Design and Study of a Convergent-Divergent Supersonic Nozzle

Announcement
Extended

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### Nomenclature

The next list describes the symbols used within the body of the document:

#### Acronyms

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>τ</td>
<td>Shear stress tensor</td>
</tr>
<tr>
<td>γ</td>
<td>Specific heat ratio</td>
</tr>
<tr>
<td>ν</td>
<td>Prandtl Meyer function</td>
</tr>
<tr>
<td>ρ</td>
<td>Density</td>
</tr>
<tr>
<td>θ</td>
<td>Flow angle with respect to the symmetry axis</td>
</tr>
<tr>
<td>⃗v</td>
<td>Velocity</td>
</tr>
<tr>
<td>C⁺</td>
<td>Left Running Characteristic</td>
</tr>
<tr>
<td>C⁻</td>
<td>Right Running Characteristic</td>
</tr>
<tr>
<td>cₚ</td>
<td>Specific heat capacity at constant pressure</td>
</tr>
<tr>
<td>h</td>
<td>Enthalpy</td>
</tr>
<tr>
<td>M</td>
<td>Mach number</td>
</tr>
<tr>
<td>N</td>
<td>Number of characteristics in the net</td>
</tr>
<tr>
<td>p</td>
<td>Pressure</td>
</tr>
<tr>
<td>q</td>
<td>Heat</td>
</tr>
<tr>
<td>R</td>
<td>Ideal gas constant</td>
</tr>
<tr>
<td>r</td>
<td>Radial coordinate</td>
</tr>
<tr>
<td>S</td>
<td>Surface</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
</tr>
<tr>
<td>V</td>
<td>Volume</td>
</tr>
<tr>
<td>x</td>
<td>Longitudinal coordinate</td>
</tr>
<tr>
<td>CDS</td>
<td>Central Difference Scheme</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>LRC</td>
<td>Left Running Characteristic</td>
</tr>
<tr>
<td>MoC</td>
<td>Method of Characteristics</td>
</tr>
<tr>
<td>ND</td>
<td>Nozzle Design</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>RRC</td>
<td>Right Running Characteristic</td>
</tr>
<tr>
<td>TDP</td>
<td>Thermal design Power</td>
</tr>
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</table>
Abstract

This thesis presents a comprehensive exploration of the design and analysis of a convergent-divergent supersonic nozzle, bridging the gap between traditional nozzle design methodologies and modern computational techniques. A custom-built nozzle design tool, developed in MATLAB, serves as the cornerstone of this research. In its core, the tool uses a finite differencing scheme of the axisymmetric Method of Characteristics to trace the contour streamline. The results obtained are compared to existing implementations of the case, and are compared to the two-dimensional analogue yielding very promising results in terms of material and weight savings for the nozzle design.

Furthermore, the thesis delves into the historical evolution of rocket nozzle designs, tracing the trajectory from rudimentary conic structures to sophisticated aerospike configurations.

The energy consumption associated to the resources allocated to the project has been calculated and determined to be negligible. In a similar fashion, the required budget for this project has been justified and comes out as a really low and affordable endeavour.

In essence, this work strives to push the boundaries of nozzle design and analysis, leveraging modern computational tools while maintaining a strong foundation in established theoretical frameworks. The insights derived promise to inform and enhance future endeavors in rocket propulsion systems design.
1 Introduction

Rocket engines are the only choice for a vast majority of space missions when it comes to current propulsion technology, especially in launch endeavours, where a combination of both solid and liquid propellant technology has been and still is the industry standard. Inside these engines, the flow is accelerated beyond supersonic speeds in a region known as the thrust chamber which, in thermochemical rockets, encompasses the combustion chamber and the nozzle, being the latter the focus of this project.

1.1 Objectives

The backbone of this thesis is an exploration of nozzle design utilizing the Method of Characteristics, a mathematical technique which can be used in supersonic flow regimes. This method, originally employed for the design of supersonic wind tunnels, has found significant application in the field of rocket propulsion, given its ability to handle the non-linear equations associated with compressible flows. The method, despite having being the basis of rocket design for more than 70 years, still has no consensus nor extensive detail on the solving procedure, which makes it a challenging problem with large variability in its results, even nowadays. The method will be implemented in MATLAB, thus creating a reusable Design Tool able to generate nozzle designs for a range of exit Mach numbers.

1.2 Scope

1.2.1 Key Points

This thesis will deal with the following key points:

1. Theoretical Principles: Fundamentals of fluid dynamics, thermodynamics, and nozzle design relevant to convergent-divergent nozzles.
2. Literature Review: Existing research and technologies on nozzle design and performance.
3. Matlab Tool Development: Creation of a computational tool using Matlab for nozzle design optimization, including details of the algorithmic implemented into the source code and subroutines workflow.

1.2.2 Out-of-scope Points

The following points fall out of the scope of this project, and therefore are not going to be dealt with:

1. Experimental Validation: Due to resource limitations, this research will not include experimental testing of the nozzle design.
2. Multi-phase Flows: The study is restricted to single-phase flows and will not consider multi-phase flow scenarios.

3. Combustion Effects: Combustion phenomena inside the nozzle will not be analyzed in this research.

4. Components: Neither the design and analysis of the Combustion Chamber and converging part of the nozzle, nor the injectors nor the nozzle cooling systems will be carried out in this thesis.

5. Material Science Aspects: The study will focus on fluid dynamics and not on material properties or thermostructural integrity of the nozzle.

1.2.3 Deliverables

The project will include the following Deliverables:

1. **D1 - Final Thesis**: A comprehensive document compiling all aspects of the research, from theoretical background to conclusions.

