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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 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.

Martin Kronberger
Vienna, 1 January 2025

Acknowledgements

Danksagung

Abtract

Kurzfassung

Contents

1. Foundational Principles

1.1. Characteristic Length

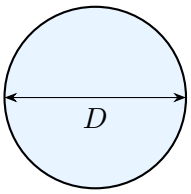
The characteristic length essentially serves the purpose of scaling physical systems. In dimensional analysis the goal is to find dimensionless quantities which describe the behavior of the system. These quantities are usually dependent on some characteristic scale, in our case the length scale, which describes the geometry of the model abstractly. For internal flows the characteristic length is defined as:

$$L_c = \frac{4A}{P_w} \quad \text{with} \quad P_w = \sum_{i=0}^{\infty} l_i$$

Where A is the cross-sectional area and P_w is the wetted perimeter, which is defined as the sum over the lengths of all surfaces in direct contact with the fluid. For gaseous fluids the whole perimeter of the cross-section must be considered, therefore the wetted perimeter reduces to the perimeter of the cross-section. The following section provides the characteristic length formulas for common duct shapes.

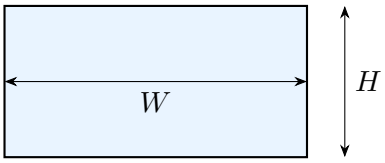
Add some more context. Why do we need to parallel plates where can we use them?

Circular duct or Nozzle



$$P_{w_\circ} = \pi D \quad \rightarrow \quad L_{c_\circ} = 2R$$

Rectangular duct



$$P_{w_\square} = 2H + W \quad \rightarrow \quad L_{c_\square} = \frac{2(HW)}{H+W}$$

Two parallel plates

These will be used in two different places.

$$\lim_{H\to\infty} L_{c_\square} = \lim_{H\to\infty} \frac{2(HW)}{H+W} = 2H$$

1.2. Dimension of the flow

The dimension describes the number of positional parameters needed to yield an exact solution for a given vector field $V(\vec{x})$, so equals essentially $n = \dim(\vec{x})$. The flow through a constant area duct is usually described as a one-dimensional flow field only depending on the position x along the length of the duct. In the case of variable area ducts the flow will be three-dimensional and has to be calculated using all spatial coordinates. But assuming only a slight change in area along the length of the duct the flow can be approximated using a one-dimensional flow field with enough precision. This is called quasi one dimensional flow. [1]

1.3. Rarefaction and the Knudsen number

In gas dynamics a flow can be categorized by its particle interaction using the Knudsen number, which represents the ratio between the mean-free-path λ of the gas and some characteristic length L_c.

$$Kn = \frac{\lambda}{L_c}$$

The characteristic length is usually chosen to be the smallest linear length in the system. For example the throat diameter of a nozzle. [2]

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 with the assumption of non-slip boundary conditions. The Navier-Stokes equations govern the calculations in this regime.

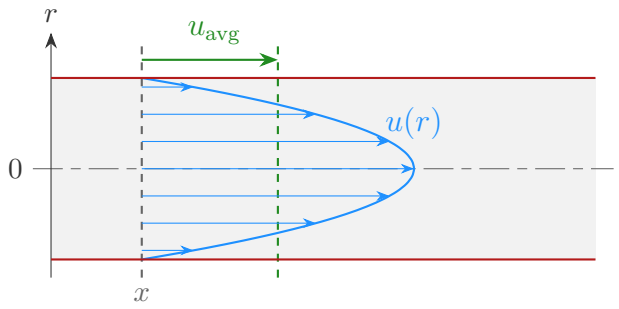


Figure 1: Velocity distribution at a point x inside a constant area duct with non-slip boundary conditions. (Continuum flow) [3]

Slip regime ($0.001 \leq Kn \leq 0.1$)

For increasing Knudsen numbers the mean free path becomes comparable to the characteristic length scale of the system. 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.

