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Title

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Declaration of Authorship

Martin Kronberger

I hereby declare that I have written this thesis independently and that I have fully acknowledged all the sources and aids used. Furthermore, I confirm that I have marked as borrowed any parts of this work (including tables, maps, and figures) that are taken from other works or from the internet, either verbatim or in spirit, giving explicit reference to the source.

I further declare that large language models (LLMs), such as ChatGPT, were used solely to assist with formatting, providing code snippets, and helping to resolve minor technical issues. These models did not contribute to the research content, analyses, interpretations, conclusions, or any intellectual substance of this thesis.

Vienna, 1 January 2025

Martin Kronberger

Abtract

test

Kurzfassung

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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

$$Re = \frac{\rho v L_c}{\mu} = \frac{v L_c}{\nu}$$

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 ($Re \leq 2300$) Laminar flow, means higher chance of encountering boundary layers. Velocity changes significantly along the radius of ducts. Low Mixing, mostly diffusion mediated.

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. More evenly distributed velocity profile. Better for mixing.

Work out pl
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same here!

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.

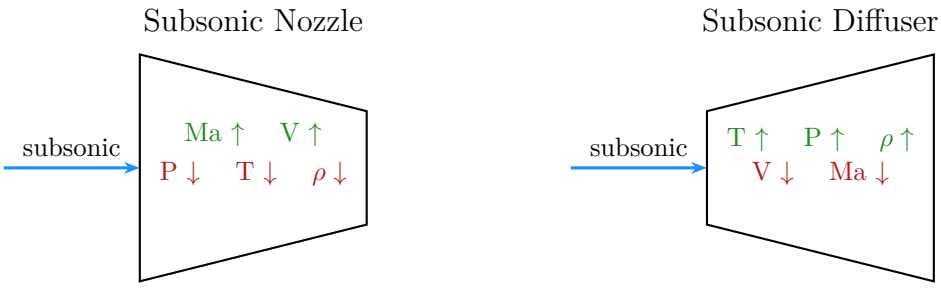


Figure 1: ToDo

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.

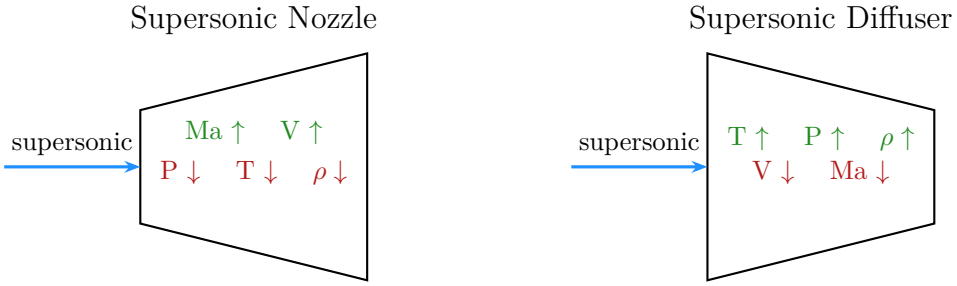
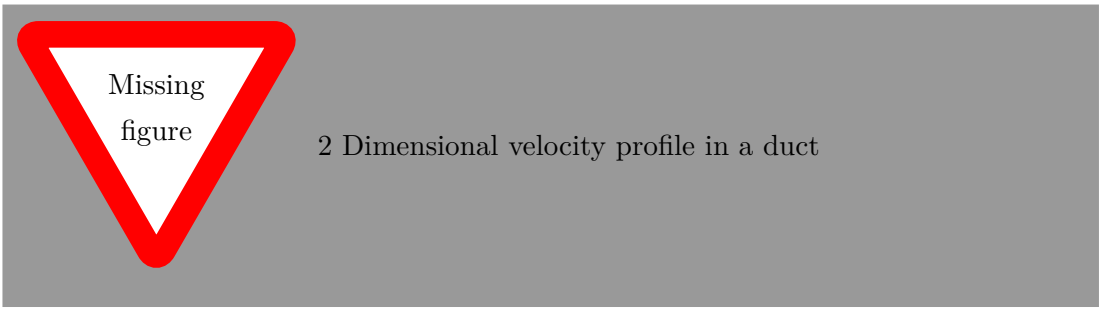