2. **D2 - Code**: The MATLAB code developed during this project.

1.3 Requirements

This project is carried out to fulfill the technical specifications detailed in table 1.

<table>
<thead>
<tr>
<th>ID</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>REQ-ND-1</td>
<td>The ND tool shall be reusable for as many times as the user requires.</td>
</tr>
<tr>
<td>REQ-ND-2</td>
<td>The ND tool shall produce identical results in multiple runs of the same set of input variables. A small computational error is granted due to software restrictions.</td>
</tr>
<tr>
<td>REQ-ND-3</td>
<td>The ND tool shall be able to generate designs for a range of exit Mach numbers of at least 1 to 3.5.</td>
</tr>
<tr>
<td>REQ-ND-4</td>
<td>The ND tool must produce as an output a &quot;.txt&quot; file containing the set of points that define the generated contour.</td>
</tr>
<tr>
<td>REQ-ND-5</td>
<td>The contour generated by the ND tool can have either an abrupt expansion or a smooth expansion at the throat.</td>
</tr>
<tr>
<td>REQ-ND-6</td>
<td>The ND tool will use the Axisymmetric Method of Characteristics formulation for supersonic compressible, inviscid, adiabatic flows.</td>
</tr>
<tr>
<td>REQ-ND-7</td>
<td>The ND tool shall take as inputs:</td>
</tr>
<tr>
<td></td>
<td>1. The diameter of the throat of the nozzle.</td>
</tr>
<tr>
<td></td>
<td>2. The exit Mach number or the expansion angle.</td>
</tr>
<tr>
<td></td>
<td>3. The specific heat ratio $\gamma$.</td>
</tr>
<tr>
<td></td>
<td>4. The number of Characteristic lines to be calculated.</td>
</tr>
</tbody>
</table>
1.4 Justification

This thesis aims to create a design tool for rocket nozzles which can be coupled with open-source CFD software to allow an integrated workflow between design and analysis. Such workflow can be used to map the design input parameters to output variables that are otherwise hard to obtain analytically, or whose experimental setup can not be carried out.

Even by today standards, rocket design is a tremendously hard task to handle which requires many inputs from very diverse areas, making it a topic of limited spread due to a lack of experience and resources. Many academic and newcomer organizations can benefit from open-source tools of this type to help them in the first steps towards developing rocket technology and supersonic hardware design.

2 State of the Art

The concept of a supersonic convergent-divergent nozzle was first proposed by Karl Gustaf Patrik de Laval, a Swedish engineer born in 1845 who worked in steam turbines, among other areas. Intuition and empiricism led him to the conception of the De Laval nozzle, which he used in his impulse steam turbine design to accelerate a steam jet to supersonic speeds and work from the kinetic energy of the fluid to rotate the turbine \[6\]. These conical-shaped nozzles were the ones used during the late XIX and during the first half of the XX centuries. In the late 1930s and early 1940s, German scientists conducted comprehensive research on nozzle design, covering all its various aspects \[36\]. They concluded that for low area-ratio nozzles, such as those used in the V-2 rocket, there was little advantage in employing highly complex contours. Due to their significant divergence losses, these simpler, conical short nozzles are typically used in small thrusters and solid rocket boosters. In these applications, the ease of fabrication takes precedence over aerodynamic efficiency.

The Method of Characteristics (MoC) was adopted as a numerical design method for supersonic nozzles during the first half of the XX century. Developed by Riemann in his 1860 paper \[56\], the method is a technique for solving hyperbolic partial differential equations. The fluid dynamics PDEs are reduced to a set of ordinary differential equations by introducing characteristic regions along which properties are indeterminate. A set of these regions is then computed, which is followed by the computation of their intersecting points, revealing the fluid properties in the process.

With the dawn of the Space race after World War II, rocket technology development experienced its apogee and new designs, manufacturing techniques and materials became available for the scientists. One of the most influential contributions to this field came from G.V.R. Rao, who
developed the concept of the "Optimum Thrust Nozzle" [51], which optimized the MoC to yield the highest possible thrust for a given length. This was achieved by integrating the mass flow rate over a set control surfaces to find the one with the highest thrust output. The contoured nozzle design continued to be optimised throughout the years, in parallel with the creation of new types of nozzles as illustrated in figure 2.

After many research conducted during the decades of the 60s, 70s and 80s of last century, the space engineering paradigm shifted towards a more pragmatic approach, focusing on the subsystems dealing with the communication and data processing of an ever expanding network of shared knowledge powered by the world wide web. The trimming of the budget of the Space Agencies were one of the main contributors to this feat, and the understanding and development of thrust chambers, inelegantly complex for many, became stagnant. In spite of all this, the worldwide regrowth of the interest in space travel during the last pair of decades is pushing the creation of initiatives, both from public and private entities, to put into practice some of the different designs proposed during the second half of the XX century. The most promising of these designs is the aerospike, which can be applied to current combustion rocket engines, as well as being the default alternative for Rotating Detonation Rocket Engines.

Nowadays, Rao’s optimization of the MoC still is a method used worldwide for designing rocket nozzles, in conjunction with CFD-based approaches in what are called multidisciplinary optimization methods [38]. The MoC per se is limited to supersonic flow, since the subsonic flow equations are elliptical. So far, the design of the whole nozzle has been carried out in three
separate parts which are somehow patched together, with the throat segment being defined by Sauer [60]. Steady techniques are currently limited to this type of solutions, contrasting with the time-dependent techniques of unsteady flow which can yield results for the elliptic and hyperbolic cases [6].