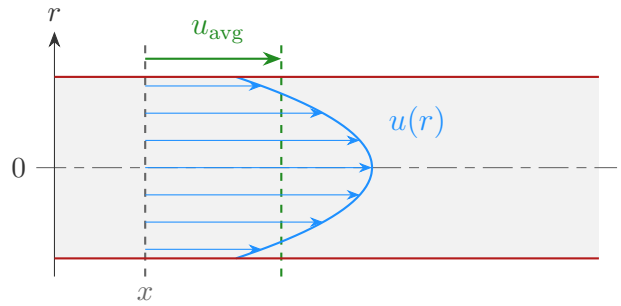


Figure 2: Velocity distribution at a point x inside a constant area duct with slip boundary conditions. [3]

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. [4]

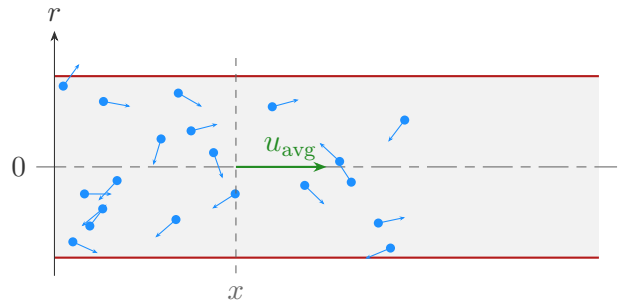


Figure 3: Mean velocity parallel to the flow at a point x inside a constant area duct in molecular flow.

1.4. Isentropic one-dimensional flow

Isentropic varying-area flow is one of the most idealized models to describe the behavior of gases flowing through a confined space. The following assumptions are made:

- steady, one-dimensional flow
- adiabatic: $\delta q = 0, ds_e = 0$
- no shaft work: $\delta w_s = 0$
- negligible change in potential energy: dz = 0
- reversible: $ds_i = 0$

Being reversible as well as adiabatic, the flow is therefore isentropic. The Mach number is defined as the ratio between the local velocity u and the local speed of sound a.

$$Ma = \frac{u}{a}$$

It is a very important metric when analyzing isentropic flow, since state variables are uniquely defined through the mach number at the corresponding location, as long as either the stagnation, or critical conditions of the flow are known.

Low subsonic regime ($Ma < 0.3$) For low Mach numbers, compressibility effects of a gas can be neglected, and the gas can be treated as an incompressible fluid.

Subsonic regime ($0.3 < Ma < 1.0$) Inside system of variable area ducts the gas flow generally stays subsonic. Once sonic speed is reached in a converging duct, the behavior reverses, and the velocity decreases, limiting the flow to subsonic or sonic speeds within converging ducts.

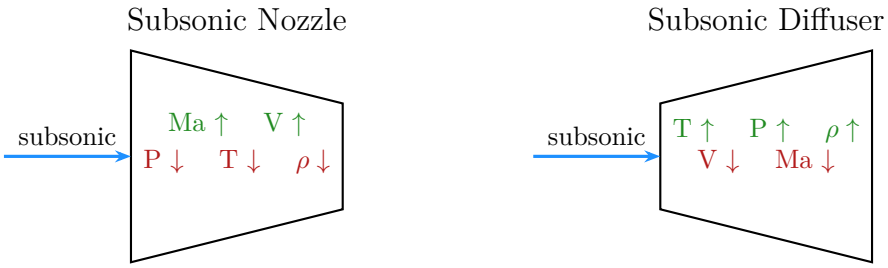


Figure 4: Change of flow properties in subsonic nozzles and diffusers

Sonic regime ($Ma = 1$) Sonic flow occurs at the exit of a converging duct, if the pressure ratio between two reservoirs becomes smaller than the following critical ratio. Which is called chocked flow and constitutes the maximum mass-flow for given stagnation conditions. This ratio is defined as:

$$\frac{P^*}{P_t} = \left(\frac{2}{\gamma + 1}\right)^{\gamma/(\gamma-1)}$$

Where P_t is the stagnation condition, P^* the critical back-pressure and γ the specific heat ratio. The ratio is derived from the isentropic flow relation (14) and can be expressed for any state variable.

