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NUMERICAL ANALYSIS AND VISUALIZATION OF SHOCK STRUCTURES IN A CONVERGENT-DIVERGENT NOZZLE

A Thesis Submitted
in Partial Fulfilment of the Requirements for the
Degree of

MASTER OF TECHNOLOGY

in
Computer Aided Analysis and Design
by

MEHARBAN ALAM
(2K24/CAD/09)

Under the supervision of
Dr. MOHAMMAD ZUNAID
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CANDIDATE'S DECLARATION

I, MEHARBAN ALAM, Roll No. 2K24/CAD/09 student of M.Tech-CAAD Engineering, hereby declare that the project Dissertation titled “Numerical Analysis and Visualization of Shock Structures in a Convergent-Divergent Nozzle” which is submitted by me to the Department of Mechanical Engineering, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Master of Technology, is original and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or other similar title or recognition.

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CERTIFICATE

I hereby certify that the Project Dissertation titled “Numerical Analysis and Visualization of Shock Structures in a Convergent-Divergent Nozzle” which is submitted by MEHARBAN ALAM, Roll No. 2K24/CAD/09, Department of Mechanical Engineering, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Master of Technology, is a record of the project work carried out by the student under my supervision. To the best of knowledge this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.

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Associate Professor
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Place: Delhi

MEHARBAN ALAM

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Date:26/05/2026

M.Tech

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ABSTRACT

High-speed gas flow through Convergent-Divergent Nozzles is a fundamental aspect of aerospace and propulsion engineering, where efficient energy conversion is critical. This study presents a detailed numerical investigation of shock structure formation and flow behaviour within a Convergent-Divergent nozzle. Although the nozzle is initially designed for a Mach number of 2.0, the analysis reveals that the exit Mach number varies significantly with nozzle pressure ratio, ranging from approximately 2.1 under over-expanded conditions ($\text{NPR} \approx 6.81$) to about 2.7 under under-expanded conditions ($\text{NPR} \approx 12.25$) based on boundary conditions.

A Computational Fluid Dynamics approach is employed using a density-based implicit solver to simulate compressible flow across different regimes, including choked, over-expanded and under-expanded conditions. The study evaluates variations in key flow parameters such as Mach number, static pressure, temperature, and velocity, highlighting their dependence on NPR and nozzle geometry.

The results provide detailed visualization of shock structures and their propagation within and downstream of the nozzle. It is observed that both the location and intensity of shock waves are strongly influenced by NPR. The findings are consistent with compressible flow theory and contribute to a better understanding of shock dynamics, offering valuable insights for optimizing nozzle design and improving performance in high-speed propulsion systems.

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NOMENCLATURE

Symbol	Description	Unit
M	Mach Number	–
p	Pressure	Pa
T	Temperature	K
ρ	Density	kg/m ³
v	Velocity	m/s
μ	Dynamic viscosity	(Pa.s)
k	Thermal conductivity	(W/m.K)
V1	Inlet Radius	mm
V2	Throat Radius	mm
V3	Exit Radius	mm
H1	Convergent Length	mm
H2	Divergent Length	mm
H3	Extended Length	mm
V4	Extra Domain Height	mm

ABBREVIATION

CFD	Computational Fluid Dynamics
CD	Convergent-Divergent
NPR	Nozzle Pressure Ratio
2D	Two Dimensional

CHAPTER 1

INTRODUCTION

1.1 Compressible Flow Fundamentals

Fluid flow can be classified into incompressible and compressible flow depending on the variation of density. In low-speed conditions, density remains nearly constant and the flow is treated as incompressible. However, when the velocity of the fluid increases and approaches the speed of sound, density variations become significant, and such flows are known as compressible flow.

Compressible flow is commonly observed in high-speed engineering applications such as jet engines, rockets, and supersonic aircraft. In these systems, parameters like pressure, temperature, velocity, and density vary simultaneously and influence the overall flow behaviour.

Table 1.1: Classification of Flow Based on Mach Number

Flow Type	Mach No.	Characteristics
Subsonic	$M < 1$	Low-speed flow
Sonic	$M = 1$	Flow velocity is equal to the speed of sound
Supersonic	$M > 1$	Shock waves and expansion waves present
Hypersonic	$M > 5$	Very high-speed flow with thermal effects

1.2 Convergent–Divergent Nozzle

By transforming pressure energy into kinetic energy, a convergent–divergent nozzle can increase fluid flow from subsonic to supersonic speeds. The converging section, neck, and diverging section are its three primary sections.

As the cross-sectional area reduces in the converging section, velocity rises and pressure falls. The flow reaches sonic conditions (Mach number = 1) near the neck, which is referred to as the choked situation. Under the right pressure circumstances, the diverging portion beyond the throat permits additional flow expansion, resulting in supersonic velocities.

The CD nozzle is used in aerospace and propulsion systems due to its ability to efficiently control high speed flows.

1.3 Flow Behaviour in CD Nozzle

The pressure conditions at the inlet and outlet have a significant impact on the flow behaviour inside a CD nozzle. The flow grows gradually and reaches supersonic speeds when the pressure ratio is appropriately maintained.

However, in real-world scenarios, disruptions in the flow field result from mismatches in pressure conditions. The nozzle's performance is greatly impacted by these disruptions, which cause complicated flow phenomena as shock waves and expansion waves.

1.4 Shock Waves in Compressible Flow

Shock waves are an important characteristic of supersonic flow. They occur when a high-speed flow is suddenly compressed, causing abrupt changes in pressure, temperature, and density.

Across a shock wave:

Pressure increases sharply

Temperature increases,

Velocity decreases.

Shock waves can be classified into different types based on their orientation;

Table 1.2: Types of Shock Waves

Type	Orientation	Key Characteristics
Normal Shock	Perpendicular to flow direction	Strong shock with sudden increase in pressure and temperature, and rapid decrease in velocity
Oblique Shock	Inclined to flow direction	Weaker than normal shock; gradual change in flow properties and flow deflection occurs

1.5 Practical Flow Conditions

In real applications, the flow inside a nozzle does not always behave ideally. Different flow conditions can occur depending on operating parameters.

Table 1.3: Flow Conditions in Nozzle

Condition	Description
Choked Flow	Mach = 1 at throat
Over-expanded Flow	Exit pressure less than ambient pressure
Under-expanded Flow	Exit pressure greater than ambient pressure
Perfectly Expanded Flow	Exit pressure equals ambient pressure

These conditions determine the location and nature of shock waves in the nozzle.

1.6 Role of Computational Fluid Dynamics

The analysis of compressible flow using experimental methods is often difficult due to high-speed conditions. Therefore, Computational Fluid Dynamics is widely used for analysing such flows.

CFD allows simulation of flow behaviour and provides detailed visualization of parameters such as pressure, velocity, temperature, and Mach number.

It also helps in identifying shock structures and understanding complex flow phenomena.

1.7 Scope of the Present Study

The present study focuses on the numerical analysis of compressible flow through a convergent-divergent nozzle. The aim is to understand the variation of flow parameters and the formation of shock structures under different operating conditions.

The study involves simulation using CFD tools to visualize flow behaviour and analyse shock wave characteristics.

CHAPTER 2

LITERATURE REVIEW

2.1 Literature Review

Several researchers have contributed to the study of compressible flow in C-D nozzles. Early studies focused on theoretical and experimental analysis of supersonic flows, while recent works emphasize numerical simulations using CFD.

Tapasvi et al. [1] carried out a detailed numerical investigation of compressible flow through a nozzle using computational fluid dynamics techniques. Their study focused on evaluating the variations of key flow parameters such as pressure, velocity, temperature, and Mach number along the nozzle axis. The results demonstrated that CFD simulations can accurately capture the acceleration of flow from subsonic to supersonic regimes and predict the formation of shock waves under off-design conditions. Their work provides a strong computational basis for analyzing nozzle flow behavior.

Rathakrishnan [2] presented an extensive theoretical framework for fluid mechanics, with a strong emphasis on compressible flow and gas dynamics. The book explains fundamental concepts such as conservation equations, isentropic flow relations, shock waves, and expansion fans. These principles are essential for understanding the physical behavior of flow in convergent-divergent nozzles and serve as the theoretical foundation for the present study.

Xu et al. [3] provided a comprehensive review of computational fluid dynamics applications in engineering, particularly in complex flow environments. Their study highlighted the ability of CFD to simulate turbulent, compressible, and multiphase flows with high accuracy. The review also emphasized the importance of proper meshing, boundary conditions, and numerical schemes in obtaining reliable simulation results, which is directly relevant to nozzle flow analysis.

Aabid et al. [4] investigated the influence of area ratio on flow development in duct flows through numerical simulations. The study showed that an increase in area ratio significantly affects pressure distribution and velocity profiles. These findings are highly relevant to convergent-divergent nozzle design, where the area ratio plays a critical role in determining flow expansion and shock formation.

Aabid and Khan [5] examined high-speed compressible flow through a convergent-divergent nozzle using CFD coupled with design of experiments (DOE) techniques. Their research focused on optimizing nozzle performance by analyzing the effects of geometric parameters and operating conditions. The study provided valuable insights into flow control, efficiency improvement, and shock wave management in supersonic nozzles.

The ANSYS Fluent Theory Guide [6] provides a comprehensive description of the governing equations, discretization methods, turbulence models, and numerical solution techniques used in CFD simulations. It explains the implementation of the finite volume method and various solver algorithms for compressible flow. This

guide serves as the primary reference for the numerical modeling approach adopted in the present study.

