relatively thick ($\Psi > 1$), the Damkhler number of the flame does not have much influence on its stability and the anchor point will just hover behind the tip even for very high turbulence, that is very high hydrogen velocities. This is related to the impossible extinction by strain mentioned earlier\cite{66}. However, if the tip is too thin, part of the flame becomes exposed to the high speed hydrogen jet and if the Damköhler number is too small, the flame can be blown off. This is not often seen experimentally for LOX-GH2 systems as flame thicknesses for H$_2$-O$_2$ systems are usually on the order of 200 microns. Even tapered injectors seldom have tips thinner than 300 microns. However, for LOX-GCH4 systems, this situation could arise more often. Further downstream, Ivancic and Mayer\cite{62} have shown that the Kolmogorov length scale grows from about 1 $\mu$m near the injector exit plane to at least 20 $\mu$m downstream of the main reacting zone. Meanwhile, they show that the integral time scale is growing at the same rate along the shear layer, from 20 $\mu$s in the recirculation
region behind the tip to about 1 ms further downstream. This confirms the fact a wide range of combustion regimes are probably occurring in a typical supercritical coaxial flame: the modeling of the combustion will be a difficult challenge.

Also, for cryogenic propellants, the possibility of periodic ice formation\[143, 88\] around the injector, effectively changing the injector geometry, should not be disregarded as it would prevent an accurate modeling of the experience. This ”natural” recess of the injector with respect to the combustion chamber can actually improve the overall performance of such single-element injector[158]. On the other hand, Smith et al.[143] report a high-frequency, periodic lifting of the flame from the injector LOX tip where it usually sits. This phenomena could be due to the ice. It it unlikely that these effects can occur in multiple-injector configurations.

Film cooling of the experimental chamber can have a strong influence on the acoustics[73], the combustion[143] and also the reformation of liquid water near the chamber boundaries[143]. This condensation of water after combustion is an important issue, especially for engines operating at supercritical conditions. Not only would this liquid water be unable to recombine with other molecules in some chain branching reactions[143] but also the water droplets, in the absence of other droplets for supercritical (with respect to oxygen) conditions, could dampen pressure fluctuations and have a stabilizing effect on the combustion[51]. Other studies such as the one by Shastri et al.[138], in gas turbines configurations, have shown the detrimental effects of this multiphase water.

An accurate geometrical representation of the injector is also very important to capture the correct physical behavior of the shear-coaxial injection. The role of recessing[70] or tapering[129] has been demonstrated under moderate, subcritical pressures but their influence is expected to be the same for supercritical operating conditions.

To summarize, it appears that even qualitative understanding is still missing for the supercritical combustion in a shear coaxial configuration. Does the propellants start reacting before the phase transition thanks to the highly diffusive nature of supercritical fluids? Under supercritical and burning conditions, what is the break-up mechanism, if any, for the compressible liquid oxygen jet? Are we really dealing with a diffusion flame or can we also
find premixed flames at some locations? Could we have triple flames structures (a fuel-rich, a
fuel-lean and a diffusion flame front starting from the same location) as in solid propellants?
In which combustion regime occurs the bulk of the heat release? Are the mechanisms at work
to make the flame stable/unstable the same for subcritical and supercritical conditions?
How the geometry of the injector impacts this flame stability? Do the previously mentioned
dimensionless parameters have the same effects on the injector performance at supercritical
pressures? All these questions do not seem to have a definite answer yet and likely will
not get one until both experimental efforts and numerical investigations benefit from each
other. We believe that for the modeling of this problem, Large Eddy Simulation can provide
valuable, additional information compared to RANS. Especially better insight of jet break-
up, combustion instability and flame characterization could help improve our understanding
of the performance of modern liquid rocket engines. Only such improvement can validate
the cost involved in performing LES, a cost that prevents unsteady, 3D simulations of a
multi-injector configuration as of today.

1.3.3 Numerical

Time accurate studies of rocket motor combustion have only recently become feasible due to
the advent of massively parallel computers. In the past, steady state studies [20, 22, 21] have
been numerous, but unsteady simulations have been very rare. Recent unsteady simulations
include the axisymmetric Large Eddy Simulation (LES) studies of supercritical mixing [166],
and the more recent rocket motor studies of single injector configurations [60, 98, 99]. In
these latter studies, the limited size of the domain of interest allowed simulation of LOX
injection under subcritical conditions for which a very high resolution was required due to
the large density gradients. Thus, the three-dimensional (3D) computational domain used
by Oefelein [98, 99] needed around 12 million grid points for a single, small-scale injector.
Since we are interested in modeling a multi-injector sub-scale rocket chamber [121], this
very high resolution appears to be out of question since such computational requirement
would be prohibitive for design studies where many simulations need to be carried out for
parametric analysis. Even more recent works have focused only on the near-field of the
injector. This very limited computational domain (a few centimeters at most) has allowed the use of DNS resolution while looking at the dynamics of a single mixing layer [84, 15, 72].

Past studies do provide some conclusions worth highlighting. The anchoring of the flame to the LOX post tip, observed experimentally by Mayer et al. [89, 86], has been confirmed with the use of the several real gas equation of state and truly subcritical injection. One of the only advantages in modeling an engine under supercritical conditions is that we do not have to worry about liquid particles. Even when the injection is subcritical ($T_{inj} < T_{crit}$ but $P_{inj} > P_{crit}$), experimental evidence by Mayer et al. suggests that no significant liquid atomization occurs and thus a gas phase modeling of the jet with an appropriate equation of state is adequate. However, there has been some attempts to produce a flow solver capable of dealing with multiphase flows. Among numerical approaches, the mixed Eulerian-Lagrangian approach used by Pourouchottamane et al. [119] is quite unique. They attempt to take into account the sharp density gradient around the LOX jet through the computation of a new scalar field, the interface density while keeping track of the secondary atomization through discrete, Lagrangian droplets. However, this method does not seem to have been further investigated.

Finally, for the last couple of years, we have observed a trend towards multiphysics solver for liquid rocket engine simulations. As mentioned before, the heat transfer from the hot gases to the chamber walls is one of the limiting factor in the design of modern liquid rocket engines and it is a measurement easily available through many experiments. Thus having a solver that can model the flow inside the chamber as well as the heat transfer through the walls and even the effect of cooling channels is a major breakthrough and is being developed by several research groups [90, 77].

### 1.3.4 Motivation and objectives

Our long term objective is to be able to model the physical processes that take place inside a liquid rocket engine, which means very high pressures, as well as a wide range of temperatures, from the cryogenic (around 100 K) injection temperature to the very high flame temperature (about 3600 K in a real engine) of the liquid oxygen-gaseous hydrogen
(LOX-GH₂) system. Under such conditions, real gas effects may be significant, especially the trans-critical (transition from subcritical liquid to supercritical fluid) phenomena during LOX injection. The use of species with very different thermo-physical properties also imposes a severe constraint since these properties have to be carefully computed for real gas flows. The current effort is focused on developing a self-consistent methodology that can be used to simulate high-pressure combustion in realistic rocket motors. One of the eventual goals of this effort is to predict unsteady dynamics in such devices, as well as the impact of such unsteadiness on the heat flux to the combustion chamber walls.

Our literature reviews shows that there is definitely a need for more validation of the CFD tools before they become useful to study these physical processes and to help design efforts. In particular, it appears that Large Eddy Simulations, although much more costly than Reynolds-Averaged Navier Stokes simulations, could provide some more insight on specific, transient processes. That is why we think the current trend of joint CFD-experimental investigations should be encouraged and expanded. The coordination of a joint CFD-experimental effort is a very complicated matter and of course the CFD side of such an investigation has also its own shortcomings. If we consider the work of Conley and Segal [27], one of the best and most thorough effort available as of today, we see that several challenges still need to be addressed on the computational side before we can validate our rocket combustion modeling effort:

- Most of the experiments have a sustained firing of only a few seconds. Thus, as shown by Conley et al. [27], the combustion chamber does not have time to reach its thermal equilibrium. This, along with the inherent unsteadiness of the physics inside the chamber, confirms the need for a multi-physics solver that includes the solution of the heat transfer inside the chamber walls. Such complex solvers are already under investigation [90,77]. But this also raises the question of the existence of a steady-state solution which a RANS simulation would try to converge towards.

- In order to preserve the chamber walls, the rocket engine is usually operated under
slightly rich conditions. This means the shear layer will likely grow as much in di-
rection of the centerline as towards the outside. This is another caveat to overwhelm
for an axisymmetric formulation and thus a full 3D simulation is likely also needed
for single injector configuration. And even for sub-scale rocket combustion chamber,
the cost of such a simulation is huge and many speed-up need to be achieved before
attempting it.

- The definition of accurate boundary conditions for the computational effort is still an
issue. There needs to be a consultation between the experimental and the computa-
tional researchers about which boundary conditions should be measured and how they
are measured. For example, for the flame anchoring mechanism, the temperature of
the tip wall is of critical importance but it is a very difficult measurement to perform.
Also, when designing the combustion chamber, there is often a compromise between
the square chamber where optical access is easier and the round chamber which is
easier to model. This leads to square chambers with rounded corners.

For now, we aim at providing the basic framework necessary to perform the simulation
of real rocket engine in the future. The objectives of the current work will follow three
guidelines:

- **Verify a modified 3D code for efficient axisymmetric computations.**

  We just need to make sure that by applying adequate boundary conditions and by
generating a sensible grid, the same general Navier-Stokes three dimensional solver
can be used to efficiently perform simulations of the rocket chamber, with or without
using the axisymmetric assumption. In this study, we will only consider the axisym-
metric assumption but we will look at the influence of the third dimension. A full
3D computation with the actual configuration is beyond our current computational
resources.

- **Apply a real gas framework to demonstrate injection of oxygen under
  subcritical temperature (compressed liquid) and start to investigate the
  importance of such a model.**
Since we are looking at limiting the computational cost of our solver, we want to implement a real gas model that provides a good compromise between accuracy and cost. The Peng-Robinson equation of state fulfills these requirements as well as providing a framework to also compute accurate transport properties that will be critical in the evaluation of the wall heat transfer. However, we will qualitatively and quantitatively compare simulations run with thermally perfect gas model and real gas model in order to estimate how critical this real gas model is. We will especially focus on the extent of the real gas effects and see how the importance of grid resolution on the modeling of the transcritical event.

- **Conduct a preliminary study on the transient heat transfer in a subscale rocket combustion chamber.**

  To the knowledge of the author, no past study has reported on the transient heat transfer of a steady operating liquid rocket engine. We will attempt to gain some insight on this phenomena with a very simple approach inside a real combustion chamber. In particular, we will investigate how it relates to the dynamics of the combustion chamber. In parallel, we will look at more simple problems involving heat transfer between a flow and a solid. We will also introduce the framework for a coupled multi-physics solver that would include the walls into the computational domain.

  Based on these objectives, we will first present the different frameworks available in our flow solver and see how they are implemented. Then we will review our analysis of a multi-injector, sub-scale liquid rocket engine and see what we can learn from it. Finally, we will present some validation cases which are the first steps towards the roadmap we will present at the end of this work. This roadmap will provide a sequential path towards the successful modeling a multi-injector, sub-scale liquid rocket engine.
CHAPTER II

FORMULATION

2.1 Governing Equations for the Fluid Mechanics in Axisymmetric Configurations

In order to maintain computational tractability, we restrict our simulations to axisymmetric configurations. Originally, the 2D-axisymmetric formulation, referred to as the 2D_AXI solver in this work, was used to perform the simulations. In the 2D-axisymmetric framework, additional source terms and special derivatives have to be added in order to artificially create the effects of the third dimension. The governing Navier-Stokes equations then become:

\[
\frac{\partial}{\partial t} \begin{pmatrix}
\rho \\
\rho u_x \\
\rho u_y \\
\rho e \\
\rho Y_k
\end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix}
\rho u_x \\
\rho u_x u_x + p - \tau_{xx} \\
\rho u_x u_y - \tau_{xy} \\
\rho u_x h - u_x \tau_{xx} - u_y \tau_{xy} + q_x \\
\rho u_x Y_k - \rho Y_k V_{x,k}
\end{pmatrix} \\
+ \frac{1}{y} \frac{\partial}{\partial y} \begin{pmatrix}
\rho u_y \\
\rho u_y u_y - \tau_{xy} \\
\rho u_y u_y + p - \tau_{yy} \\
\rho u_y h - u_x \tau_{xy} - u_y \tau_{yy} + q_y \\
\rho u_y Y_k - \rho Y_k V_{y,k}
\end{pmatrix} = \begin{pmatrix}
0 \\
0 \\
- \frac{\tau_y}{y} \\
0 \\
\omega_k
\end{pmatrix}
\]

where \( x \) and \( y \) represent respectively, streamwise and radial coordinates and the subscripts \( x \) and \( y \) denote of course streamwise and radial quantities. Equation 3 neglects any motion in the circumferential direction. Here, \( \rho, u_x, u_y, e \) and \( Y_k \) represent respectively, the mixture density, the axial velocity, the radial velocity, the massic total energy and the mass fraction of species \( k \). Also, \( h \) represents the massic total enthalpy \( h = e + p/\rho \). The species equation has been written for the \( k^{th} \) species, with \( k \) varying between 1 and \( N_S \), the total number of species. Also, \( \tau_{ij} \) represents the viscous stress tensor, \( V_{i,k} \) the diffusion velocity.
of species $k$ in the direction $i$ and $\mathbf{q}_i$ the heat flux vector in the direction $i$. Finally, on the right side of the equation, we note the tangential stress $\tau_\theta$ of the axisymmetric formulation and the chemical source terms $\dot{\omega}_k$ representing the reaction rates of each species $k$.

We later moved to a more flexible solver that was capable of handling full 3D simulations. This was motivated by the possibility to easily extend the thermodynamic framework to more complex geometries. However, we were also faced with a choice of the axisymmetric implementation in this solver. Two solutions were possible:

- A straight port of the 2D AXI framework with 2D-axisymmetric metrics and source terms. This solution, labeled 3D_AXI_SRC, is more computationally efficient.

- Implementation of a more unusual solution involving the computation of the tangential fluxes while applying axisymmetric boundary conditions in the transverse direction. This framework, dubbed here 3D_AXI_FLUX, requires only minimum change to the full 3D solver and is more flexible since it allows the extension of the computational domain from an infinitely thin slice to a full 3D sector. This approach has already been successfully employed in astrophysics. However, the computational cost is expected to be greater than for 3D_AXI_SRC, even when considering only one slice.

More details on the numerical implementations are given in Chapter 3. But since neither of these solutions require too much coding compared to the port of the thermodynamic framework from the 2D-solver to the 3D-solver, we will investigate quantitatively the costs and benefits of each one.

Also since the 3D LES formulation can be easily found, we will only detail the 2D-axisymmetric LES formulation. We follow the framework laid out by Erlebacher et al. where the resolved, supergrid scales, denoted by a tilde ($\tilde{\sim}$), are computed using Favre averaging. Together with the unresolved, subgrid scales denoted by a double prime ($\overset{\prime\prime}{\sim}$), they give an exact decomposition of a flow variable $f = \tilde{f} + f''$. The Favre averaging is obtained through a spatial filtering (superscript $-$) expressed as:

$$\bar{f}(x_i, t) = \int_D f(z_i, t)G(x_i - z_i, \Delta)dz_i.$$  \hspace{1cm} (4)
with $D$ the domain of the flow and $\Delta$ the filter size, defined as $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$, where $\Delta x$, $\Delta y$ and $\Delta z$ are the grid size in axial, transverse and spanwise directions, respectively.

The filter kernel $G$ is defined as:

$$G = \begin{cases} \
1/\Delta & -\frac{\Delta}{2} \leq (x - z) \leq \frac{\Delta}{2} \\
0 & \text{otherwise} 
\end{cases}$$

(5)

The supergrid variable is then obtained through $\tilde{f} = \rho f / \bar{\rho}$. The filtering of the Navier-Stokes equations for the axisymmetric configuration yields:

$$\frac{\partial}{\partial t} \begin{pmatrix} \tilde{\rho} \\
\tilde{\rho} u_x \\
\tilde{\rho} u_y \\
\tilde{\rho} \tilde{\omega}_k \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \tilde{\rho} u_x \\
\tilde{\rho} u_x \tilde{u}_x + \tilde{\rho} - (\tilde{\tau}_{xx} - \tau_{xx}^{sgs}) \\
\tilde{\rho} u_x \tilde{u}_y - (\tilde{\tau}_{xy} - \tau_{xy}^{sgs}) \\
\tilde{\rho} u_x \tilde{h} - \tilde{u}_x (\tilde{\tau}_{xx} - \tau_{xx}^{sgs}) - \tilde{u}_y (\tilde{\tau}_{xy} - \tau_{xy}^{sgs}) + \tilde{q}_x + H_x^{sgs} + \sigma_x^{sgs} \\
\tilde{\rho} u_x \tilde{Y}_k - \tilde{\rho} \tilde{Y}_k \tilde{V}_{x,k} + Y_{x,k}^{sgs} + \theta_{x,k}^{sgs} \end{pmatrix} + \frac{1}{y} \frac{\partial}{\partial y} \begin{pmatrix} \tilde{\rho} u_y y \\
\tilde{\rho} u_y \tilde{u}_x y - (\tilde{\tau}_{xy} - \tau_{xy}^{sgs}) y \\
\tilde{\rho} u_y \tilde{u}_y y + \tilde{p} y - (\tilde{\tau}_{yy} - \tau_{yy}^{sgs}) y \\
(\tilde{\rho} u_y \tilde{h} - \tilde{u}_x (\tilde{\tau}_{xy} - \tau_{xy}^{sgs}) - \tilde{u}_y (\tilde{\tau}_{yy} - \tau_{yy}^{sgs}) + \tilde{q}_y + H_y^{sgs} + \sigma_y^{sgs}) y \\
(\tilde{\rho} u_y \tilde{Y}_k - \tilde{\rho} \tilde{Y}_k \tilde{V}_{y,k} + Y_{y,k}^{sgs} + \theta_{y,k}^{sgs}) y \end{pmatrix} = \begin{pmatrix} 0 \\
0 \\
-\frac{(\tilde{\tau}_{y} - \tau_{y}^{sgs})}{y} \\
0 \\
\tilde{\omega}_k \end{pmatrix}$$

(6)

The resolved parts of the viscous stress tensor can be expressed as:

$$\tilde{\tau}_{xx} = 4 \frac{\mu}{3} \left( \frac{\partial \tilde{u}_x}{\partial x} - 2 \frac{\mu}{3} \left( \frac{\partial \tilde{u}_y}{\partial y} + \frac{\tilde{u}_y}{y} \right) \right)$$

(7)

$$\tilde{\tau}_{yy} = 4 \frac{\mu}{3} \left( \frac{\partial \tilde{u}_y}{\partial y} - 2 \frac{\mu}{3} \left( \frac{\partial \tilde{u}_x}{\partial x} + \frac{\tilde{u}_x}{y} \right) \right)$$

(8)

$$\tilde{\tau}_{xy} = \tilde{\tau}_{yx} = \mu \left( \frac{\partial \tilde{u}_y}{\partial x} + \frac{\partial \tilde{u}_x}{\partial y} \right)$$

(9)
while the axisymmetric stress source term is:

\[
\tau_\theta = \frac{4}{3}\bar{\mu}\frac{\ddot{u}_y}{y} - \frac{2}{3}\bar{\mu}\left(\frac{\partial \ddot{u}_x}{\partial x} + \frac{\partial \ddot{u}_y}{\partial y}\right)
\]  

The computation of the dynamic viscosity \(\bar{\mu}\) is dealt with in Section 2.3.1.

The heat flux vector components are given by:

\[
\bar{q}_x = \bar{\lambda}\frac{\partial \bar{T}}{\partial x} + \bar{\rho} \sum_{k=1}^{N_s} \bar{h}_k \bar{Y}_k \bar{V}_{x,k} + \sum_{k=1}^{N_s} q_{x,k}^{gs}
\]

\[
\bar{q}_y = \bar{\lambda} \frac{1}{y} \frac{\partial \bar{T}}{\partial y} + \bar{\rho} \sum_{k=1}^{N_s} \bar{h}_k \bar{Y}_k \bar{V}_{y,k} + \sum_{k=1}^{N_s} q_{y,k}^{gs}
\]

with \(\bar{\lambda}\) the mixture thermal conductivity, \(\bar{h}_k\) the massic enthalpy of formation of species \(k\) and the unclosed subgrid heat flux \(q_{x,y}^{gs}\).

The modeling of the diffusion velocities under our operating conditions is more complex. On top of the classical Fickian diffusion, we also consider the cross-diffusion Soret and Dufour effects. The Soret, or "thermal-diffusion", effect corresponds to the diffusion of species because of temperature or pressure gradients whereas the Dufour, or "diffusion-thermo", effect refers to the diffusion of temperature due to species concentration or pressure gradients. Some recent Direct Numerical Simulation (DNS) studies of non-reacting temporal mixing layers (TML) of real gases [93, 78, 53, 52] have reported that Soret and Dufour cross-diffusion effects are important. However, Oefelein [98] finds only a small influence of these effects on the minor species in a reacting flow study while Palle et al. [110] report only important Soret effect in laminar flames when the molecular weights of the reactant are very different. In any event, modeling of these terms for LES studies remains to be properly developed and validated [102, 103, 153]. Therefore, we have not included these effects in the present study:

\[
\bar{V}_{x,k} = -\frac{\bar{D}_{k,m}}{\bar{Y}_k} \frac{\partial \bar{Y}_k}{\partial x}
\]

\[
\bar{V}_{y,k} = -\frac{\bar{D}_{k,m}}{\bar{Y}_k} \frac{1}{y} \frac{\partial \bar{Y}_k}{\partial y}
\]

The computation of the diffusion coefficient \(\bar{D}_{k,m}\) of species \(k\) into the mixture is investigated in Section 2.3.3.
The remaining governing equation for the fluid mechanics is the one that defines pressure. The pressure is determined from the filtered equation of state. Depending on the temperature and pressure conditions in the combustion chamber, a different equation of state is necessary to describe the behavior of the flow. A general form containing the compressibility factor $Z$ is used in this section and will be further explained in the next sections.