Supersonic regime ($Ma > 1$) If there are critical conditions at the end of a converging duct and a diverging duct follows. The flow continues to accelerate and reaches supersonic speeds. The location where the flow reaches critical condition is called throat and represents the minimal diameter of the duct.
In supersonic flows, state variables change rapidly causing phenomenons like shock waves and expansion fans.

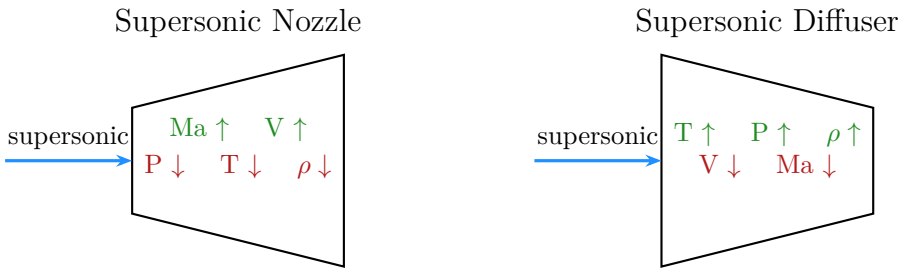


Figure 5: Change in flow properties in supersonic nozzles and diffusers

1.5. Flow behaviors in micro channels

Going from macro scale channels to microscales has some major implications for the behavior of the gas. The primary factor for these differences is slipping at the boundary of the surfaces. This is due to the fact that at small characteristic length scales the Knudsen number (Kn), whose value describes the interaction of the molecules in the gas and its boundaries, becomes relatively high ($Kn > 0.001$). Which usually puts the gas flow in the category of compressible flow with slip at the boundaries.

Most of these behaviors have to be studied using complex simulations or experimental results and are sometimes not fully explained. Therefore, this section is not intended to give concrete definitions or formulations, but to provide as many relevant references regarding behaviors in microfluidics as possible. It will be mainly based on the review study conducted by Amit Agrawal. [5]

Phenomenon of Slip

Slip, in comparison to non-slip, refers to the fact that the tangential velocity close to a surface is non-zero. Determining this velocity at the boundary is the main focus when slip is to be included in future calculations.

Slip models Maxwell suggested that on a control surface s, at distance half the mean free path away from the surface, one half of the molecules come in from one mean free path away with the tangential velocity u_λ, the other half is reflected from the surface. Assuming a fraction σ of the molecules are reflected diffusively (average velocity corresponds to velocity at the wall u_w)at the walls, with the remainder $(1-\sigma)$ being reflected specularly (no change in their impinging velocity u_λ). When expanding u_λ in a second order Taylor series this yields:

$$u_g - u_w = \left[\frac{2-\sigma}{\sigma} Kn \left(\frac{\partial u}{\partial n}\right)_s + \frac{Kn^2}{2}\left(\frac{\partial^2 u}{\partial n^2}\right)_s\right]$$

Where u stands for the streamwise velocities, where the subscripts g, w and s refer to gas, wall and control surface, with n being the normal to the control surface. And most importantly σ is the tangential momentum accommodation coefficient, or short TMAC.

The TMAC can be expressed in terms of tangential momentum of the incident molecules τ_i and the tangential momentum of the reflected ones τ_r:

$$\sigma = \frac{\tau_i - \tau_r}{\tau_i}$$

The tangential momentum accommodation coefficient

Surface Roughness

Numerical simulations

Sudden expansion or contraction

2. Scope and objectives

Short introduction of the goal of the machine in general. What is it trying to do? Why do we even try to answer following questions? Maybe even try to focus on finding out if what is measured is even what we expect to measure. Simulations To be able to establish reliable performance metrics for a given single atom catalyst

2.1. Geometry of the components

The geometry can be explained in three simple sections: gas from a reservoir flows over the inlet into the micro-reactor where it leaves through the outlet into a vacuum. 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.