Al-Khalifah et al. [7] conducted a regression-based analysis of flow parameters at high Mach numbers to establish relationships between pressure, temperature, and velocity in supersonic regimes. Their work contributes to understanding the nonlinear behavior of compressible flow and provides empirical correlations that can support validation of numerical results.

Khan et al. [8] performed a detailed CFD analysis of compressible flow through a convergent-divergent nozzle. Their study demonstrated the formation of normal and oblique shock waves, expansion fans, and flow separation under different pressure ratios. The results validated the capability of CFD in capturing complex shock structures, which is a key focus of the present research.

Anderson [9] provided an in-depth treatment of modern compressible flow theory, including isentropic relations, normal and oblique shocks, and expansion wave phenomena. The book also explains nozzle flow behavior under design and off-design conditions. It is one of the most authoritative references for understanding the physics of supersonic flow in CD nozzles.

Liepmann and Roshko [10] discussed the fundamental principles of gas dynamics with a focus on high-speed flows. Their work explains the mechanisms of flow acceleration, shock formation, and compressibility effects, which are crucial for analyzing flow behavior in convergent-divergent nozzles.

Oosthuizen and Carscallen [11] presented analytical solutions for compressible flow problems, including nozzle flow equations and isentropic relations. These solutions are widely used for validating CFD results and ensuring the accuracy of numerical simulations.

White [12] provided a comprehensive introduction to fluid mechanics, covering conservation of mass, momentum, and energy. The book also discusses dimensional analysis and flow properties, which form the fundamental basis for computational modeling of fluid flow.

Ferziger and Perić [13] described advanced numerical methods used in CFD, including finite difference, finite volume, and finite element techniques. Their work emphasizes the importance of grid generation, discretization accuracy, and convergence criteria in obtaining reliable simulation results.

Patankar [14] introduced the finite volume method, which is the most widely used numerical technique in CFD solvers such as ANSYS Fluent. The method ensures conservation of physical quantities and provides stable solutions for complex flow problems, including compressible flows.

Wilcox [15] focused on turbulence modeling approaches, particularly the $k-\omega$ turbulence model. This model is well-suited for simulating boundary layer flows and high-speed compressible flows, making it highly relevant for nozzle flow analysis.

Cebeci and Bradshaw [16] discussed the physical and computational aspects of convective heat transfer and boundary layer development. Their work is important for understanding thermal effects and viscous interactions in nozzle flows.

Goldstein [17] presented various experimental techniques for measuring fluid flow parameters such as velocity, pressure, and turbulence intensity. These techniques are essential for validating CFD simulations and ensuring the reliability of numerical predictions.

Zucrow and Hoffman [18] provided a detailed analysis of gas dynamics, including nozzle flow equations, shock waves, and expansion processes. Their work serves as a classical reference for understanding compressible flow behavior.

Shapiro [19] discussed the thermodynamic aspects of compressible fluid flow, including energy transfer, entropy changes, and shock wave phenomena. This book is fundamental for understanding the thermodynamic processes occurring in CD nozzles.

Godunov [20] developed a numerical method for solving discontinuous flow problems, particularly those involving shock waves. This method forms the foundation of modern shock-capturing schemes used in CFD solvers for accurately predicting discontinuities in compressible flows.

RESEARCH GAPS AND OBJECTIVES

2.2 Research Gaps

1. Most studies isolate either over-expanded or under-expanded regimes. There is a notable absence of comparative research that evaluates both conditions within a singular, controlled computational framework using identical nozzle geometry.
2. Existing literature often focuses on one or two isolated flow parameters. A holistic, simultaneous visualization of all five major flow parameters Mach number, pressure, temperature, density, and velocity is currently lacking, obscuring the complex interactions between these variables.
3. While advanced techniques like Large Eddy Simulation and Design of Experiments exist, the application of polyhedral meshing for stability in high-speed nozzle flow remains limited. Polyhedral elements offer superior convergence and accuracy over traditional tetrahedral meshes, yet remain underutilized in comparative expansion studies.

2.3 Research Objectives

1. To perform a systematic analysis of both over-expanded ($NPR = 6.81$) and under-expanded ($NPR = 12.25$) flow regimes using the same convergent-divergent nozzle geometry, while varying only the duct size to ensure consistent data benchmarking.
2. To generate and analyze high-fidelity, contour-level visualizations of the five core flow parameters simultaneously, providing a detailed understanding of how pressure, temperature, density, velocity, and Mach number evolve across nozzle sections.
3. To apply a polyhedral mesh approach to enhance numerical stability and accuracy, enabling more reliable simulation of complex flow physics compared to conventional mesh techniques.
4. To visualize and compare shock structures and flow behaviour between over-expanded and under-expanded conditions to better understand shock dynamics in high-speed propulsion applications.

CHAPTER 3

METHODOLOGY AND MODEL DESCRIPTION

3.1 Geometrical Modelling

The objective of the present study is to analyse compressible flow through a two-dimensional convergent-divergent nozzle using the Computational Fluid Dynamics approach. The analysis is carried out using ANSYS software, which provides a robust platform for simulating high-speed compressible flows. In this study, important parameters such as nozzle pressure ratio, Mach number, and flow characteristics are evaluated using a density-based implicit solver.

The convergent-divergent nozzle is specifically chosen due to its ability to accelerate fluid flow from subsonic to supersonic speeds. This makes it highly relevant for applications in aerospace propulsion systems, jet engines, and high-speed aerodynamic devices. The geometry of the nozzle plays a crucial role in determining the flow behaviour, especially in the formation of shock waves and expansion regions.

The geometrical modelling of the nozzle is carried out using ANSYS design tools. Initially, the nozzle profile is constructed by drawing a series of line segments that represent the different sections of the nozzle. These sections include the converging section, throat, and diverging section. The converging section is designed to gradually reduce the cross-sectional area, which results in an increase in velocity and a decrease in pressure. The throat represents the minimum cross-sectional area, where the flow reaches Mach 1 under choked conditions. Beyond the throat, the diverging section is designed to increase the cross-sectional area, allowing the flow to expand and accelerate to supersonic velocities.

Each segment of the nozzle is carefully defined based on the design parameters to ensure smooth transition between sections. Proper continuity between the segments is maintained to avoid any geometric discontinuities, which may lead to numerical instability during simulation. The lines are then connected to form a closed profile, which represents the complete geometry of the C-D nozzle.

The schematic representation of the nozzle geometry is shown in Figure 3.1. This figure illustrates the different sections of the nozzle, including the inlet, converging section, throat, diverging section, and the extended duct region. The extended duct is included in the model to capture the downstream flow behaviour and to analyse the formation of shock structures outside the nozzle.

All the geometrical dimensions used in the present study are defined based on a design Mach number of 2. The inlet diameter, throat diameter, exit diameter, and lengths of different sections are selected carefully to achieve the desired flow characteristics. The convergent and divergent angles are also chosen to ensure smooth acceleration and expansion of the flow.

Once the two-dimensional profile of the nozzle is created, a surface is generated using the surface creation tool available in ANSYS. This step converts the line geometry into

a computational domain suitable for CFD analysis. The generated surface represents the flow region through which the fluid will pass during simulation.

The final two-dimensional CFD model of the nozzle is shown in Figure 3.2. This model is used as the computational domain for further analysis. The simplicity of the two-dimensional model helps in reducing computational cost while still capturing the essential flow features such as pressure variation, velocity distribution, and shock wave formation.

The geometrical modelling process is a critical step in CFD analysis, as the accuracy of the simulation results largely depends on the quality of the geometry. A well-defined geometry ensures proper meshing, stable numerical solution, and reliable prediction of flow characteristics. Therefore, careful attention is given to the design and construction of the nozzle geometry in this study.

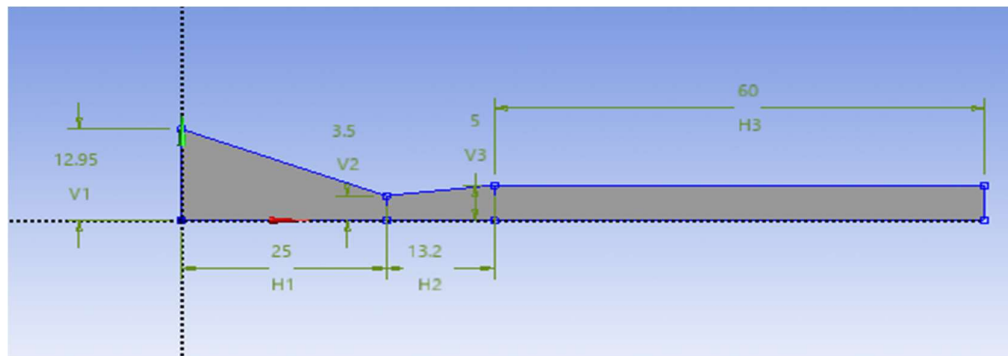


Fig. 3.1 Axisymmetric Convergent -Divergent nozzle geometry for over-expanded flow condition with notation

