

ME 605 | Computational Fluid Dynamics

Project 3

Due: 11:59 pm, November 7th

Instructions

1. You can choose any programming language of your choice.
2. Do not use any in-built or intrinsic functions, as you are expected to write your computer program (including for solving the system of algebraic equations).
3. Discussion among students is permitted;
4. Your report must consist of:
 - (a) Problem statement
 - (b) Mesh details and approach for discretization
 - (c) Derivation and presentation of the final form of the discretized equations
 - (d) Solution methodology
 - (e) Results and discussion
 - (f) Concluding remarks

Note that an in-depth analysis and discussion of results is required.

5. The report must be prepared using WORD or LaTeX. Handwritten reports will not be accepted.
6. Submit the project report and the code using the link/form that will be provided before the submission deadline.
7. Usage of any artificial intelligence (AI) tools to write project reports or develop code modules is a violation of the course policy

Project Statement

Fluid Flow through Converging-Diverging Rocket Nozzles

Background and Assumptions

Nozzles are devices that are used to increase the velocity of the flow. They find numerous applications; one such application that is relevant to this project is rocket propulsion. In this case, the products of combustion are expanded through a convergent-divergent (CD) nozzle to extremely high velocities (typically supersonic speeds) to generate thrust.

The goal of this project is to computationally analyze fluid flow through a converging-diverging nozzle. To avoid excessive complexity, the following assumptions are invoked:

1. The flow is assumed to be quasi one-dimensional. In other words, flow properties are uniform across the cross-sectional area of the nozzle and therefore vary only along the axial direction.

2. The flow can be assumed to be inviscid, since the objective of the project is *not* to study the effect of walls on the fluid flow. Further, at high speeds, the convective terms in the governing equations are more important than the diffusive terms.
3. The fluid flow is assumed to be unsteady, laminar, and compressible.
4. The wall is assumed to be adiabatic. The radiative heat transfer and body forces are neglected.

Flow Regimes in Nozzle

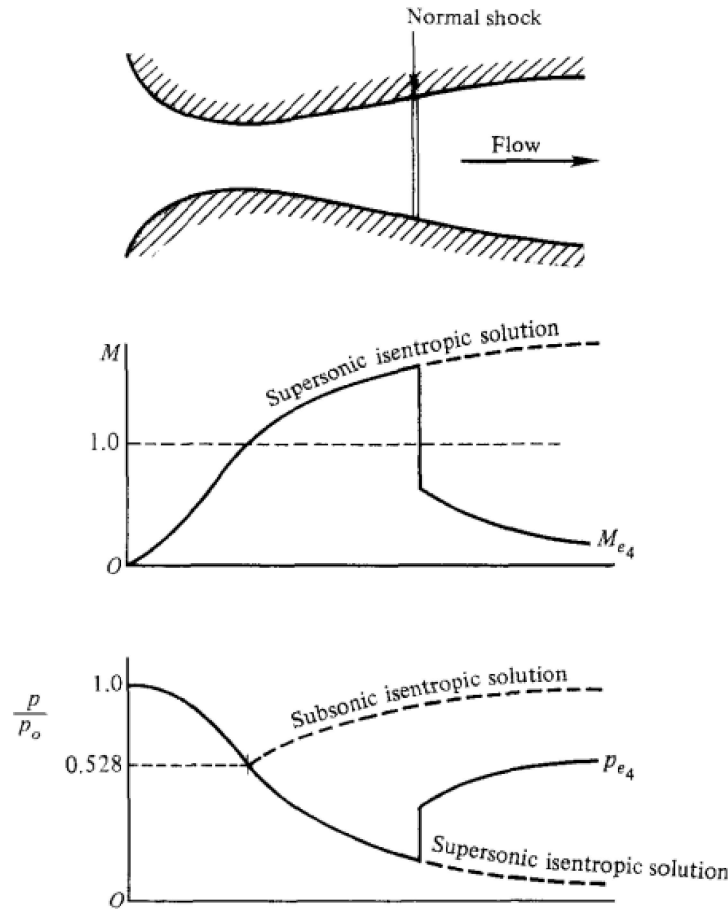


Figure 1: Flow regimes in a converging-diverging nozzle flow. From *Modern Compressible Flow* by John D. Anderson Jr.