3 Theoretical background

In this section, the details of the isentropic flows will be described followed by an in-depth mathematical look at the Method of Characteristics.

The design of conventional converging-diverging nozzles resides within the classical fluid dynamics
equations, namely the laws of conservation of mass, momentum and energy, which form a system of equations that can be both in partial and in integral forms. The principle of conservation of mass asserts that mass is neither created nor destroyed in a fluid system. For incompressible flows, this is encapsulated by the continuity equation 1. The left term contains the sum of the variation in the total mass of the fluid encapsulated in certain volume \( V \) and the flux of fluid matter through the surface \( S \) of said volume, which is always equal to zero.

Rooted in Newton’s second law, the momentum equations 2 describe the balance of forces acting on a fluid element. These are a set of vectorial equations which relate the variation on the momentum of the fluid with the pressure, viscous and external forces, as well as describing turbulence by means of a convective term.

Lastly, the energy equation 3 dictates that energy can neither be created nor destroyed; it only changes forms. Similarly to the momentum equation, it relates the variation of the total energy within the fluid with the temperature and pressure, as well as with the external energy sources.

\[
\frac{d}{dt} \int_V \rho \, dV + \oint_S \rho \vec{v} \cdot \vec{n} \, dS = 0
\]  

\[
\frac{d}{dt} \int_V \rho \vec{v} \, dV + \oint_S \rho \vec{v}(\vec{v} \cdot \vec{n}) \, dS = \oint_S (- (p - p_a)) \vec{I} + \vec{r} \cdot \vec{n} \, dS + \vec{F}_{ext}
\]  

\[
\frac{d}{dt} \int_V e \, dV = \oint_S ((e + p)\vec{v} - k\nabla T) \cdot \vec{n} \, dS + \oint_V \dot{q} \, dV
\]

The present study will focus on the isentropic relations and on the Method of Characteristics as tools for modelling the fluid flow inside rocket nozzles.

### 3.1 The isentropic relations

The isentropic relations are a common, one-dimensional model of a fluid, which can be obtained from the integrated equations of continuity 1, momentum 2 and energy 3. They can be obtained upon the assumptions that the fluid behaves as an adiabatic and inviscid substance, which flows without discontinuities (shocks) in a steady state. Integrating 1 over a closed control volume with an inlet of area \( A_1 \) and an outlet of area \( A_2 \) (as illustrated in figure 4), and applying the hypothesis above mentioned, the equation becomes:

\[
\rho_1 u_1 A_1 = \rho_2 u_2 A_1
\]  

Where \( \rho \) and \( u \) denote the density and the velocity in the \( x \) direction of the fluid, respectively.
Integrating in a similar manner equations 2 and 3, their respective one-dimensional isentropic forms are obtained:

\[ p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \]  
\[ h_1 + \frac{u_1^2}{2} + q = h_2 + \frac{u_2^2}{2} \]

Where \( p, h \) and \( q \) denote pressure, enthalpy and added heat, respectively. The speed of sound \( a \) can be defined for a calorically perfect gas as

\[ a = \sqrt{\gamma RT} \]  

where \( \gamma \) is the specific heats ratio \( c_p/c_v \). Furthermore, the enthalpy of such a gas can be expressed as

\[ h = c_p T \]

Taking these relations, and defining the stagnation magnitudes as those corresponding to a hypothetical condition where a fluid element in point A of the fluid flow is brought to rest isentropically at point B, one can manipulate the above described expressions to obtain the isentropic relations for a one dimensional flow:

\[ \frac{T_0}{T} = \left( \frac{p_0}{p} \right)^{\frac{\gamma - 1}{\gamma}} = \left( \frac{\rho_0}{\rho} \right)^{\gamma - 1} = 1 + \frac{\gamma - 1}{2} M^2 \]  

Equation 9 relates the stagnation magnitudes (denoted with the subscript 0) with the magnitudes at any point of the flow. The former are constant all over the domain, and thus it is possible to obtain all fluid variables as functions of the Mach number if the stagnation conditions are known.
Further insight into these relations provides new equations that can help define the properties of a rocket nozzle, which will be discussed in section 4.

### 3.2 Nozzle design

The Method of Characteristics (MoC) can be used to solve the ideal flow field case inside a nozzle. With this method, characteristic lines are computed from the throat region by means of a set of compatibility equations which will be now deduced. These characteristic lines are defined as regions of the fluid domain along which the fluid variables are continuous, but the derivatives are indeterminate. Mach lines and expansion waves are an example of characteristic lines. Let’s first begin by understanding the mathematical deduction of these lines.

The continuity equation can be expressed in its differential form as

$$\mathbf{\nabla} \cdot (\rho \mathbf{\vec{v}}) = 0$$  \hspace{1cm} (10)

Let $[x, r, \phi]$ be a cylindrical system coordinate for the flowfield, which complies with the axisymmetric conditions $\frac{d}{d\phi} = 0$, $w = 0$, where $w$ is the tangential velocity. Thus, 10 can be rewritten as

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial r} + \frac{\rho v}{r} = 0$$  \hspace{1cm} (11)

![Superposition of Cylindrical and rectangular coordinate systems for supersonic flows](image)

**Figure 5:** Superposition of cylindrical and rectangular coordinate systems for supersonic flows

Equation 11 is then coupled with Euler’s equation for irrotational flow to derive the MoC

$$d\rho = -\frac{\rho}{a^2}(udu + vdv)$$  \hspace{1cm} (12)

Where $a = \left(\frac{\partial p}{\partial \rho}\right)_S$ is the speed of sound.
Taking the derivative of equation 12 with respect to $x$ and $r$, one obtains