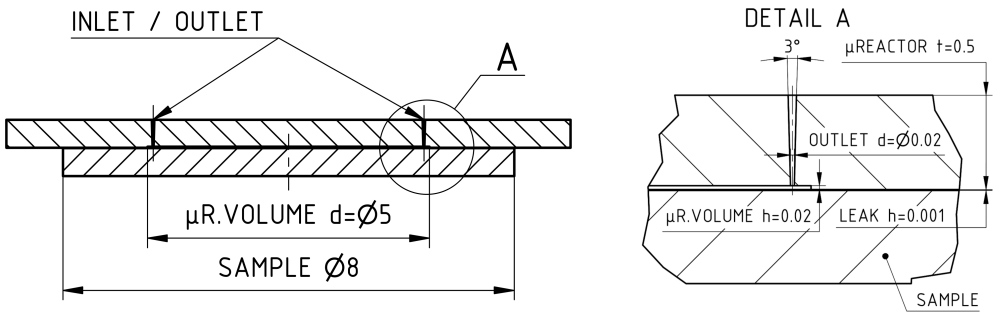


Figure 6: A descriptive caption for the figure.

Inlet Reservoir

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 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

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.

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

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,

2.2. 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 type of flow has major implications on which mathematical formulations and simulations are applicable, as well as the way the gas particles interact with each other and the walls of the assembly. 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 mass-flow and therefore some pressure drop ΔP_L inside the reactor. This can lead to major changes to the steady state of the system, therefore influencing the velocity distribution at the outlet. 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 and use them to predict probable behaviors.

Behavior of the gas around the sample

Knowing more about the state the gas is in close to the sample is very helpful. These can be used to estimate values for diffusion rates to and from the surface, boundary layer thickness, and mean velocities and momentum of particles reaching the reactive surface. Important metrics are the velocity, pressure and temperature of the gas and the type of flow.

Velocity distribution at the outlet

After the gas leaves the outlet nozzle, it expands into a vacuum chamber where the gas atoms are ionized by an electron beam and picked up by the mass-spec, to measure the ratio of different products. This won't be the case for all atoms, since for an atom to be ionized it has to cross the electron beam, which is localized in space. The remaining gas has to be pumped out and doesn't contribute to the ratio measured by the mass-spec. Therefore, it is important to approximate, how much of the gas leaving the outlet actually is able to reach the region of influence of the electron beam and will contribute to the measurement of the mass-spec. To answer this the velocity distribution of the expansion after the gas is fully rarefied is needed. This distribution can then essentially be treated as a source like surface, with no interaction between gas particles, and can

therefore be directly correlated to the amount of atoms reaching the sphere of influence of the electron beam.
Knowing what determines the distribution of the outlet can also help identify changes to be made to the geometry or the reservoir conditions to increase the amount of atoms reaching the mass-spec.

3. Analytical work

We will be using nitrogen as our gas for the whole section, therefore $\gamma = 1.470$ *and* $M = 28.0134 g/mol$

3.1. Expected Flow Regimes

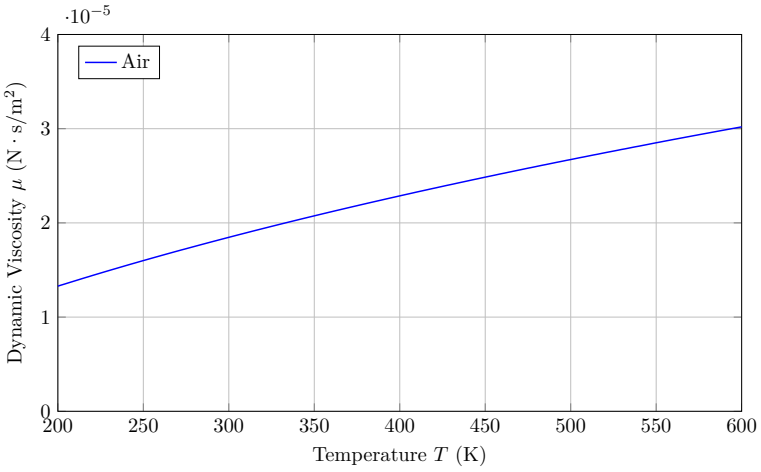
Continuum Regime

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 and use these state variables to calculate the Knudsen number.
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:

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

Where λ is the mean free path, L_c is the characteristic length, k_B is the Boltzmann constant, R is the specific gas constant, T is the temperature of the fluid, p is the pressure of the fluid, m is the molecular mass and μ is the dynamic viscosity.
The dynamic viscosity can be calculated using Sutherland's formula.

$$\mu(T) = \mu_0 \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_\mu}{T + S_\mu}$$



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.

This argument makes more sense than calculating some ratio which can be tested, since it is the same as just checking Knudsen number. This is something we can always check during the calculations, since we will calculate p and T anyway. But we can still improve this argumentation and maybe state that checking the Knudsen number at different sections makes sense, but only while calculating, not in advance.

Knudsen Number in low pressure Zones As the gas is leaving the outlet geometry and expands into the vacuum the characteristic length looses its significance. This is because the walls of the vacuum chamber are very far away in comparison to the length-scales of the flow geometry, while the gas expands it will lose pressure to conform to the vacuum and in that process will transition into free molecular flow. This leads to formulations using the mach number also loosing its significance. Therefore, it makes sense to identify a much more elegant way of calculating the local Knudsen number Kn_L which will be much more applicable in this situation.

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

Where λ is the mean free path, ϕ is some state variable of the flow. This way the Knudsen number can be calculated throughout the expansion of the gas and can be used to find the contour lines where the transition between continuum and molecular flow will happen. *Add reference!*

Laminar Flow

The Reynolds number itself does not bare any real significance for the applicability of the formulations used. Nonetheless, deviations in Reynolds number can in reality shape great parts of how the flow behaves and therefore effects important state variables.
Reynolds numbers per unit length for isentropic expansion range $10^{-2} < Re/l < 1$, whereas the characteristic length is constant at $L_c = 20 \cdot 10^{-6}$ and will therefore dominate the equation forcing low Reynolds numbers. [6]
Therefore the flow will stay laminar as long as it is contained inside the assembly and therefore mixing will be most likely diffusion mediated. [7]

Dimension of the Flow

Inside - pseudo 1D 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.

Outside - radial symmetric 3D 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 the amount of gas which will reach the mass spec and the velocity distribution. [1]

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.

3.2. One-dimensional isentropic variable area flow

By assuming the flow through the assembly will be fully isentropic and pseudo one-dimensional it is possible to calculate the state variables at every point knowing the stagnation conditions and the ratio between the cross-sectional area at the point of interest A_i and the at throat of the assembly A^*.
It must be noted that this is a very radical approximation since for the flow to be considered pseudo one-dimensional the problem must be reduced to consist purely of variable area ducts. This clearly overlooks the fact that when entering and leaving the reactor the gas has to perform a right angle turn to follow the flow path. Another constraint on the duct geometry to achieve reasonable solutions assuming pseudo one-dimensional flow is that the duct must change its cross-sectional area gradually. [1] This won't be the case inside the reactor, since there is no way of slicing the reactor chamber to achieve a gradual change in cross-section, especially around the inlet and outlet.

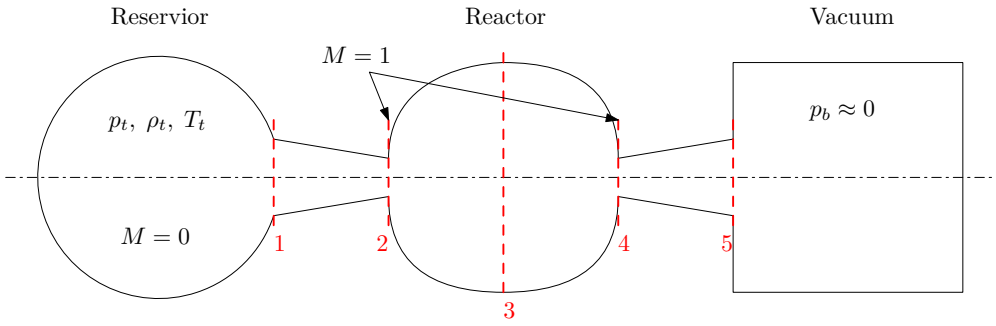


Figure 7: A descriptive caption for the figure.