The flow regime in a converging-diverging nozzle is dictated by the conditions at the inlet and the outlet. In a typical experiment, the nozzle is connected to a reservoir where stagnation conditions prevail. A flow is established when the pressure at the outlet (commonly referred to as back pressure) is lowered below the pressure in the reservoir (commonly referred to as stagnation/total pressure). For a given stagnation pressure, different flow regimes are established depending on the back pressure:

1. **Isentropic subsonic flow:** Here, the back pressure is only slightly lower than the stagnation pressure. The flow accelerates in the converging section and decelerates in the

diverging section of the nozzle, as one would expect in an incompressible flow conserving the volumetric flow rate. The pressure follows an opposite trend. This is shown in fig.1. Note the the Mach number is always lower than 1, ensuring subsonic conditions throughout the nozzle. As viscous effects are neglected and the walls are assumed to be adiabatic, the flow can be regarded as isentropic.

2. **Isentropic subsonic-supersonic flow:** Here, the back pressure is significantly lower than the stagnation pressure. The flow accelerates in the converging nozzle, reaches sonic condition at the throat, and supersonic conditions at the outlet. The pressure decreases monotonically, as shown in fig.1. As viscous effects are neglected and the walls are assumed to be adiabatic, the flow can be regarded as isentropic.
3. **Non-isentropic flow with shock wave:** Here, the back pressure is in between the above two cases. That is, it is not sufficiently low for the flow to be fully supersonic in the diverging section of the nozzle. To meet the unexpectedly high back pressure at the outlet, a shock wave is established in the diverging section. Across the shock wave, pressure jumps abruptly and the flow transitions from supersonic to subsonic conditions. The pressure evolution is shown in fig.1. The shock wave renders the flow to be highly non-isentropic due to irreversible processes occurring inside the shock wave.

Nozzle Geometry

A converging–diverging nozzle is a classic one-dimensional compressible flow problem and is commonly used as a validation case in CFD code and software development. It illustrates key flow features such as choking, supersonic expansion, and shock formation within the nozzle. For this project, the converging–diverging verification nozzle case developed by the National Program for Application-Oriented Research in CFD ([NPARC](#)) is provided for study. This case was used to validate the WIND CFD code developed by NASA and AEDC, and details of those studies can be found here:[CVD Nozzle](#).

The nozzle geometry is described by the area (m^2) function as given below, and a schematic of the nozzle is shown in the fig.2.

$$A = \begin{cases} 0.0444 - 0.019 \cos \left(\left(\frac{0.2x}{0.0254} - 1 \right) \pi \right) & \text{if } 0 \leq x < 0.127 \\ 0.0318 - 0.0063 \cos \left(\left(\frac{0.2x}{0.0254} - 1 \right) \pi \right) & \text{if } 0.127 \leq x \leq 0.254 \end{cases}$$

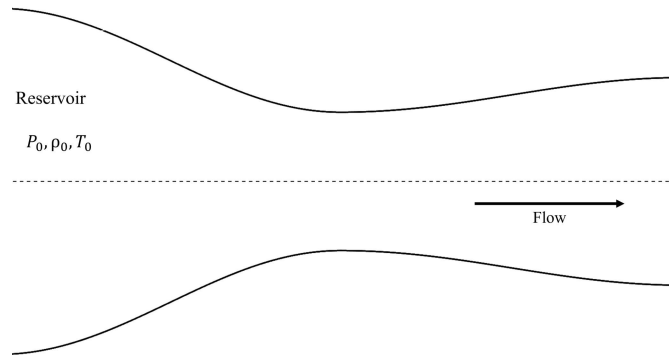


Figure 2: Converging-Diverging nozzle to be considered in the present study

Governing Equations

Since the flow is assumed to be unsteady, compressible, and inviscid, the time-dependent Euler equations must be solved. While the objective of the project is to compute the steady-state solution, the time-dependent Euler equations must be solved to ensure hyperbolicity of the governing equations across the entire Mach number regime of concern. The mass, momentum, and energy conservation equations for the quasi-one-dimensional flow are given below:

Continuity

$$\frac{\partial(\rho A)}{\partial t} + \frac{\partial(\rho AV)}{\partial x} = 0 \quad (1)$$

where ρ is the density, A is the cross-sectional area, and V is the velocity.