$\frac{\partial \rho}{\partial x} = -\frac{\rho}{a^2} \left( u \frac{\partial u}{\partial x} + v \frac{\partial v}{\partial x} \right)$, \hspace{1cm} (13)

$\frac{\partial \rho}{\partial r} = -\frac{\rho}{a^2} \left( u \frac{\partial u}{\partial r} + v \frac{\partial v}{\partial r} \right)$. \hspace{1cm} (14)

When these results are incorporated into Equation 11 and simplified, the following expression results

\[ \left( 1 - \frac{u^2}{a^2} \right) \frac{\partial u}{\partial x} - \frac{uv}{a^2} \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial r} \right) + \left( 1 - \frac{v^2}{a^2} \right) \frac{\partial v}{\partial r} = -\frac{v}{r}. \] \hspace{1cm} (15)

Recalling the condition for irrotational flow in cylindrical coordinates:

$\nabla \times V = \begin{vmatrix} e_r & re_\phi & e_x \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \phi} & \frac{\partial}{\partial x} \\ v & rw & u \end{vmatrix} = 0 \implies \frac{\partial u}{\partial r} = \frac{\partial v}{\partial x}$, \hspace{1cm} (16)

Substituting equation (16) into equation (15) results in

\[ \left( 1 - \frac{u^2}{a^2} \right) \frac{\partial u}{\partial x} - 2uv \frac{\partial v}{\partial x} + \left( 1 - \frac{v^2}{a^2} \right) \frac{\partial v}{\partial r} = -\frac{v}{r}. \] \hspace{1cm} (17)

Next, differentials for $u$ and $v$ are introduced to form a system of equations,

$du = \frac{\partial u}{\partial x} dx + \frac{\partial u}{\partial r} dr$, \hspace{1cm} (18)

$dv = \frac{\partial v}{\partial x} dx + \frac{\partial v}{\partial r} dr$. \hspace{1cm} (19)

Several authors have linearised equations (17)–(19) and solved them using methods like Cramer’s rule. For example, $\frac{\partial v}{\partial x}$ can be expressed as

$\frac{\partial v}{\partial x} = \frac{N}{D}$, \hspace{1cm} (20)

where $N$ and $D$ are determinants of appropriate matrices.

From the requirement that the derivative must be indeterminate, it is deduced that $D$ must be zero, yielding

$\left( \frac{dr}{dx} \right)_{\text{char}} = \frac{-uv/a^2 \pm \sqrt{(u^2 + v^2)/a^2 - 1}}{1 - u^2/a^2}$. \hspace{1cm} (21)

This insight explains why the Method of Characteristics is typically applied only to supersonic flows, as only in this case do the compatibility equations produce real solutions. This is illustrated
by the term \( \sqrt{(u^2 + v^2)/a} * 2 - 1 \), which is equivalent to \( \sqrt{M^2 - 1} \) for the axisymmetric case.

After enough algebraic manipulation, the system of compatibility equations is obtained

\[
\frac{dr}{dx} = \tan (\theta + \mu) \quad \text{for a } C^+
\]

\[
\frac{dr}{dx} = \tan (\theta - \mu) \quad \text{for a } C^-
\]

\[
d(\theta - \nu) = -\frac{1}{\sqrt{M^2 - 1} + \cot \theta} \frac{dr}{r} \quad \text{for a } C^+
\]

\[
d(\theta + \nu) = \frac{1}{\sqrt{M^2 - 1} - \cot \theta} \frac{dr}{r} \quad \text{for a } C^-
\]

The actual compatibility equations are 24 and 25, whereas 22 and 23 define the slopes of the characteristics. In these equations, \( \mu \) is the Mach angle

\[
\mu = \arcsin \frac{1}{M}
\]

\( \theta \) is the flow angle with respect to the symmetry axis and \( \nu \) is the Prandtl-Meyer function:

\[
\nu(M) = \sqrt{\frac{\gamma + 1}{\gamma - 1}} \tan^{-1} \left( \frac{\frac{\gamma - 1}{\gamma + 1} (M^2 - 1)}{\gamma + 1} \right) - \tan^{-1} \left( \sqrt{M^2 - 1} \right)
\]

The \( C^+ \) and \( C^- \) respectively denote left running an right running characteristics. For every location in the fluid domain, a left-running characteristic and a right running characteristic, which intersect at such point, define the upstream region of influence over the point, as well as the region of influence of that point downstream, as can be illustrated in figure 6. This is useful for defining the the flow regions inside the nozzle, explained further on.

The inner nozzle can be divided into two regions: the kernel and the straightening segment, as depicted by figure 7.

The kernel, or non-simple region, is defined as the space inside the nozzle which the gases undergo
Figure 7: Nozzle regions and example of a characteristics net

the initial expansion. Here, for a fixed position along the axis $x$, the flow angle increases as the radial distance with respect to the axis of symmetry $r$ becomes larger upon reaching the nozzle wall, in which the flow angle is the maximum for that axial position. Each characteristic line emanating from the contour expansion region intersects with the characteristic emanating from the opposite side across the symmetry axis, which causes them to curve. The boundary of the kernel is traced by the characteristic emanating from the point of maximum expansion angle $\theta_{\text{max}}$ on the wall of the expansion section contour. This initial expansion section wall can be arbitrarily defined and is usually a circular segment with a radius in the order of the throat radius.

The point out of which that characteristic emanates is the same point which marks the beginning of the straightening region. The wall angle of the contour in this region decreases as the axial position increases, until reaching a null value at the exit. The contour shape is such that the characteristic lines are cancelled at the wall.