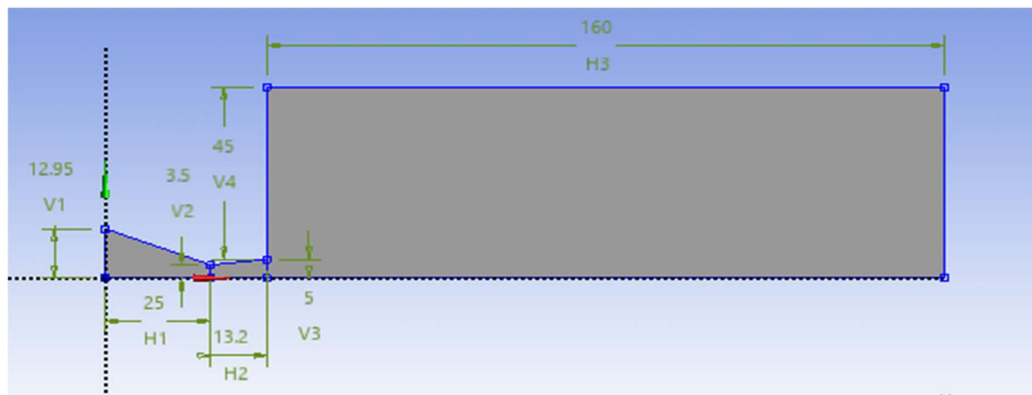


Fig. 3.2 Axisymmetric Convergent -Divergent nozzle geometry for under-expanded flow condition with notation

Table 3.1: Geometrical Parameters of C-D Nozzle

S. No.	Parameters	Over-expanded (mm)	Under-expanded (mm)
1	Inlet Radius (V1)	12.95 mm	12.95 mm
2	Throat Radius (V2)	3.5 mm	3.5 mm
3	Exit Radius (V3)	5 mm	5 mm
4	Convergent length(H1)	25 mm	25 mm
5	Divergent length (H2)	13.2 mm	13.2 mm
6	Extended length (H3)	60 mm	160 mm
7	Extra Domain Height (V4)	0 mm	45 mm

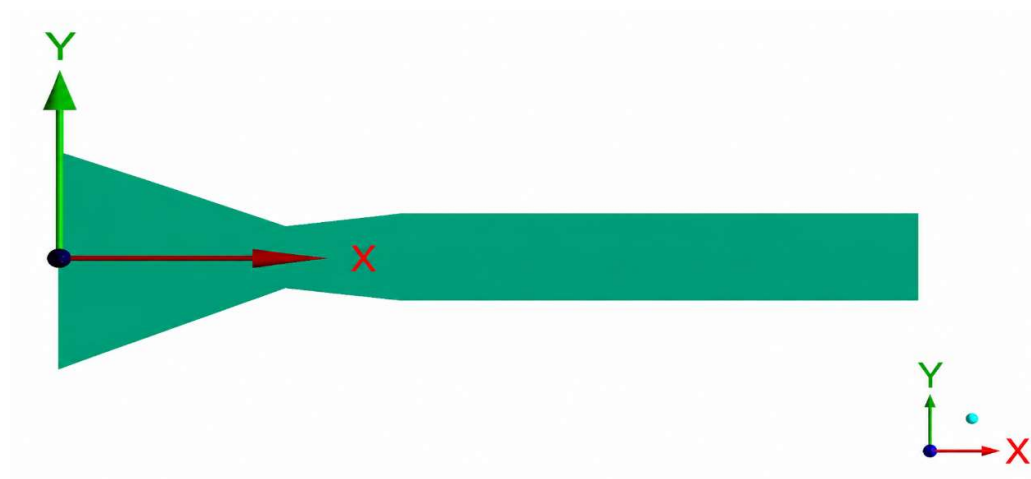


Fig. 3.3 Two-dimensional axisymmetric CFD model of the convergent-divergent nozzle for Over-Expanded flow condition

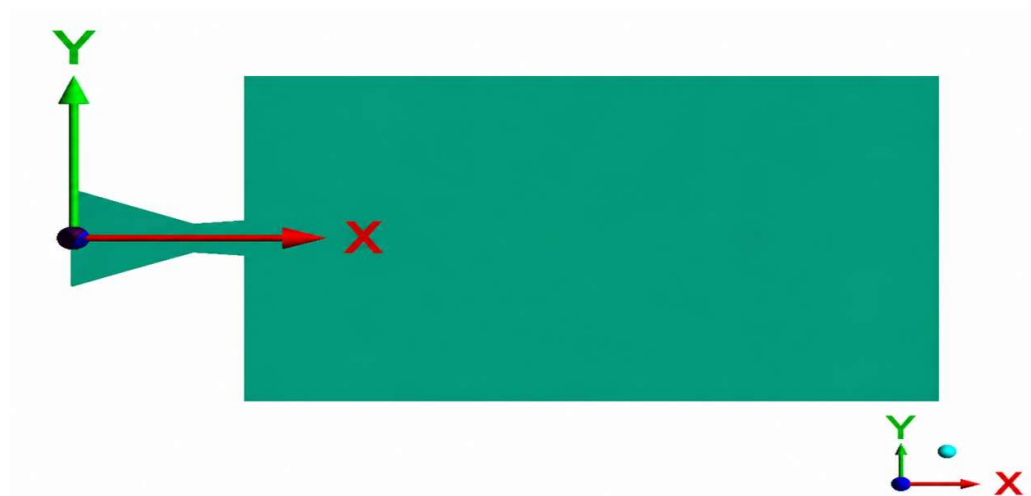


Fig. 3.4 Two-dimensional axisymmetric CFD model of the convergent-divergent nozzle for under-expanded flow condition

3.2 Governing Equations

The governing equations of fluids consist of:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad 3.1$$

Momentum equation:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \left(\frac{2}{3} \right) \mu \delta_{ij} \left(\frac{\partial u_k}{\partial x_k} \right) + \rho(f_i) \quad 3.2$$

Energy balance equation

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial[u_j(\rho E + p)]}{\partial x_j} = \frac{\partial(u_i \tau_{ij})}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{k \partial T}{\partial x_j} \right) + S_E \quad 3.3$$

Where,

ρ = Density (kg/m³)

u_i, u_j = Velocity components (m/s) in x and y direction

p = Pressure (Pa)

T = Temperature (K)

μ = Dynamic viscosity (Pa·s)

k = Thermal conductivity (W/m·K)

E = Total energy is $E = e + (u^2/2)$

$u^2/2$ = kinetic energy

e = internal energy

δ_{ij} = Kronecker delta

(f_i) is a force applied on the fluid,

(S_E) is the energy source term, and

the tensor (τ_{ij}) is:
$$\tau_{ij} = \mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] - \frac{2}{3} \mu \delta_{ij} \left(\frac{\partial u_k}{\partial x_k} \right) \quad 3.4$$

Equations of state relate pressure $p = p(\rho, T)$ and internal energy $e = e(\rho, T)$ to the variables ρ and T .

An example of this relation is the equation of state for an ideal gas:

$$p = \rho R T \quad 3.5$$

where, R is a gas constant

Assumptions:

- Flow is compressible
- Fluid is Newtonian
- Ideal gas assumption
- Steady Flow
- No-slip condition at walls
- Two-dimensional flow

3.3 Boundary Conditions

In order to accurately simulate compressible flow via a convergent–divergent nozzle, boundary conditions are essential. Appropriate boundary conditions are used in the current work to simulate actual flow behavior inside the nozzle. A density-based solver that is appropriate for high-speed compressible flow analysis is used to run the simulation.

The inlet boundary is characterized as a pressure inlet with a total pressure of 690000 Pa and an inlet temperature of 300 K. These circumstances guarantee that the flow has enough energy when it enters the nozzle to accelerate through the converging portion and achieve sonic conditions at the throat.

A pressure outlet boundary condition is applied at the outlet. The atmospheric pressure of 101325 Pa is equivalent to the gauge pressure of 0 Pa. To keep boundary conditions consistent, the outflow temperature is likewise adjusted to 300 K. A nozzle pressure ratio (NPR) of roughly 6.81 is produced by this pressure differential between the inlet and output, which is adequate to generate supersonic flow in the diverging portion.

The flow can smoothly accelerate from subsonic conditions at the intake to sonic conditions at the throat and then to supersonic conditions in the diverging section thanks to the chosen boundary conditions. Additionally, the pressure differential promotes the development of expansion zones and shock waves inside the nozzle, two crucial components of compressible flow analysis.

Careful selection of boundary conditions ensures numerical stability and convergence of the solution. Any improper specification may lead to inaccurate results or divergence of the simulation. Therefore, the boundary conditions are chosen based on theoretical considerations and validated reference data.

Table 3.2: Initial Boundary Conditions for Over-Expanded & Under-Expanded condition

Parameter	Over-expanded (NPR~6.81)	Under-expanded (NPR ~12.25)
Inlet Pressure	690000 Pa	490000 Pa
Inlet Temperature	300 K	300 K
Outlet Pressure	101325 Pa	40000 Pa
Operating Pressure	0 Pa (Gauge)	0 Pa (Gauge)
Wall Condition	Adiabatic (No-slip)	Adiabatic (No-slip)

Source: Adapted from Aabid et al. [4]

CHAPTER 4

VALIDATION AND GRID INDEPENDENCE TEST

4.1 Mesh Generation

Mesh generation is a crucial step in Computational Fluid Dynamics, as it directly influences the accuracy and stability of the numerical solution. In the present study, the computational domains for both over-expanded and under-expanded flow conditions are discretized using ANSYS meshing tools. A two-dimensional axisymmetric mesh is generated for the convergent-divergent nozzle geometry. Special refinement is applied near critical regions such as the throat, nozzle wall, and downstream region where shock waves and expansion fans are expected.

