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SURFACE SCIENCE

Bachelors Thesis

Title

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1 Theory

1.1 Formulary

1.1.1 Thermodynamics

1.1.2 Continuous one-dimensional flow

Thermal equation of state:

$$\frac{p}{\rho} = RT \quad \text{[term perf]} \tag{1}$$

Dynamic equation:

$$\frac{1}{\rho}dp + VdV = 0 \tag{2}$$

Speed of Sound:

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\gamma\left(\frac{\partial p}{\partial \rho}\right)_T} \tag{3}$$

$$a = \sqrt{\gamma\frac{p}{\rho}} = \sqrt{\gamma RT} \quad \text{[term perf]} \tag{36}$$

Mach Number:

$$M = \frac{V}{a} \tag{4}$$

Dynamic Pressure:

$$q = \frac{1}{2}\rho V^2 \tag{5}$$

$$q = \frac{\gamma}{2}pM^2 \tag{6}$$

From the dynamic equation and the speed of sound relation:

$$\frac{p}{\rho^\gamma} = \text{constant} = \frac{p_t}{\rho_t^\gamma} \quad \text{[isen, perf]} \tag{34}$$

From which:

$$\frac{p}{p_t} = \left(\frac{\rho}{\rho_t}\right)^\gamma = \left(\frac{T}{T_t}\right)^{\frac{\gamma}{\gamma-1}} = \left(\frac{a}{a_t}\right)^{\frac{2\gamma}{\gamma-1}} \quad \text{[isen, perf]} \tag{35}$$

Combining the above equations gives Bernoulli's equation for compressible flow:

$$\frac{\gamma}{\gamma-1}\left(\frac{p_t}{\rho_t}\right)^{\frac{\gamma-1}{\gamma}}\left(\frac{p}{p_t}\right)^{\frac{1}{\gamma}} + \frac{V^2}{2} = \frac{\gamma}{\gamma-1}\frac{p_t}{\rho_t} \quad \text{[isen, perf]} \tag{36}$$

Usefull Ratios

$$\frac{T}{T_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-1} \quad \text{[adiab, perf]} \tag{43}$$

$$\frac{p}{p_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\frac{\gamma}{\gamma-1}} \quad \text{[isen, perf]} \tag{44}$$

$$\frac{\rho}{\rho_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\frac{1}{\gamma-1}} \quad \text{[isen, perf]} \tag{45}$$

$$\frac{a}{a_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\frac{1}{2}} \quad \text{[adiab, perf]} \tag{46}$$

1.2 Foundational principles

1.2.1 Idealized flow regimes

There are different idealized flow regimes which can be distinguished by the value of their Knudsen number (Kn).

Continuum regime ($Kn \leq 0.001$) In this regime, the interactions of particles in the medium are much more frequent than the interactions of particles with the boundaries of the duct. This makes it possible to describe the fluid itself as a continuous medium. The Navier-Stokes equations govern the calculations in this regime.

Slip regime ($0.001 \leq Kn \leq 0.1$) Increasing Knudsen numbers mean the mean free path becomes comparable to the characteristic length scale. In this regime, the assumptions for continuum flow still hold, but there are deviations, especially near the boundaries. While continuum mechanics assumes no-slip conditions on the boundary, in this regime, slip on the boundary must be factored in.

Transition regime ($0.1 \leq Kn \leq 10$) This regime is a middle ground between continuum and fully molecular flow. Neither the continuum assumptions of fluid dynamics nor the free molecular flow assumptions hold completely. The interactions between the gas molecules and the boundaries are significant, and the flow characteristics may vary widely.

Molecular regime ($Kn \geq 10$) In this regime, the mean free path is much larger than the dimensions of boundaries. This leads to particle interactions themselves becoming negligible in comparison to the interaction of particles with the boundary.

1.2.2 Turbulence

This dimensionless number can be used to predict if it is probable to encounter turbulent flow or laminar flow in some region of the flow studied.

Laminar Flow ($Re \leq 2300$)

Turbulent Flow ($Re > 2300$) Having high Reynolds numbers means viscous forces are dominated by inertial forces. In this situation eddies and vortices begin to form.

1.2.3 Mach regimes

Low subsonic regime ($Ma < 0.3$)

Subsonic regime ($0.3 < Ma < 1.0$) In this regime, the flow throughout the duct, except at the throat, remains subsonic. The velocity increases as the gas flows through the duct.

Missing figure

Subsonic nozzle and diffuser

Sonic regime ($Ma = 1$) Sonic flow occurs at the throat of a converging-diverging duct. It is a limiting phenomenon in converging ducts, achievable only if a diverging section follows, creating a minimum cross-sectional area referred to as the throat.