4 Methodology

The system of equations from 22 to 25 can be used to generate an ideal contour in which the flow exits the nozzle parallel to the axis of symmetry. By employing the Method of Characteristics, one can obtain the streamline that leads from the end of the supersonic expansion region up to the exit section, defined by the exit Mach number.

The MoC can be solved numerically with the use of first-order finite differences, leading to the following sets of equations

$$
C^+ \left\{
\begin{array}{l}
\frac{r_{i,j+1} - r_{i,j}}{x_{i,j+1} - x_{i,j}} = \tan (\theta_{i,j} + \mu_{i,j}) \\
\theta_{i,j+1} - \theta_{i,j} - \nu_{i,j+1} + \nu_{i,j} = -\frac{1}{\sqrt{\frac{1}{2} (M_{i,j+1} + M_{i,j})^2 - 1 + \cot \frac{1}{2} (\theta_{i,j+1} + \theta_{i,j})}} \frac{r_{i,j+1} - r_{i,j}}{\frac{1}{2} (r_{i,j+1} + r_{i,j})}
\end{array}
\right.
$$

(28)
28 and 29 define the slope and the compatibility equation for each characteristic. The domain inside the nozzle is discretised in $N \times (N + 1)$ nodes. Sub-index $i$ of each node indicates the numeration of the characteristic line, beginning from 1 at the throat and going up to $N$ at the maximum expansion angle point on the predefined contour. Sub-index $j$ indicates the point along the discretised characteristic, as illustrated in figure 8.

The algorithm for this first-order finite difference scheme of 28 and 29 is as follows:
Algorithm 1 Kernel algorithm structure

Require: $M_e, \theta_{\text{expansion}}, N, r_a$

0: for $l = 1$ to $N$ do
0: \[ [x, r]_{1,1} \leftarrow F_1(\Delta \theta_l) \]
0: \[ [M]_{1,1} \leftarrow F_2(\Delta \theta_l) \]
0: \[ [x, r]_{1,2} \leftarrow F_3((M, \theta, x, r)_{1,1} + (M, \theta, x, r)_{1,2}) \]
0: \[ [M, \theta]_{1,2} \leftarrow F_4((M, \theta, x, r)_{1,1} + (M, \theta, x, r)_{1,2}) \]
0: for $l = 2$ to $N$ do
0: \[ [x, r]_{l,k} \leftarrow F_5([[l, k-1], [l-1, k]]) \]
0: \[ [M, \theta]_{l,k} \leftarrow F_6([[l, k-1], [l-1, k]]) \]

0: = 0

The user initiates the process by defining a set of initial input parameters, specifically the exit Mach number ($M_e$) or the initial expansion angle ($\theta_{\text{max}}$), the heat capacity ratio ($\gamma$), the number of characteristics ($N$), and the throat and agreement radii ($r_t$ and $r_a$). The agreement radius is that of the initial expansion circumference, as illustrated in figure 9. These parameters serve as the foundational elements for establishing the nozzle’s initial expansion section. On this initial section lie the first points from which the characteristics will be traced. In order to ensure a uniform and well-controlled layout of these lines, particularly for the first set of Left Running Characteristics (LRC), a growth rate function 30 is utilized. This function determines the angular increment ($\Delta \theta$) between successive characteristics. By doing so, it minimizes the scattering or dispersion among the initial characteristics, thereby allowing for a more accurate and efficient computational process for tracing subsequent flow properties within the nozzle. If this growth rate function is not used, the characteristic net density is concentrated downstream the nozzle, leaving the throat area largely empty of grid points. This provides an inaccurate solution of the flow near the initial expansion region.

\[
\theta_{\text{max}} = \sum_{n=1}^{n} \Delta \theta_0 b^{n-1}
\]

(30)

Where $\Delta \theta_0$ is the increment at the first point, $b$ is the growth rate and $\theta_{\text{max}}$ is the maximum expansion angle, given by the following expression

\[
\theta_{\text{max}} = \frac{\nu(M_e)}{2}
\]

(31)

To establish the Mach number at various points along this initial contour, the Prandtl-Meyer relation 27 is employed. This equation is a cornerstone in compressible flow theory and offers an accurate means for determining $M$ based on the given flow conditions. Once the Mach numbers are determined, the focus shifts to calculating the first RRC. To achieve this, Equation 23 is
The resulting expression serves as the basis for calculating the RRC, thereby facilitating the subsequent steps in the nozzle design process:

$$\frac{r_{1,2} - r_{1,1}}{x_{1,2} - x_{1,1}} = \tan(\theta_{1,1} - \mu_{1,1})$$  (32)

The algorithm described in this study is fundamentally constructed based on a first-order discretization approach. While this offers the advantage of computational simplicity and speed, it may compromise the accuracy and robustness of the results, especially for complex flow fields or intricate nozzle geometries. To enhance these crucial parameters—robustness and accuracy—a transition to a second-order discretization approach is highly desirable.

The implementation of a second-order approach necessitates the use of more sophisticated numerical schemes, such as the central difference scheme, which is widely recognized for its second-order accuracy. Unlike the first-order rearward finite difference method, which relies primarily on upstream points to approximate derivatives, the central difference scheme uses both upstream and downstream points. This enables the capturing of higher-order terms in the Taylor series expansion, thereby providing a more accurate representation of the underlying continuous function.