For the **over-expanded case**, a relatively compact domain is used, and mesh refinement is concentrated within the nozzle where shock formation occurs.

For the **under-expanded case**, a larger domain with extended duct height is considered to capture jet expansion and shock cell structures. Accordingly, finer mesh is applied in the downstream region to accurately resolve expansion and shock patterns.

Mesh quality parameters such as skewness and aspect ratio are carefully maintained to ensure numerical stability and convergence.

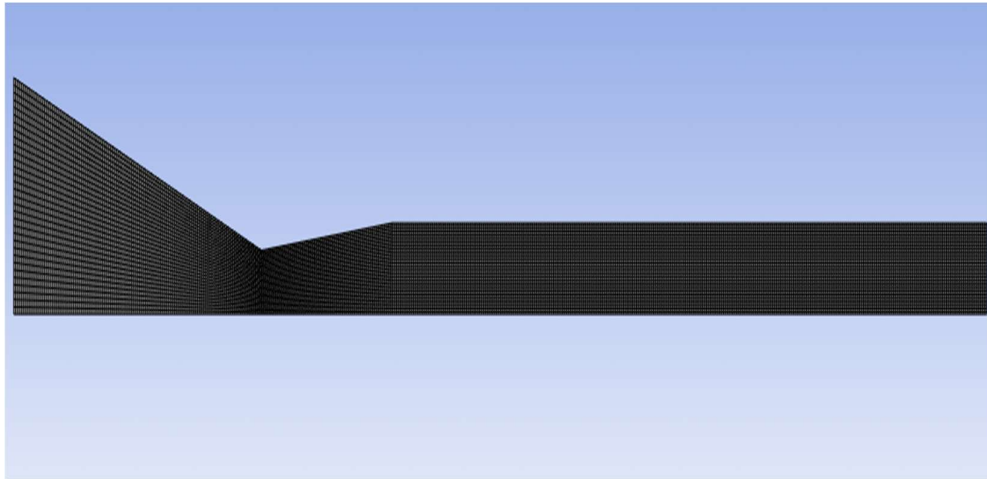


Figure 4.1: Mesh Generation of the C-D Nozzle for Over-Expanded Flow Condition

4.2 Mesh Information (Over-Expanded Case)

The computational domain for the over-expanded flow condition was discretized using a polyhedral mesh with the following technical specifications:

- Total Node Count: The simulation was performed using 15,675 nodes.
- Total Cell Count: The computational grid consists of 15,168 cells, representing the control volumes used for numerical calculations.
- Total Face Count: The mesh comprises 30,842 faces, representing the interfaces between adjacent control volumes.
- Element Distribution: All 15,168 elements are classified as polyhedral, with no tetrahedral, wedge, pyramidal, or hexahedral elements used in this mesh configuration.
- Mesh Independence: A mesh independence study was conducted by refining the grid, and it was observed that further refinement resulted in negligible changes in the solution, confirming that the selected mesh is sufficiently fine and accurate.
- Mesh Advantage: The use of a polyhedral mesh enhances numerical stability and improves convergence behaviour, making it suitable for simulating compressible over-expanded flow in a convergent-divergent nozzle.

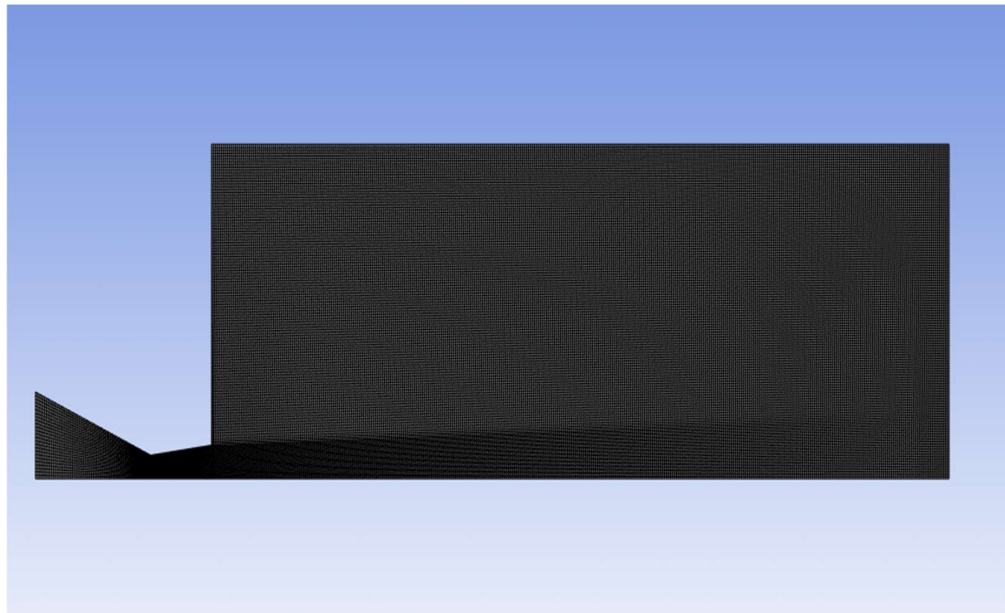


Figure 4.2: Mesh Generation of the C-D Nozzle for Under-Expanded Flow Condition

4.3 Mesh Information (Under-Expanded Case)

The computational domain for the under-expanded flow condition was discretized using a polyhedral mesh with the following technical specifications:

- **Total Node Count:** The simulation was performed using 52,314 nodes.
- **Total Cell Count:** The computational grid consists of 51,710 cells, representing the control volumes used for numerical calculations.
- **Total Face Count:** The mesh comprises 104,023 faces, representing the interfaces between adjacent control volumes.
- **Element Distribution:** All 51,710 elements are classified as polyhedral. No tetrahedral, wedge, pyramidal, or hexahedral elements were utilized in this mesh configuration.
- **Mesh Independence Study:** A mesh independence study was conducted by refining the grid, and it was observed that further refinement resulted in negligible changes in the solution, confirming that the selected mesh is sufficiently fine and provides accurate results.
- **Mesh Type:** The use of a polyhedral mesh enhances numerical stability and improves convergence behavior, making it suitable for simulating compressible under-expanded flow in a convergent-divergent nozzle.

4.4 Grid Independence Test

A grid independence test is carried out for both over-expanded and under-expanded cases to ensure that the numerical results are independent of mesh size. In Computational Fluid Dynamics, the accuracy of the solution is strongly influenced by the discretization of the computational domain. Therefore, it is essential to verify that further refinement of the mesh does not significantly alter the results.

In the present study, three different mesh densities coarse, medium, and fine are generated by varying the element size. Simulations are performed for each mesh configuration, and key flow parameters such as pressure, temperature, velocity, and Mach number are analyzed. The exit Mach number is selected as the primary reference parameter for comparison.

The results obtained using the coarse mesh show noticeable variations, particularly in critical regions such as the throat and shock zones. As the mesh is refined, the solution becomes more stable and accurate. It is observed that the variation between the medium and fine mesh results is negligible for both over-expanded and under-expanded cases.

This indicates that the solution has achieved grid independence, as further mesh refinement does not significantly influence the results. Therefore, the medium mesh is selected for subsequent simulations, as it provides an optimal balance between computational accuracy and computational efficiency.

The grid independence study confirms that the selected mesh is sufficiently accurate for capturing the flow characteristics, including shock structures and expansion behavior, in both over-expanded and under-expanded conditions.

4.5 Validation

The numerical results obtained in the present study are validated by comparing them with the reference research works of Aabid et al. [4] for a nozzle pressure ratio (NPR) of 6.81. A good agreement between the present simulation and the reference data confirms the accuracy of the numerical method, boundary conditions, and solver settings used in this study.

4.5.1 Validation of Temperature Distribution

The validation is carried out by analyzing the variation of temperature along the nozzle length. The fluid enters the nozzle at approximately 300 K, and as it passes through the converging section, the temperature gradually decreases due to an increase in velocity caused by the reduction in flow area.

The flow reaches sonic conditions near the throat region, and further expansion occurs in the diverging section. This expansion leads to a significant drop in temperature. At the nozzle exit, the temperature is observed to be approximately 120–130 K, indicating a substantial reduction from the inlet condition.

This decrease in temperature is a direct result of the conversion of thermal energy into kinetic energy, which is a fundamental characteristic of compressible flow. The overall trend closely matches the reference data, thereby validating the numerical model.