Supersonic regime ($Ma > 1$) Supersonic flow cannot occur inside a purely converging duct. In subsonic conditions, the velocity increases while the cross-sectional area decreases. Once sonic speed is reached, the behavior reverses, and the velocity decreases, limiting the flow to subsonic or sonic speeds within converging ducts.

Missing figure

Supersonic nozzle and diffuser

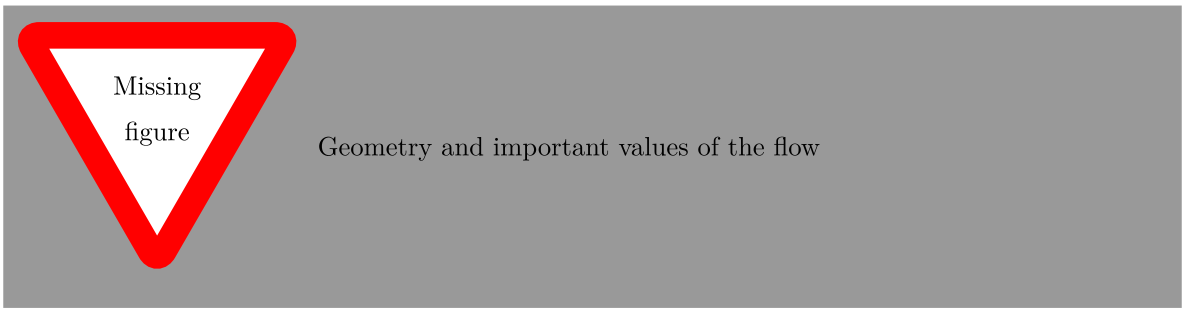
1.2.4 Dimensionality of the flow

2 Analytical work

2.1 Scope and objectives

2.1.1 Geometry and components

The geometry can be explained in three simple sections: gas from a reservoir (1) flows over a duct into the reactor (2) where it leaves through another duct into a vacuum (3). This is a stark simplification, but for a great part of this thesis, this is how we will imagine our flow path. This is because the only important thing we left out is any kind of leaks in the system. Those leaks will be most influential around the reactor, since this is the only part not held at a constant pressure by any external part of the system.



Inlet Reservoir (1) It is held at a constant pressure P_0 and a constant temperature T_0 and contains only one gas which is defined by its specific heat ratio γ and by its molar mass M_m. These are all parameters which are set in advance and won't change after being set, which constraints us to a steady flow.

Inlet Nozzle The duct connecting the inlet reservoir with the reactor will actually be a slightly narrowing duct, due to production constraints. Therefore, it will act like a Nozzle, accelerating the gas until it expands into the reactor.

Reactor (2) The reactor resembles a very small but broad cylinder shape which is opened at the bottom. The sample will be pressed into the opening, which will lead to some leakage out of the system, this will actually force us to decouple the system at the chamber (more about that later). The gas itself reaches the chamber at some velocity and will decelerate rapidly while expanding into the chamber. Therefore, a great part of the chamber will have very slow moving gas inside. Very close to the outlet nozzle the gas will start to accelerate again and will enter it at very high speeds.

Outlet Nozzle With the same geometry as the inlet, but the gas flowing in opposite directions, one would suspect the outlet to act as a subsonic nozzle which could logically be the case, since without a converging section in front it would be impossible to reach sonic velocities and therefore will choke the flow and keep them at subsonic velocities. But actually it is possible for the flow to create a converging section by itself, which will force the flow to be sonic at the beginning of the outlet and will further accelerate into the supersonic regimes, creating a supersonic nozzle. Which of these two possibilities is most likely will be discussed at a later point.

Vacuum (3) After leaving the outlet the gas will first expand into a small cylindrical section after which it will expand freely into the vacuum. The exact pressure left in the vacuum will be very low and small changes won't have great influence onto the flow itself. Therefore,

2.1.2 Motivation and goals

The general goal of this thesis is to create a relatively simple, analytical framework to be able to make predictions on how the flow through the system behaves and to approximate values at different positions in the flow to be later used as initial values for more complex numerical simulations. The following section will state specific questions we will then try to answer in the following Sections.

Type of Flow:

Impact of the leak:

Flow in the reactor and around the sample:

Velocity distribution at the outlet:

2.2 Framework for Analysis

2.2.1 Important assumptions

Dimension of the Flow

Gas

Idealized flow regime

2.2.2 Limits of the theory

2.3 Analytical Descriptions

2.3.1 Fully isentropic flow

leads to supersonic flow in the reactor

2.3.2 The reactor as a reservoir

2.3.3

3 Discussion

4 Conclusion

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