Momentum

$$\frac{\partial(\rho AV)}{\partial t} + \frac{\partial(\rho AV^2)}{\partial x} = -A \frac{\partial P}{\partial x} \quad (2)$$

where P is the pressure.

Total energy equation

$$\frac{\partial}{\partial t} \left[\rho A \left(e + \frac{V^2}{2} \right) \right] + \frac{\partial}{\partial x} \left[\rho AV \left(e + \frac{V^2}{2} \right) \right] = - \frac{\partial(PAV)}{\partial x} \quad (3)$$

where e is the internal energy.

Note that the above equations are in the **conservative** form. It is referred to as the conservative form, since the equations describe the evolution of mass, momentum, and energy, which are typically conserved. The non-conservative form is highly susceptible to numerical instabilities and conservation issues and should be avoided in general. It is bound to fail in situations where there are shock waves in the solution domain, since the primitive variables change abruptly across the shock wave, while the conserved variables do not change. Henceforth, you are required to solve the conservative form of the governing equations, only, and the governing equations in the conservative form can be simply represented as below:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{J} \quad (4)$$

where

$$\mathbf{Q} = \begin{bmatrix} \rho A \\ \rho AV \\ \rho A \left(e + \frac{V^2}{2} \right) \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho AV \\ \rho AV^2 + pA \\ \rho AV \left(e + \frac{V^2}{2} \right) + pAV \end{bmatrix}, \quad \mathbf{J} = \begin{bmatrix} 0 \\ p \frac{\partial A}{\partial x} \\ 0 \end{bmatrix} \quad (5)$$

To solve the above governing equations, all the fluxes (\mathbf{F}) and source terms (\mathbf{J}) also need to be represented in terms of conservative variables(\mathbf{Q}). For that purpose, fluxes and source terms in terms of conservative variables are given below:

$$\mathbf{F} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = \begin{bmatrix} Q_2 \\ \frac{Q_2^2}{Q_1} + (\gamma - 1) \left(Q_3 - \frac{Q_2^2}{2Q_1} \right) \\ \frac{Q_2}{Q_1} \left[Q_3 + (\gamma - 1) \left(Q_3 - \frac{Q_2^2}{2Q_1} \right) \right] \end{bmatrix} \quad (6)$$

$$\mathbf{J} = \begin{bmatrix} 0 \\ J_2 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ (\gamma - 1) \frac{\partial(\ln A)}{\partial x} \left(Q_3 - \frac{Q_2^2}{2Q_1} \right) \\ 0 \end{bmatrix} \quad (7)$$

where γ is the specific heat ratio.

Boundary conditions

The following guidelines may be considered to ensure correct implementation of boundary conditions:

1. At the inlet, one can assume that reservoir conditions prevail. The pressure is equal to the stagnation pressure, density is equal to the stagnation density, and temperature is equal to the stagnation temperature. Velocity should NOT be set as zero!. The outlet pressures for different flow regimes are given in the table.1.
2. Check the sign of the Eigenvalues at the inlet and outlet to decide the number of boundary conditions to be specified at the inlet and outlet for each simulation case. In other words, let characteristics guide the treatment of boundary conditions. If you are solving for N governing equations and characteristics dictate that the number of boundary conditions to be n , you should implement $N - n$ auxiliary conditions. The auxiliary conditions are commonly implemented using extrapolation techniques.
3. Since you are solving the conservative form of governing equations, the boundary conditions should also be implemented in terms of conserved variables instead of primitive variables.

Table 1: Flow conditions in SI units.