Table 4.1: Validation of Temperature Distribution with Aabid et al. [4]

x (m)	Present [K]	Reference [K]	Error (%)
0.0000	300	300	0.00
0.0109	299	297	0.67
0.0218	292	285	2.45
0.0327	201	210	4.28
0.0436	131	140	6.43
0.0546	155	150	3.33
0.0655	170	165	3.03
0.0764	159	155	2.58
0.0873	157	152	3.28
0.0982	159	158	0.63

Source: Reference data adapted from Aabid et al. [4]

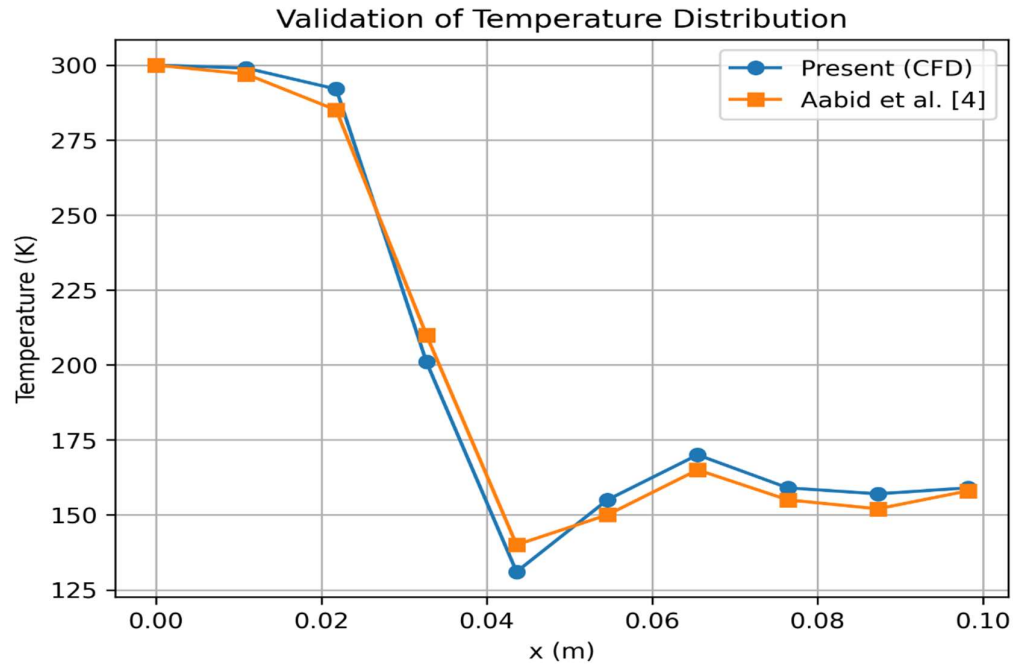


Figure 4.3: Temperature distribution along the nozzle axis (Present vs Aabid et al. [4])

4.5.2 Validation of Velocity Distribution

The velocity distribution is analyzed for validation, showing a gradual increase in the converging section, reaching sonic conditions at the throat and further accelerating to supersonic speeds in the diverging section. The trend shows good agreement with the reference data, thereby validating the numerical model.

Table 4.2: Validation of Velocity Distribution with Aabid et al. [4]

x (m)	Present [m/s]	Reference [m/s]	Error (%)
0.0000	20.1	18	11.67
0.0109	34.1	32	6.56
0.0218	127	120	5.83
0.0327	448	460	2.61
0.0436	583	600	2.83
0.0546	540	530	1.89
0.0655	512	500	2.40
0.0764	532	520	2.31
0.0873	536	525	2.09
0.0982	533	530	0.57

Source: Reference data adapted from Aabid et al. [4]

The higher error near the inlet is due to the low velocity magnitude, where small absolute differences result in relatively higher percentage deviations.

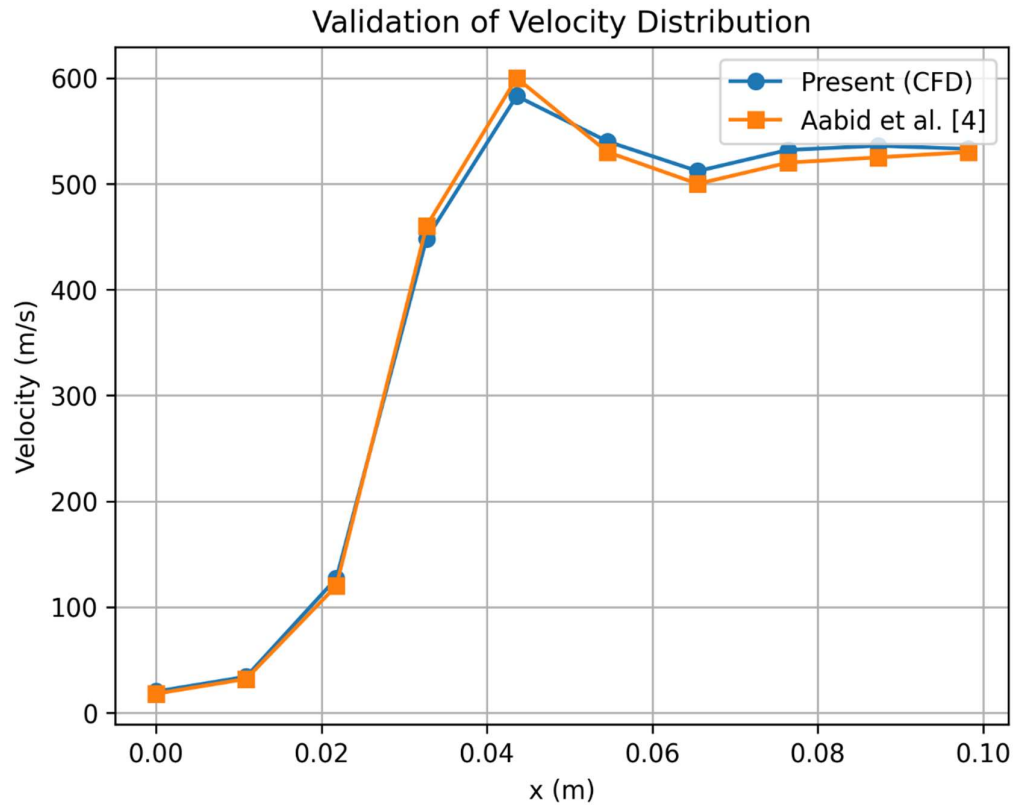


Figure 4.4: Velocity distribution along the nozzle axis (Present vs Aabid et al. [4])

The agreement of the obtained results with the fundamental principles of compressible flow provides further support for the validation. The expected flow acceleration, temperature drop, and corresponding increase in velocity confirm that the governing equations and numerical methods have been applied appropriately.

The close agreement between the present results and the reference data demonstrates the capability of the numerical model to accurately predict compressible flow behavior in a convergent–divergent nozzle.

CHAPTER 5

Results and Discussion

5.1 Over-Expanded Flow

The simulation is run for a lower pressure ratio of $NPR = 6.81$ in order to further analyze the flow behavior. In this scenario, the flow is over-expanded because the exit pressure is lower than the surrounding pressure. Internal shock waves are created in the diverging region as a result of the flow being compressed inside the nozzle. The overall flow parameters are impacted by these shock structures, which produce an abrupt rise in pressure and a fall in velocity. Compression shocks show that the flow adapts to the increased surrounding pressure before leaving the nozzle.

5.1.1 Over-Expansion Contours

The contours for velocity, temperature, and density under over-expanded conditions are shown in figures 5.1–5.6.

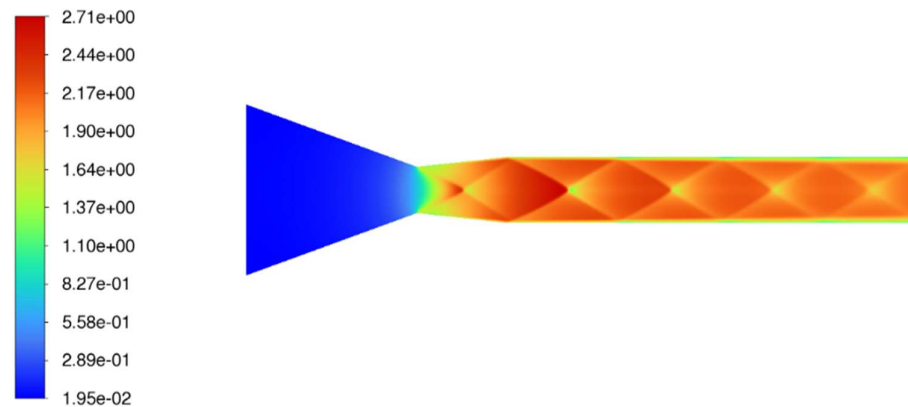
The flow exhibits:

- Flow compression inside the nozzle due to exit pressure being lower than ambient pressure
- Formation of compression shock waves within the divergent section
- Non-uniform and disturbed flow behaviour
- The velocity increases after the throat but decreases across shock regions, while density and temperature show sudden increases due to compression effects.

5.1.1.1 Mach Number Contour

- The Mach contour of Figure 5.1 shows that the flow begins in the subsonic area at the entrance (Mach ~ 0.02 – 0.3), where the velocity is comparatively low, according to the Mach number contour.
- The flow accelerates and achieves sonic state (Mach ≈ 1) as it gets closer to the throat, signifying choked flow at the nozzle throat
- The flow continues to develop into the supersonic area in the diverging segment, reaching Mach numbers between approximately 2.4 and 2.7.
- There are alternating areas of high and low Mach numbers downstream of the nozzle exit, which are indicative of shock cells (shock diamonds) created by under-expanded flow conditions.
- The jet core maintains high supersonic values (~ 1.8 – 2.5), while the surrounding region shows lower Mach numbers (~ 0.5 – 1.2) due to mixing with ambient air.
- The periodic variation between compression and expansion waves confirms the presence of complex supersonic flow structures governing the nozzle exhaust behavior.