This geometry can now be characterized as a double throat, and therefore isentropic flow can result in one of two fundamental solutions. One predicting subsonic flow and one predicting supersonic flow after the first throat (2). [8] [9]

Calculations

The first step is to define the critical locations, where the flow fill be chocked. Since the outlet is expanding into vacuum, resulting in a pressure ratio tending towards zero, therefore the flow therefore must be chocked and can be recognized as a critical point. Maximum mass-flow occurs if the flow is chocked. Therefore, to keep up with the mass-flow of the outlet, the inlet must also be chocked:

$$A_{2,4},\ p_{2,4},\ \rho_{2,4},\ T_{2,4} \quad \xrightarrow{M=1} \quad A^*,\ p^*,\ \rho^*,\ T^*$$

The second reference location corresponding to the stagnation or total conditions is at the entry of the inlet nozzle (1), which can be defined afterward to get quantitative solutions.

$$A_1,\ p_1,\ \rho_1,\ T_1 \quad \xrightarrow{M=0} \quad A_t,\ p_t,\ \rho_t,\ T_t$$

Next step is to calculate the cross-sectional areas for every location:

$$A_i = \pi \left(\frac{D_i}{2} \right)^2 \quad \text{for} \quad i = \{1, 2, 4, 5\} \quad \text{and} \quad A_3 = H_{\text{reactor}} \cdot D_{\text{reactor}}$$

Followed by solving the equation for the ratio of cross-sectional area for M numerically which, should yield one subsonic and one supersonic solution.

$$\frac{A}{A^*} = \frac{1}{M}\left[\frac{2}{\gamma+1}\left(1+\frac{\gamma-1}{2}M^2\right)\right]^{\frac{\gamma+1}{2(\gamma-1)}} \tag{10}$$

Afterward the ratios of state variables can be determined, which after defining the total conditions can be used to calculate the local variables for every point. [10]

$$\frac{T}{T_t} = \left(1+\frac{\gamma-1}{2}M^2\right)^{-1} \tag{14}$$

$$\frac{p}{p_t} = \left(1+\frac{\gamma-1}{2}M^2\right)^{-\frac{\gamma}{\gamma-1}} \tag{15}$$

$$\frac{\rho}{\rho_t} = \left(1+\frac{\gamma-1}{2}M^2\right)^{-\frac{1}{\gamma-1}} \tag{16}$$

Where $p,\ \rho,\ T$ are the local gas conditions, $p_t,\ \rho_t,\ T_t$ the total gas conditions, γ the specific heat ratio and M the local mach number. This leads to the following solutions:

i	$\frac{A_i}{A^*}$	M	$\frac{p_i}{p_t}$	$\frac{\rho_i}{\rho_t}$	$\frac{T_i}{T_t}$
1	4	0	1	1	1
2	1	1	0.52	0.64	0.81
3	318.31	∼0	∼1	∼1	∼1
		10.55	$3.28 \cdot 10^{-5}$	$8.90 \cdot 10^{-4}$	$3.68 \cdot 10^{-2}$
4	1	1	0.52	0.64	0.81
5	4	0.15	0.983	0.988	0.994
		3.06	0.02629	0.08415	0.31245

Table 1: Isentropic flow properties for different conditions.

Mass flow must be conserved along the flow and can be calculated using following equation, which derives from the general equation for mass-flow, the isentropic relations and the ideal gas law. [11]

$$\dot{m} = A \cdot P_t \cdot \sqrt{\frac{\gamma}{RT_t}} \cdot M \cdot \left(1+\frac{\gamma-1}{2}M^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

Where A is the local cross-sectional area, P_t the total pressure, T_t the total temperature, γ the specific heat ratio, R the specific gas constant and M the mach number. [12]

Interpretation

Go more into the solutions. Especially into the non physicality of the high mach numbers inside. Also mention non isentropic processes. Calculate the mass flow for all the points, to check validity.