The equation of state is written $p = Z \rho RT$, with $R$ the specific gas constant. In the case of thermally perfect gases (TPG), $Z$ is 1 and the equation of state reduces to the well known $p = \rho RT$. The filtered form of the real gas equation of state is:

\[
\bar{p} = \bar{\rho} R_u \sum_{k=1}^{n} \left( \tilde{Z}_k \tilde{Y}_k \tilde{T}_k \right) + \bar{\rho} R_u \sum_{k=1}^{n} \left( \tilde{Z}_k \frac{\tilde{Y}_k \tilde{T} - \tilde{Z}_k \tilde{Y}_k \tilde{T}}{W_k} \right) \quad (16)
\]

Here, $R_u$ is the universal gas constant and $M_k$ is the molecular weight for the $k$-th species. The first term on the right hand side contains only resolved values: $\tilde{Z}$, $\tilde{Y}_k$, $\tilde{T}$. The second term includes a triple correlation of the temperature, compressibility and species terms and is a term that requires closure. As mentioned earlier, for thermally perfect gases, the filtered equation of state is the same as Eqn. (16) except that $Z = 1$. Details about the definition of $Z$ in the current study are given in the next Section. It has been shown that the subgrid term in the above equation is negligible for low heat release in a perfect gas, and it seems to be also the case for real gases even though this has not been clearly demonstrated for a reacting case as yet. Actually, more closure terms appear because of the modified equation of state as discussed by Schweitzer et al. but because of the lack of physical understanding of the processes involved, we choose to neglect all of them for the current study. More details about the EoS will be given in the next sections.

The subgrid terms, denoted by the superscript $s gs$ in Eqn. 6, require closure:

\[
\tau_{s gs}^{x y} = \tau_{s gs}^{y x} = \bar{\rho} [\tilde{u}_x \tilde{u}_y - \tilde{u}_x \tilde{u}_y] \\
\tau_{s gs}^{x x} = \bar{\rho} [\tilde{u}_x \tilde{u}_x - \tilde{u}_x \tilde{u}_x] \\
\tau_{s gs}^{y y} = \bar{\rho} [\tilde{u}_y \tilde{u}_y - \tilde{u}_y \tilde{u}_y] \quad (17)
\]
\begin{align}
H_{sgs}^x &= \bar{\rho} [\bar{c_u} u_x - \bar{c} \bar{u}_x] + [\bar{p u}_x - \bar{p} \bar{u}_x] \\
H_{sgs}^y &= \bar{\rho} [\bar{c_u} u_y - \bar{c} \bar{u}_y] + [\bar{p u}_y - \bar{p} \bar{u}_y]
\end{align}

\begin{align}
\sigma_{sgs}^x &= [\bar{u}_y \bar{r}_{yx} - \bar{\bar{u}}_y \bar{r}_{yx}] \\
\sigma_{sgs}^y &= [\bar{u}_x \bar{r}_{xy} - \bar{\bar{u}}_x \bar{r}_{xy}]
\end{align}

\begin{align}
Y_{s_{gs},x,k} &= \bar{\rho} [\bar{u}_x \bar{Y}_{k} - \bar{u}_x \bar{Y}_{k}] \\
Y_{s_{gs},y,k} &= \bar{\rho} [\bar{u}_y \bar{Y}_{k} - \bar{u}_y \bar{Y}_{k}]
\end{align}

\begin{align}
q_{s_{gs},x,k} &= \big[ h_{k} D_{k,m} \partial \bar{Y}_k / \partial x - \bar{h}_k \bar{D}_{k,m} \partial \bar{Y}_k / \partial x \big] \\
q_{s_{gs},y,k} &= \big[ h_{k} D_{k,m} \frac{1}{y} \partial \bar{Y}_k / \partial y - \bar{h}_k \bar{D}_{k,m} \frac{1}{y} \partial \bar{Y}_k / \partial y \big]
\end{align}

\begin{align}
\theta_{s_{gs},x,k} &= \bar{\rho} [\bar{V}_{x,k} \bar{Y}_k - \bar{V}_{x,k} \bar{Y}_k] \\
\theta_{s_{gs},y,k} &= \bar{\rho} [\bar{V}_{y,k} \bar{Y}_k - \bar{V}_{y,k} \bar{Y}_k]
\end{align}

\begin{align}
T_{s_{gs},k} &= \frac{\bar{Z} \bar{Y}_k \bar{T} - \bar{Z} \bar{Y}_k \bar{T}}{W_k}
\end{align}

They represent, respectively, the subgrid stress, the subgrid enthalpy flux, the subgrid viscous work, the subgrid species flux, the subgrid heat flux, the subgrid diffusive species flux and the subgrid temperature.

Here, a closure based on a transport model for the subgrid kinetic energy \( k_{s_{gs}} \) (\( k_{s_{gs}} = \frac{1}{2} \bar{[\bar{u}_k u_k - \bar{u}_k \bar{u}_k]} \)) is used to close the momentum and energy subgrid fluxes, \( \tau_{s_{gs}} \) and \( H_{s_{gs}} \).
respectively. In this approach, a one-equation model for $k^{\text{sgs}}$ is solved along with the LES equations\cite{16}:

$$\frac{\partial \rho k^{\text{sgs}}}{\partial t} + \frac{\partial}{\partial x} \left( \rho \tilde{u}_x k^{\text{sgs}} \right) + \frac{1}{y} \frac{\partial}{\partial y} \left( \rho y \tilde{u}_y k^{\text{sgs}} \right) = P^{\text{sgs}} - \varepsilon^{\text{sgs}} + \frac{\partial}{\partial x} \left( \rho \nu_t Pr_t \right) \frac{\partial k^{\text{sgs}}}{\partial x} + \frac{1}{y} \frac{\partial}{\partial y} \left( \rho y \nu_t Pr_t \right) \frac{\partial k^{\text{sgs}}}{\partial y}$$

(25)

Here, $\nu_t$ is the turbulent viscosity, also called eddy viscosity, given as $\nu_t = C_{\nu} \sqrt{k^{\text{sgs}}} \Delta$ with $C_{\nu}$ a model coefficient and $\Delta$ the local grid filter width. The turbulent Prandtl number $Pr_t$ is fixed at 0.9. Also, $P^{\text{sgs}}$ is the subgrid kinetic energy production and $D^{\text{sgs}}$ is the subgrid kinetic energy dissipation, and are defined as

$$P^{\text{sgs}} = -\tau_{xy}^{\text{sgs}} \frac{1}{y} \frac{\partial y \tilde{u}_x}{\partial y} - \tau_{yy}^{\text{sgs}} \frac{1}{y} \frac{\partial y \tilde{u}_y}{\partial y} - \tau_{xx}^{\text{sgs}} \frac{\partial \tilde{u}_x}{\partial x} - \tau_{yx}^{\text{sgs}} \frac{\partial \tilde{u}_y}{\partial x}$$

(26)

$$D^{\text{sgs}} = C_{\nu} \bar{\rho} \left( k^{\text{sgs}} \right) \frac{k^{\text{sgs}}}{\Delta}$$

(27)

Like $C_{\nu}$, $C_{\epsilon}$ is also a model coefficient. Given $\nu_t$, the subgrid stresses are closed as follows:

$$\tau_{xy}^{\text{sgs}} = \tau_{yx}^{\text{sgs}} = -\bar{\rho} \nu_t \left( \frac{1}{y} \frac{\partial y \tilde{u}_x}{\partial y} + \frac{\partial \tilde{u}_x}{\partial x} \right)$$

(28)

$$\tau_{xx}^{\text{sgs}} = -\frac{4}{3} \bar{\rho} \nu_t \left( \frac{1}{y} \frac{\partial y \tilde{u}_x}{\partial y} \right) + \frac{2}{3} \bar{\rho} \left( \nu_t \frac{\partial \tilde{u}_x}{\partial x} + k^{\text{sgs}} \right)$$

(29)

$$\tau_{yy}^{\text{sgs}} = -\frac{4}{3} \bar{\rho} \nu_t \left( \frac{\partial \tilde{u}_x}{\partial x} \right) + \frac{2}{3} \bar{\rho} \left( \nu_t \frac{1}{y} \frac{\partial y \tilde{u}_y}{\partial y} + k^{\text{sgs}} \right)$$

(30)

We close the energy and species subgrid fluxes using a gradient assumption. We are aware that this assumption might not be valid under supercritical conditions but preliminary studies\cite{104} seem to indicate that the gradient assumption is at least reasonable for mixing of subcritical and supercritical fluids. However, the model coefficients might need to be adjusted under supercritical burning conditions. The best solution, which we will consider for further studies, is to compute these coefficients using the Localized Dynamic (LDKM) subgrid model:

$$H_x^{\text{sgs}} = -\bar{\rho} \nu_t \frac{\partial \tilde{h}}{\partial x}$$

(31)

$$H_y^{\text{sgs}} = -\bar{\rho} \nu_t \frac{1}{y} \frac{\partial y \tilde{h}}{\partial y}$$

(32)

$$Y_{x,k}^{\text{sgs}} = -\bar{\rho} \nu_t \frac{1}{Sc_t} \frac{\partial \tilde{Y}_k}{\partial x}$$

(33)

$$Y_{y,k}^{\text{sgs}} = -\bar{\rho} \nu_t \frac{1}{y} \frac{1}{Sc_t} \frac{\partial \tilde{Y}_k}{\partial y}$$

(34)
The turbulent Schmidt number $\text{Sc}$ is fixed at 0.7.

The subgrid viscous work, $\sigma^{gs}$, has been neglected in the past \cite{74, 94}. This assumption is justified in the case of a high Reynolds number flow, where the viscous terms are generally small compared to the convective terms. As a consequence, the viscous subgrid transport term is considered negligible. Similar logic can be applied to the subgrid heat flux $q^{gs}$ and the subgrid species diffusive flux $\theta_k^{gs}$. However, the importance of these terms for real gas mixing and burning is not clear at present and needs further investigation that is beyond the scope of this work. An earlier study \cite{16} have shown that the two model coefficients $C_\nu$ and $C_\epsilon$ have constant values of 0.067 and 0.916. The derivation of those constants did not imply any assumptions of incompressibility or ideal gas behavior and are consequently used as is for both thermally perfect and real gas studies. The current flow solver is also capable of dynamically computing the model coefficients as shown earlier by Kim and Menon \cite{74}, as well as turbulent quantities denoted by the subscript $t$ (such as $\text{Pr}_t$). The influence of the resolution in the tangential direction and the behavior of the turbulence in an axisymmetric supercritical configuration could thus also be studied with the 3D_AXI_FLUX framework.

2.2 Governing Equations for the Thermodynamics

Operating at high pressures does not always imply that the gases will exhibit a very different behavior from what is predicted by the ideal gas assumption. Consider, for example, the injection of supercritical hydrogen into a rocket combustion chamber at pressure of about 100 bar. In this case, the reduced pressure $p_r = p/p_c$ is around 10, and on any compressibility chart \cite{95}, it is seen that the non-ideality of hydrogen is quite small. In the following, subscript $c$ represents a critical property and the subscript $r$ represents a reduced property (i.e. $T_r = T/T_c$). So using the ideal gas law in this case would not be inappropriate but this is, of course, a very specific case. For most practical applications (and especially those involving combustion), at least one species (oxygen, in the case of a liquid rocket engine) will behave as a non-ideal gas under supercritical conditions. Therefore, this effect is included by using a real gas equation of state.

Several equations of state have been developed to describe the behavior of a supercritical
fluid. It has been noted [98] that the cubic Peng-Robinson equation of state (PR EoS) is an acceptable choice from accuracy and cost considerations. Other studies [26] have shown that the PR EoS is the most accurate cubic equation for rocket motor application. It can also be applied to model sub-critical injection of liquid oxygen due to its accuracy in the compressed liquid domain. The PR EoS also reduces to the thermally perfect EoS when the conditions change and therefore, this approach could allow us to simulate supercritical to subcritical states in the combustor without switching the EoS model.

Table 4: Values of the critical properties needed for the PR EoS for the species used here.

<table>
<thead>
<tr>
<th>Species</th>
<th>$T_c$(K)</th>
<th>$p_c$(bar)</th>
<th>$v_c$(cm$^3$.mol$^{-1}$)</th>
<th>$Z_c$</th>
<th>$\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>O$_2$</td>
<td>154.581</td>
<td>49.771</td>
<td>73.37</td>
<td>0.287886</td>
<td>0.0222</td>
</tr>
<tr>
<td>H$_2$</td>
<td>33.19</td>
<td>12.978</td>
<td>66.93</td>
<td>0.315</td>
<td>-0.214</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>647.14</td>
<td>220.64</td>
<td>55.95</td>
<td>0.229</td>
<td>0.3443</td>
</tr>
<tr>
<td>OH</td>
<td>100.7</td>
<td>57.6</td>
<td>39.3</td>
<td>0.27</td>
<td>0.329</td>
</tr>
<tr>
<td>H</td>
<td>182.6</td>
<td>251.9</td>
<td>16.3</td>
<td>0.27</td>
<td>0.329</td>
</tr>
</tbody>
</table>

The general PR EoS is:

$$p = \frac{R_u T}{v - B_m} - \frac{A_m}{v^2 + 2vB_m - B_m^2}$$  \hspace{1cm} (35)

with the molar volume $v$ in m$^3$.mol$^{-1}$, $A_m$ in Pa.(m$^3$.mol$^{-1}$)$^2$ and $B_m$ in m$^3$.mol$^{-1}$. The mixture parameters $A_m$ and $B_m$ are [92]:

$$A_m = \sum_i \sum_j X_i X_j A_{ij} \quad B_m = \sum_i X_i B_i$$  \hspace{1cm} (36)

$X_k$ is the $k$-th species mole fraction. The mixture parameters are given as:

$$A_{ij} = 0.457236 \frac{R_u^2 T_{c(ij)}^2}{p_{c(ij)}} \alpha(T_{r(ij)})$$  \hspace{1cm} (37)

and

$$B_i = 0.077796 \frac{R_u T_{c(ii)}}{p_{c(ii)}}$$  \hspace{1cm} (38)

where
\[ \alpha(T_{ij}) = \left[ 1 + f(\omega_{ij}) \left( 1 - \sqrt{T_{ij}} \right) \right]^2 \tag{39} \]

\[ f(\omega_{ij}) = 0.379642 + 1.48503 \, \omega_{ij} - 0.164423 \, \omega_{ij}^2 + 0.016666 \, \omega_{ij}^3 \tag{40} \]

This expression for \( f(\omega_{ij}) \) is based on modifications made by Peng and Robinson\[113\] to the initial formulation, and validated later \[156\]. Except for \( \alpha(T_{ij}) \), all these terms are computed once at the beginning of a simulation. The mixture critical properties are determined by following the standard mixing rules\[54\]:

\[
\begin{align*}
T_{c(ii)} &= T_{ci} \\
T_{c(ij)} &= (1 - \kappa_{ij}) \sqrt{T_{c(ii)} T_{c(jj)}} \\
p_{c(ii)} &= p_{ci} \\
p_{c(ij)} &= Z_{c(ij)} \frac{R_u T_{c(ij)}}{v_{c(ij)}} \\
v_{c(ii)} &= v_{ci} \\
v_{c(ij)} &= \frac{1}{8} \left( v_{c(ii)}^{1/3} + v_{c(jj)}^{1/3} \right)^3 \\
M_{ii} &= M_i \\
M_{ij} &= \frac{2M_i M_j}{M_i + M_j} \\
Z_{c(ii)} &= Z_{ci} \\
Z_{c(ij)} &= \frac{1}{2} (Z_{c(ii)} + Z_{c(jj)}) \\
\omega_{c(ii)} &= \omega_{ci} \\
\omega_{c(ij)} &= \frac{1}{2} (\omega_{c(ii)} + \omega_{c(jj)})
\end{align*}
\tag{41}
\]

where \( \kappa \) is an interaction parameter which is non-zero only for polar molecules such as water. More details are given in Sec. 2.3.3. Table 4 summarizes the critical properties of the species used in our simulations.

Finally, an equivalent form of this EoS, using a cubic equation in \( Z \), is employed. The compressibility factor \( Z \) defines the deviation of a real gas from ideal gas behavior and links directly \( T, P \) and \( \rho \) with \( Z = p/\rho RT \). This form allows computation of \( Z \) analytically when \( T \) and \( p \) are known:
\[ Z^3 + \alpha Z^2 + \beta Z + \gamma = 0 \] (42)

with

\[
\begin{align*}
\alpha &= -1 + \frac{B_m p}{R_u T} \\
\beta &= \frac{A_m P - 3(B_m p)^2}{(R_u T)^2} - \frac{2B_m p}{R_u T} \\
\gamma &= \frac{-A_m B_m p^2}{(R_u T)^3} + \frac{(B_m p)^2}{(R_u T)^2} + \frac{(B_m p)^3}{(R_u T)^3}
\end{align*}
\] (43)

Such general cubic equation, since the coefficients are real, has at least one real root and may have three real roots. An efficient root-finding algorithm is available and is detailed here. First we compute the following quantities:

\[
Q = \frac{\alpha^2 - 3\beta}{9} \\
R = \frac{2\alpha^3 - 9\alpha\beta + 27\gamma}{54}
\]

If \( Q^3 - R^2 \geq 0 \), then the cubic equation has three real roots. We then compute:

\[ \theta = \arccos \left( \frac{R}{Q^{3/2}} \right) \] (44)

and assume \( Z \) is the largest positive root among:

\[
\begin{align*}
Z_1 &= -2\sqrt{Q} \cos \left( \frac{\theta}{3} \right) - \frac{\alpha}{3} \\
Z_2 &= -2\sqrt{Q} \cos \left( \frac{\theta + 2\pi}{3} \right) - \frac{\alpha}{3} \\
Z_3 &= -2\sqrt{Q} \cos \left( \frac{\theta + 4\pi}{3} \right) - \frac{\alpha}{3}
\end{align*}
\]

On the other hand, if \( Q^3 - R^2 < 0 \), the only real root is:

\[
Z_1 = -\text{sign}(R) \left\{ \left[ (R^2 - Q^3)^{1/2} + |R| \right]^{1/3} + \frac{Q}{\left[ (R^2 - Q^3)^{1/2} + |R| \right]^{1/3}} \right\} - \frac{\alpha}{3} \] (45)

This is the kind of equation that needs to be solved when one uses a real gas framework, another example is given in the Appendix.

For our formulation to be consistent, we must also use the PR EoS to compute the thermodynamic properties of the flow. Usually, this is done using the concept of the departure function. Let \( \Psi \) be the value of some thermodynamic property of a pure component (or a
mixture with a fixed composition) at some \( P \) and \( T \). If \( \Psi^\circ \) denotes the value of \( \Psi \) at the same temperature but in an ideal-gas state and at a reference pressure \( P^\circ \), then we call \( \Psi - \Psi^\circ \) the departure function.