Quantity	Value
Total Pressure at Inlet (Pa)	6894.76
Total Temperature at Inlet (K)	55.56
Exit Static Pressures (Pa)	6136.34 (Subsonic)
	5171.07 (Shock)
	1103.16 (Supersonic)

Initial conditions

Since the goal of the project is to compute steady-state solutions, the initial condition can be creatively chosen to ensure convergence. You are encouraged to understand the evolution of flow variables for different simulation cases to arrive at intelligent initial conditions. For example, for the isentropic subsonic-supersonic flow case, it is known the density decreases monotonically with spatial coordinate. You could therefore assume a linear density profile (or piece-wise linear density profile) as an initial condition to ensure fast convergence. A similar approach can be adopted for other flow variables. Needless to say, using the analytical solution as the initial condition is NOT permitted.

Numerical Schemes

You should use the Finite Difference method (FDM) to discretize the governing equations. It is sufficient to use explicit method in this project. You should use MacCormack's scheme to ensure second order accurate discretization in both space and time. Since you will implement an explicit scheme, the Courant (CFL) number should be sufficiently small to ensure stability. Note that the CFL number should be calculated based on the maximum wave speed (Eigenvalue) for the problem.

Action Items

1. You will need to write a computer program to solve the governing equations and compute the steady-state solution for two cases: (1) isentropic subsonic flow and (2) isentropic subsonic-supersonic flow. You do not need to solve for Non-isentropic flow with a shock wave case. Take the specific heat ratio (γ) to be 1.4.
2. Plot the variation of the following quantities with the axial coordinate and compare with the analytical solution:
 - (a) Pressure (P/P_0)
 - (b) Density (ρ/ρ_0)
 - (c) Temperature (T/T_0)
 - (d) Mach number (M)
3. Plot the variation of Pressure and Mach number along the axial direction with the experimental data of NASA. For the experimental data, refer to Table 2 in the [CDV-NASA](#) website.
4. Discuss the results in detail and provide physics-based reasons to explain the trends.

Analytical solutions

Isentropic Flow Solutions

$$\frac{P}{P_0} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{\gamma}{\gamma - 1}} \quad (8)$$

$$\frac{\rho}{\rho_0} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{1}{\gamma - 1}} \quad (9)$$

$$\frac{T}{T_0} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-1} \quad (10)$$

$$\frac{A}{A^*} = \frac{1}{M} \left[\frac{2}{\gamma + 1} \left(1 + \frac{\gamma - 1}{2} M^2\right) \right]^{\frac{\gamma + 1}{2(\gamma - 1)}} \quad (11)$$

$$C = \sqrt{\gamma R T} \quad (12)$$

where A^* represents the throat area and the subscript 0 refers to the reservoir state. C is the speed of sound.

Extra Credits Problem

- *The extra credit problem is optional for the students*
- *The students who fully complete and submit the extra credits problem will be awarded an extra 25% marks.*

You are required to write a code to simulate non-isentropic flow through a converging–diverging nozzle, where a shock wave forms in the diverging section. The presence of the shock makes the flow non-isentropic because there is an abrupt, irreversible change in flow properties such as pressure, density, and temperature. You need to compute the pressure, density, temperature, and Mach number profiles along the axial direction and compare them with the analytical solutions. The shock wave is a discontinuity in the flow field across which the flow properties change. The analytical solution for the properties change across the shock wave is given below.

Formulas for property change across the shock wave

$$\frac{P_{0_2}}{P_{0_1}} = \left(\frac{(\gamma + 1) M_1^2}{(\gamma - 1) M_1^2 + 2} \right)^{\frac{\gamma}{\gamma - 1}} \left[\frac{(\gamma + 1)}{2\gamma M_1^2 - (\gamma - 1)} \right]^{\left(\frac{1}{\gamma - 1}\right)} \quad (13)$$

$$\frac{P_2}{P_1} = 1 + \frac{2\gamma}{\gamma + 1}(M_1^2 - 1) \quad (14)$$

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)M_1^2}{(\gamma - 1)M_1^2 + 2} \quad (15)$$

$$M_2 = \left\{ \frac{1 + \left[\frac{(\gamma - 1)}{2} \right] M_1^2}{\gamma M_1^2 - \frac{(\gamma - 1)}{2}} \right\}^{1/2} \quad (16)$$

where the subscript 1 denotes the state before the shock wave, and the subscript 2 denotes the fluid state after the shock wave.