3.3. Further simplifications and impact of the leak

There is no reasonable analytical solution for the leakage. Use measurements of pressure drop inside the chamber as reference and interpolate it to get solutions for higher pressure values. This forces the reactor to be treated as a reservoir with some static pressure. Does this still make sense in terms of conservation of mass? Do we need to create some region of expansion and contraction around inlet and outlet to make the equations work?

Since there is no way to make the equations work sensibly the goal of this section will be to use the middle of the chamber as the pressure input for the leakage calculation. Calculating mass flow for one pressure or maybe two. Then let the mass flow of the leak get bigger and bigger and see when the inlet turns supersonic.

3.4. Under-expanded nozzle plume at outlet

After the gas reaches sonic speeds at the throat of the outlet nozzle, it expands in the diverging outlet nozzle. This leads to a steady pressure drop as the gas reaches the exit plane of the nozzle. There are three distinctive expansion patterns characterized by the difference in pressure between the exit of the nozzle and the back pressure of the chamber.

If these values match, this is called fully expanded, which leads to a straight column of gas leaving the nozzle and no shock waves being created. Is the pressure of the gas leaving the nozzle lower than the back-pressure. The gas inside gives way to the back-pressure, leading to oblique shockwaves forming at the exit, compressing the column of gas, this is called under-expanded. If the back-pressure is now lower than the pressure of the gas, in this over-expanded state the gas leaving the nozzle further expands over the edges of the exit, creating what is called expansion fans.

These fans are often called prandl-meyer fans and occur when super-sonic flow has to turn around a sharp edge. *brandl-meyer angle and maximum angle. More information about connection with caracteristic lines, also explanation on the process of rarification and transistion regime.*

Method of characteristics

Use for nozzle design The method of characteristics is a mathematical technique used to design supersonic nozzles so that gas flows expand smoothly from sonic to supersonic speeds without generating internal shocks. It works by tracing characteristic lines—paths along which flow properties remain constant—through the nozzle region. By aligning the walls with these lines it ensures that each incremental flow turn occurs through a series of controlled expansion waves, rather than abrupt angle changes that could cause shocks. If fully expanded this leads to a straight column of gas leaving the nozzle, where all of its energy is converted into kinetic energy without significant losses due to shocks.

Navier-Stokes Equations

Fundamental equations for solving continuum flow problems. No information about boundary layer thickness and boundary conditions. These need simulations like DSMC to define boundary layer

Direct simulation Monte Carlo (DSMC)

Fundamentals of montecarlo simulations in general. How does it solve continuum regime even tho it uses molecular simulations. Use for boundary layer approximations. [2] [13] [14]

4. Discussion

Further work to be done:

- *Better formulation of the leakage.*
-

5. Conclusion

Symbols and Notation

Primary Symbols and Definitions

a speed of sound
A cross-sectional area of a duct
ξ pressure ratio across a shock wave, $\frac{p_2}{p_1}$
ρ mass density
c_p specific heat at constant pressure
c_v specific heat at constant volume
h enthalpy per unit mass, $u + pv$
L_c characteristic reference length
M Mach number, $\frac{V}{a}$
p pressure
q dynamic pressure, $\frac{\rho V^2}{2}$
R gas constant
s entropy per unit mass
T absolute temperature
u internal energy per unit mass
v specific volume, $\frac{1}{\rho}$
u velocity components parallel to flow
v velocity components perpendicular to flow
V speed of flow
V_∞ maximum speed at absolute zero
β $\sqrt{M^2 - 1}$
γ $\frac{c_p}{c_v}$ (ratio of specific heats)
θ shock-wave angle from upstream direction
μ Mach angle, $\sin^{-1} \frac{1}{M}$
μ absolute viscosity
ν Prandtl-Meyer angle