Incorporating a central difference scheme into the algorithm changes the nature of the discretized equation system. The equations that result from this discretization are generally more accurate,
but they may also be more sensitive to numerical instabilities, particularly in regions where the flow field exhibits sharp gradients or discontinuities. Therefore, while the second-order approach enhances the fidelity of the simulation, it also necessitates more rigorous stability checks and may require the introduction of artificial diffusion or other stabilization techniques.

The transition to a second-order approach is not merely a technical refinement; it has substantial implications for the entire simulation process. For instance, the improved accuracy could reveal subtleties in the flow field that are not captured by a first-order scheme, thereby providing deeper insights into the physical phenomena under study. This could be particularly beneficial in the design and analysis of rocket nozzles, where small differences in flow properties can translate into significant variations in performance metrics like thrust and efficiency.

Moreover, a second-order accurate scheme can potentially reduce the computational grid requirements. In other words, to achieve the same level of accuracy, fewer grid points might be needed compared to a first-order scheme. This could lead to faster simulations, thereby offsetting the increased computational cost per grid point that generally comes with higher-order methods.

Thus, the CDS discretization of 22 to 25 yields:

\[
C^+ \begin{cases} 
W_w \frac{r_p-r_w}{x_p-x_w} + W_e \frac{r_e-r_p}{x_e-x_p} = \tan(\theta_p + \mu_p) \\
W_w \frac{(\theta_p-\nu_p)-(\theta_w-\nu_w)}{r_p-r_w} + W_e \frac{(\theta_e-\nu_e)-(\theta_p-\nu_p)}{r_e-r_p} = -\frac{1}{\sqrt{M^2_p-1}} \cot \theta_p \frac{1}{r_p} 
\end{cases} 
\]

\[
C^- \begin{cases} 
W_n \frac{r_p-r_n}{x_p-x_n} + W_s \frac{r_s-r_n}{x_s-x_p} = \tan(\theta_p - \mu_p) \\
W_n \frac{(\theta_p+\nu_p)-(\theta_n+\nu_n)}{r_p-r_n} + W_s \frac{(\theta_s+\nu_s)-(\theta_p+\nu_p)}{r_s-r_p} = \frac{1}{\sqrt{M^2_p-1}} \cot \theta_p \frac{1}{r_p} 
\end{cases} 
\]

Where the influence of a neighbouring point \(i\) is associated to its respective weight \(W_i\), calculated as a function of the distance which separates it from point \(p\):

\[
W_w = \frac{\sqrt{(r_p-r_e)^2 + (x_p-x_e)^2}}{\sqrt{(r_w-r_e)^2 + (x_w-x_e)^2}} 
\]

\[
W_e = \frac{\sqrt{(r_p-r_w)^2 + (x_p-x_w)^2}}{\sqrt{(r_w-r_e)^2 + (x_w-x_e)^2}} 
\]
\[ W_n = \sqrt{\frac{(r_p - r_n)^2 + (x_p - x_n)^2}{(r_n - r_n)^2 + (x_n - x_n)^2}} \]  
\[ W_s = \sqrt{\frac{(r_p - r_n)^2 + (x_p - x_n)^2}{(r_n - r_n)^2 + (x_n - x_n)^2}} \]

To obtain the coordinates and flow variables of the neighbouring points of point \( i \), the algorithm initially calculates a series of characteristics extending to the immediate eastward point, labeled as point \( e \), from point \( i \). This is done using a first-order forward finite differences approach. Once these preliminary characteristics are computed, the algorithm proceeds to iterate over these points to refine the calculated variables and coordinates further. The algorithmic is as follows:

**Algorithm 2 Kernel algorithm structure using a CDS**

Require: \( M_e, \theta_{expansion}, N, r_a \)
0: for \( l = 1 \) to \( N \) do
  0: \( [x, r]_{1,1} \leftarrow F_1(\Delta \theta_l) \)
  0: \( [M]_{1,1} \leftarrow F_2(\Delta \theta_l) \)
  0: \( [x, r]_{1,2} \leftarrow F_3((M, \theta, x, r)_{1,1}) \)
  0: \( [M, \theta]_{1,2} \leftarrow F_4((M, \theta, x, r)_{1,1}) \)
  0: \( [x, r]_{2,2} \leftarrow F_3((M, \theta, x, r)_{2,1}, (M, \theta, x, r)_{1,2}) \)
  0: \( [M, \theta]_{2,2} \leftarrow F_5((M, \theta, x, r)_{2,1}, (M, \theta, x, r)_{1,2}) \)
  0: \( [x, r]_{2,3} \leftarrow F_3((M, \theta, x, r)_{2,2}) \)
  0: \( [M, \theta]_{2,3} \leftarrow F_4((M, \theta, x, r)_{2,2}) \)
  0: for \( k = 2 \) to \( l \) do
    0: \( [x, r]_{l,k} \leftarrow F_5((M, \theta, x, r)_{l,k-1}, (M, \theta, x, r)_{l-1,k}) \)
    0: \( [M, \theta]_{l,k} \leftarrow F_6([l, k - 1], [l - 1, k]) \)

Initialization Step: For \( l \) ranging from 1 to \( N \):
- Calculate the initial \( x \) and \( r \) values using function \( F_1 \) and store them in the matrix at the location \([1, 1]\).
- Calculate the initial Mach number \( M \) using function \( F_2 \) and store it at \([1, 1]\) as well.

First Iteration Step:
- \([x, r]_{1,2}\) and \([M, \theta]_{1,2}\) are computed using \( F_3 \) and \( F_4 \) respectively, using the values at \([1, 1]\).
- \([x, r]_{2,2}\) and \([M, \theta]_{2,2}\) are computed using \( F_3 \) and \( F_5 \) respectively, using the values at \([2, 1]\) and \([1, 2]\).
- \([x, r]_{2,3}\) and \([M, \theta]_{2,3}\) are computed using \( F_3 \) and \( F_4 \) respectively, using the values at \([2, 2]\).