By deriving the Helmholtz and Gibbs free energies as given by \([123]\) and \([92]\), we get the departure functions for the internal energy per unit mass and the enthalpy per unit mass:

\[
e - e^\circ = K_1 \left( A_m - T \frac{\partial A_m}{\partial T} \right) \tag{46}
\]

\[
h - h^\circ = e - e^\circ + \frac{p}{\rho} - R_m T \tag{47}
\]

The constant volume heat capacity \( c_v = (\partial e/\partial T)_V \) is directly obtained from the previous expression:

\[
c_v - c_v^\circ = -K_1 T \frac{\partial^2 A_m}{\partial T^2} \tag{48}
\]

with:

\[
K_1 = \frac{1}{2\sqrt{2}B_m} \ln \left( \frac{1 + (1 - \sqrt{2})\rho B_m}{1 + (1 + \sqrt{2})\rho B_m} \right)
\]

whereas the constant pressure heat capacity \( c_p = (\partial h/\partial T)_p \) is related to \( C_v \) through:

\[
c_p = c_v - T \frac{\left( \frac{\partial p}{\partial v} \right)_{v,X}^2}{\left( \frac{\partial p}{\partial v} \right)_{T,X}} \tag{49}
\]

This yields:

\[
c_p - c_p^\circ = -T \frac{\left( \frac{\partial p}{\partial v} \right)_{v,X}^2}{\left( \frac{\partial p}{\partial v} \right)_{T,X}} - R_m - K_1 T \frac{\partial^2 A_m}{\partial T^2} \tag{50}
\]

with the following partial derivatives:

\[
\left( \frac{\partial p}{\partial v} \right)_{T,X} = \frac{-\rho^2 R_m T}{(1 - \rho B_m)^2} \left[ 1 - \frac{2\rho A_m}{R_m T(1 + \rho B_m) \left( \frac{1}{1 - \rho B_m} + \frac{\rho B_m}{1 + \rho B_m} \right)^2} \right] \tag{51}
\]

\[
\left( \frac{\partial p}{\partial T} \right)_{V,X} = \frac{\rho R_m}{1 - \rho B_m} - \frac{\rho^2 \frac{\partial A_m}{\partial T}}{1 + 2\rho B_m - \rho^2 B_m^2} \tag{52}
\]

\[
\frac{\partial A_m}{\partial T} = -\frac{1}{T} \sum_i \sum_j X_i X_j A_{ij} G_{ij} \tag{53}
\]

\[
G_{ij} = \frac{f(\omega_{ij}) \sqrt{T_c(ij)}}{1 + f(\omega_{ij})(1 - \sqrt{T_c(ij)})} \tag{54}
\]
\[
\frac{\partial^2 A_m}{\partial T^2} = \frac{0.457236 R_m^2}{2T} \sum_i \sum_j X_i X_j f(\omega_{ij}) (1 + f(\omega_{ij})) \frac{T_{c(ij)}}{p_{c(ij)}} \sqrt{\frac{T_{c(ij)}}{T}} \tag{55}
\]

The partial molar enthalpy is evaluated using the relation:

\[
h_{i} = h_{i}^0 + p v_{i} - R_{m} T + (A_{m} - T \frac{\partial A_{m}}{\partial T}) v_{i} - v B_{i}/B_{m} + K_{1} \left[ \frac{\partial A_{m}}{\partial X_{i}} - T \frac{\partial^2 A_{m}}{\partial X_{i} \partial T} - (A_{m} - T \frac{\partial A_{m}}{\partial T}) \frac{B_{i}}{B_{m}} \right] \tag{56}
\]

The partial molar volume used in the previous equation is given by:

\[
v_{i} = \frac{-1}{(\partial p/\partial v)_{T,X}} \left[ \frac{R_{m} T}{v - B_{m}} + \frac{R_{m} TB_{i}}{(v - B_{m})^2} + \frac{2A_{m}(v - B_{m})B_{i}}{(v^2 + 2vB_{m} - B_{m}^2)} - \frac{2 \sum_{j} A_{ij} X_{j}}{v^2 + 2vB_{m} - B_{m}^2} \right] \tag{57}
\]

and the needed derivatives are:

\[
\frac{\partial A_{m}}{\partial X_{i}} = 2 \sum_{j} A_{i,j} X_{j} \tag{58}
\]

\[
\frac{\partial^2 A_{m}}{\partial X_{i} \partial T} = -\frac{2}{T} \sum_{j} A_{i,j} X_{j} G_{ij} \tag{59}
\]

The speed of sound is defined by:

\[
c = (\rho \kappa_{s})^{-1/2} \tag{60}
\]

where \(\kappa_{s}\) is the isentropic compressibility with:

\[
\kappa_{s} = \kappa_{T} - v T \frac{\alpha_{V}^2}{C_{p}} \tag{61}
\]

The expansivity \(\alpha_{V}\) and the isothermal compressibility \(\kappa_{T}\) are defined as:

\[
\alpha_{V} = -\frac{(\partial P/\partial T)_{V,X}}{v(\partial P/\partial v)_{T,X}} \tag{62}
\]

\[
\kappa_{T} = \frac{-1}{v(\partial P/\partial v)_{T,X}} \tag{63}
\]

Details of the iterative process performed in the main solver to compute temperature and pressure from density and energy are detailed in the Appendix. This iterative process is very similar to the one described by Okong’o et al. [105].
2.3 Transport properties

The transport properties are computed using the methodology developed by Chung et al. [23], which is considered most effective in terms of computational cost and accuracy [26]. Before going into the computational details, it should be noted that the thermodynamic framework and the transport properties framework are independent and thus it is possible, as demonstrated later, to run any EoS (CPG, TPG or RG) with any transport properties framework such as the multi-species Sutherland’s law model used for perfect gas computations or Chung’s model.

2.3.1 Viscosity

The most simple approach to compute the viscosity $\mu$ of a gas is the Sutherland’s law [159]:

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S}{T + S}$$

(64)

where:

- $\mu$ = viscosity in $\mu$P
- $M$ = molecular weight in g.mol$^{-1}$
- $\Sigma$ = hard-sphere diameter in Å
- $\Omega_v$ = collision integral. Equal to 1 if molecules do not attract each other (perfect gas).

If we consider molecules interacting through a Lennard-Jones potential, the following correlation [57] has been proposed in order to evaluate the collision integral $\Omega_v$:

$$\Omega_v = A(T^*)^{-B} + Ce^{-DT^*} + Ee^{-FT^*}$$

(66)
where subscript $*$ denotes a dimensionless temperature $T^*$, $k$ is the Boltzmann’s constant and $\varepsilon$ is the minimum potential energy between two molecules. The constants are:

\[
A = 1.16145 \\
B = 0.14874 \\
C = 0.52487 \\
D = 0.77320 \\
E = 2.16178 \\
F = 2.43787
\]

However, this is also hardly transferable to dense gases and we will prefer other techniques that can be applied to both dilute and dense regimes. Following the discussion by Poling et al.\[117\], we choose the Chung et al.\[23\] method which is designed to use temperature and molar volume, i.e. density, as input:

\[
\mu = \mu^* 3.6344 \times 10^{-10} \frac{\sqrt{MT_c}}{v_c^{2/3}}
\]

where:

\[
\mu^* = \sqrt{T^*} \Omega_v \left( F_c \left[ G_2^{-1} + E_{6y} \right] \right) + \mu^{**}
\]

It has to be noted that this estimation doesn’t use the usual Lennard-Jones parameter database but rather relate them to the critical properties. So we have:

\[
\varepsilon = \frac{T_c}{k} = \frac{1.2593}{1.2593} \\
\Sigma = 80.9v_c^{1/3}
\]

which yields:

\[
T^* = 1.2593T_r
\]

Also, $\Omega_v$ has already been defined whereas $F_c$, which is still used in the limit of dilute gas, is:

\[
F_c = 1 - 0.2756\omega + 0.059035\eta_r^4 + \kappa
\]
We have also:

\[ y = \frac{v_c}{6v} \]
\[ G_1 = \frac{1 - 0.5y}{(1 - y)^3} \]
\[ G_2 = \frac{E_1 \left[ (1 - e^{-E_4y}) / y \right] + E_2G_1e^{E_5y} + E_3G_1}{E_1E_4 + E_2 + E_3} \]
\[ \mu^{**} = E_7y^2G_2e^{E_8 + E_9 + E_{10} / (\tau^2)} \]

\( F_c \), as well as the parameters \( E_1 \) to \( E_{10} \), is a linear function of the accentric factor \( \omega \), of the fourth power of a dimensionless dipole moment \( \eta_r \) and of the association factor \( \kappa \). The reduced dipole moment is computed from the physical dipole moment \( \eta \) in debyes:

\[ \eta_r = 0.1313 \frac{\eta}{\sqrt{v_cT_c}} \]  

(71)

Table 5 summarizes the values of these coefficients in our simulations.

Table 5: Values of the parameters used for the viscosity computations for the species used in this work.

<table>
<thead>
<tr>
<th>Species</th>
<th>( \mu_r )</th>
<th>( \kappa )</th>
</tr>
</thead>
<tbody>
<tr>
<td>O(_2)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>H(_2)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>H(_2)O</td>
<td>0.076</td>
<td>1.8</td>
</tr>
<tr>
<td>OH</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>H</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
We note that the low-pressure viscosity is readily available if we set $y$ to 0, it will be useful for the computation of the thermal conductivity.

\[
E_1 = 6.324 + 50.412\omega \\
E_2 = 0.00121 - 0.001154\omega \\
E_3 = 5.283 + 254.209\omega \\
E_4 = 6.623 + 38.096\omega \\
E_5 = 19.745 + 7.630\omega \\
E_6 = -1.9 - 12.537\omega \\
E_7 = 24.275 + 3.45\omega \\
E_8 = 0.7972 - 1.117\omega \\
E_9 = -0.2382 + 0.06770\omega \\
E_{10} = 0.06863 + 0.3479\omega
\]

### 2.3.2 Thermal conductivity

The same discussion can be led for thermal conductivity and once again, the Chung et al.\cite{23} method is very useful here since its validity goes from low pressure to high pressure. The computation of the viscosity and the thermal conductivity are actually linked as one can see in the following estimation:

\[
\lambda = \frac{31200\mu^0\Psi}{M} \left( \frac{1}{G_2} + B_6y \right) + qB_7y^2\sqrt{T_r}G_2
\]

(72)

where $\lambda$ is the thermal conductivity in W.(m.K)$^{-1}$, the superscript $0$ in $\mu$ denotes the low-pressure viscosity mentioned earlier and $q$ is defined as:

\[
q = 1.134 \times 10^{-5} \sqrt{\frac{T_c}{Mv_c^4/3}}
\]

and $\Psi$ is a function of the specific heat at constant volume $C_v$, the accentric factor $\omega$ and the reduced temperature $T_r$:

\[
\Psi = 1 + \alpha \frac{0.215 + 0.28288\alpha - 1.061\beta + 0.26665Z}{0.6366 + \beta Z + 1.061\alpha\beta}
\]

(73)
with:

\[ \alpha = \frac{C_v}{R_u} - \frac{3}{2} \]
\[ \beta = 0.7862 - 0.7109\omega + 1.3168\omega^2 \]
\[ Z = 2.0 + 10.5T_r^2 \]

The other parameters are very similar to the ones used for the viscosity, allowing an easy implementation:

\[ y = \frac{V_c}{6v} \]
\[ G_1 = \frac{1 - 0.5y}{(1 - y)^3} \]
\[ G_2 = \frac{B_1 \left[ (1 - e^{-B_4y}) / y \right] + B_2G_1e^{B_3y} + B_3G_1}{B_1B_4 + B_2 + B_3} \]

\[ B_1 = 2.4166 + 0.74824\omega \]
\[ B_2 = -0.50924 - 1.5094\omega \]
\[ B_3 = 6.6107 + 5.6207\omega \]
\[ B_4 = 14.543 - 8.9139\omega \]
\[ B_5 = 0.79274 + 0.82019\omega \]
\[ B_6 = -5.8634 + 12.801\omega \]
\[ B_7 = 91.089 + 128.11\omega \]

### 2.3.3 Diffusion coefficients

For low pressure binary gas systems, we can apply the Chapman and Enskog theory straightforwardly and use the Lennard-Jones potential to evaluate the binary diffusion coefficient \( D_{AB} \) and the collision integral \( \Omega_D \):

\[ D_{AB} = \frac{0.0266T^{3/2}}{pM_{\Sigma}^{3/2}g_{\Sigma}^{2}\Omega_D} \]
\[ \Omega_D = \frac{A}{(T^*)^B} + \frac{C}{e^{DT^*}} + \frac{E}{e^{FT^*}} + \frac{G}{e^{HT^*}} \]  

(75)

where:

\[ D_{AB} \text{ = diffusion coefficient in m}^2\text{s}^{-1} \]
\[ M_{AB} = 2 \left( \frac{1}{M_A} + \frac{1}{M_B} \right) \]
\[ \Sigma_{AB} = \frac{\Sigma_A + \Sigma_B}{2} \]
\[ \varepsilon_{AB} = \sqrt{\varepsilon_A \varepsilon_B} \]
\[ T^* = \frac{kT}{\varepsilon_{AB}} \]
\[ A = 1.06036 \]
\[ B = 0.15610 \]
\[ C = 0.19300 \]
\[ D = 0.47635 \]
\[ E = 1.03587 \]
\[ F = 1.52996 \]
\[ G = 1.76474 \]
\[ H = 3.89411 \]

For high pressure, even for binary diffusion, the experimental data are very scarce and no extensive method exists at that point. That is why we choose to use species-dependent but conditions-independent Schmidt numbers \[ \text{Sc} \] to compute, from the viscosity, the diffusion coefficient \[ D_{k,m} \] of species \( k \) into the mixture:

\[ \text{Sc}_i = \frac{\mu_m}{\rho_m D_{i,m}} \]  

(76)

Table displays the values used in the present work.

### 2.4 Chemistry

The following one-step reduced mechanism[122], suggested by Astrium Corporation, is used for the simulations reported in the first part of the results section:
Table 6: Values of Schmidt number for the species used in this work

<table>
<thead>
<tr>
<th>Species</th>
<th>Schmidt number</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>1.25</td>
</tr>
<tr>
<td>H₂</td>
<td>0.22</td>
</tr>
<tr>
<td>H₂O</td>
<td>1.6</td>
</tr>
<tr>
<td>OH</td>
<td>40.0</td>
</tr>
<tr>
<td>H</td>
<td>1.25</td>
</tr>
</tbody>
</table>

\[
H₂ + 0.5145 \, O₂ \rightarrow 0.9310 \, H₂O + 0.040 \, H + 0.0980 \, OH
\]

(77)

However, we limit the infinite chemical rate by a mixing rate computed using the subgrid Eddy Break-Up (EBU) model [144]. This mixing rate depends on the dissipation rate of turbulent eddies which mix reactants at the smallest scales, and is expressed here as:

\[
R_{mixing} = \min(Y_{O₂}, Y_{H₂}) \frac{\sqrt{2k_{sgs}}}{C_{EBU} \Delta}
\]

(78)

The nominal value of \(C_{EBU}\) is unity. At present, there is no way to assess the validity of this subgrid EBU approach for RG simulations, especially to account for very high pressure combustion. We expect the kinetics to be enhanced at high pressures, and so we looked at the sensitivity of prediction to \(C_{EBU}\) and report on some of these studies in this paper.

Another mechanism is used for the final comparison between TPG and RG simulations. This two-step reduced mechanism is the one proposed by Rogers and Chinitz [128] and for which accurate rates are given by Drummond [32]:

\[
H₂ + O₂ \rightleftharpoons 2 \, OH
\]

(79)

\[
2 \, OH + H₂ \rightleftharpoons 2 \, H₂O
\]

(80)

The forward reaction rates are computed from the Arrhenius law:

\[
k_{f₁} = A₁T^{-10}e^{-4865/R⁰T}
\]

(81)

\[
k_{f₂} = A₂T^{-13}e^{-42,500/R⁰T}
\]

(82)
where

\[ A_1 = (8.917 \phi + 31.433/ \phi - 28.95)(10^{4.7}) \text{ cm}^3/\text{mol.s} \]  \hspace{1cm} (83)

\[ A_2 = (2.0 + 1.333/ \phi - 0.833 \phi)(10^{6.4}) \text{ cm}^6/\text{mol}^2.\text{s} \]  \hspace{1cm} (84)

The equilibrium constants are given by:

\[ K_1 = 26.164 \exp^{-8992/T} \]  \hspace{1cm} (85)

\[ K_2 = 2.682 \times 10^{-6}T \exp^{69415/T} \]  \hspace{1cm} (86)

The EBU model is also used here as a way to limit the reaction rate to the regions of very high shear. However, a lower, non-zero bound is adopted for the mixing rate so that there is some reaction in regions where the sub-grid kinetic energy is zero.

Finally, we would like to point out the fact that detailed understanding is still missing with the chemical mechanisms and their reaction rates under typical operating conditions. As mentioned earlier, the typical environment inside a LRE is very difficult to reproduce experimentally, even for mixing studies where only a cold flow setup is required. So not only are the real diffusion processes barely understood, but it is mostly unknown whether and how the chemical paths are affected by such a dense environment. In the context of LREs, some recent studies have been conducted using the GRI mechanism at high pressure for methane\textsuperscript{[111]}, but the work on the hydrogen/oxygen is limited. So, due to the lack of experimental and theoretical backgrounds, usual global mechanisms are used in most of the work reviewed by the author. A recent review on laminar flames at high pressures\textsuperscript{[75]} underlines the difficulty of choosing an appropriate mechanism under such conditions and calls for further investigations. For example, a comprehensive model like the one proposed by Conaire et al. \textsuperscript{[25]} needs to be tested in typical LRE configurations.
CHAPTER III

NUMERICS

3.1 Numerical implementation

The governing equations are solved using a finite volume, predictor-corrector scheme, that is second-order accurate in time and between second and fourth-order accurate in space. The complete formulation can be found elsewhere\cite{130}, we do not detail here for brevity. The Astrium chamber simulations were conducted using a Turkel-Gottlieb\cite{47} scheme whose accuracy is up to fourth-order in space where the grid is uniform but whose accuracy drops as grid stretching increases. To suppress initial transients explicit artificial dissipation is included using a combined second-fourth-order dissipation scheme \cite{65}.

Profiling of the code performance highlights the computational cost of the real gas formulation, for the thermodynamics as well as for the transport properties. It involves many complex operations such as real-powers, square roots, logarithms or iterative computations. It appears that more than 20% of the computation time is spent on these various operations. There is definitely a need to speed up the calculations, either by trying to simplify the formulation, by using more robust mathematical methods for the iterative process or by making simplifying assumptions. For example, analysis has shown that the transport properties vary very slowly with time and that we do not have to compute them at every time step. For the same baseline flow, the error introduced over a thousand iterations by computing the transport properties only every third time step is negligible (less than 0.1% of deviation over main flow variables such as the temperature). There might be more significant gains to be made for the thermodynamics, especially for reacting flows. In most combustion configurations, the region where thermodynamic real gas effects are significant is quite limited: an example is given later with Figure\cite{22}. Thus, we could envision some kind of hybrid TPG-RG scheme that would limit the number of computational cells where the full RG computations are performed. The switch for this scheme would be the value of

49
the local compressibility which is relatively inexpensive to compute. Also, the enthalpy and constant-pressure specific heat for each species are computed, under perfect gas assumptions, using standard curve-fit approximations[45], i.e. polynomials function of temperature. Typically, the range of temperature for these curve-fit coefficients is 300 K - 5000 K. This is an issue for our cryogenic simulations where we have injection temperatures as low as 100 K. However, most of the correlations are well behaved just outside their range of validity and we had no issues using the same coefficients for temperatures between 100 K and 300 K. A check is done at the beginning of each simulation to make sure this extrapolation is valid for each species.

3.2 Grid generation for axisymmetric configuration

The main issue is the generation of the grid at the centerline. For the 2D-axisymmetric formulation and the 3D_AXI_SRC, there is a special treatment in the metrics computation and in the source terms computation to make sure no singularity appears at the centerline. For the 3D_AXI_FLUX, we wish to change the formulation the least possible and thus we decide to slightly modify the grid generation. The only limitation is to actually start the grid slightly off the centerline in order to avoid a singularity. This could have been a problem if we had to keep the size of the ghost cells equal to the size of the flow cells. For example, that would have meant that if we wanted to start the computational domain very close from the centerline in order to minimize the size of the area not computed, we would have had to use a very small grid spacing. As shown on Fig. 4(a), with \( r_0 \) the distance from the last gridpoint to the centerline and \( \Delta r \) the grid spacing at the centerline, to avoid any singularity at the centerline, we need to have: \( \Delta r < \frac{r_0}{2} \). However, even this constraint does not satisfy the conservation of volume between the flow cell and the ghost cell. To respect this condition, we would need a grid like the one shown on Fig. 4(b). However, this latter grid raises another issue. In fact, it looks impossible to rotate this grid around the centerline as it is no longer axisymmetric. But since our implementation of the wall boundary conditions explicitely enforces the fluxes to be zero across the boundary, the equality of the cell volumes is not needed and we can use a grid similar to the one showed
on Fig. 4(c). Then, one just needs to carefully generate the ghost cells in the tangential direction. A simple rotation of an angle $\theta$ from the computational cell around the centerline is required. By copying the values of the computational cell in these ghost cells, we actually enforce the axisymmetric condition. The computation of the tangential fluxes using the ghost cells reproduces the effects produced by the additional terms of Eq. 3 and we can use the governing equations for the Navier-Stokes equations in three cartesian dimensions.

![Figure 4: Issues with the grid generation near the centerline.](image)

Figure 4: Issues with the grid generation near the centerline. Grids shown in (a) and (b) are not practical to use while the grid (c) allows an arbitrary grid spacing near the centerline while remaining axisymmetric (unlike (b)). Note that the letter FF represents a flow cell and the letter G represents ghost cells.

A last issue with the axisymmetric grid concerns the very high aspect ratio that can be obtained for the cells far away from the centerline. This is also only a concern for the 3D_AXI_FLUX methodology. As we move away from the centerline, the transverse dimension increases linearly with the radius while the radial resolution might be very small if we are trying, for example, to capture boundary layer profiles along a wall. This high aspect ratio $Y/Z$ might cause a completely wrong extrapolation of the face values since
the grid is turning in the K-direction. Basic geometry considerations yield the following condition if we want the extrapolated value at the face to actually be the value from a point belonging to the cell interface:

\[ \sqrt{1 + \tan^2 \theta} > \frac{1}{2} \left( \frac{Y(J + 1)}{Y(J)} + 1 \right) \]  

(87)

This restriction did not prove to reduce significantly the angular size of our axisymmetric slice (usually between 3° and 5°) but this condition is checked before each run to be on the safe side.

### 3.3 Boundary conditions

For inflow and outflow boundary conditions, the derivation of the real gas formulation can be found in Appendix [B.4](#). The previous section discusses about the slip-wall boundary condition applied along the centerline. Additional discussion on wall boundary conditions can be found in Sections [4.1.3](#).
CHAPTER IV

ASTRIUM SUB-SCALE CHAMBER

4.1 Geometry and operating conditions

4.1.1 From the actual chamber to the axisymmetric configuration

Figure 5: Axial view of a nineteen elements coaxial injector plate schematic. We notice the 60° axisymmetry of the configuration, highlighted here by the red lines.