Subscripts

∞	free-stream conditions
t	total conditions (isentropic rest conditions)
$*$	critical conditions (local speed equals local sound speed)
r	reference (or datum) values
perf	thermally and calorically perfect gas
therm perf	thermally perfect, calorically imperfect gas

Notations

`[perf]`	thermally and calorically perfect gas.
`[therm perf]`	thermally perfect but calorically imperfect gas.
`[isen]`	isentropic flow process (not valid for shock waves).
`[adiab]`	adiabatic process (no heat transfer, may or may not be isentropic).

Formulary

Thermodynamics

Thermal Equations of State

Is in general an equation of the form

$$p = p(v,\ T) \tag{1}$$

Commonly used equations of state for thermally perfect gases

$$p = \frac{RT}{\rho} \quad \texttt{[therm perf]} \tag{2}$$

$$\frac{1}{\rho}dp + VdV = 0 \quad \texttt{[therm perf]} \tag{3}$$

Control Volume Analysis

Continuity Equation:

$$\frac{d}{dt}\int_V \rho\, dV + \int_S \rho V \cdot dA = 0 \tag{4}$$

Momentum Equation:

$$\frac{d}{dt}\int_V \rho V\, dV + \int_S \rho V(V \cdot dA) = -\int_S p\, dA + \int_V \rho g\, dV \tag{5}$$

Energy Equation:

$$\frac{d}{dt}\int_V \rho e\, dV + \int_S \rho h V \cdot dA = \dot{Q} - \int_S pV \cdot dA \tag{6}$$

Continuous one-dimensional

Speed of Sound:

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\gamma\left(\frac{\partial p}{\partial \rho}\right)_T} \tag{7}$$

$$a = \sqrt{\gamma\frac{p}{\rho}} = \sqrt{\gamma RT} \quad \texttt{[therm perf]} \tag{8}$$

Mach Number:

$$M = \frac{V}{a} \tag{9}$$

Area-ratio in terms of mach number:

$$\frac{A}{A^*} = \frac{1}{M}\left[\frac{2}{\gamma+1}\left(1 + \frac{\gamma-1}{2}M^2\right)\right]^{\frac{\gamma+1}{2(\gamma-1)}} \quad \texttt{[isen, perf]} \tag{10}$$

Isentropic Relations:

$$\frac{p}{\rho^\gamma} = \text{constant} = \frac{p_t}{\rho_t^\gamma} \quad \texttt{[isen, perf]} \tag{11}$$

From this:

$$\frac{p}{p_t} = \left(\frac{\rho}{\rho_t}\right)^\gamma = \left(\frac{T}{T_t}\right)^{\frac{\gamma}{\gamma-1}} = \left(\frac{a}{a_t}\right)^{\frac{2\gamma}{\gamma-1}} \quad \texttt{[isen, perf]} \tag{12}$$

Bernoulli's Equation for Compressible Flow

$$\frac{\gamma}{\gamma-1}\left(\frac{p_t}{\rho_t}\right)^{\frac{\gamma-1}{\gamma}}\left(\frac{p}{p_t}\right)^{\frac{1}{\gamma}} + \frac{V^2}{2} = \frac{\gamma}{\gamma-1}\frac{p_t}{\rho_t} \quad \texttt{[isen, perf]} \tag{13}$$

Stagnation Relations

$$\frac{T}{T_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-1} \quad \texttt{[adiab, perf]} \tag{14}$$

$$\frac{p}{p_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\frac{\gamma}{\gamma-1}} \quad \texttt{[isen, perf]} \tag{15}$$

$$\frac{\rho}{\rho_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\frac{1}{\gamma-1}} \quad \texttt{[isen, perf]} \tag{16}$$

$$\frac{a}{a_t} = \left(1 + \frac{\gamma-1}{2}M^2\right)^{-\frac{1}{2}} \quad \texttt{[adiab, perf]} \tag{17}$$

List of Figures

List of Tables

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