Figure 2: To-Do

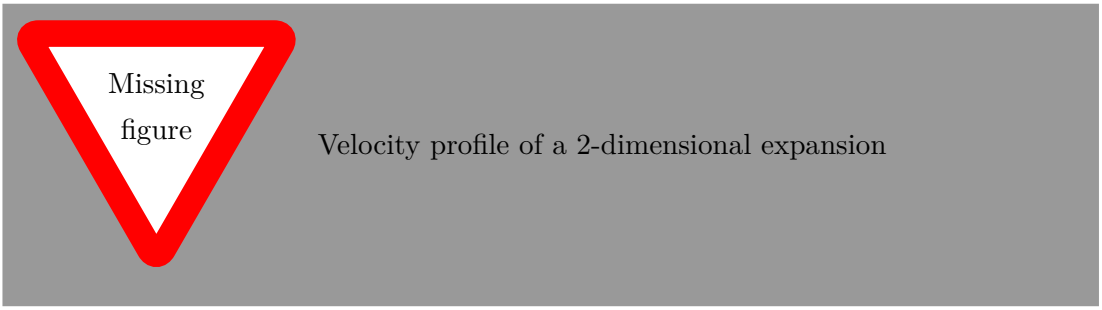
1.2.4 Dimensionality of the flow

Dimensionality of the flow describes on how many location parameters the velocity depends on. For example, it makes total sense to describe the velocity $V(\vec{x})$ of a gas flowing through a variable diameter duct only by its x coordinate, so where we are inside the duct. And also how close the point sits to the boundary of the duct since boundary conditions given by the interaction with the wall will restrain the velocity to different values than at locations in the free stream. Radial symmetry will take care of the 3rd dimension and left will be a velocity field $V(x, r)$, only dependent on x and r. It's important notice that even tho the velocity at a point is a vector, in a duct we are only interested in the velocity component along the length of the duct. This is because the gas can either flow in or out of the duct and will do this with some velocity. So essentially it constitutes a scalar value, usually depicted in a velocity profile like this:



2 Dimensional velocity profile in a duct

This also poses the problem, how to treat the velocity once it leaves such a duct and the following geometry lacks any useful symmetries. Essentially, the 2 dimensionality of the flow doesn't make sense anymore and the velocity has to be explicitly dependent on all 3 spacial coordinates, and it has to be dealt with proper field equations since not even the general direction of movement of the flow will be clearly defined. This will be the case for the flow expanding into reactor after leaving the inlet. Since the reactor has no symmetric boundaries in relation to the inlet position. This will make it hard to describe the flow into, inside and out of the reactor in any simple way, among other problems discussed in Section 2.3.1. Luckily this won't be the case for the expansion into the vacuum, after leaving the outlet. Since there the gas leaves a symmetric geometry and won't be forced by any boundaries, making the assumption of a radial symmetric expansion into the vacuum plausible, but this time with a velocity profile which must include some kind of direction of the flow. Which could look like this:



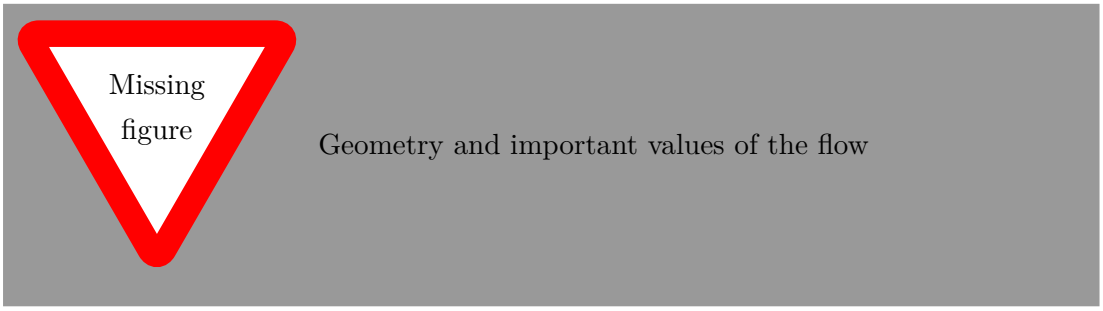
Velocity profile of a 2-dimensional expansion

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 thing we left out is any kind of leak in the system. Those leaks will be the most influential around the reactor, since this is the only part that is not held at a constant pressure by any external part of the system.



Geometry and important values of the flow

Inlet Reservoir (1) It is kept at constant pressure P_0 and 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 will not change after being set, which constrains us to a steady flow.

Inlet Nozzle The duct connecting the inlet reservoir with the reactor will actually be a slightly converging 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. However, it is actually 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 will not 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 about the behavior of the flow through the system and approximate values at different positions in the flow to later be 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: The first and most important question to answer is which type of flow will be expected inside the assembly. This has major implications on which equations are applicable and down the line which type of numerical simulations will lead to the best results. The main focus here is the Knudsen number and the idealized flow regimes connected to it. With the main goal being to assess the most likely flow regime governing the inside of the assembly and therefore determine the equations applicable to calculate the state variables at different points in the system and the throughput of the system as a whole.
In preparation for numerical simulations it is also important to find a way to calculate Knudsen numbers and other flow parameters using given datasets of state variables without having to rely on flow regime specific methods. This will help to analyze transient regimes, encountered when the gas expands into the vacuum, using one generally applicable method.