The actual configuration of a typical rocket motor of current interest is very complex and highly three-dimensional. Figure 5 shows a typical (head-on) view of a multi-injector configuration. The injector plate consists of 19 coaxial injection elements. As noted earlier, because of the configuration of the injector, the whole combustion chamber is not axisymmetric but it does have 3 planes of symmetry. This means that a 60 degrees slice including 1 full injector (outer row), 4 half-injectors and a slice of the centerline injector is probably an accurate representation of the full injector plate. However, it would involve special treatment for the outer injectors such as embedded boundary conditions, and this is beyond the scope of the current effort. But we believe the rest of the framework would be in place for
such a simulation. An example of how the grid would look like is displayed on Fig. 6. The resolution for this grid is $300 \times 200 \times 100$ but we think the actual grid needed for accurate results would be at least 10 million points.

However, in order to maintain computational tractability, we do need to restrict our simulations to axisymmetric configurations and therefore we have to make some major assumptions. To summarize, we model the injector plate as made of concentric injector slots. So we geometrically transform the injector plate from Fig. 5 into either a 2D-axisymmetric computational grid or a slice of the full 3D configuration with the concentric annuli as shown on Fig. 7.

Because of the limitations of our approach where slots are replacing the actual injectors, the choices we make on the approximate axisymmetric configuration have a direct influence on the boundary conditions. The initial data provided by ASTRIUM are summarized on Table 8. The velocities given here are valid for the oxygen post exit but we need the values further upstream in the injector since we hint that both the recess and the taper of the injector will play an important role in the dynamics of the flow. For the conversion from the rows of injectors to the slots, we would like to make the following assumptions:

- We conserve the respective areas for the injection of oxygen and hydrogen.
Figure 7: Required transformation: from the real injector plate with 19 elements (Fig. 5) to a 3D, axisymmetric slice grid with multiple points in the tangential direction.
• We conserve the wall thickness at the post exit.

• We conserve the recess length, the taper length and the taper angle.

However, in the axisymmetric slot configuration, the oxygen openings are much narrower than in reality for the outer rows and we cannot keep the same taper without actually obstructing the oxygen channels. Assuming the taper angle is the most important factor for the mixing between the “coaxial” streams, we shorten the taper by a factor 3.

The consequences of these choices are unfortunately difficult to evaluate and add to the complexity of the analysis of the results. Especially since we are interested in the dynamics between the injectors, there is a distinct possibility that these dynamics will be strongly affected by our geometrical approximations.

A major restriction of the axisymmetric assumption is that the behavior at the centerline is different from the full 3D case. In the former case, flow motion across the centerline is not allowed. Although this is not realistic, for the conditions simulated here, this restriction may not be of great importance since the centerline injector only represents 1/19 of the flow-rate. Note that this would still be problem for the 60 degrees slice mentioned earlier, but not for the outer rows since the periodic boundary conditions could allow the coaxial streams to display any three-dimensional instability. The other issues as far as the grid generation is concerned have been addressed in Section 3.2.

For the rest of the geometry, Fig. 8 from Preclik et al.\cite{121} shows a schematic of the calorimeter chamber and nozzle of interest. The combustor consists of two pieces, a calorimeter cylinder with an inner diameter of 80.0 mm and a calorimeter nozzle with a throat diameter of 50.6 mm. The calorimeter chamber consists of 20 independently cooled segments, of which 11 belong to the 245 mm long cylinder section and 9 to the 144 mm long nozzle section. The total length of the combustor (injector face plate to nozzle exit) amounts to 409 mm and includes a 20 mm long igniter ring flanged between the injector and the calorimeter cylinder (see Figure 2). Additional details can be found in the mentioned reference.

Following earlier work on real gas combustion LES modeling in rocket motor \cite{167}, it
Figure 8: Schematic of the DASA calorimeter chamber cylinder and nozzle throat.
is well understood that a true LES will require simulation in full 3D but we justify this
approach here for five major reasons: (a) the computational cost of full 3D LES of a multi-
injector configuration is prohibitive at this time for parametric studies needed in a design
process, (b) there are many unknowns in the subgrid closure that remain to be resolved
before full 3D LES can be attempted, (c) a somewhat fine resolution can be used in a
axisymmetric approach, thereby resolving all important scales of motion without enormous
combutional overhead, (d) the 3D effects dominate in the regions where the large-scale
vortical structures break down into small-scale turbulence, however, this happens further
downstream away from the regions of interest near the injector, and (e) in the axisymmetric
LES approach (as opposed to steady state methods) the grid scale is used as a characteristic
length scale in the eddy viscosity, thus, the modeled dissipation scales with the local grid
size. In spite of the limitation of the axisymmetric approach, we believe it contains sufficient
physics of mixing and combustion to be useful for study of multi-injector rocket motors. As
mentioned above, a moderate increase in the computational resources (less than an order of
magnitude if we consider less than 10 points in the tangential direction) is only needed to
give our simulations a more pronounced three dimensional component and maybe alleviate
some of the concerns expressed here about a Large Eddy Simulation in an axisymmetric
configuration.

4.1.2 Computational grid

Figure 9 shows the grid used for the real gas simulations close to the injector plate while
Table 7 gives the precise dimensions for the different injectors. The tip walls between the
oxygen and hydrogen channels are resolved with only a few points, as are the hydrogen
channels. Due to the small dimensions (less than half a millimeter) of these channels, this
resolution still leads to a $\Delta y$ of the order of 50 microns. Near the motor wall a grid resolution
of $\Delta y = 20$ microns is used. The grid near the injectors is nearly uniform and is slowly
stretched away from the injector region. The maximum grid stretching is 5% axially and
7% radially. Earlier, some grid resolution issues were investigated primarily to ensure that
all the features near the injector lips were well resolved. Based on these studies we employ
a grid of 601 \times 382 in (x,y) directions for all the reported RG simulations.

![Grid Image](image_url)

(a) Overall view  
(b) Injector detail

Figure 9: Details of the computational grid near the injection plane.

<table>
<thead>
<tr>
<th></th>
<th>Centerline injector</th>
<th>Outer injectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial O$_2$ channel radius (Exp.)</td>
<td>2.15 mm</td>
<td>2.15 mm</td>
</tr>
<tr>
<td>Initial O$_2$ channel radius (2D-axi)</td>
<td>2.8643 mm</td>
<td>1.129 mm</td>
</tr>
<tr>
<td>Initial O$_2$ channel grid points (2D-axi)</td>
<td>26</td>
<td>16</td>
</tr>
<tr>
<td>Exit O$_2$ channel radius (Exp.)</td>
<td>3.15 mm</td>
<td>3.15 mm</td>
</tr>
<tr>
<td>Exit O$_2$ channel radius (2D-axi)</td>
<td>3.15 mm</td>
<td>1.8604 mm</td>
</tr>
<tr>
<td>Exit O$_2$ channel grid points (2D-axi)</td>
<td>26</td>
<td>16</td>
</tr>
<tr>
<td>Tip wall width (Exp.)</td>
<td>0.325 mm</td>
<td>0.325 mm</td>
</tr>
<tr>
<td>Tip wall width (2D-axi)</td>
<td>0.325 mm</td>
<td>0.325 mm</td>
</tr>
<tr>
<td>Tip wall grid points (2D-axi)</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Lower H$_2$ channel width (Exp.)</td>
<td>None</td>
<td>0.475 mm</td>
</tr>
<tr>
<td>Lower H$_2$ channel width (2D-axi)</td>
<td>None</td>
<td>\approx 0.444 mm</td>
</tr>
<tr>
<td>Lower H$_2$ channel grid points (2D-axi)</td>
<td>None</td>
<td>7</td>
</tr>
<tr>
<td>Upper H$_2$ channel width (Exp.)</td>
<td>0.475 mm</td>
<td>0.475 mm</td>
</tr>
<tr>
<td>Upper H$_2$ channel width (2D-axi)</td>
<td>0.585 mm</td>
<td>\approx 0.386 mm</td>
</tr>
<tr>
<td>Upper H$_2$ channel grid points (2D-axi)</td>
<td>9</td>
<td>6</td>
</tr>
</tbody>
</table>

The simulation model is implemented in parallel using MPI and employs a multi-block implementation. On an Intel Xeon cluster with an Infiniband interconnect, a single flow-through time for the RG simulation requires approximately 1500 single-processor hours. The RG simulations are carried out for around 3 flow-through time (after the initial transients have been washed out) to obtain properties for statistical analysis. The TPG simulations
have been carried out much further, typical 5-6 flow-through times after initial transients. In general, it has been determined that the mean properties are well converged after 3 flow-through times and the second-order moments converge within 6 flow-through times. Since, we are primarily interested in the mean properties (such as the mean heat flux) and in the transient features, the chosen simulation length is considered sufficient.

4.1.3 Operating conditions and boundary conditions

Table 8 also shows the boundary conditions used in the real gas (RG) and thermally perfect gas (TPG) simulations. Please note that for the oxygen velocities, the values displayed for the simulations correspond to the upstream part of the injector, before the taper. So, if compared at the same locations, the values are in fact closer. But there is still a significant difference because we originally chose to inject the oxygen under supercritical conditions (201 K instead of 101 K) in order to avoid any issue with the transcritical phenomena. Since then, transition from sub-critical to supercritical has been simulated with the current flow solver with a very high resolution but much closer to the critical point than in the current conditions. Details are given in Section 5.3. Since the geometrical assumptions in the current study seem to prevent any definitive conclusion to be made on the physics inside the combustion chamber, we have chosen not to include sub-critical injection of the oxygen in this work. We firmly believe this is an available capability of this solver, although maybe not a very efficient or stable one.

Boundary conditions are very important in numerical simulation and have to be implemented with great care. We employ no-slip, isothermal conditions on all walls and characteristic based inflow/outflow boundary conditions for real gas, as described in Appendix B.4. These boundary conditions reduce to the thermally perfect conditions when $Z = 1$, and therefore, can be used for both perfect and real gas flows.

The current engine configuration uses a choked nozzle at the exit so outflow is supersonic. Studies showed that the choking process from an arbitrary initialization, while the LOX-GH$_2$ mixture is burning and heat is being released, is a complex process that can lead to numerical instability. To achieve choking, and at the same time maintain combustion
at the required chamber pressure, we enforce a constant flow-rate condition at the inflow. For this purpose, we set the flowrate, the temperature and the mixture composition at the inflow, and solve for the density. However, by preventing any fluctuation in the flow-rate, we are in fact assuming a steady-state operation that eliminates one of the main sources of combustion instability in liquid rocket engines. While no combustion instability has been reported for this particular experiment, this boundary condition might be too restrictive in other configurations.

The isothermal wall boundary condition for temperature is problematic since we are interested in wall heat flux prediction. The actual motor Fig. 8 employed external cooling jackets around the combustion chamber. The exact wall temperature on the inside wall of the motor is not known. This wall temperature is extrapolated from the amount of heat absorbed by the water in the cooling channels and the temperature of the wall in these same cooling channels. Furthermore, the real motor had multiple injector elements while we are simulating an axisymmetric configuration. Therefore, our estimate for the wall heat flux is limited by these unknowns.

We implement an isothermal no-slip wall with the wall cell temperature set to a fixed value so that the temperature at the interface between the flow cell and the ghost cell remains constant through time, assuming a linear temperature gradient:

\[ \frac{1}{2} (T_j + T_{j+1}) = T_{\text{wall}}. \]

An alternate, second-order accurate, approach for the temperature gradient at the wall was also considered. For a uniform grid at the wall, this yields:

\[ \left( \frac{\partial T}{\partial y} \right)_{\text{wall}} = \frac{-9T_j + 8T_{\text{wall}} + T_{j-1}}{3\Delta y} \quad (88) \]

The main shortcoming of both these approaches is that the gas-side wall temperature is probably not constant in time. In the actual experiment, the steady state temperature measured is the temperature of the wall on the coolant side. For proper modeling of the wall condition, it would be necessary to solve the heat conduction through the wall, including the effect of the coolant flow so that the internal wall temperature does not have to be specified. The first steps towards such a coupled, multiphysics solver are given in Section 5.5.
Table 8: Physical conditions at the inflow of the combustion chamber

<table>
<thead>
<tr>
<th></th>
<th>Experiment</th>
<th>Simulation (TPG)</th>
<th>Simulation (RG)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber pressure</td>
<td>100 bar</td>
<td>100 bar</td>
<td>100 bar</td>
</tr>
<tr>
<td>Mixture ratio</td>
<td>5.964</td>
<td>5.964</td>
<td>5.964</td>
</tr>
<tr>
<td>Oxygen velocity</td>
<td>11 m.s(^{-1})</td>
<td>66 m.s(^{-1})</td>
<td>41 m.s(^{-1})</td>
</tr>
<tr>
<td>Liquid Oxygen Temperature</td>
<td>101.3 K</td>
<td>201.3 K</td>
<td>201.3 K</td>
</tr>
<tr>
<td>Hydrogen velocity</td>
<td>270 m.s(^{-1})</td>
<td>150 m.s(^{-1})</td>
<td>164 m.s(^{-1})</td>
</tr>
<tr>
<td>Hydrogen Temperature</td>
<td>106.4 K</td>
<td>106.4 K</td>
<td>106.4 K</td>
</tr>
<tr>
<td>Total Propellant Flow-rate</td>
<td>8.81 kg.s(^{-1})</td>
<td>8.81 kg.s(^{-1})</td>
<td>8.81 kg.s(^{-1})</td>
</tr>
</tbody>
</table>
4.2 Results and discussion

4.2.1 Sensitivity to grid and model parameters

Due to the computational costs of the real gas computations, all the studies mentioned in this subsection have been conducted with the thermally perfect gas assumption in the thermodynamic framework.

4.2.1.1 Grid independence

We conducted some grid independence studies using the TPG setup. Axial grid was changed from 326 to 404 and the radial grid was varied from 226 to 326. The key focus of these grid resolution studies was again the near-injector region where mixing and most of the combustion takes place. All in all, beyond the grid of $354 \times 276$ points, very little overall change was observed. Maximum variation of some variables was less than 5 percent, while most of the resolved features looks identical. Therefore, reported TPG simulations in the the results section are for the grid of $354 \times 276$.

4.2.1.2 Sensitivity to Model Parameters

As noted earlier, the subgrid model coefficients $C_\nu$ and $C_\epsilon$, and the EBU model coefficient all can be either determined using the dynamic procedure or need to be adjusted for the high pressure conditions simulated in this study. We use the TPG approach to evaluate the sensitivity of the results to changes in these model parameters since it is computationally efficient. We discuss only some representative results, for brevity.

Figure 10 shows the influence of the mixing time scale constant ($C_{EBU}$) on the radially-averaged mean temperature along the axis. Near the inlet, the temperature increases slightly with decreasing $C_{EBU}$, although the change is very marginal. Accordingly, the mass concentration of the combustion product $H_2O$ will also increase (not shown). This is consistent since smaller $C_{EBU}$ implies faster mixing and this leads to more complete combustion. Figure 11 shows the temperature distribution at two typical axial locations, 0.058m and 0.256m from the injector. The temperature has some differences at $x = 0.058m$, which is likely due to the interaction between the multiple injectors (see further discussion on the
However, by $x = 0.256m$ there is no noticeable difference in the temperature profiles for different values of $C_{EBU}$. These results suggest that the variation of the combustion process is only weakly affected by the changes in the model coefficient $C_{EBU}$.

![Figure 10: Influence of $C_{EBU}$ on the cross-section average temperature.](image)

The influence of $C_{\nu}$ and $C_{\epsilon}$ in the subgrid model were also analyzed (not shown, for brevity). There is very little change in the profile and/or the mean temperature magnitude for different values (within 20 percent of the nominal values) of these coefficients. These results are not surprising since the grid resolution is fine enough to resolve all important scales, especially in the injector region of high shear mixing. Furthermore, since the grid scale $\Delta$ is used as the characteristic scale, dissipation scales with the grid size and therefore, does not overwhelm the flow physics.

We conclude from these studies that although the model coefficients can impact some of the local physics, the time-averaged profiles show little or no sensitivity to the changes in the model parameters, within a nominal range. It is not clear at this time if this insensitivity is due to the other underlying assumptions used in this study. Nevertheless, it appears that the results discussed below should be self-consistent and relatively insensitive to the model constants used in the closure. This being said, we can now focus on general flow field observations such as the study of the instantaneous data, the analysis of time-averaged quantities and the flame structure.
Figure 11: Influence of $C_{EBU}$ on the temperature distribution at two sections.
4.3 Unsteady flow features

Figure 12 shows a time sequence of the density and temperature contours in the near field of the injectors for the RG simulation. The density contours show the state of the oxygen jet. Due to the supercritical injection condition, the incoming oxygen jet is not liquid but the density is close to the one of a liquid jet, as indicated by the dark areas in these figures. Further downstream, the jet seems to have a mixed liquid-gas behavior.

Closer examination shows that each of the three injectors exhibits different flow and combustion patterns. The jet at the centerline cannot flap due to the centerline restriction. Thus, it looks very stable, and even though a shear mixing layer is present near it, the core stays mostly unperturbed for several diameters downstream. Combustion occurs in the mixing layer around the oxygen jet. However, since the mixing region is very thin, the combustion region is also limited.

All the three injectors interact with each other. However, the behavior of the flow near each of them is different due to their relative locations. To understand this behavior, we show in Fig. 13 a time sequence of the vorticity contours superimposed with the velocity vector field. The velocity vectors have been uniformly resampled on the computational domain and although they represent cell center values, are displayed on a grid based on grid points, leading to a small discrepancy as can be seen on the centerline, where the velocity vectors should not have a radial component. These figures closely correspond to the figures shown in Fig. 12 but are chosen to highlight the flow motion. Comparison of both these figures show that the middle injector interacts significantly with the other two. The shear layers from both sides of each of the injectors shed vortices that grow and interact with the vortices from the shear layer of the adjacent injector. Both the vorticity and velocity vector fields show that the shear layers from the two edges of each injector undergo a periodic shedding process. The low pressure region at the base of the steps between the three injectors offer a mechanism to create and maintain the vortex shedding process.

Since the three step planes are of different height, the interaction and vortex sizes are also different. However, there is similarity in the interaction between the upper shear layer
of an injector with the lower shear layer of the adjacent injector, and vice versa. These interactions occur behind the base walls and result in alternate shedding of vortices from the upper and lower shear layers. The size of these vortices ranges between 20-60 mm depending on the local state.

This vortex shedding process is related to the instability in the shear layers from each of the injectors. Overall, the interaction for the middle injector is the most dramatic. This is because, the central injector is restricted by the centerline condition and the upper injector is next to the combustor wall, both of which inhibit the flapping of the shear layers closer to these walls.
Figure 13: Instantaneous tangential vorticity and velocity vector fields at 6 different instants for the near-field of the three rows of injectors.
Analysis of the time sequence of the vortex motion for the middle injector shows a frequency of 3.6 KHz (the other shedding frequency is similar). This corresponds to a Strouhal number $St = fD/U$ of 1.24 (using $D = 0.102$ m, the hydrogen step height, and $U = 300$ m.s$^{-1}$, characteristic velocity of the hydrogen jet), which is in the jet preferred mode for a free jet \[49\].

Thus, the flow from all the injectors is periodically controlled by alternate vortex shedding. This in turn causes the flapping of the jets from the upper and lower injector. Since the lower jet is more stable, the upper jet motion appears to dominate. As shown in Fig. 12, this flapping instability leads to a pinch-off of the jet, with a pocket of dense, unburned oxygen being convected downstream.

The outermost shear layer next to the combustor wall also shows some shedding, however the flapping is constrained by the wall. We will see later that the impingement of this jet on the chamber wall is critical for the transient heat flux.

The oxygen jet instability is controlled by both thermodynamic (e.g., specific heat, heat release from combustion) and transport (e.g., viscosity, thermal conductivity, molecular diffusion) properties and these properties must be computed accurately. Figures 14(a)-(c) show respectively, the molecular viscosity, thermal conductivity and specific heat at constant pressure for the RG simulation. All values are normalized by their representative perfect gas (constant) value. As can be seen, all properties show a wide range of values in the combustor. For both viscosity and conductivity, we can have gradients of one order of magnitude between each reactant stream, or between the reactants and the burned products. Also, these large variations extend quite far downstream, further than the variations of the compressibility parameter, which are mostly limited to the oxygen jets inner core. This justifies our emphasis of getting an accurate estimate of these transport properties, since these large gradients probably play an important role in the overall flow behavior. This will be emphasized in the last part of this results section.
Figure 14: Instantaneous snapshot of the normalized dynamic viscosity (top), thermal conductivity (middle) and constant pressure specific heat (bottom) in the combustion chamber. The quantities have been normalized by their thermally perfect values at the same local temperature.
4.4 Analysis of time averaged quantities

The statistical averaging has been performed over a time of about 2 ms, which corresponds to a little more than a flow-through time. Although this is probably not long enough for a true statistically stationary average, we believe this gives a reasonable estimate of the time-average solution. In particular, we do not believe that any of our qualitative conclusions could be altered by a longer averaging.

The average pressure field (not shown here) is smooth without large fluctuations, and close enough to the nominal conditions in the bulk of the chamber. This has required some adjustment of the nominal throat size once it has been choked. There is also a low pressure region caused by recirculation of vortices behind the injector walls. The centerline pressure is within 5% of the nominal conditions even though some small oscillations occur, probably due to the centerline condition and the grid resolution there. However, these oscillations do not impact the results.