Mach Number



contour-13

Figure 5.1: Mach Number Contour of Flow Through the Nozzle

5.1.1.2 Pressure Flow Contour

- The pressure contour of Figure 5.2 shows that the highest pressure ($\sim 6.3 \times 10^5 - 6.7 \times 10^5$ Pa) exists at the inlet region, where the flow is in subsonic condition.
- As the flow accelerates towards the throat, a continuous pressure drop is observed, reaching lower values at the throat corresponding to sonic flow.
- In the divergent section, the pressure initially decreases but due to over-expanded condition, the flow experiences compression shocks inside the nozzle, causing a sudden rise in pressure locally.
- These internal shock structures create non-uniform pressure distribution, with alternating high and low-pressure regions along the flow direction.

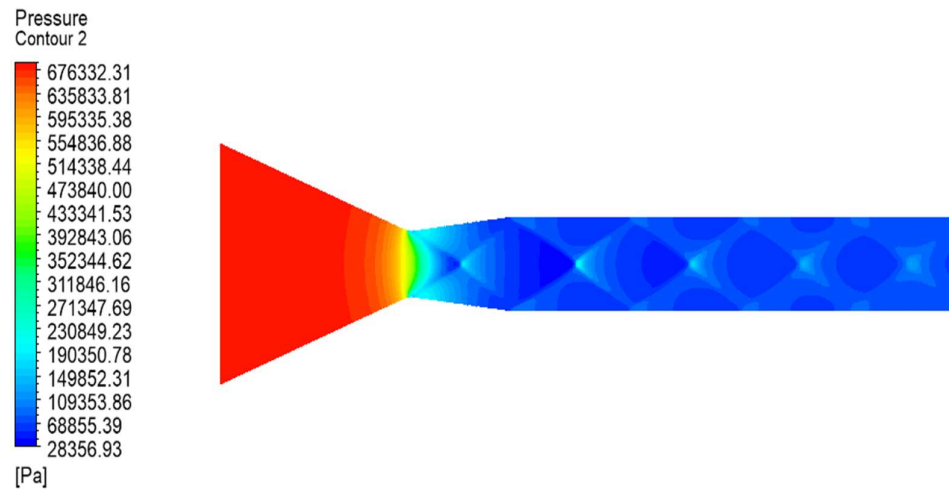


Figure 5.2 Pressure Contour of Flow Through the Nozzle

5.1.1.3 Temperature Flow Contour

- The temperature contour of Figure 5.3 shows that the maximum temperature (~296 K) is observed at the inlet region before the flow accelerates.
- As the flow approaches the throat, the temperature decreases due to increase in velocity and reaches lower values near the sonic condition.
- In the divergent section, a reduction in temperature is observed (~130–200 K), but compared to under-expanded flow, the drop is relatively moderate due to compression effects in over-expanded flow.
- The presence of shock waves inside the nozzle leads to localized temperature rise in certain regions, forming non-uniform temperature distribution.
- Downstream of the nozzle, the temperature gradually increases (~200–270 K) due to mixing with the surrounding ambient air.

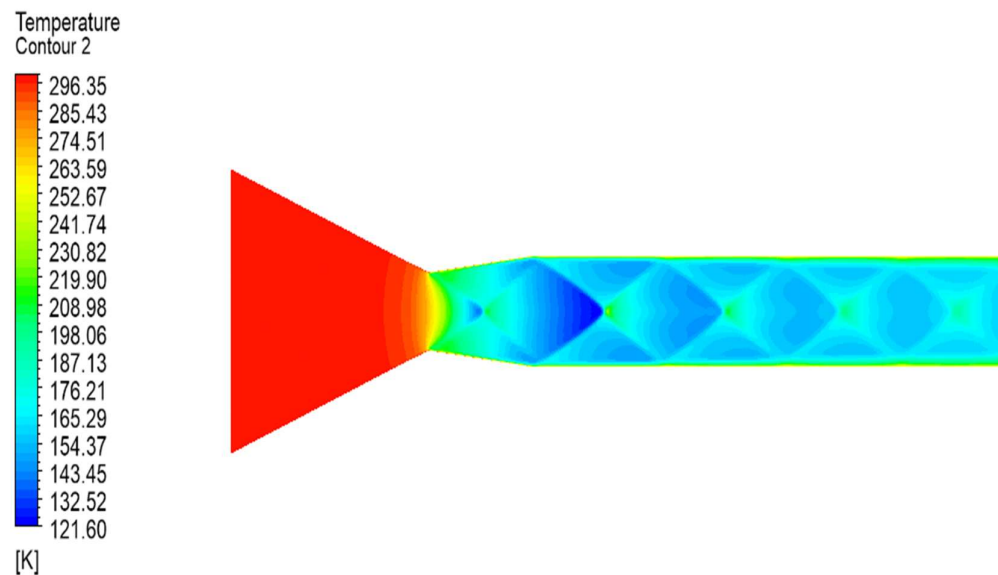


Figure 5.3 Temperature Contour of Flow Through the Nozzle

5.1.1.4 Density Flow Contour

- The density contour of Figure 5.4 shows that the maximum density ($\sim 7.0\text{--}7.8\text{ kg/m}^3$) is observed at the inlet region, where the flow is subsonic and pressure is high.
- As the flow accelerates towards the throat, the density decreases significantly due to increase in velocity and reduction in pressure.
- In the divergent section, the density further drops to lower values of about $\sim 1.2\text{--}3.5\text{ kg/m}^3$, indicating expansion of the flow into the supersonic region.
- Due to over-expanded flow condition, shock waves are formed inside the nozzle, causing local increases in density and resulting in non-uniform distribution.
- Downstream of the nozzle, alternating regions of high and low density are observed, representing compression and expansion effects, followed by gradual mixing with the ambient fluid.

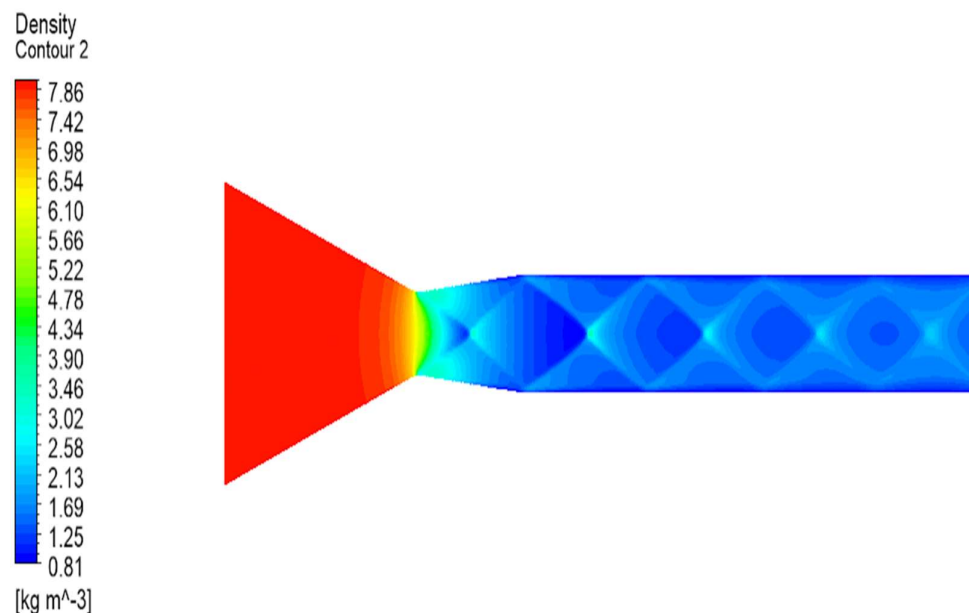


Figure 5.4: Density Contour of Flow Through the Nozzle

5.1.1.5 Velocity Flow Contour

- The velocity contour of Figure 5.5 shows that the flow enters the nozzle with low velocity (~ 0 – 100 m/s) at the inlet region, indicating subsonic conditions.
- As the flow moves through the converging section, the velocity increases steadily due to the reduction in cross-sectional area.
- The velocity rises sharply near the throat region (~ 300 – 400 m/s), indicating the approach to sonic conditions.
- In the diverging section, the flow accelerates further and becomes supersonic, reaching high velocities in the range of ~ 450 – 600 m/s, as indicated by the red region.
- The downstream region shows periodic variations in velocity, indicating the presence of expansion waves and shock cell structures.
- The jet core maintains maximum velocity (~ 550 – 600 m/s), while slight reductions near the edges indicate mixing with the surrounding fluid.