Main Loop:
- For \( l \) ranging from 3 to \( N \):
  - A nested loop for \( k \) from 2 to \( l \) calculates \([x, r]_{l,k}\) and \([M, \theta]_{l,k}\) using \( F_5 \) and \( F_6 \).
The nozzle contour is drawn by first tracing a straight line from the last point of the expansion region contour, illustrated as the yellow point in figure 10, with an equal slope to that of the point. This line intersects with the left running characteristic coming from the second point of the last kernel characteristic, illustrated by the green point, which is the boundary of the kernel. The flow variables in the simple region are preserved alongside characteristics, and thus the Mach number and flow angle at the intersection point are known. Such intersection point (illustrated in red) belongs to the contour. The subsequent contour points are traced by following the same logic, taking at each time the last point of the contour and the LRC emanating from the successive point alongside the kernel boundary, and computing their intersection. The Mach value at the last point on the kernel boundary is that of the exit value, and the flow angle is 0. Thus, the length and shape of the nozzle is entirely defined by its kernel.

5 Results

The findings generated by the nozzle design tool developed in Matlab are presented. To assess the validity and applicability of the tool, its results are compared with established data and theories in existing nozzle design literature. This comparative analysis serves both to validate the tool’s effectiveness and to identify potential areas for further refinement.

5.1 Nozzle design tool - grid sensitivity

A grid density sensitivity analysis is carried out using the first order discretization scheme. An expansion angle of 0.3327 radians is chosen as the initial design point, for which a net of 80 characteristics yields an exit mach of 3.

The results shown in figures 11 to 15 correspond to an expansion angle of 0.3327 radians. Figures (A) illustrate the variation of the Mach number along each $C^{-}$ characteristic line, whereas figures (B) illustrate the contour in red, and the net of $C^{-}$ characteristics in several colours.
A remarkable increment in the Mach number from points $k = 1$ to $k = 2$ is observed in every case, being the higher such increment the lower the number of characteristics. The increment is also observed to be of greater magnitude as the expansion angle of the corresponding characteristic increases. This only happens for the increment between the first couple of points, whereas the increments between the following pairs of points are of smooth variation with respect to one another.

At first insight on this might suggest that the rapid expansion at the throat induced by an agreement radius of $r_a = 0$ is causing a large gradient of the Mach field near this area. However, the same effect is observed when utilizing large agreement radii, i.e. $r_a = r_t$, as illustrated in 16.
Figure 13: Grid of 20 characteristics, with an exit Mach of 3.0147

Figure 14: Grid of 40 characteristics, with an exit Mach of 3.0047

Figure 16: Variation of the Mach number along each $C^-$ characteristic line for an $r_a = r_t$ and $M_e = 2.8953$
Figure 15: Grid of 80 characteristics, with an exit Mach of 3.0000

Figure 17: Nozzles comparison for an exit Mach of 3

Figure 18: Nozzles comparison for an exit Mach of 3
5.2 Comparison with literature cases

When compared to literature cases ([70], [65], figures 17 and 18), the obtained nozzle shares similarity with them for low exit Mach numbers (< 1.5). However, as the exit Mach increases, the nozzle hereby designed seems to take longer shapes. The variation on the exit area among results obtained by other authors is of around 4%. When comparing the results obtained in this thesis with those results, the obtained variation is of around 20%.

The tool is compared to a two-dimensional planar case implementation of the Method of Characteristics for supersonic nozzle design [59]. For this case, the system of compatibility and slope equations is greatly simplified with respect the axisymmetric case (22 to 25). The planar system takes the form of systems 39 and 40:

\[
\begin{align*}
C^+ & \quad \left\{ \begin{array}{l}
\left( \frac{dr}{dx} \right)_{\text{char}} = \tan (\theta + \mu) \\
\theta - \nu(M) = \text{const.} = K^+
\end{array} \right. \\
C^- & \quad \left\{ \begin{array}{l}
\left( \frac{dr}{dx} \right)_{\text{char}} = \tan (\theta - \mu) \\
\theta + \nu(M) = \text{const.} = K^-
\end{array} \right.
\end{align*}
\]

Figure 19: Nozzles comparison between the planar and the axisymmetric MoC an exit Mach of 3. The \( C^+ \) characteristics have not been traced for the axisymmetric case.
The exit radius of the planar case is 2.3 times larger when compared to the axisymmetric case, making the total area ratio 5.29 times larger for the former. The length is also a 215% larger for the planar case.

6 Budget

This project has been developed using the commercial MATLAB software, and it is thought to be continued with (and ported to) open-source software.

The only practical cost identified during the elaboration of this project is the MATLAB license, which has been provided by the Universitat Politècnica de Catalunya. Such license is of the type "Student", and has a base cost of €69 granted a lifetime of use [47].

The remaining resources necessary for the execution of this project as it are common for most households, companies, institutions, etc. nowadays. In particular, only a computer complying with the minimum specifications to run MATLAB is required. These are the OS Windows 10 (version 21H2 or higher), 8 GB of RAM and 4 GB of disk space to install MATLAB and the required modules [47]. A computer such as the HP Z240 SFF in the €260 bracket is enough to run the program [31]. Taking into account the allocation of resources for this project, the estimated coding time is of around 80 hours. In order to calculate a wage cost and an energy consumption cost, a net €15 an hour salary of a formed professional and a 62 € a month electricity flat rate are assumed, based on usual performance metrics and on the author’s electricity bill. The total cost of the wage sums up to

\[ 15 \cdot 80 = 1200 \] (41)

Whereas the total electricity cost is €62, assuming that the code is developed in two 40 hours working weeks.