Impact of the leak: As described in the leading section there will be some leakage expected at the boundary between the reactor casing and the sample holder. This leak will inevitably lead to some leakage and therefore some pressure drop ΔP_L inside the reactor. This can lead to mayor changes in the flow into and out of the reactor. If the pressure drop is high enough it could even be possible to dominate over the outlet with regard to the mass flow out of the system. Thus leading to mayor differences in the velocity distribution calculated at the outlet. Which is without doubt one of the major questions tried to answer in this work. In summary the goal is finding the pressure drop ΔP_L caused by the leak and the effective mass flow $\dot{m}_L$ through it.

Flow in the reactor and around the sample:

Velocity distribution at the outlet:

2.2 Framework for Analysis

2.2.1 Important assumptions

Let's first identify two regions in the flow analysis, for which we will make different assumptions. The first one being everything from the gas reservoir until the exit of the outlet. This will be referred as the inside of the assembly. The second one being everything after the exit plane of the outlet, which will be referred as the outside of the assembly.

Steady Flow Steadiness of the flow is essentially given by the fact that the temperature T_0 and the pressure p_0 of the reservoir will be held constant during measurements. Thus, the flow will be driven by the pressure differential between the vacuum and the reservoir alone. So there is no reason for the flow to establish any dynamic behaviors after reaching some equilibrium state, after gas is first released into the system. This is true for regions inside as well as outside the assembly.

Dimension of the Flow

Inside In this section of the flow a further simplification of the two-dimensional flow through a duct will be used called "quasi one-dimensional" flow. This is possible by reducing the velocity distribution present at any point in a duct to its mean velocity. Therefore, reducing the velocity from a distribution $V(r)$ at every point in the duct to a scalar value V at every point of the duct. This is a general simplification which can be made when using continuum flow analysis inside of ducts and is only bound by the applicability of continuum flow. This makes sense, because approximations of state variables and mass flow is the main goal here. Taking mean values still yield sensible solutions and won't leave us with less information per se.

Outside Any further simplification from the radially symmetric expansion into vacuum described in section ..., would not make sense since it would eliminate important information on how the flow behaves when leaving the outlet. Like how much of the gas will actually reach the mass spec and how fast it will be.

Perfect Gas

Isentropic, adiabatic Flow

2.2.2 Limits of the theory

It is important to state for which situations the assumptions made earlier are applicable and for which they are not. In the leading section we already made clear which assumptions we made and on which values they rely on. The goal is now to provide a range of state variables, in which using the following framework makes sense. Also, to show a way to calculate important dimensionless numbers like the Knudsen Number without relying on the continuum model.

Knudsen Number The whole Theory relies heavily on the continuum model. For every location of the flow, but the vacuum, it will suffice to approximate the state variables at certain locations using a simple continuum model like the one described in section 2.3.1 and use these state variables to calculate the Knudsen number. link
A sensible question to ask at this point is: Where in the flow it is the most probable encounter the highest Knudsen number. Because this will reduce the locations to check for high Knudsen numbers and therefore will simplify the process. To find such most probable Location, given the Definition of the Knudsen number:

$$Kn(p,T) = \frac{\lambda}{L_c} = \frac{\mu(T)R}{pL_c}\sqrt{\frac{\pi m T}{2k_B}}$$

L_c can be assumed constant since the height of the reactor and the smallest diameter of the ducts match. And by assuming μ to be close to constant the Knudsen number becomes a simple proportionality relation.

$$Kn(p,T) \approx \frac{\mu R}{L_c}\sqrt{\frac{\pi m}{2k_B}} \cdot \frac{\sqrt{T}}{p} = \alpha \cdot \frac{\sqrt{T}}{p} \quad \rightarrow \quad Kn \propto \frac{\sqrt{T}}{p}$$

This makes it obvious that areas with low pressure will lead to higher Knudsen numbers and will come closest to the limit of $Kn = 0.1$ where continuum regime formulations stop to yield sensible solutions. Therefore, calculating the Knudsen number where the gas leaves the outlet nozzle will be useful to identify the flow regime that governs the gas flow inside the whole assembly.

Knudsen Number in low pressure Zones When the gas is leaving the outlet the pressure will steadily drop until the method of determining Pressure and Temperature themselves will fail and force us to rely on numerical calculations. Therefore, it makes sense to identify a much more elegant way of calculating the Knudsen number which will be much more applicable in this situation.

$$Kn_L = \frac{\lambda}{\phi}\left|\frac{d\phi}{dx}\right|$$

Reynolds Number

2.3 Analytical Descriptions

2.3.1 The reactor as a reservoir

2.3.2 Full Continuum description with leak

2.3.3 Approximating outlet distribution

3 Discussion

4 Conclusion

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