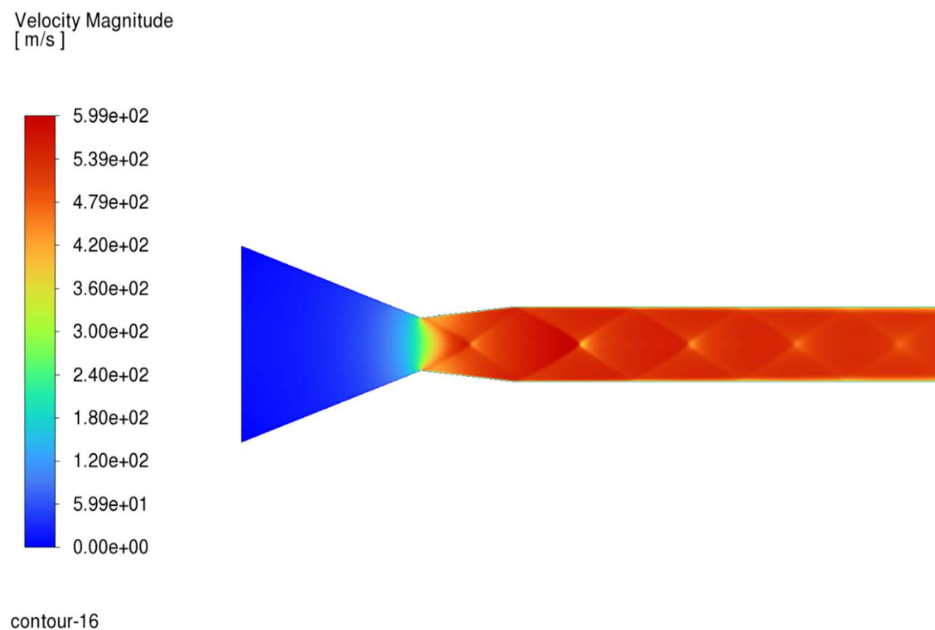


Figure 5.5 Velocity Contour of Flow Through the Nozzle

5.1.1.6 Velocity Streamline Contour

- The velocity contour of Figure 5.6 shows that Velocity Scale: The color-coded legend represents velocity in meters per second with a maximum velocity of 599.34 m/s (dark red) and a minimum velocity of 0.00 m/s (dark blue).
- Acceleration Phase: The streamlines show low velocity at the inlet (blue region), which increases significantly as the fluid passes through the nozzle throat.
- Flow Characteristics: Upon exiting the nozzle, the fluid maintains a high velocity (red region), with distinct patterns indicating the acceleration and downstream flow stability of the jet.
- This visualization effectively demonstrates the transformation of internal energy into kinetic energy, highlighting the nozzle's performance in accelerating the fluid to high speeds.

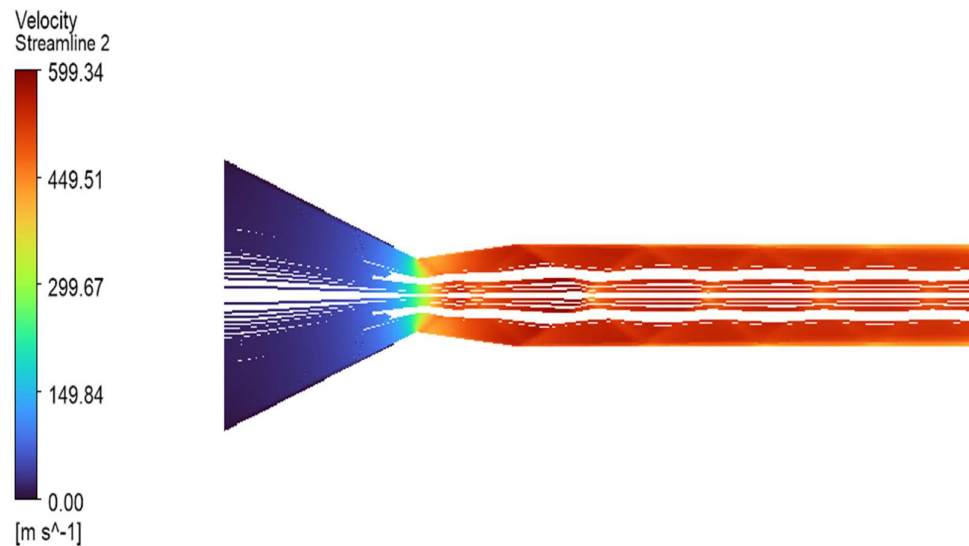


Figure 5.6 Velocity Streamline Contour of Flow Through the Nozzle

Table 5.1: Summary of Flow Parameters

The following table summarizes the average values calculated at the inlet and outlet sections of the nozzle:

Parameter	Inlet Average	Outlet Average
Pressure (Pa)	689,136	77,666.2
Velocity (m/s)	14.1688	491.771
Density (kg/m ³)	8.00561	1.53588
Temperature (K)	299.893	177.645

5.2 Under-Expanded Flow

The simulation is expanded at a higher-pressure ratio of $NPR = 12.25$ in order to further examine the flow behavior. Under these circumstances, the flow is under-expanded because the exit pressure is higher than the ambient pressure. Shock diamonds are created as the flow keeps growing outside the nozzle.

5.2.1 Under-Expansion Contours

The contours for velocity, temperature, and density under under-expanded conditions are shown in Figures 5.7–5.12.

The flow exhibits:

- Rapid expansion at the nozzle exit
- Formation of shock waves and expansion fans
- Oscillatory flow behaviour
- The velocity reaches maximum values at the exit, while density and temperature show periodic variations.

5.2.1.1 Velocity Flow Contour

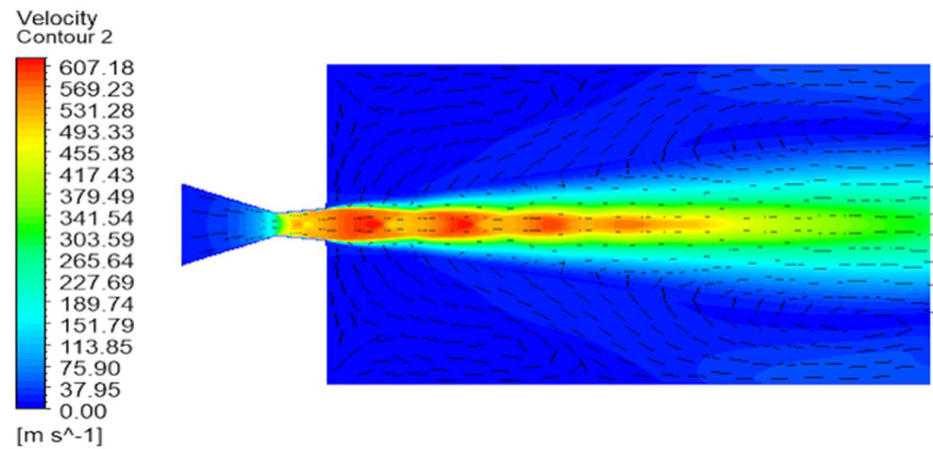


Figure 5.7: Velocity Contour Under-Expanded Condition

- The velocity contour of Figure 5.7 represents the flow characteristics under under-expanded nozzle conditions.
- The flow accelerates at the throat, attaining maximum velocity along the jet core region.
- After exiting the nozzle, the jet continues to expand, forming high-velocity zones downstream.
- Low-velocity regions around the jet indicate mixing with ambient fluid and shear layer development.

5.2.1.2 Pressure Flow Contour

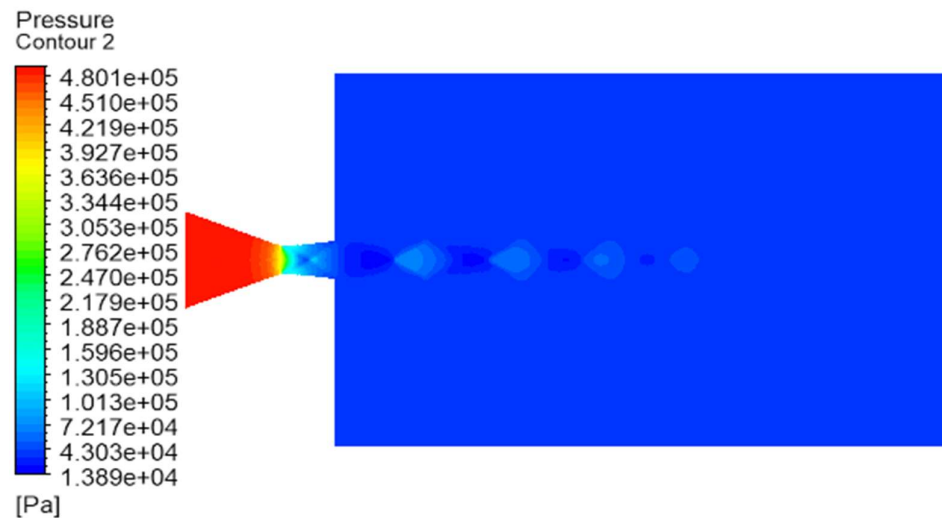


Figure 5.8: Pressure Contour Under-Expanded Condition

- The pressure contour of Figure 5.8 shows how the pressure is distributed in the nozzle under under-expanded flow circumstances.
- Due to flow acceleration, high pressure is seen at the entrance region and progressively drops near the throat.
- The under-expanded situation is confirmed at the nozzle exit, where the pressure is still higher than the surrounding air.
- Periodic pressure changes suggest the development of expansion waves and shock structures downstream of the exit.