Thus, the total cost of the project is summarized in table 2

<table>
<thead>
<tr>
<th>Material</th>
<th>Cost (€)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Computer</td>
<td>260</td>
</tr>
<tr>
<td>MATLAB Student license</td>
<td>69</td>
</tr>
<tr>
<td>Wage</td>
<td>1200</td>
</tr>
<tr>
<td>Electrical energy</td>
<td>62</td>
</tr>
<tr>
<td>Total</td>
<td>1591</td>
</tr>
</tbody>
</table>

Table 2: Cost breakdown of the project
7 Environmental Impact

The creation of a thesis, like any academic or research endeavor, has an associated environmental impact, albeit typically minimal when compared to industrial activities. To understand the footprint of this particular thesis on "Design and Study of a Convergent-Divergent Supersonic Nozzle," one must comprehend that the associated electrical power is very low when compared to most of everyday tasks. The runtime takes up to 80% of the TDP (Thermal Design Power) whereas the actual coding takes only a 20%. The programming was carried out using an 85 W TDP power supply unit feeding to the Windows Machine. The runtime represents around 4% of the total working time, which is estimated to be around 80 hours. Thus, the total energy consumption can be calculated with

\[
E = \left( \frac{\% \text{runtime}}{\% \text{TDP}} \cdot \frac{\% \text{runtime}}{t_{\text{total}}} + \frac{\% \text{programming}}{\% \text{TDP}} \cdot \frac{\% \text{programming}}{t_{\text{total}}} \right) \cdot TDP \cdot t_{\text{total}}
\]

(0.8 \cdot 0.04 + 0.2 \cdot 0.96) \cdot 85 W \cdot 288000 s = 5483520 J

The total energy consumed is around 5.5 megajoules, which is what a single wind turbine produces in a second.

The most direct environmental impact arises from the electricity used to power computers, servers, and other electronic equipment. Whether it’s for the execution of simulations, data storage, or the actual writing process, these activities consume power. If this electricity comes from non-renewable sources, such as coal or natural gas, it contributes to greenhouse gas emissions and global warming. However, the impact of this particular project is minimal and the associated emissions can be neglected. According to the Catalan Authorities [26], the 2022 mix of the Spanish electrical grid, at the date of May 3rd, 2023, is of 273 grams of CO₂ per kWh. Taking this as a reference, the total emissions of CO₂ associated to this project are:

\[
\frac{5483520 J}{3600000 J} \cdot \frac{1 \text{ kWh}}{273 g \text{CO}_2} = 415 g \text{CO}_2
\]

415 grams of CO₂ have a minimal if any impact whatsoever on the current environmental status.

8 Conclusions and future work

This thesis has taken on the endeavour of creating an automated tool for the design of a rocket nozzle using the Method Of Characteristics. Not much information is publicly available on this topic, and it is difficult to find already designed tools that carry out these types of design to
compare to.

An insight on the results of the here produced code first order has shed light onto a possible flaw of the code which causes large increments in the Mach number in the calculation of the first points of the characteristics. The two first points are calculated in a separated subroutine from the rest of the net, since they require different boundary conditions to be computable. This leads to a conflict which must be resolved either by modifying the algorithmic of this scheme or by ensuring the proper implementation of the higher order scheme. Despite this, the method comes in as a large improvement when compared to the 2D MoC, with the latter producing nozzle designs with notably longer and wider dimensions, which negatively impacts the performance of the rocket engine by adding substantia weight.

Nevertheless, the design methodology is based on the ideal gas hypothesis, which is a common feature on all the available bibliography found. Even if it is true that the results hereby obtained differ from those obtained in the bibliographic sources, these bibliographic results differ in many cases among each other. No direct comparison could be found with experimental data, and thus it is difficult to determine what is the right approach when determining the degree of validity of a source.

The future improvements for this thesis include:

- Improvement of the algorithmic of the ND tool
- Comparison with numerical results obtained with powerful, well-established CFD solvers
- Comparison with experimental data

Being the use of numerical CFD tools an actual affordable approach, a concept of workflow for the implementation on the open-source OpenFOAM suite is proposed below in figure 20. The idea is to carry out a simulation of the supersonic exhaust of the obtained nozzle design to identify and analyze the key performance metrics, such as exit Mach, exit pressure, subexpansion or overexpansion and possible separation zones.

The workflow is designed to automate the mesh generation process to be able to test many different designs created by the ND tool so that only the output .txt file is required to generate the mesh. The solver does not need to be automated, since the chamber conditions are user input. This can be a good extension to compare the flowfield obtained by means of the MoC to, and thus identify which zones of the fluid domain diverge from the more acceptable results provided by a CFD solver.

Overall, the design tool yields acceptable results up to Mach 3.5, pending to be validated with reliable data.
Figure 20: Meshing algorithm workflow

MATLAB Algorithm

Contour.txt

ContourRead.sh

Input.sh → Contour2BlockMeshDict.sh

blockMeshDict.template

Domainer.sh

blockMeshDict

→ OpenFOAM
References


“Design of Interconnecting Components and Mounts”. In: Modern Engineering for Design of Liquid-Propellant Rocket Engines. Progress in Astronautics and Aeronautics. American


[58] Anxo del Río Otero. “Final Assignment”. In.