The difference between the centerline injector and the two other slots is obvious in Fig. 15. We see that the centerline jet is much longer than the outer ones for two reasons: (a) the diameter of the centerline injector is more than twice the outer slots, 5.728 mm against 2.578 mm, and (b) because of the axisymmetric assumption, there is no flapping of the centerline jet, whereas flapping seems to enhance the mixing for the outer two inlets.

Figure 16 shows the density profiles against a non-dimensional coordinate $x/D$, where $D$ is the diameter of the LOX inlet before the expansion of the coaxial injector. These profiles are taken along the x-axis, from the radial coordinate that correspond to the "center" of each row of injectors. These coordinates are respectively 0 m, 0.016 m and 0.032 m for the centerline injector and the two outer rows. The origin is taken at the tip plane. It has to be noted that in this coordinate system, the injector plane does not have the same location for all injectors. The physical distance between the tip and the injector planes is 3.19 mm, which represents 1.24 $x/D$ for the outer rows, and 0.56 $x/D$ for the centerline injector. This explains the shift to the right of the outer profiles. Also, the lack of combustion along the centerline probably explains the slower decay further downstream for the centerline injector.

Taking into account these two features, we look at the dependence in $x/D$ of the density
Figure 15: Mean density field near the injection plane. The statistical averaging is done over about 2 ms.
Figure 16: Density decay downstream of the centerline injector and of the two rows of outside injectors.

Profiles. In the region where they follow a power-law of the type:

$$\rho \alpha \left( \frac{x}{D} \right)^n$$

(89)

the exponents are found to be close to the values given by Oschwald et al. [106], who report values below -1 for supercritical jets without combustion.

Figures 17(a) and (b) show respectively, the time-averaged axial and radial velocity profiles in the combustor downstream of the inlet plane. The axial distance is normalized by the step height of $H = 0.0102$ m. Note that the scale for the x-axis and the y-axis are different. The dimensions are stretched in the axial direction as obviously 1 unit in the x-direction is not equivalent to 0.01 m in the radial direction. This allows us to have a better view of the near-field velocity profiles. The velocity profiles are plotted every 0.1 H and the profiles have been normalized by the maximum value of the axial velocity at the inflow, that is 542 m.s$^{-1}$. Thus, a speed of 542 m.s$^{-1}$ is represented by a point 0.1H away from the profile plane. It appears that the hydrogen flows actually attain higher speeds as
they expand right after the injection plane. As can be seen, the shear layers are clearly
evident for at least one step height downstream of the dump plane. The axial profiles also
show the spreading of the jets as well as the extent of the recirculation regions downstream
of the injector steps. It seems that we observe mean negative axial velocities until a distance
of about 0.6 H.

Figures 18(a) and (b) show respectively, the axial and the radial velocity fluctuation
profiles in the combustor. Regions of high axial velocity fluctuations are seen in the shear
layers whereas, the radial fluctuations are larger in the regions where the adjacent vortex
shedding causes interaction between the two shear layers. The fluctuations persist for
quite a distance downstream and probably play an active part in the final mixing of the
reactants. We also observe that the recirculation region between the two outer rows displays
a symmetric flow field as expected since the conditions on each side are identical. This seems
to show that our time averaging, although not perfect, is sufficient. On the other hand, the
flow between the centerline injector and the first row of injector is asymmetric since the
flow conditions are different on each side because of our geometrical assumptions.
Figure 17: Profiles of the mean velocity components in the region close to the injector plate. Note that dimensions are stretched in the x-direction.
Figure 18: Profiles of the velocity fluctuations in the region close to the injector plate. Note that dimensions are stretched in the x-direction.
4.4.1 Flame structure

The location of the flame is of course a very valuable information which has been the subject of much debate for this configuration. Very limited reliable measurements are available for supercritical combustion in a coaxial injector. Using new visualization techniques on subcritical LOX/GH2 flames, Herding et al. [56] claimed that the flame is established in the outer boundary of the LOX jet, in a region of low velocity. Even though the interpretation of OH concentration data (LIF, planar laser light scattering, emission imaging) is difficult, this has been later confirmed using tomography (see Herding et al. [55]). However, Mayer et al. [89] reported that a pilot flame is anchored at the tip of the tube between the oxygen and the hydrogen under supercritical conditions. The most recent studies [85, 98] seem to confirm this observation.

Figure 19 shows the instantaneous contour of the stoichiometric flame surface, that is where $Y_{O_2}/Y_{H_2} = 8$. It can be seen that the flame is anchored at the lip between the hydrogen and oxygen injectors. This agrees with earlier observations [85] where the flame was indeed observed in the recirculation region behind the tip. Whether the flame is in reality attached to the wall seems unlikely, but to prove it would require much better resolution as well as an isothermal boundary condition at the tip. We chose not to do this for simplicity. We can also notice an independent flame around a pocket of unburned oxygen. We know this pocket is composed of oxygen by comparing Fig. 19 with Fig. 12. Although Fig. 19 shows the instantaneous flow field at a slightly later instant, we can see that the pockets of dense ($\rho > 50 \text{ kg.m}^{-3}$) gas can only be oxygen and corresponds to the closed flame observed on Fig. 19. This seems to be a characteristic of the RG simulations as this is not observed for the TPG runs.

Figure 20 shows the time-averaged temperature contours. It can be seen that the flame is indeed attached to the sleeve that separates the two coaxial jets. The mixing layer created in the wake of this wall is resolved in the current simulation with enough accuracy so that a continuous region of high temperature is always present. Additional analysis shows that this flame anchoring location is in a region of high strain rates ranging from 30 m.s$^{-1}$ to 300 m.s$^{-1}$. It is possible that such a high strain can cause flame extinction and lift-off,
and could result in a lifted flame structure. However, flame extinction/re-ignition is a very complex process and relatively detailed kinetics will be needed to understand this process.

Figure 21 compares the temperature fields of the present study with previous numerical results [122] using RANS and an axisymmetric configuration as well. These simulations were performed assuming that both reactants were injected as sprays in the combustion chamber. Whereas the hydrogen was allowed to evaporate immediately, a supercritical LOX gasification model controlled the behavior of the oxygen spray. There are similarities and differences between these two fields. Both computations show temperature fields reaching close to their maximum values after approximately 0.08 m. Also the overall range of temperature is pretty similar in both cases. But the LES simulation shows even less combustion along the centerline than the RANS, probably because of the lack of extra radial dissipation in the LES.
Figure 20: Time-averaged temperature field near the injection plane. The arrows show the anchoring of the flame at the tip of the sleeve between the oxygen and the hydrogen.
(a) Current study using Large Eddy Simulation

(b) ASTRIUM results using Reynold-Averaged Navier-Stokes

Figure 21: Time-averaged temperature field
4.5 Comparison of TPG and RG models

Three cases are considered here. The classical TPG and RG models as well as the TPG model with the real gas transport properties. This simulation combines Chung’s methodology described previously and including high-pressure effects with the thermally perfect gas framework. All simulations are started from the same initial real gas solution and run on the same grid of $601 \times 382$. They use the 2-step mechanism instead of the global mechanism. Since we have inlet boundary conditions that ensure that the mass flow-rate remains constant in time, the inflow conditions for both runs are similar in terms of flow-rate, temperature and mass fractions. However, we expect the inlet densities and velocities to differ, especially for the oxygen jet that is injected under supercritical conditions for which its compressibility is significantly smaller than 1.

Only instantaneous results are discussed here, mainly because our interest is centered on the dynamics of the flow and on how the choice of the model can impact them. We have attempted to show characteristic figures that closely compare the flow features at (nearly) the same instant of flow development (identified here as the vortex shedding process from the injector tip).

On Fig. 22 which displays the instantaneous oxygen concentration for both cases, one can clearly see the different behavior that occurs under the thermally perfect gas assumption. As stated before, the density of the oxygen jets is much lower for the TPG case (around 250 kg.m$^{-3}$) than for the RG case (around 380 kg.m$^{-3}$) and thus the inlet velocity for the oxygen is 50% higher in the TPG case. This has of course a direct impact on the dynamics of the jets since the velocity ratios have been changed. The breaking-up of the oxygen jets for the RG case seems to occur earlier than for the TPG case, leading to large, round pockets of unburned oxygen being convected downstream. The oxygen jets in the TPG case appear thinner and extend further in the flow without pinching. As a result, although both jets seem to flap in a similar fashion, the jet in the TPG case will impinge the wall further away from the injector plate. This will have a consequence on the wall heat flux. Furthermore, we can notice one of the shortcomings of our simulation on this figure by taking a closer look at the centerline jets. Because of the axisymmetric assumption, this jet
is constrained to remain along its principal axis and cannot flap like the outer rows. Thus, we experience poor mixing along the centerline of the combustion chamber. The behavior is the same for both TPG and RG models: even the very different transport properties computed in both cases (inlet dynamic viscosities are about twice as large in the RG case as shown on Fig. 14) do not seem to have any influence on these constrained jets.

Figure 22: Instantaneous oxygen concentration fields for the TPG run (top) and RG run (bottom). The figure for the RG also includes a dotted area where the compressibility is in the range 0.6-0.9, i.e. where the real gas effects are significant.

Also, the Figure 22 for the RG case allows us to look at the extent of the real gas effects in the combustion chamber in terms of the compressibility $Z$. As mentioned before, the axisymmetric configuration and our assumptions to keep the velocity and momentum ratios
close to the experimental values prevent us from having identical injectors. This explains why the real gas effects can be felt over a much larger region for the centerline injector. We even see that unburned pockets of oxygen, after having broken up from the jet, can experience significant departures from perfect gas behavior. This feature is not present in our simulation for the outer rows probably because their apparent diameter is smaller than what it should be in reality. For all jets, we can see that our RG model allows for a smooth transition between regions where the perfect gas model is not valid and where the compressibility is almost 1. Since the real gas model is very expensive in terms of computational resources, there is a need in the future to look at ways to bypass most of the RG computations when Z is sufficiently close to 1.

In relation with these pockets of unburned oxygen, there is another significant difference between the TPG computations and the RG computations, illustrated by Fig. 23. The two snapshots shown here have been taken at the same instants than in Fig. 22. It seems that the flames for each row of injectors are not interconnected in the TPG case whereas they appear contiguous for the RG case. Although this is just a snapshot, these different behaviors have been observed over a lengthy period of time. It seems like the pockets of oxygen that are breaking up more easily in the RG case are in fact burning in a manner analogous to the “group combustion” observed among liquid droplets. On the other hand, the more continuous oxygen jets in the TPG simulation appear to burn independently. This striking difference might be explained by the very different transport properties in the two cases.

The average wall heat flux for both cases is shown in Fig. 24. Several features are interesting to discuss. First, the absolute level of heat flux, several tens of mega-watts per meter-square, is characteristic of those encountered in actual rocket engines. It is important that our simulations can represent such high values of heat transfer. Only looking at the laminar (or molecular) conduction of heat at the wall, such high rates of heat flux represent a temperature gradient of approximately 1000 K over 20 microns, the characteristic distance of our first cell center to the wall. This plot seems to show that for both RG and TPG models, the sub-grid model is able to capture at least part of the physics occurring along the
Figure 23: Instantaneous temperature fields for the TPG run (top) and RG run (bottom).
Comparing both RG and TPG heat flux profiles, we can see that the peak value for the TPG model is higher and occurs further downstream compared to the RG simulation. This can be related to the jet dynamics described in the previous paragraphs, which showed that the jet flapping is different between the two cases. This flapping causes the heat transfer to the wall to be a very transient phenomena.

![Figure 24: Time-averaged heat flux through the combustion chamber wall for the RG case (dotted line) and the TPG case (full line).](image)

Finally, the profile obtained for the simulation using the TPG model with the real gas transport properties is also shown on Fig. 24. We can see once again the influence of the transport properties on the jets dynamics with the difference between the pure TPG profile and the mixed TPG/RG profile. The oxygen jets for this mixed case have less inertia than for the RG case but are more viscous than the pure TPG case. As a result, the oxygen jets are much more constrained by the hydrogen annulus and the flapping is reduced. Thus, the smaller value of the initial maximum on the heat flux profile. Even though this local behavior is different, we are still injecting the same quantity of reactants.
in the same conditions as for the TPG case. Since far downstream from the injection, the RG formulation and RG transport properties recover to their TPG counterpart, it is logical that the profiles for the TPG simulation and the mixed simulation are the same. For the RG, the lower inlet velocity for the oxygen seems to lead to less turbulent subgrid energy far downstream and thus to a lesser heat transfer in the later part of the chamber.

A region of particular interest is where the upper flapping jet impinges on the wall. Figure 25 shows the instantaneous maximum heat flux and the location of this maximum. If we compare the $k_{sgs}$ field in the region of impingement with locations further downstream, it can be seen that the unsteady impingement process generates small-scale turbulence and increases turbulent kinetic energy in that area. However, this increase in turbulent kinetic energy cannot by itself explain the increase in heat flux. Indeed, the flame is also impinging on the wall and increases the temperature gradient. Combined, these two effects explain the very large magnitude of the unsteady peak that occurs at a frequency of approximately 3 kHz, which is close to the frequency observed in the vorticity spectra. This frequency is characteristic of the vortex shedding observed at the exit of the hydrogen jet and appears to control the flame impingement on the wall.

Analysis of the data shows that unsteady flapping of the jets will result in transient high heat flux on the combustor wall. However, this may not be observed on the outer walls that are being cooled (and where data is being obtained). Assuming the wall is made of stainless steel, we obtain a thermal thickness of approximately $6.5\sqrt{\frac{\kappa}{\omega}} \approx 2.4cm$. Thus, if the wall is more than 2 cm thick, the cooling channel is not affected by the unsteady heat flux. In order to reach better agreement, we may have to reconsider our current assumption of fully isothermal wall. Assuming the temperature is constant on the coolant side, it may be necessary to solve the full heat equation in the domain with the heat flux boundary conditions provided by the computation of the full chamber. This is an issue that will need additional effort in the future.
Figure 25: Time history of maximum heat flux in the combustion chamber.
4.6 What we have learned

The unsteady numerical simulation of a sub-scale liquid rocket engine with multiple injectors has been attempted for the first time to our knowledge. However, because of the various assumptions that have been necessary to make, the relationship between our simulation and the actual flow conditions of the experimental chamber is probably distant. For example, our modifications to the actual geometry prevents us from conserving non-dimensional parameters such as the momentum ratio between the two coaxial streams. Also, the active cooling of the chamber has been neglected and we used a much simpler isothermal wall boundary condition. This does not necessarily mean that our modeled physical processes are incorrect but rather than our simulated configuration and the actual configuration are too different to be able to conclude definitely on why our heat flux (the only experimental data available for that case) is so far off the reality. Simply put, it is too possible to compare the Astrium results and our simulated results with our current set of assumptions, but our results do not appear to be a correct representation of the observed experimental behavior. We think that before we can come back to this very complex case, we need to isolate most (if not all) of the issues that have hampered the current effort.

However, limited experimental data are available in order to verify the validity of our different assumptions. Especially, no flow visualization of a multi-injector configuration is available, only more global quantities have been measured as of today. Thus, the current LES simulations, with a reasonable qualitative agreement with the available experimental observations, give us an idea of the dynamics of a typical rocket combustion chamber. It is shown that vortex shedding and flame dynamics are intrinsically linked. Influence of various parameters and model choices is examined through the evaluation of both steady-state and instantaneous results. The comparison between RG and TPG computations shows that real gas effects have an overall influence despite being limited to the core of the oxygen jets. The transport properties have also a strong influence and should not be neglected in any effort to model such system. Finally, current simulations predict a lower heat flux in the cylindrical portion of the chamber and a higher heat flux in the near-injector region, with some new insight gained on the unsteady nature of heat flux due to the transient impingement of
the jet flame on the wall. Transient motion causes a wide variation in the heat flux on the gas side, even though, the high frequency associated with these transient events might prevent it from affecting the coolant side. Solving the heat equation in the chamber walls could help resolve this issue. Although our heat flux profile for the ASTRIUM sub-scale chamber does not match the experimental data, the same shape has already been observed experimentally for a similar 19-element sub-scale configuration [46]. They do not provide any physical explanation for this heat flux profile so we cannot confirm or contradict our claim that this is due to major impinging of the flame on the chamber walls. While not dismissing all the assumptions that the current work has made, this might be a hint in order to explain this behavior when other possibilities will be eliminated.
CHAPTER V

CODE VERIFICATION AND VALIDATION

For an introduction to the verification and validation of CFD solvers in the context of liquid rocket engines, we refer the reader to the discussion provided by Lin et al. [76]. For more details on this topic, we recommend the exhaustive work by Roache [127] and more recently Oberkampf et al. [97, 155]. The cases presented in this chapter are low-level cases but represent necessary building blocks for a full liquid rocket engine simulation.

5.1 Traveling waves

In order to validate the boundary conditions mentioned in Section 3.3 and described in Appendix B.4, we reproduce the numerical simulations of Baum et al. [6] using a 3D grid with 2 processors in each direction in order to verify that MPI communication is working as well for the ghost cells at the domain boundaries. We use the same physical dimension as in the original paper, that is a domain of length \( L = 2 \) mm. The overall grid size is \( 129 \times 33 \times 33 \) and the timestep is fixed at \( 1.25 \times 10^{-8} \) s. We initialize our computational domain with a propagating acoustic wave using the following conditions:

\[
\begin{align*}
    u &= u_0 + A \exp \left( - \left( \frac{B x - L/2}{L} \right) \right) \\
    p &= p_0 \pm \rho_0 c_0 (u - u_0) \\
    \rho &= \rho_0 \pm \frac{\rho_0 (u - u_0)}{c_0} \\
    T &= \frac{p}{\rho R}
\end{align*}
\]

The wave propagates either towards the inflow or the outflow depending on the signs of the pressure and velocity perturbations. If they are of same sign, the wave moves towards the outflow whereas it moves towards the inflow if the pressure and velocity perturbations have different signs. This allows us to easily test both the subsonic reflecting inflow and the non-reflecting outflow. Figures 26 and 27 display the perfect propagation of the waves according
to theory. In Fig. 26, the wave bounces on the inflow reflecting boundary condition as the pressure disturbance doubles on the boundary and the velocity disturbance changes sign. Note that the reflected wave is almost a perfect copy of the incoming wave. For the outflow test in Fig. 27 we observe the wave exiting the domain without any significant disturbance being reflected inside the computational domain.

Figure 26: Reflection of an incoming acoustic wave on an inflow boundary condition. Time evolution of the pressure (a) and velocity (b) profiles. The black profile corresponds to the initial conditions. Each subsequent profile (red, green, blue, yellow and grey) is taken at a time interval of 1.25 µs.

Figure 27: Exit of an acoustic wave through an outflow boundary condition. Time evolution of the pressure (a) and velocity (b) profiles. The black profile corresponds to the initial conditions. Each subsequent profile (red, green, blue, yellow and grey) is taken at a time interval of 1.25 µs.
5.2 Annular pipe

Another test case relevant to the rocket configuration is the annular pipe flow, that is the flow between two concentric pipes. This is representative of the typical flow in an outer annulus of a coaxial injector as shown on Fig. 28. Because of its simplicity, it is a good case for validation and evaluation of the numerical cost of the different methods for axisymmetric configurations.

![Figure 28: Annular pipe flow configuration.](image)

We consider a pipe of length 1 meter, with the outer radius $a = 2 \times 10^{-3}$ m and the inner radius $b = 1 \times 10^{-4}$ m, dimensions similar to the ones we can find in a laboratory for a sub-scale rocket injector setup. These small dimensions in an axisymmetric configuration also allow significant departures from the classical 2D solution (Poiseuille flow). We are interested in the developing laminar flow in this pipe in order to compare the numerical results with the analytical solution of the steady state, fully developed flow in an annular pipe. This can be found in the classical literature [159]:

$$u(r) = \frac{-dp/dx}{4\mu} \left( a^2 - r^2 + (a^2 - b^2) \frac{\ln(a/r)}{\ln(b/a)} \right)$$ (90)

Here $u$ represents the axial velocity, $r$ the radial coordinate and $-dp/dx$ the pressure gradient. We apply a flat profile at the entrance of our 1 meter long pipe. The mean velocity...
of this flat profile is determined by the flowrate $Q$ that will theoretically go through this pipe under a given pressure gradient:

$$Q = \frac{\pi}{8\mu} \left( -\frac{dp}{dx} \left( a^4 - b^4 - \frac{(a^2 - b^2)^2}{\ln(a/b)} \right) \right)$$

(91)

The dynamic viscosity $\mu$ has no influence on the turbulent character of our flow since we enforce a laminar solution by not perturbing the flow. On the other hand, the pressure gradient is the main unknown variable in this case since it is not strictly enforced in the simulation. With the use of the characteristics boundary conditions, the pressure difference between the inflow and the outflow will slightly evolve during the simulation. However, this small change does not influence much the resulting velocity profile.

The reference grid have dimensions $401 \times 41 \times 2$ with a stretched grid normal to the wall that yields a laminar $y^+$ of about 3 for the first cell center. Figure 29 presents the evolution of the velocity profile in the middle of the pipe for the 3D AXI FLUX code. After the initial numerical transients, it tends towards the analytical, skewed solution and becomes notably different from the Poiseuille profile.