5.2.1.3 Temperature Flow Contour

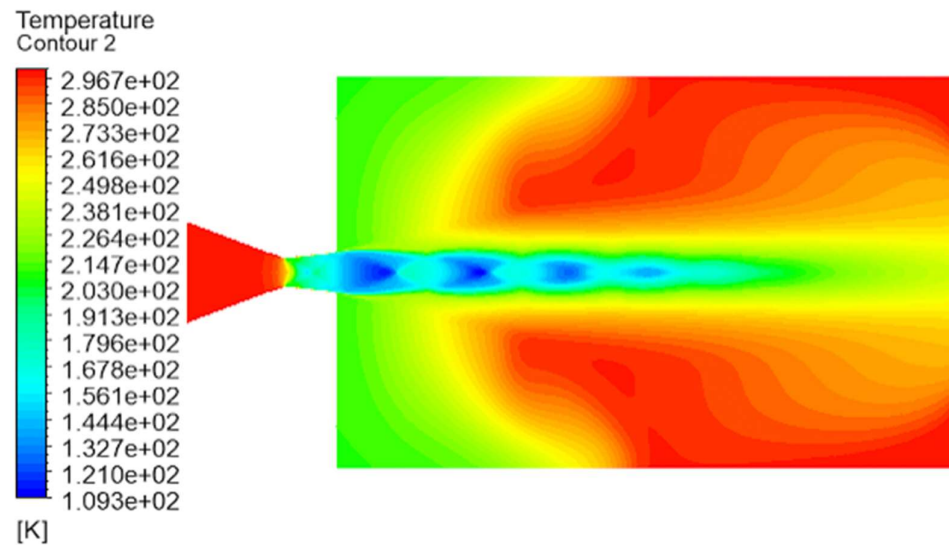


Figure 5.9: Temperature Contour Under-Expanded Condition

- The temperature contour of Figure 5.9 shows that the maximum temperature (~ 296 K) is observed at the inlet region before expansion.
- A sharp decrease in temperature occurs at the throat and jet core, reaching values as low as ~ 110 – 150 K due to rapid expansion.
- The downstream jet region exhibits low-temperature zones (~ 120 – 180 K), indicating strong expansion and cooling effects.
- Higher temperature regions (~ 250 – 290 K) surrounding the jet represent mixing with the ambient fluid and gradual thermal recovery.

5.2.1.4 Density Flow Contour

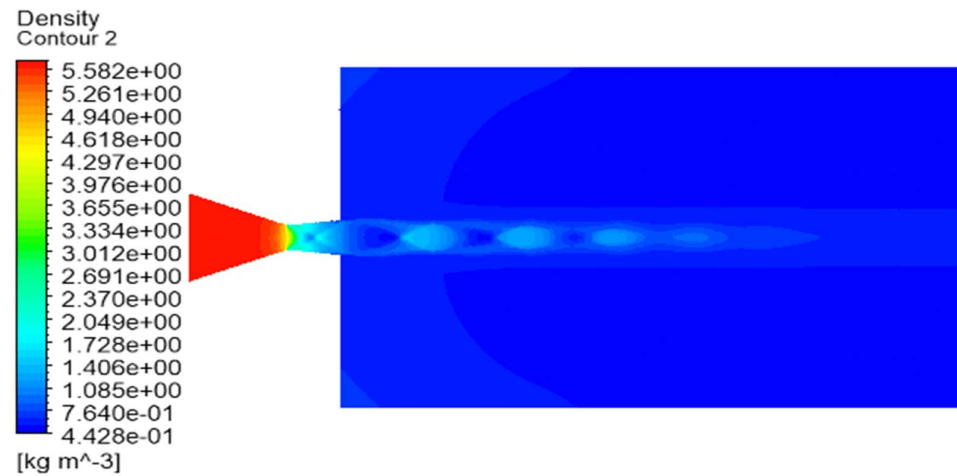


Figure 5.10: Density Contour Under-Expanded Condition

- The density contour of Figure 5.10 shows that the maximum density ($\sim 5.58 \text{ kg/m}^3$) is observed at the inlet region before expansion.
- A sharp decrease in density occurs at the throat and along the jet core, reaching values as low as $\sim 0.44\text{--}1.0 \text{ kg/m}^3$ due to rapid expansion.
- The downstream jet region exhibits low-density zones ($\sim 0.5\text{--}1.5 \text{ kg/m}^3$), indicating strong expansion effects in the under-expanded flow.
- Higher density regions ($\sim 3\text{--}5 \text{ kg/m}^3$) near the inlet and surrounding areas represent compressed flow and interaction with ambient conditions.

5.2.1.5 Mach Number Contour

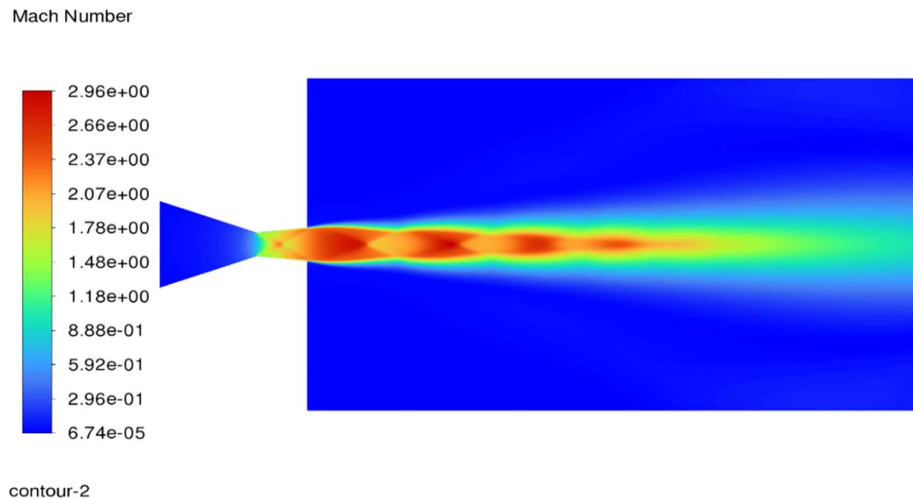


Figure 5.11: Mach Contour Under-Expanded Condition

- The Mach contour of Figure 5.11 represents the flow characteristics under under-expanded nozzle conditions.
- The flow accelerates at the throat, attaining maximum velocity along the jet core region.
- After exiting the nozzle, the jet continues to expand, forming high-velocity zones downstream.
- Low-velocity regions around the jet indicate mixing with ambient fluid and shear layer development.
- The flow accelerates from subsonic conditions at the inlet to supersonic conditions at the nozzle exit, as indicated by the Mach number contour.
- In the jet core, the maximum Mach number reaches roughly 2.9–3.0, signifying extremely supersonic flow.
- Shock cells and expansion waves are shown downstream by alternating areas of high and low Mach numbers.
- The core region (~ 1.5 – 3.0) verifies under-expanded jet behavior, but the surrounding low Mach number region (~ 0 – 0.5) implies ambient fluid.

5.3 Overall Discussion

The results clearly demonstrate the behaviour of compressible flow through a convergent–divergent nozzle.

Key observations include:

- Significant pressure drops ($676332 \text{ Pa} \rightarrow 28357 \text{ Pa}$)
- Temperature reduction ($297 \text{ K} \rightarrow 122 \text{ K}$)
- Increase in velocity to supersonic levels
- Formation of shock waves and expansion regions
- Presence of shock diamonds in under-expanded flow
- These results are consistent with theoretical predictions and confirm the accuracy of the CFD simulation.

CHAPTER 6

Conclusions and Future Directions

6.1 Conclusions

In the present study, a detailed numerical analysis of compressible flow through a convergent–divergent nozzle has been carried out using Computational Fluid Dynamics. The objective of visualizing shock structures and analyzing flow behaviour under different operating conditions has been successfully achieved.

The results show that the flow accelerates from subsonic conditions at the inlet to sonic conditions at the throat and further to supersonic conditions in the diverging section. The exit Mach number is found to vary with nozzle pressure ratio (NPR), with values of approximately 2.1 for the over-expanded condition ($\text{NPR} \approx 6.81$) and around 2.7 for the under-expanded condition ($\text{NPR} \approx 12.25$).

In the over-expanded case, shock waves are observed inside the nozzle due to higher ambient pressure, resulting in a sudden increase in pressure and decrease in velocity. In contrast, for the under-expanded case, expansion waves and shock cell structures are formed downstream of the nozzle, indicating that the exit pressure is higher than the ambient pressure.

The variation of flow parameters such as pressure, temperature, velocity, density, and Mach number clearly demonstrates the strong dependence of flow behaviour on NPR. The contour plots effectively capture the formation and propagation of shock structures, fulfilling the primary objective of this study.

Furthermore, the numerical results are validated with available literature, showing good agreement and confirming the accuracy and reliability of the CFD model. The use of a polyhedral mesh and density-based solver ensures stable convergence and accurate prediction of compressible flow characteristics.

Overall, the present study provides a clear understanding of shock dynamics and flow behaviour in a convergent–divergent nozzle, which is essential for the design and optimization of high-speed propulsion systems.

6.2 Future Directions

The present study provides a detailed analysis of compressible flow behaviour; however, further research can be carried out to extend and enhance the work.

One important extension is the analysis of three-dimensional nozzle geometry. The current study is based on a two-dimensional model, whereas real-world applications involve three-dimensional flow effects. Incorporating these effects would provide more realistic and accurate results.

The use of advanced turbulence models is another important area for future work. Techniques such as Large Eddy Simulation or Direct Numerical Simulation can be employed to capture complex flow characteristics and improve the accuracy of shock prediction.

Experimental validation of the numerical results is also essential. Conducting experiments and comparing them with CFD results would enhance the credibility of the study and provide deeper insight into flow behaviour.

Further analysis can be performed for different Mach numbers and nozzle pressure ratios to better understand their influence on flow characteristics and to optimize nozzle performance for various applications.

In addition, the inclusion of heat transfer and real gas effects can improve the accuracy of simulations, particularly in high-speed flow conditions.

Optimization of nozzle geometry by varying parameters such as nozzle length, divergence angle, and throat diameter can also be explored to achieve improved performance.

Finally, advanced approaches such as flow control techniques and integration of machine learning with CFD may be investigated for better prediction, optimization, and efficiency of high-speed flow systems.

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