![Figure 29: Velocity profiles for a concentric annulus with $a = 2$ mm and $b = 0.1$ mm.](image-url)
Table 9: Timing comparison for the different axisymmetric frameworks available for our flow solver. The simulations have been performed with 1 to 32 1.5 GHz power4 processors on an IBM p655+, the quantity expressed in CPU s/cell/step remaining essentially constant. The problem modeled is the DNS of a two-dimensional \( (401 \times 41 \times 2) \) annular pipe with 1 species (air). The physical timestep is \( 2 \times 10^{-8} \) s and the run is completed after 10000 iterations. The 1D exchange corresponds to a vectorized method to exchange information between processors.

<table>
<thead>
<tr>
<th></th>
<th>3D_AXI_FLUX</th>
<th>3D_AXI_FLUX 1D exchange</th>
<th>3D_AXI_SRC</th>
<th>2D_AXI</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU s/cell/step</td>
<td>9.2 \times 10^{-6}</td>
<td>7.0 \times 10^{-6}</td>
<td>4.2 \times 10^{-6}</td>
<td>1.5 \times 10^{-6}</td>
</tr>
</tbody>
</table>

This simple case allows us to time the different frameworks available for our flow solver. Table 9 presents the computational cost in CPU\(^s\)/cell/step, an invariant quantity for a given flow solver on a given machine. It compares the 2D-axisymmetric approach, 3D-axisymmetric approach with source terms and the 3D-axisymmetric approach with tangential fluxes. Note that two different methods for message passing are compared in the case of the 3D_AXI_FLUX method, showing the influence of processor mapping even for simple configurations. We see that there is quite an overhead with the 3D flow solver, even when we are using essentially the same exact framework: the 3D_AXI_SRC is almost 3 times as slow as the 2D-axisymmetric code. This is the price to pay for a much more generic flow solver, capable of switching easily from one geometry to another and boasting many more features than the 2D solver which can only model really simple geometries such as a pipe or the ASTRIUM chamber for which it has fine-tuned. We also see that the 3D_AXI_SRC formulation is about twice as fast as the 3D_AXI_FLUX approach which is clearly not justified in such a simple case.
5.3 Transcritical injection

We model the injection of a liquid nitrogen jet above the critical pressure into a chamber at ambient temperature filled with quiescent gaseous nitrogen. Under these conditions, the liquid nitrogen is a compressible liquid and the gaseous nitrogen is supercritical. The test conditions are somewhat arbitrary but are similar to the conditions expected in the Georgia Tech high pressure experimental facility where experiments are being carried out\textsuperscript{[154]}. The inlet target temperature is 120 K and the chamber temperature is 298 K. The pressure is 100 bar. The target velocity of the liquid jet is $100 \text{ m/s}$. The target value refer to those used for the non-reflective boundary conditions: velocity and temperature are allowed to vary around a target value to ensure non reflectivity of incoming acoustic waves.

The inlet diameter is $2.2\text{mm}$ ($D_0$). The axial length of the inlet pipe is $11D_0$ for a total axial length of $54D_0$. The diameter of the combustion chamber is $9D_0$. The axial resolution is 1952 points (60 points for the inlet pipe) and the transverse resolution is 361 points. For this simulation, a pure two-dimensional formulation with no axisymmetric or three-dimensional component. The grid is stretched towards the dump wall in the axial direction and towards the shear layer in the transverse direction. The current study can be categorized as 2D DNS similar to the DNS studies by Miller and Bellan\textsuperscript{[91, 92]}. However, our studies focus on spatially evolving jets whereas these studies dealt with temporal mixing layers.

A very important feature of the our solver is that it must handle the transition from compressible liquid to supercritical gas. We recall here some specific thermodynamics to illustrate the usefulness of this test case. According to its pressure and temperature, a pure fluid undergoes different state changes. As we can see on Fig. 30 if the pressure is above the critical pressure but below the critical temperature, the fluid is called a compressible liquid. If the temperature is raised above the critical temperature, the fluid becomes a supercritical gas. Between those two regions, no real phase change occurs, just a change of state without discontinuities (for example, the density and the specific heats change but smoothly). Even if our real gas \textsuperscript{EoS} is not able to deal with the near-critical region or the transition between subcritical liquid to compressible liquid, it is still able to handle
perfectly the change from compressible liquid to supercritical gas (and vice-versa) as well as the transition from supercritical gas to subcritical gas (and vice-versa). This is shown on Fig. 30. The phase transition between compressible liquid and supercritical fluid is often called transcritical transition and this is the phase transition we demonstrate with the current simulation.

Figure 30: Phase diagram of nitrogen. The dashed arrows represent the possible state changes developed in this study.

Figure 31 displays some flow features of our jet flow near the injection plane. We see the onset of instabilities as soon as the flow enters the main chamber whereas the shear layer starts rolling up after about a length of about $2 D_0$. These individual vortices are similar to the ones studied in temporal mixing layers. Here they end up pairing with each other after a length of at least $4 D_0$, forcing the nitrogen jet to pinch and to "break up". Also shown in Fig. 31, the constant pressure specific heat depicts the transition described earlier: the liquid jet has a $C_p$ of about 2500 $J/(Kg.K)$ whereas the supercritical gas has a $C_p$ of 1200 $J/(Kg.K)$. As the compressible liquid heats up, it reaches the critical
temperature, the value of the $C_p$ increases. As the temperature keeps on increasing, the fluid becomes a supercritical gas and the value of the $C_p$ decreases. It has to be noted that the peak of $C_p$ does not actually occur at the critical temperature if the pressure is different from the critical pressure. The fluid actually crosses what is called the "pseudo-boiling" line which is a continuation of the liquid-gas line of equilibrium. Figure 32 illustrates this "pseudo-boiling" line with a P-T diagram for oxygen generated with our Peng-Robinson formulation. The sharp discontinuity at the bottom-left of the diagram is the liquid-gas line of equilibrium that our equation of state cannot actually resolve. The specific heat on this line is actually non-defined theoretically while our formulation yields values of up several to several hundred of thousands of J. kg$^{-1}$.K$^{-1}$. These values are not displayed since our range of displayed values has been scaled down in order to clearly show the pseudo-boiling curve, where the change in $C_p$ is smooth and of decreasing amplitude as we go further from the critical point.

![Diagram](image)

**Figure 31:** Instantaneous contours of constant pressure specific heat for the injection of subcritical nitrogen into supercritical nitrogen. The red line indicates where the profiles for Fig. 33 have been taken.

The spatial evolution of $C_p$ in the transverse direction is shown in Fig. 33 at an axial location corresponding to one diameter from the wall. On this same graph, we have plotted the $C_p$ profile that we would obtain for the ideal mixing of two fluids. One of the fluid would have the same $C_p$ as the compressible liquid nitrogen and the other would have the $C_p$ of supercritical nitrogen. We clearly see, by comparing these two profiles, the bulge in $C_p$ due to the change of state as the compressible liquid turns into supercritical gas. We evaluate
Figure 32: P-T diagram for pure oxygen generated with the Peng-Robinson equation of state. The filled color contours represent the values of specific heat at constant pressure in J.kg$^{-1}$.K$^{-1}$ for a given temperature and pressure. The white lines indicate the critical temperature (154.6 K) and pressure (50.4 bar) for oxygen.

the thickness of this thin layer to about 150 microns. This thickness is obviously dependent of our idealized $C_p$ profile but we do not think another definition would have a strong influence on our evaluation, maybe 30% at most. This layer, that we call the transcritical layer and that is likely dependent on transport properties as well as thermodynamic state, is resolved here using about twenty points over 150 microns. This highlights the very high resolution requirements of the current formulation. However, it also shows the capability of our flow solver to handle subcritical injection of a fluid in a supercritical environment.
Figure 33: Plot of the constant pressure specific heat versus transverse direction.
5.4 **Temporal Mixing Layers with density gradients.**

Towards our goal of evaluating the performance of our current solver for simulation of liquid rocket engine combustion chamber, we take a look at some features of temporal mixing layers (TML) with a large density gradient. We consider a two-dimensional temporal mixing layer between a stream of heptane (C$_7$H$_{16}$) and nitrogen (N$_2$), whose different molecular weights, respectively 100 and 28, ensure large density gradients in the shear layer. The ambient pressure is 100 bar and the initial temperature is uniform at 500 K. High-pressure transport properties are used for the perfect gas computations in order to provide an easier comparison of the results. The dynamics of the temporal mixing layer, especially in 2D, is that the species, and thus the density gradients grow in time. Due to the temporal nature of this mixing layer, the physical relevance of a simulation is only valid over a finite range of time. Moreover, as the gradients become larger, the grid resolution requirements grow in time as well. Here, we are not interested in an accurate description of a particular mixing layer but rather we want to highlight some features of the McCormack predictor-corrector scheme that we think need to be addressed before moving further with the real gas modeling. In fact, with the MacCormack predictor-corrector scheme, we get slight temperature oscillations at the location of density gradients, even for a perfect gas equation of state as shown on Fig. 34. There is almost a perfect superposition between the location of the density gradients and the location of the temperature anomalies.

Of course, this same behavior is reproduced with the real gas formulation, with even higher temperature anomalies as shown on Fig. 35. We reach a peak temperature of over 700 K at a location which does not actually coincide with the peak of density gradient. More insight can be gained if we also observe the density fields for both simulations, shown on Fig. 36. First of all, we see that the range of densities for the RG simulation (from 46 kg.m$^{-3}$ to 506 kg.m$^{-3}$) is more than twice as large than the range of densities for CPG simulations (from 67 kg.m$^{-3}$ to 242 kg.m$^{-3}$), thanks to a compressibility as low as 0.4 in the heptane stream under the operating conditions. This implies a larger magnitude for the density gradients as well. Looking at the flow features on Fig. 36 we can distinguish smaller scales structures for the real gas simulation, especially near the center of the vortex.
Figure 34: Density gradient magnitude (a) and temperature (b) fields at $t = 6.62 \times 10^{-4}$ s for the calorically perfect gas simulation. The computational domain corresponds to the highlighted central frame, the two other vortices are just mirror images, here to help put the mixing layer into its environment.
where small threads of heptane are getting entrained by the vorticity. This seems to create additional gradients in a direction 45° from the coordinates axis, direction in which the spatial resolution is course less. This might explain the additional peak of temperature observed and the subsequent instability experienced, eventually leading to a crash of the simulation. As mentioned before, since at that point, the mixing layer has completed its roll-up, the physical relevance of the latter stages of the simulation might not be significant. Such a crash in the simulation does not necessarily mean our models are not predicting accurately the physical processes, as mentioned before, there are other parameters at stake. For example, Figure 37 shows the influence of grid resolution and artificial dissipation. The time evolution of the temperature anomalies, both average and maximum, is represented on this graph. It appears that both perfect gases behave very similarly while the real gas is significantly more unstable. Increasing the grid resolution does delay the onset of the instabilities but does not prevent it. Adding artificial dissipation does not seem to affect the instability significantly at all but it does allow the code to run a little bit longer. In any case, this seems to show that the McCormack scheme has some difficulty in handling these gradients and might not be suited in the long run for real gas modeling where density will be even larger. In order to improve the robustness of the solution, preliminary studies have been conducted using a Monotone Upstream-centered Scheme for Conservation Laws (MUSCL) formulation and we do observe a smoother behavior for the perfect gases simulations. However, this robustness should not come at the expense of accuracy and the choice of the adequate limiter will be a key component of future studies.

Finally, Table 10 presents some quantitative data on the cost of each framework. We see that TPG simulations are about 50% more expensive that comparative CPG runs. Also, the heavy cost of real gas modeling is illustrated by the multiplication by at least a factor 6 of the time from the CPG simulation. Note that for the inclusion of the Jameson artificial dissipation, the added cost is due in great part to the increase in communication requirements required by the scheme. In any case, this stresses the immediate need of improving the efficiency of the real gas formulation. We firmly believe that a two-fold gain could be easily reached.
Figure 35: Density gradient magnitude (a) and temperature (b) fields at $t = 6.62 \times 10^{-4}$ s for the real gas simulation.
Figure 36: Comparison of the density fields for the CPG simulation (a) and the RG simulation (b).

Figure 37: Comparison of the density fields for the CPG simulation (a) and the RG simulation (b).

Table 10: Timing comparison for the different thermodynamic frameworks available for our flow solver. The simulations have been performed with 32 1.5 GHz power4 processors (4 nodes) on an IBM p655+. The problem modeled is the LES of a two-dimensional ($129 \times 257 \times 2$) TML with 2 species ($C_7H_{16}$). The physical timestep is $7 \times 10^{-8}$ s and the roll-up is completed after 10000 iterations. Results are shown in CPU s/cell/step. The RG Jameson case corresponds to the real gas formulation with an artificial, fourth-order dissipation added.
5.5 Heat transfer

5.5.1 Flat plate

We try here to reproduce a classical flow as given by White[159]. We consider a flat-plate flow with \( \text{Ma}_e = 3.0 \). The freestream air temperature is 300 K and the Prandtl number is assumed to be 0.71. Using crude inflow conditions (flat profile) and Sutherland law instead of the power laws for the transport properties, we still expect to get a solution very close to the analytical one. Our grid is quite fine with a spacing of 2 microns at the wall and obviously, an unsteady simulation is not the most efficient tool to take on such a problem. Moreover, in order to avoid reflections of the compression wave that develops at the inflow, the dimension of our computational domain in a direction normal to the wall is quite large. Thus, the simulation takes about 100 CPU hours to converge for a grid of computational size \( 301 \times 184 \times 2 \) and of physical dimensions \( 0.5 \times 0.01 \) m. We investigate both adiabatic and isothermal wall configuration. In the isothermal case, the wall temperature is set to be equal to the freestream air temperature, i. e. 300 K. Figure 38 displays the convergence of the velocity profile at the downstream end our computational domain for a simulation using the calorically perfect gas framework. Figure 39 confirms the consistency of the thermally perfect gas approach which yields very similar results than the calorically perfect gas approach. For the cold wall case, the thermally perfect approach actually yields slightly superior results than the calorically perfect model, but both are in relative agreement with analytical solution, correctly predicting the location and the amplitude of the temperature peak. Figure 40 emphasizes the achievement of self-similarity along the flat plate as both the non-dimensional temperature and velocity profiles get closer to the analytical solution as we go further downstream.

The cold, isothermal wall results are even better, with both the location and amplitude of the peak correctly predicted.
Figure 38: Calorically perfect results for non-dimensional velocity profile with adiabatic wall. Convergence towards the steady-state, analytical solution represented by the black crosses.

Figure 39: Comparison between the calorically perfect and the thermally perfect solutions for velocity (a) and temperature (b) profiles.
Figure 40: Thermally perfect results for velocity (a) and temperature (b) profiles with cold, isothermal wall.
5.5.2 Development of a multi-physics solver

It appears that for steady-state problems, the simplified isothermal wall boundary condition is enough to correctly model the heat transfer of simple flows. However, for unsteady flows, we will need a coupled fluid mechanics-heat conduction solver as the isothermal boundary conditions will not be accurate enough.

As a preliminary stage, we quickly introduce an idea of architecture for this coupled solver and we demonstrate the validity of the stand-alone solver. The solution provided here assume memory is not so much of an issue for our typical computations. The heat conduction module is able to take care of any domain with six faces, with at least one face being contiguous with the flow region. We will call such a domain a heat block, compared to the traditional flow block. The connectivity between the flow block and the heat block(s) is assured by an input file that can be modified before each run without the need to recompile the whole solver.

For each face of a heat block, three kinds of boundary conditions can be applied: Dirichlet (temperature imposed at the boundary), Neumann (heat flux imposed at the boundary) or a two-way coupling with the flow. Either way, the boundary condition values are stored in arrays such as $BC\_BLOCK\_I(J1:J2,K1:K2,1:NBLOCK,1:2)$ and they contain either temperature or heat flux values. The dimensions $J1$, $J2$, $K1$, $K2$ are determined by the maximum dimensions among different blocks which can lead to large arrays if the heat blocks span in various directions. Inside each heat block, the same finite volume scheme used for the solver is applied, with obviously a different stability criterion which would lead, in typical computations, to a heat conduction time step larger than the fluid dynamics time step. The exact temporal coupling between the two solvers has not been picked yet so we assume for our example that we use the straightforward but inefficient method of picking as overall time step the smaller time step.

Figure 41 presents an example of the algorithm that could be used to couple the conduction module with the fluid mechanics module:

1. On the gas side, we solve the usual Navier-Stokes equations, using the values stored
in BC_BLOCK arrays as boundary condition values for the wall temperature.

2. Using for example a second order, one-sided differencing, we compute the new value of the heat flux using updated gas-side values of temperature.

3. We perform one iteration of the heat conduction module, assuming the fluid mechanics time step is the limiting time step.

4. We update the BC_BLOCK arrays with the updated temperatures from the solid side and we iterate the procedure.

Figure 41: A possible algorithm for the heat conduction module. The blue cells represent the flow cells while the gray cells represent the material in contact with the flow.

A quick test has been performed with the heat conduction module in order to verify it. We consider a one-dimensional copper bar whose ends are maintained at constant temperature while the middle of the bar is being heated. Once the middle of the bar has reached a certain temperature (325 K in our case, to be compared with the 300 K of the isothermal boundary conditions), the bar is left to evolve by itself. Figure 42 displays the evolution of the temperature profiles along the bar in time. We can see the gradual diffusion of heat that follows exactly the analytical solution. It takes several minutes for the copper bar to regain a near-equilibrium state, illustrating the kind of time scale we might be experiencing later with the coupled solver.
Figure 42: A simple problem to verify the heat conduction solver: the cooling of a preheated copper bar.
5.6 Conclusion

Two different approaches for axisymmetric flow configurations have been implemented and validated in our current flow solver framework. As mentioned before, the 3D_AXI_SRC is significantly less expensive in terms of computational resources while the 3D_AXI_FLUX can be directly extended to quasi-3D in order to include for example more realistic turbulence. The question is of course whether the additional cost is worth paying. In the case of a spatially developing layer, the 3D_AXI_FLUX appears like a good compromise between a full 3D simulation and a single-plane, axisymmetric one. Fig. 43 presents the grid used for simulating a 45 degree slice of a typical coaxial injector flow. For this simple and limited configuration, we are using a grid containing 540,000 cells with 501, 61 and 19 grid points in the axial, radial and tangential directions. Also, in order to have a relatively large timestep for this simulation, we have scaled up the physical dimensions of our injector so that the inner diameter of the central pipe is about 30 cm and the inner diameter of the annulus is about 60 cm while the convective velocity \( U_C \) remains low at 6.4 m.s\(^{-1}\). As it is the case with most of the coaxial flows in rocket configurations, the outer flow is faster with \( U_2 = 8 \) m.s\(^{-1}\) and the inner flow velocity \( U_1 = 4.8 \) m.s\(^{-1}\). The initialization of the inflow profile is based on the work by Wilson and Demuren\[160\]: we adopt a hyperbolic tangent velocity profile with a vorticity thickness \( \delta_\omega_0 = 0.008 \). Then we excite the most unstable wave number according to linear stability analysis with a time-varying perturbation of the inflow. Although our limited domain length does not allow us to observe complete pairing, the inflow perturbation we have adopted\[61, 58\] is a multi-frequency perturbation that promotes the pairing of the growing vortices:

\[
u' = A_0 \sin(2\pi f_0 t) + A_1 \sin(2\pi f_1 t + \beta)
\]

where \( u' \) is the axial velocity perturbation, \( f_0 \) is the most unstable frequency from the linear stability analysis, \( f_1 \) is the first subharmonic frequency and \( A_0 \) and \( A_1 \) are the amplitudes of the fundamental and subharmonic perturbations, respectively 5% and 2.5% of the convective velocity \( U_C \). The non-dimensional, fundamental frequency is \( \frac{f_0 \delta_\omega_0}{U_1 + U_2} = 0.02 \). Finally, in
order to promote three-dimensional effects, we also superimpose white, random noise perturbations for the radial and tangential velocities. The magnitude of these perturbations is 10% of the local inflow axial velocity.

Fig. 44 shows the growth of the mixing layer. The isosurface of tangential vorticity is drawn for a value of $-50 \, \text{s}^{-1}$. This isosurface is colored by the value of axial vorticity, thus displaying the onset of three-dimensionality. We see that the initial random disturbances do not really grow until about 3 inner-pipe diameters downstream of the inlet. In a short distance, vortices began to appear very clearly. As these vortices are rolling between the two streams, we can distinguish the apparition of a characteristic feature of 3D mixing layers, the braids between two consecutive vortices. The braids link the vortices as they are being from the mixing layer and disappear once each vortex becomes independent. Further downstream (our computational domain is not long enough), we would see vortices paired with each other and these braids would likely reappear between pairing vortices. Note that the amplitude of the tangential velocities (not shown here) has at least doubled between the inflow and the maximum observed downstream, a clear sign that three-dimensionality is starting to appear.

![Figure 43: Example of application for the 3D_AXI_FLUX code. For this spatially developing mixing layer, we model a 45 degree slice using 19 grid points. Note the hole around the centerline.](image)

This shows that there are applications where the 3D_AXI_FLUX formulation can provide...
Figure 44: Example of application for the 3D_AXI_FLUX code. The isosurface of tangential vorticity is drawn for a value of \(-50\, \text{s}^{-1}\). This isosurface is colored by the value of axial vorticity, thus displaying the onset of three-dimensionality.

additional physics and justify its double computational cost. However, these applications are limited and for real combustion chambers, it appears that neither the 3D_AXI_SRC nor the 3D_AXI_FLUX are satisfactory\[133\, \text{[135].} Only full 3D simulations will reliably give accurate results in these configurations.
CHAPTER VI

CONCLUSION AND FUTURE WORK

6.1 Conclusion

The applications of high-pressure combustion are more and more common as technology and needs evolve and are no longer limited to liquid rocket engines. Solid rocket motors and gas turbines are also fields where higher efficiency in a more compact volume is required. But as the systems get smaller and the combustion more intense, understanding of the heat transfer becomes critical. The combination of real gas and heat transfer effects makes the study of such systems very difficult, from the experimental as well as the numerical point of view. A new real gas/thermally perfect gas LES code using an axisymmetric approximation has been used to simulate unsteady combustion and dynamics in a representative LOX-GH2 rocket motor consisting of three slot injectors that attempts to match the actual motor conditions. The purpose of this work was to prove the feasibility of such simulations and to pave the way for further improvements. The axisymmetric LES formulation allows such computations for a moderate cost. Different models for thermodynamic and transport properties can be used with this solver. Also, the implementation of these models into a full 3D flow solver enables us to quickly and easily switch between:

- A pure axisymmetric formulation through the modification of the governing equations to include axisymmetric derivatives and source terms. This allows us to reproduce the 2D axisymmetric results for about the same cost.

- A more complex axisymmetric implementation that allows us to perform simulations of 3D sectors. Modifying only the boundary conditions and keeping the original 3D Navier Stokes equations, we can model more realistic 3D turbulence or include the effect of swirl. However, this implementation is only useful when the centerline plays no role in the flow (for example, in the near-field of a coaxial injector).
Although not presented in this work, this flow solver is fully capable of performing full 3D simulations of a combustion chamber using the "butterfly grid" [34] technique to solve the centerline grid issue. Obviously much more computationally expensive, this method removes many geometrical assumptions and is needed for the simulation of realistic configurations.

However, limited experimental data are available in order to verify the validity of our different assumptions. Especially, no flow visualization of a multi-injector configuration is available, only more global quantities have been measured as of today. Thus, the current LES simulations, with a reasonable qualitative agreement with the available experimental observations, only give us an idea of the dynamics of a typical rocket combustion chamber. We need to develop, implement and validate many features in order to improve this crude first modeling effort. Some of these features are in place and require only some improvements. This is the case for the numerical scheme and the thermodynamic framework. They appear to be able to accomplish their objective but not with enough stability or robustness to become a reliable design tool. On the other hand, there is much more work required on the heat transfer and the combustion modeling in LES simulations of typical LRE configurations. These are standalone research topics that will be necessary to incorporate in our design tool once it will have reached a certain stage of maturity. We will now detail how to reach this stage.
6.2 Future Work

As of now, a full 3D LES simulation of a multi-injector sub-scale liquid rocket engine is not affordable in terms of computational resources nor would it be immediately valuable to the understanding of the physics inside the combustion chamber. There are too many assumptions on the numerical modeling and too few experimental data to compare with to justify the cost of such simulation. That being said, we believe the current study is an important stepping stone towards such future simulation, although many tasks still need to be accomplished to approach this goal:

- There is a critical need to improve the stability of the current numerical scheme. It appears that the straightforward McCormack predictor-corrector scheme might not be the best suited to deal with the very large density gradients involved in high pressure, cryogenic environments. Since the thermodynamic framework is already quite expensive, it is difficult to imagine using successful but expensive solutions such as the adaptation of the shock-capturing Piecewise-Parabolic Method[24]. Instead, simpler solutions such as the Monotone Upstream-centered Schemes for Conservation Laws (MUSCL) or the implementation of a Total Variation Diminishing (TVD) limiter in the base McCormack scheme should provide us with a good balance between stability and dissipation. Preliminary testing with MUSCL schemes stresses the influence of the limiters on the amount of dissipation generated. We believe these schemes should be investigated first in temporal mixing layers[92, 105] and spatially developing mixing layers[100, 163].

- There is a critical need to improve the efficiency of the current thermodynamic framework. Based on the timing results provided in this work, even the thermally perfect gas framework could be sped up. For the fast resolution of these systems of one (TPG) or two (RG) non-linear equations, more advanced mathematical methods could be implemented. Our current formulation using basic Newton’s method is not as robust or efficient than the Brent’s method[10] or more advanced multi-dimensional algorithms[120]. Fortran libraries for such methods are readily available in the public
domain and it should be straightforward to test whether they bring significant improvement to this costly iterative process. If this does not appear satisfactory, we could try to implement curvefits\cite{92}, table look-up\cite{162} or even some modified In-Situ Adaptive Tabulation\cite{118}.

- Studies of temporal mixing layers and spatially developing mixing layers in an axisymmetric configuration are not common and there might some interesting insight to be gained in studying these flows, under both perfect gas or real gas assumptions. Such studies could be combined with the development of the more stable numerical scheme. Since such flows do not interact with the centerline, the axisymmetric assumption is valid and should allow us to study three-dimensional turbulence at reduced cost. This could definitely settle the argument between the 3D AXI_SRC framework and the 3D AXI_FLUX framework. These studies could also include the evaluation of the closure terms for the energy and pressure equations and the influence of the cross-diffusion Soret and Dufour effects as well as heat release effects.

- On parallel to these efforts focused on the real gas formulation, there should be some work conducted around the gas-gas coaxial configurations. Some quantitative experimental data are readily available\cite{39} for moderate pressures and could give us an indication on the validity of our numerical scheme as well as a definite answer on the influence of the axisymmetric assumption in such simple configuration. If such tests yields satisfactory results, then one could move to a multi-physics simulation in order to reproduce experimental wall heat transfer in similar gas-gas configurations.

- In order to reduce the computational cost of LES simulations in complex geometries, a multi-block solver capable of dealing with multi-grids and hanging nodes is being developed in the Computational Combustion Laboratory. This should reduce the grid requirements for all simulations, no matter which thermodynamic framework is used. On the other hand, this will probably necessitate some additional development to test the interaction between the multi-block solver and the real gas framework. This step is required for our solver to be efficient in terms of computational cost when compared
to unstructured solvers in complex geometries.

- The need for a multi-physics solver is apparent when looking at the latest solvers from various groups interested in modeling realistic gas turbines or liquid rocket engines\(^9^0\)\(^9^1\). This is an issue that can be treated in parallel in the early stages using steady and unsteady problems for which we know the analytical solutions. To complete the validation of such solver, we will need relevant test cases for which reliable experimental data are available and computational cost is not too large. For steady heat transfer, the nozzle experiment by Back\(^5\) has already been used as a benchmark\(^7^7\) and seems to be a good choice to assess the influence of the multi-physics solver as active cooling is present in the experiment. For unsteady problems, the backward-facing step is a classical problem \(^4\)\(^6^9\) but the flow conditions are very different from our applications of interest. Ideally, we would like an experiment with a hot flow of non-reacting gas in a dump combustor configuration. The flow should have a Reynolds number based on the step height slightly above 1000, which corresponds to the turbulent regime. The flow could possibly be pulsed to increase the unsteadiness of the heat transfer. The walls of the combustor downstream of the dump plane would be cooled and some basic flow visualization (including the measurement of the reattachment length) should be performed along with the recording of the unsteady heat transfer. To our knowledge, no such experiment, even in a two-dimensional configuration, has been performed.

These different tasks are summarized in Fig. 45. We want to stress the important computational resources required for almost every single step. That is why the numerical developments located at the beginning of the roadmap are very important and need to achieve significant performance gains in order to be able to conduct the following validations in a reasonable amount of time. Further down the road, some additional experimental data would be welcomed. For example, an extension to high pressures of the work by Boniface et al.\(^8\), already mentioned earlier, would be very beneficial. Ideally, subcritical or supercritical oxygen could be injected through the central jet while gaseous hydrogen
would be injected around that jet in a typical coaxial configuration. A rather thick high-speed co-flow of inert gas (preferably helium or argon) would embrace that coaxial flow and simulate the presence of surrounding injectors. Not only would this configuration be closer to the actual injection in a multi-injectors combustion chamber, it would also eliminate some issues for the numerical simulations. A co-flow with a large enough flow rate would eliminate the need to model the isothermal walls and also make the throat at the end of the combustion chamber larger. This could reduce the complexity and the computational cost of the simulation. Figure 46 is a very basic representation of this experimental setup. It should also be mentioned that we have seen this year the first attempts to model multi-injectors configuration with a 3D LES simulation. Although the work of Richecoeur et al.[126] extends only to moderate-pressure, non-reactive cases, the prospects of their modeling efforts using unstructured grid are very good and could be a viable solution to the computational costs issues mentioned previously.

Finally, we also believe this work can be beneficial to the field of gas turbine combustion. For both non-reacting and reacting coaxial configurations, the vast majority of the work has been done for gas turbines configurations, where the dimensions of the coaxial injectors are much larger than in typical liquid rocket engines. For non-reacting flows, the experimental work by Dellenback et al.[31], which studied the mixing of coaxial air and water flows, provides an interesting set of validation data that has been used for example by Schlüter et al.[134] or Akselvoll et al.[1]. A relevant example of experimental data available for reacting flows is the work by Owen et al.[108]. Pitsch et al.[115], Pierce[114] and Mahesh et al.[81] have used these data to validate their LES approach in realistic gas turbines. As the pressure increase in modern gas turbines in order to increase performance, real gas effects could become significant although probably not as much as in liquid rocket engines. Also, the development of a multi-physics solver could be very useful for gas turbine simulation in order to model heat losses and their influence on stability and emissions[139].
Figure 45: Roadmap for the future work towards the full 3D LES multi-physics simulation of a multi-element sub-scale liquid rocket engine under real operating conditions.
Figure 46: Schematic of the proposed experimental setup involving high-pressure coaxial combustion with a large co-flow.
APPENDIX A

ADDITIONAL DETAILS ON THE EOS FORMULATION

A.1 Temperature equation

Starting from the cubic equation in $Z$, we can derive an equation isolating the temperature by first replacing $Z$ by $\frac{pv}{R_u T}$:

\[
\left(\frac{pv}{R_u T}\right)^3 + \left(\frac{B_m p}{R_u T} - 1\right)\left(\frac{pv}{R_u T}\right)^2 + \left(\frac{A_m(T) p - 3B_m^2 p^2}{R_u^2 T^2}\right) - \frac{2B_m p}{R_u T} - \frac{A_m(T) B_m p^2}{R_u^3 T^3} + \frac{B_m^2 p^2}{R_u^2 T^2} + \frac{B_m^3 p^3}{R_u^3 T^3} = 0
\]

We then multiply this equation by $R_u^3 T^3$, develop the different terms and rearrange to isolate the temperature. We obtain the following equation:

\[
R_u T \rho^2 (v - B_m)^2 + A_m(T) \rho^2 (v - B_m) + p^3 (v^3 + B_m^3 + B_m v^2 - 3B_m^2 v) = 0 \quad (93)
\]

Unfortunately, because of the complex expression of $A_m$ in function of temperature, only an iterative, root-finding method can efficiently solve this equation. Solving this equation is not needed in the current implementation of the McCormack predictor-corrector scheme but it would be needed for a MUSCL scheme for example. Some numerical methods are suggested in the future work section (Section 6.2).

A.2 Iterative computation of pressure and temperature

From the UPDATE subroutine, we know the new internal energy (through total energy) and the new molar volume (through density). By "new", we mean the value corresponding to the next stage of the McCormack scheme. Those values will be superscripted with a "N+1" like $e^{N+1}$. So, $e^{N+1}$ and $v^{N+1}$ are computed at the beginning of the CALC_TEMP subroutine (variables EINEW and VVNEW) and expressed respectively in J.kg\(^{-1}\) and cm\(^3\).mol\(^{-1}\).
The procedure consists in updating P and T at each iteration using the following algebraic expression:

\[ T^k = T^{k-1} + dT \quad \quad p^k = p^{k-1} + dp \]  

(94)

The 2 convergence criteria will be \( de/e \) and \( dv/v \), with a tolerance fixed at \( 10^{-6} \):

\[ de = e^{N+1} - e^k(X^{N+1}, p^k, T^k) \quad \quad dv = v^{N+1} - v^k(X^{N+1}, p^k, T^k) \]  

(95)

The differentiation of pressure and temperature yields:

\[ dT = \left( \frac{\partial T}{\partial v} \right)_{e,X}^{k-1} dv + \left( \frac{\partial T}{\partial e} \right)_{v,X}^{k-1} de + \sum_i \left( \frac{\partial T}{\partial X_i} \right)_{v,e,X_{i\neq j}}^{k-1} dX_i \]  

(96)

\[ dp = \left( \frac{\partial p}{\partial v} \right)_{e,X}^{k-1} dv + \left( \frac{\partial p}{\partial e} \right)_{v,X}^{k-1} de + \sum_i \left( \frac{\partial p}{\partial X_i} \right)_{v,e,X_{i\neq j}}^{k-1} dX_i \]  

(97)

The required derivatives are:

\[ \left( \frac{\partial T}{\partial v} \right)_{e,X_i} = \frac{1}{\nu \alpha_v} \left( 1 - \frac{C_p}{C_v} \right) + \frac{p}{C_v} \quad \quad \left( \frac{\partial T}{\partial e} \right)_{v,X_i} = \frac{m}{C_v} \]  

\[ \left( \frac{\partial p}{\partial v} \right)_{e,X_i} = \frac{1}{\kappa_T} \left( -\frac{C_p}{C_v} + \alpha_v \frac{p}{C_v} \right) \quad \quad \left( \frac{\partial p}{\partial e} \right)_{v,X_i} = \frac{m \alpha_v}{C_v \kappa_T} \]  

(98)

\[ \left( \frac{\partial p}{\partial T} \right)_{v,X} = \frac{R}{v - B_m} - \frac{(\partial A_m / \partial T)}{v^2 + 2vB_m - B_m^2} \]  

(101)

\[ \left( \frac{\partial p}{\partial v} \right)_{T,X} = \frac{-RT}{v - B_m^2} \left[ 1 - \frac{2A_m}{RT(v + B_m) \left( \frac{v}{v - B_m} + \frac{B_m}{v + B_m} \right)^2} \right] \]  

(102)

In the iterative process (for which the \( k^{th} \) iteration will correspond to the \( "k" \) superscript), the first task is to compute the molar volume based on the new composition of the mixture \( X^{N+1} \) from the equations of motion and the guessed properties \( T^k \) and \( P^k \). This molar volume, expressed in \( \text{cm}^3 \cdot \text{mol}^{-1} \), is the \( \text{VVGUESS} \) variable. It is obtained by solving the cubic equation of the compressibility.

Then we have to compute the expansivity \( \alpha_v \) (in \( \text{K}^{-1} \)) and the isothermal compressibility \( \kappa_T \) (in \( \text{bar}^{-1} \)):

\[ \alpha_v = \frac{(\partial p/\partial T)_{v,X}}{v(\partial p/\partial v)_{T,X}} \quad \quad \kappa_T = -\frac{1}{v(\partial p/\partial v)_{T,X}} \]  

(100)

Through differentiation of the EOS, one can obtain:
Then we start evaluating the different thermodynamic derivatives, such as $\frac{\partial^2 A_m}{\partial T^2}$, expressed in bar.cm$^6$.mol$^{-2}$.K$^{-2}$:

$$\frac{\partial^2 A_m}{\partial T^2} = \frac{0.457236 R_w^2}{2T} \sum_i \sum_j X_i X_j f(\Omega_{ij})(1 + f(\Omega_{ij})) \frac{T_c(ij)}{p_c(ij)} \sqrt{\frac{T_c(ij)}{T}}$$ (103)

We then compute the departure functions for the internal energy and the specific heats following the methodology described in [2.2]. With those, we have everything needed to compute the $dT$ and $dP$ described in Eqs. [96,97] and see if the convergence criteria have been reached.
APPENDIX B

BOUNDARY CONDITIONS

Many mechanisms in turbulent reacting flows are strongly coupled with acoustic waves. Flame produces noise which itself can perturb the flame. Also, turbulence interacts with acoustic waves in different manners. For example, velocities induced by acoustic oscillations can be of the same order as turbulent velocities. As a consequence, proper description of acoustic wave behavior through the boundaries of the domain is primordial.

This chapter presents the method used to prescribe accurate boundary conditions.

**B.1 Description of the Method**

As Thompson[152] wrote, the central concept of the treatment of boundary conditions "is that hyperbolic systems of equations represent the propagation of waves and that at any boundary some of the wave are propagating into the computational domain while other are propagating out of it. The outward propagating waves have their behavior defined entirely by the solution at and within the boundary and no boundary can be specified for them. The inward propagating waves depend on the solution exterior to the [domain] and therefore require boundary conditions to complete the specification of their behavior.” This section describes how to write the conservation equations into a set of wave equations which represents the waves propagating at characteristic velocities.

The conservation equations are:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{104}
\]

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p) u_i}{\partial x_i} = \frac{\partial \rho u_j u_i}{\partial x_i} - \frac{\partial \tau_{ji}}{\partial x_i} \tag{105}
\]

\[
\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_j u_i + p \delta_{ji}}{\partial x_i} = -\frac{\partial \tau_{ji}}{\partial x_i} \tag{106}
\]

\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u_i}{\partial x_i} = \dot{w} \tag{107}
\]

where \( \rho \) is the mass density, \( p \) is the pressure, \( E \) is the total energy per unit mass, \( u_i \) is the
velocity vector, \( q_i \) is the heat flux vector, \( Y_k \) is the mass fraction of the kth species, \( \dot{\omega} \) is the reaction rate and \( \tau_{ij} \) is the stress tensor. The total energy can be divided as:

\[
E = e_i + \frac{1}{2} u_k u_k,
\]

(108)

where \( e_i \) is the internal energy and \( \frac{1}{2} u_k u_k \) is the kinetic energy.

Let us call \( \tilde{U} \) the vector of conservative variables, which obey the equation

\[
\frac{\partial \tilde{U}}{\partial t} + \frac{\partial F^1}{\partial x^1} + \frac{\partial F^2}{\partial x^2} + \frac{\partial F^3}{\partial x^3} + \tilde{D} = 0
\]

(109)

where \( F^k \) is the vector of fluxes in the k direction and \( D \) is a vector of inhomogeneous terms.

Consider now the characteristic analysis of the \( x_1 \) direction. We are interested only by derivatives with respect to the \( x_1 \) direction, so we gather all the other terms together:

\[
\frac{\partial \tilde{U}}{\partial t} + \frac{\partial F^1}{\partial x^1} + \tilde{C} = 0, \quad \tilde{C} = \frac{\partial F^2}{\partial x^2} + \frac{\partial F^3}{\partial x^3} + \tilde{D}
\]

(110)

Let now define \( U \) a vector of primitive variables, selected for convenience. The arrays \( \tilde{U} \) and \( U \) are:

\[
\tilde{U} = \begin{pmatrix}
\rho \\
\rho E \\
\rho u_j
\end{pmatrix}, \quad \tilde{F} = \begin{pmatrix}
\rho u_j \\
(\rho E + p)u_i \\
\rho u_j u_i
\end{pmatrix}, \quad U = \begin{pmatrix}
\rho \\
p \\
u_j
\end{pmatrix}
\]

(111)

It is possible to write (109) in such a way that only the primitive vector appears:

\[
\frac{\partial \tilde{U}}{\partial t} = \rho \frac{\partial U}{\partial t}
\]

(112)

where \( P \) is a Jacobian matrix of elements:

\[
p_{ij} = \frac{\partial \tilde{U}_i}{\partial U_j}
\]

(113)

And

\[
\frac{\partial \tilde{F}^1}{\partial x^1} = Q^1 \frac{\partial U}{\partial x^1}
\]

(114)
where
\[ q^1_{ij} = \frac{\partial \tilde{F}^1_{ij}}{\partial U_i} \quad (115) \]

We finally obtain
\[
\begin{align*}
\frac{\partial U}{\partial t} + A^1 \frac{\partial U}{\partial x^1} + C &= 0 \quad C = A^2 \frac{\partial U}{\partial x^2} + A^3 \frac{\partial U}{\partial x^3} + D \quad (116)
\end{align*}
\]

where
\[
A^1 = P^{-1} Q^k, \quad C = P^{-1} \tilde{C}, \quad D = P^{-1} \tilde{D} \quad (117)
\]

Let \( \lambda_i \) be the m eigenvalues of \( A^1 \), \( l_i \) the left eigenvectors of \( A^1 \) and \( r_i \) the right eigenvectors of \( A^1 \). Applying a diagonalizing similarity transformation to (116) gives:
\[
\begin{align*}
l_i \frac{\partial U}{\partial t} + \lambda_i l_i \frac{\partial U}{\partial x^1} + l_i C &= 0 \quad i = 1, .., m \quad (118)
\end{align*}
\]

If we define
\[
L_i = \lambda_i l_i \frac{\partial U}{\partial x^1} \quad (119)
\]

(116) becomes:
\[
\frac{\partial U}{\partial t} + S L_i + C = 0 \quad (120)
\]

where \( S \) is a matrix whose columns are the right eigenvectors \( r_i \).

Once the values of the \( L_i \) are defined, we find the rate of change of the primitive variables.

The rate of change of the conservative variables can then be expressed.

**B.2 Application to a perfect gas**

Following the previous method, we obtain the \( P \) and \( Q \) matrices for a calorically perfect gas:
\[
P = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
\frac{1}{2} \sum_{i=1}^{3} (u_i^2) & \frac{1}{\gamma-1} \rho u_1 & \rho u_2 & \rho u_3 \\
u_1 & 0 & \rho & 0 & 0 \\
u_2 & 0 & 0 & \rho & 0 \\
u_3 & 0 & 0 & 0 & \rho
\end{pmatrix} \quad (121)
\]
The primitive equations are then found to be:

\[
\begin{align*}
\frac{\partial\rho}{\partial t} + u_1 \frac{\partial\rho}{\partial x_1} + u_2 \frac{\partial\rho}{\partial x_2} + u_3 \frac{\partial\rho}{\partial x_3} + \rho \left( \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) &= 0 \\
\frac{\partial p}{\partial t} + u_1 \frac{\partial p}{\partial x_1} + u_2 \frac{\partial p}{\partial x_2} + u_3 \frac{\partial p}{\partial x_3} + \gamma p \left( \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right) &= 0 \\
\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_1}{\partial x_1} + u_2 \frac{\partial u_2}{\partial x_2} + u_3 \frac{\partial u_3}{\partial x_3} + \frac{1}{\rho} \frac{\partial p}{\partial x_1} &= 0 \\
\frac{\partial u_2}{\partial t} + u_1 \frac{\partial u_1}{\partial x_1} + u_2 \frac{\partial u_2}{\partial x_2} + u_3 \frac{\partial u_3}{\partial x_3} + \frac{1}{\rho} \frac{\partial p}{\partial x_1} &= 0 \\
\frac{\partial u_3}{\partial t} + u_1 \frac{\partial u_1}{\partial x_1} + u_2 \frac{\partial u_2}{\partial x_2} + u_3 \frac{\partial u_3}{\partial x_3} + \frac{1}{\rho} \frac{\partial p}{\partial x_1} &= 0
\end{align*}
\]  

(123)

In order to proceed on the boundary conditions analysis, we want to write the preceding set of equation in the form of (116). The matrix \( A^1 \) being given by:

\[
A^1 = \begin{pmatrix}
u_1 & 0 & \rho & 0 & 0 \\
0 & u_1 & \gamma p & 0 & 0 \\
0 & \frac{1}{\rho} & u_1 & 0 & 0 \\
0 & 0 & 0 & u_1 & 0 \\
0 & 0 & 0 & 0 & u_1
\end{pmatrix}
\]  

(124)
The eigenvalues of $A^1$ are:

\[
\begin{align*}
\lambda_1 & = u_1 - c \\
\lambda_2 & = u_1 \\
\lambda_3 & = u_1 \\
\lambda_4 & = u_1 \\
\lambda_5 & = u_1 + c
\end{align*}
\]

$\lambda_1$ is the relative velocity of sound waves moving in the negative $x_1$ direction. $\lambda_5$ is the relative velocity of sound waves moving in the positive $x_1$ direction. $\lambda_2$ is the velocity for entropy advection. $\lambda_3$ and $\lambda_4$ are the velocities at which $u_2$ and $u_3$ are advected in the $x_1$ direction.

The left eigenvectors may be written:

\[
\begin{align*}
l^r_1 & = (0, 1, -\rho c, 0, 0), \\
l^r_2 & = (c^2, -1, 0, 0, 0), \\
l^r_3 & = (0, 0, 0, 1, 0), \\
l^r_4 & = (0, 0, 0, 0, 1), \\
l^r_5 & = (0, 1, \rho c, 0, 0)
\end{align*}
\]

The matrix $S$ is:

\[
S = \begin{pmatrix}
\frac{1}{2c^2} & \frac{1}{c^2} & 0 & 0 & \frac{1}{2} \\
\frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\
-\frac{1}{2\rho c} & 0 & 0 & 0 & \frac{1}{2\rho c} \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0
\end{pmatrix}
\]
The vector $\mathcal{L}$ is then found to be:

\[
\mathcal{L}_1 = \lambda_1 \left( \frac{\partial p}{\partial x_1} - \rho c \frac{\partial u_1}{\partial x_1} \right), \\
\mathcal{L}_2 = \lambda_2 \left( c^2 \frac{\partial p}{\partial x_1} - \frac{\partial p}{\partial x_1} \right), \\
\mathcal{L}_3 = \lambda_3 \left( \frac{\partial u_2}{\partial x_1} \right), \\
\mathcal{L}_4 = \lambda_4 \left( \frac{\partial u_3}{\partial x_1} \right), \\
\mathcal{L}_5 = \lambda_5 \left( \frac{\partial p}{\partial x_1} + \rho c \frac{\partial u_1}{\partial x_1} \right)
\]

(127)

The product $S \mathcal{L}$ is the vector $\mathbf{d}$:

\[
\mathbf{d} = S \mathcal{L} = \begin{pmatrix}
\frac{1}{c^2} [\mathcal{L}_2 + \frac{1}{2} (\mathcal{L}_5 + \mathcal{L}_1)] \\
\frac{1}{2} (\mathcal{L}_5 + \mathcal{L}_1) \\
\frac{1}{2 \rho c} (\mathcal{L}_5 - \mathcal{L}_1) \\
\mathcal{L}_3 \\
\mathcal{L}_4
\end{pmatrix} = \begin{pmatrix}
d_1 \\
d_2 \\
d_3 \\
d_4 \\
d_5
\end{pmatrix}
\]

(128)

The set of primitive of primitive equation (123) can now be written in the form of (120) (excluding the derivatives with respect to $x_2$ and $x_3$).

\[
\frac{\partial p}{\partial t} + \frac{1}{c^2} \left[ \mathcal{L}_2 + \frac{1}{2} (\mathcal{L}_5 + \mathcal{L}_1) \right] = 0 \\
\frac{\partial p}{\partial t} + \frac{1}{2} (\mathcal{L}_5 + \mathcal{L}_1) = 0 \\
\frac{\partial u_1}{\partial t} + \frac{1}{2 \rho c} (\mathcal{L}_5 - \mathcal{L}_1) = 0 \\
\frac{\partial u_2}{\partial t} + \mathcal{L}_3 = 0 \\
\frac{\partial u_3}{\partial t} + \mathcal{L}_4 = 0
\]

(129)
By combining the previous equations, the rate of variation of conservative variable is expressed as:

\[
\frac{\partial \rho}{\partial t} + d_1 + \frac{\partial \rho u_2}{\partial x_2} = 0
\]

\[
\frac{\partial \rho E}{\partial t} + \frac{d_2}{\gamma - 1} + \rho u_1 d_3 + \rho u_2 d_4 + \rho u_3 d_5 + \frac{\partial (\rho E + p) u_2}{\partial x_2} + \frac{\partial (\rho E + p) u_3}{\partial x_3} = \frac{\partial \tau_{ij} u_j}{\partial x_i} - q_i
\]

\[
\frac{\partial \rho u_1}{\partial t} + u_1 d_1 + \rho d_3 + \frac{\rho u_1 u_2}{x_2} + \frac{\rho u_1 u_3}{x_3} = \frac{\partial \tau_{1j} u_j}{\partial x_i}
\]

\[
\frac{\partial \rho u_2}{\partial t} + u_2 d_1 + \rho d_4 + \frac{\rho u_2 u_2}{x_2} + \frac{\rho u_2 u_3}{x_3} + \frac{\partial p}{\partial x_2} = \frac{\partial \tau_{2j} u_j}{\partial x_i}
\]

\[
\frac{\partial \rho u_3}{\partial t} + u_3 d_1 + \rho d_5 + \frac{\rho u_3 u_2}{x_2} + \frac{\rho u_3 u_3}{x_3} + \frac{\partial p}{\partial x_3} = \frac{\partial \tau_{3j} u_j}{\partial x_i}
\]

### B.3 Application to a real gas

When dealing with a real gas, the derivation of the P and Q matrices is far from straightforward. Especially because the total energy depends on both volume and temperature. However, if we can prove that the conservation equation reduce to the same set of primitive equation for a real gas and for a perfect gas, then the eigenvalues are identical.

Density being both a conservative and a primitive variable, the mass conservation equation is the same in the conservative and primitive form. Transforming the momentum equation does not require the use of the perfect gas equation of state so the primitive equations for the velocities will be recovered in real gas. This statement is also valid for the primitive species conservation equation:

\[
\frac{\partial Y_k}{\partial t} + u_j \frac{\partial Y_k}{\partial x_j} = 0
\]

Following the analysis by Okongo'o et al.\[101\], the energy equation implies the use of some internal energy derivatives.

\[
\left(\frac{\partial e}{\partial p}\right)_{\rho,Y_k} = \frac{1}{\rho} \left[ \frac{p}{\rho} - \frac{C_p}{\alpha_v} \right]
\]

\[
\left(\frac{\partial e}{\partial p}\right)_{\rho,Y_k} = \frac{1}{\rho c^2 \alpha_v}
\]

\[
\left(\frac{\partial e}{\partial Y_k}\right)_{\rho,p} = \frac{h_k}{m_k} - \frac{\rho C_p v_\alpha}{\alpha_v m_k}
\]
The terms of \((106)\) can be written (if we do not consider the viscous and heat release terms):

\[
\frac{\partial \rho E_k}{\partial t} = \frac{\partial \rho e}{\partial t} + \frac{1}{2} \rho u_i u_i
\]

\[
\frac{\partial \rho E_i u_j}{\partial x_j} = \frac{\partial \rho e u_j}{\partial x_j} + \frac{1}{2} \rho u_i u_i u_j
\]

Using continuity:

\[
e \frac{\partial \rho}{\partial t} + e \frac{\partial \rho u_j}{\partial x_j} = 0 \quad \text{and} \quad \frac{1}{2} u_i u_i \frac{\partial \rho}{\partial t} + \frac{1}{2} u_i u_i \frac{\partial \rho u_j}{\partial x_j} = 0
\]

Using the momentum equation enables us to simplify some other terms:

\[
\frac{1}{2} \rho \left( \frac{\partial u_i u_i}{\partial t} + u_j \frac{\partial u_i u_i}{\partial x_j} \right) = \left( \rho u_i \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} \right) =
\]

\[
u_i \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = -u_i \frac{\partial \rho}{\partial x_i}
\]

The equation energy becomes:

\[
\rho \frac{\partial e}{\partial t} + \rho u_j \frac{\partial e}{\partial x_j} - u_j \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho u_j}{\partial x_j}
\]

The pressure derivatives can be simplified:

\[
-u_j \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho u_j}{\partial x_j} = -(\frac{\partial \rho u_j}{\partial x_j} - p \frac{\partial u_j}{\partial x_j}) + \frac{\partial \rho u_j}{\partial x_j} = p \frac{\partial u_j}{\partial x_j}
\]

Which in turns gives, for the energy equation:

\[
\rho \frac{\partial e}{\partial t} + \rho u_j \frac{\partial e}{\partial x_j} + p \frac{\partial u_j}{\partial x_j}
\]

Let us now make the previous derivatives for internal energy \((130 \ 131 \ 132)\) appear:

\[
\rho \left( \frac{\partial e}{\partial p} \frac{\partial p}{\partial t} + \rho \frac{\partial e}{\partial p} \frac{\partial p}{\partial x_j} \right) + \rho u_j \left( \frac{\partial e}{\partial p} \frac{\partial p}{\partial t} + \rho \frac{\partial e}{\partial p} \frac{\partial p}{\partial x_j} \right) + \rho \frac{\partial e}{\partial Y_k} \frac{\partial Y_k}{\partial t} + \rho \frac{\partial e}{\partial Y_k} \frac{\partial Y_k}{\partial x_j} + p \frac{\partial u_j}{\partial x_j} =
\]

\[
\left( \frac{\partial e}{\partial p} \frac{\partial p}{\partial t} + \rho u_j \frac{\partial p}{\partial x_j} \right) + \left( \frac{\partial e}{\partial \rho} \frac{\partial \rho}{\partial t} + \rho u_j \frac{\partial \rho}{\partial x_j} \right) + \left( \frac{\partial e}{\partial Y_k} \frac{\partial Y_k}{\partial t} + \rho u_j \frac{\partial Y_k}{\partial x_j} \right)
\]

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Using the primitive equation for density in (123):

\[
\rho \frac{\partial \rho}{\partial t} + \rho u_j \frac{\partial \rho}{\partial x_j} = -\rho^2 \frac{\partial u_j}{\partial x_j}
\]

and using the primitive equation for species (B.3)

\[
\rho \frac{\partial Y_k}{\partial t} + \rho u_j \frac{\partial Y_k}{\partial x_j} = 0
\]

The remaining terms are:

\[
\left( \frac{\partial e}{\partial p} \right) \left[ \rho \frac{\partial p}{\partial t} + \rho u_j \frac{\partial p}{\partial x_j} \right] - \rho^2 \frac{\partial u_j}{\partial x_j} \left( \frac{\partial e}{\partial \rho} \right) + p \frac{\partial u_j}{\partial x_j} = 0
\]

(134)

Using (130), (131), (132) and simplifying:

\[
\frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \rho c^2 \frac{\partial u_j}{\partial x_j} = 0
\]

(135)

For a perfect gas, \( \rho c^2 = \gamma p \). Thus the primitive equations in real gas recover the primitive equations for a perfect gas. As a consequence, the eigenvalues are identical. So are the wave amplitudes (127). The species are advected in the \( x_1 \) direction but \( u_1 \). Their corresponding eigenvalues are:

\[
\lambda_{(5+k)} = u_1 \quad \text{for } k = 1, \ldots, N
\]

(136)

with \( N \) the total number of species. The wave amplitudes are:

\[
L_{(5+k)} = u_1 \left( \frac{\partial Y_k}{\partial x_1} \right) \quad \text{for } k = 1, \ldots, N
\]

(137)

The total set of wave amplitudes for a real gas is:

\[
\begin{align*}
L_1 &= \lambda_1 \left( \frac{\partial p}{\partial x_1} - \rho c \frac{\partial u_1}{\partial x_1} \right), \\
L_2 &= \lambda_2 \left( c^2 \frac{\partial \rho}{\partial x_1} - \frac{\partial p}{\partial x_1} \right), \\
L_3 &= \lambda_3 \left( \frac{\partial u_2}{\partial x_1} \right), \\
L_4 &= \lambda_4 \left( \frac{\partial u_3}{\partial x_1} \right), \\
L_5 &= \lambda_5 \left( \frac{\partial p}{\partial x_1} + \rho c \frac{\partial u_1}{\partial x_1} \right),
\end{align*}
\]

(138)

\[
L_{(5+k)} = u_1 \left( \frac{\partial Y_k}{\partial x_1} \right) \quad \text{for } k = 1, \ldots, N
\]
Those wave amplitude are then included in the primitive equations:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{1}{c^2} \left[ L_2 + \frac{1}{2} (L_5 + L_1) \right] &= 0 \\
\frac{\partial p}{\partial t} + \frac{1}{2} (L_5 + L_1) &= 0 \\
\frac{\partial u_1}{\partial t} + \frac{1}{2pc} (L_5 - L_1) &= 0 \\
\frac{\partial u_2}{\partial t} + L_3 &= 0 \\
\frac{\partial u_3}{\partial t} + L_4 &= 0 \\
\frac{\partial Y_k}{\partial t} + L_{(5+k)} &= 0 \quad \text{for } k = 1, \ldots, N
\end{align*}
\]

To obtain the conservative equations from the primitive equation for density, velocity and species is straightforward and not explained here. The conservative equations are:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + d_1 + \frac{\partial \rho u_2}{\partial x_2} &= 0 \\
\frac{\partial \rho u_1}{\partial t} + u_1 d_1 + \rho d_3 + \frac{\rho u_1 u_2}{x_2} + \frac{\rho u_1 u_3}{x_3} &= \frac{\partial \tau_{1j}}{\partial x_j} \\
\frac{\partial \rho u_2}{\partial t} + u_2 d_1 + \rho d_4 + \frac{\rho u_2 u_2}{x_2} + \frac{\rho u_2 u_3}{x_3} + \frac{\partial p}{\partial x_2} &= \frac{\partial \tau_{2j}}{\partial x_j} \\
\frac{\partial \rho u_3}{\partial t} + u_3 d_1 + \rho d_5 + \frac{\rho u_3 u_2}{x_2} + \frac{\rho u_3 u_3}{x_3} + \frac{\partial p}{\partial x_3} &= \frac{\partial \tau_{3j}}{\partial x_j} \\
\frac{\partial \rho Y_k}{\partial t} + Y_k d_1 + \rho d_{5+k} &= \dot{w}
\end{align*}
\]

With:

\[
d = \begin{pmatrix}
d_1 \\
d_3 \\
d_4 \\
d_5 \\
d_{5+k}
\end{pmatrix} = \begin{pmatrix}
\frac{1}{c^2} [L_2 + \frac{1}{2} (L_5 + L_1)] \\
\frac{1}{2pc} (L_5 - L_1) \\
L_3 \\
L_4 \\
L_{5+k}
\end{pmatrix}
\]

But the energy equation requires some manipulations developed thereafter:

\[
\frac{\partial \rho E}{\partial t} = \rho \frac{\partial E}{\partial t} + E \frac{\partial \rho}{\partial t} = \rho \frac{\partial e}{\partial t} + \frac{1}{2} \rho \frac{\partial u_i u_i}{\partial t} + E \frac{\partial \rho}{\partial t}
\]
Let us look at each term one by one:

\[
\rho \frac{\partial e}{\partial t} = \rho \left( \frac{\partial e}{\partial \rho} \frac{\partial \rho}{\partial t} + \left( \frac{\partial e}{\partial p} \frac{\partial p}{\partial t} + \left( \frac{\partial e}{\partial Y_k} \frac{\partial Y_k}{\partial t} \right) \right)
\]

\[
= - \left( \frac{\rho - C_p \alpha_v}{\rho} \right) d_1 - \frac{1}{\rho c^2} \left( \frac{C_p}{\alpha_v} \left( L_1 + L_5 \right) \right) - \rho d_{5+k} \left( \frac{\partial e}{\partial Y_k} \right)
\]

\[
= - \left( \frac{\rho}{\rho^2} \right) d_1 - \frac{C_p}{\alpha_v} \left( L_2 \right) - \rho d_{5+k} \left( \frac{\partial e}{\partial Y_k} \right)
\]

\[
= - \frac{\rho}{\rho^2} d_1 - \frac{C_p}{\alpha_v} d_5 - \rho d_{5+k} \left( \frac{\partial e}{\partial Y_k} \right)
\]

\[
\frac{1}{2} \rho \frac{\partial u_i u_i}{\partial t} = \rho u_i \frac{\partial u_i}{\partial t}
\]

\[
= -\rho u_i d_{i+2}
\]

\[
E \frac{\partial \rho}{\partial t} = -Ed_1
\]

Finally the energy equation is:

\[
\frac{\partial \rho E}{\partial t} + \left( E + \frac{p}{\rho} \right) d_1 + \rho u_i d_{i+2} + \rho d_{5+k} \left( \frac{\partial e}{\partial Y_k} \right) + \frac{C_p}{\alpha_v} d_5
\]

\[
+ \frac{\partial (\rho E + p) u_2}{\partial x_2} + \frac{\partial (\rho E + p) u_3}{\partial x_3} = \frac{\partial \tau_{ij}}{\partial x_i} \frac{u_j}{x_i} - \frac{q_i}{x_i}
\]

B.4 Specification of the Boundary Conditions

According to Thompson[152], the number of boundary conditions which must be specified at a point of the boundary is equal to the number of incoming waves. For an inflow, only \( \lambda_1 \) is less than zero, which means that all the other waves are propagating inside the domain. On the contrary, for an outflow, only \( L_1 \) is an incoming waves.

B.4.1 Subsonic reflecting inflow

For a subsonic inflow, we need to define \((5 + k - 1)\) boundaries, the last one will be defined by the characteristic analysis. In general, velocities, temperature and species are specified at the inflow and the density is computed. The procedure to follow at the inflow is:

1. Compute \( L_1 \) using (138) and forward differences.

2. As \( u_2 \) is fixed, then \( L_3 \) is known.

3. As the species mass fraction are fixed, the \( L_{5+k} \) are known.
Similarly, if $u_1$ is fixed, and using $L_1$, one can compute $L_5$, $L_2$ still needs to be computed. One way is to express the wave amplitude in terms of temperature:

$$\frac{\partial T}{\partial t} + \frac{T\alpha_v(L_{5+k} + L_1)}{2\rho C_p} + \frac{L_2}{\rho \alpha_v c^2} - \frac{1}{\alpha_v} \sum_{k=1}^{N} \frac{\rho v_k}{m_k} L_{5+k}$$

(151)

Now that all the wave amplitudes are determined, the element $d_1$ is easily computed and the density is defined.

### B.4.2 Subsonic non reflecting outflow

In the case of a subsonic outflow, $L_2$, $L_3$, $L_4$, $L_5$, $L_{5+k}$, are computed using backward differences. As Baum et al.\[6\] suggested a value of $L_1$ ensuring well-posed problems:

$$L_1 = K(p - p_{\infty})$$

where $K$ is a parameter which determines the speed at which the average pressure in the domain relaxes towards the imposed infinity pressure. Either $K$ is set constant or it is determined by:

$$K = \sigma_p (1 - \mathcal{M}) \frac{c}{L}$$

where $\mathcal{M}$ is the maximum Mach number in the flow, $L$ is a characteristic longitudinal length scale and $\sigma_p$ is the reflection coefficient which the sets the amplitude of the reflected waves.
REFERENCES


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