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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. 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?

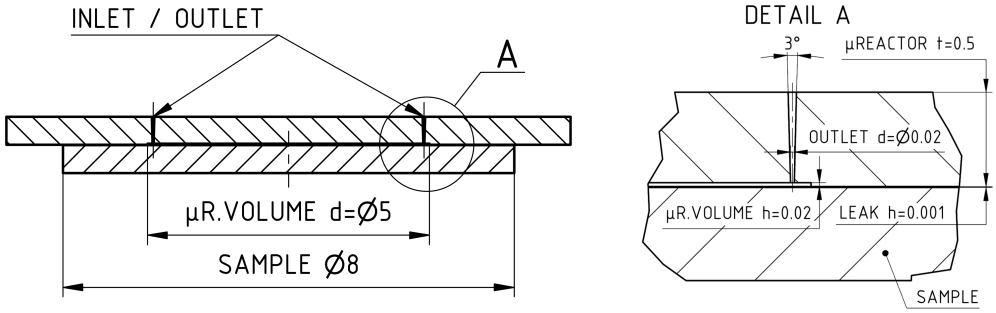


Figure 1: Dimensions of the micro-reactor assembly [1].

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.

1.1. 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.

1.2. 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.

1.3. 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.

1.4. 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.

2. Foundational Principles

When dealing with advanced fluid dynamical systems, before being able to formulate models to solve them, they have to be categorized. This is usually done by determining dimensionless numbers which values ought to describe more the behavior of the gas and its interaction with its surrounding. Essentially the values of these dimensionless numbers give a clue on which formulations are applicable and if additional boundary conditions or considerations have to be taken into account. This first chapter will go into the details of how to calculate some of the most important dimensionless numbers and give insight on what the values of them imply.

Maybe the following text is actually a little too much?

Even tho not a dimensionless number, the characteristic length L_c is an important value used to determine how length scales of the geometry and the molecules compare. It sits at the basis of both dimensionless numbers used in this work.

One way to characterize a flow of gas is by how regular the flow behaves. The Reynolds number serves this purpose by comparing viscous and inertial forces inside a fluid, therefore determining if a flow is either laminar for low values or turbulent for high ones.

Another very important dimensionless number is the Knudsen number, other than the Reynolds number it tries not to encompass flow behavior, but essentially its values decides which models and formulations can be used to solve a specific flow. It describes the ratio between the mean free path of the molecules in the gas and the characteristic length of a system. High values lead to essentially no interaction between molecules, whereas low numbers hint at particle interaction being much more important.

If the Knudsen number is significantly low, the influence of another dimensionless number becomes significant, describing the ratio between the velocity of the gas and the local speed of sound, called Mach number.

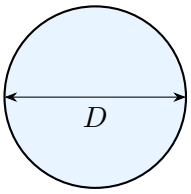
2.1. Characteristic Length

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:

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

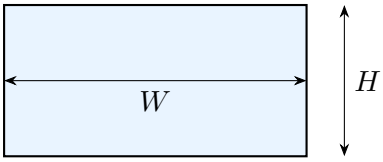
Where A is the cross-sectional area and P_w is the wetted perimeter, which is defined as the sum over the lengths of all surfaces in direct contact with the fluid. For gaseous fluids the whole perimeter of the cross-section must be considered, therefore the wetted perimeter reduces to the perimeter of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

Circular duct or Nozzle



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

Rectangular duct



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

Two parallel plates

If the height H of a rectangular duct is very small compared to its width W, it is more convenient to view it as an asymptotic case where the width approaches infinity ($W \rightarrow \infty$).

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

2.2. Turbulence and the Reynolds number

To distinguish between different kinds of flow behaviors in fluid mechanics a dimensionless quantity is introduced, which describes the ratio between inertial forces and viscous forces inside a fluid. This quantity is called the Reynolds number and is defined as:

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

Where ρ is the fluid density, u is the flow speed, L is a characteristic length (such as pipe diameter), μ is the dynamic viscosity, and ν is the kinematic viscosity. These flow behaviors can be sorted into three categories depending on the value of the Reynolds number:

- Laminar flow $Re < 2000$: where fluid moves in smooth layers, with minimal mixing between those layers.
- Transitional flow $2000 \geq Re \geq 4000$: marks the transition between the main regimes.
- Turbulent flow $Re > 4000$: where the fluid moves chaotic and mixes irregularly due to formation of eddies.

2.3. Rarefaction and the Knudsen number

In fluid 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 the characteristic length L_c of the flow geometry.

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

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.

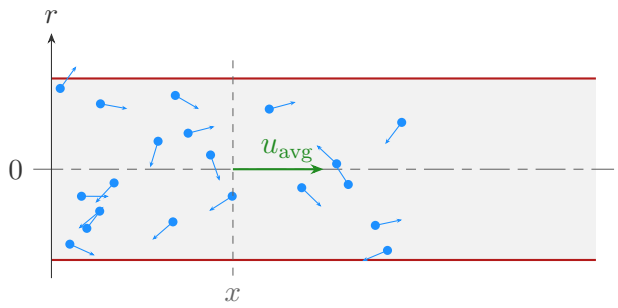


Figure 2: Mean velocity parallel to the flow at a point x inside a constant area duct in molecular flow.

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.

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.

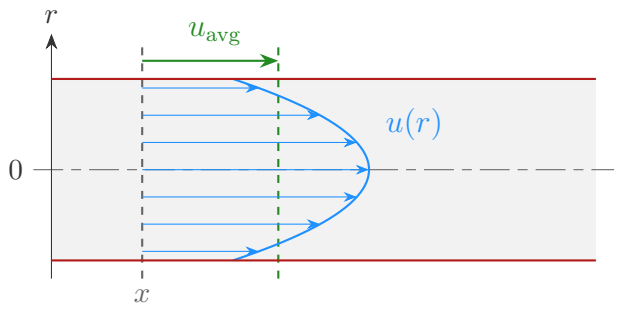


Figure 3: Velocity distribution at a point x inside a constant area duct with slip boundary conditions. [2]

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.

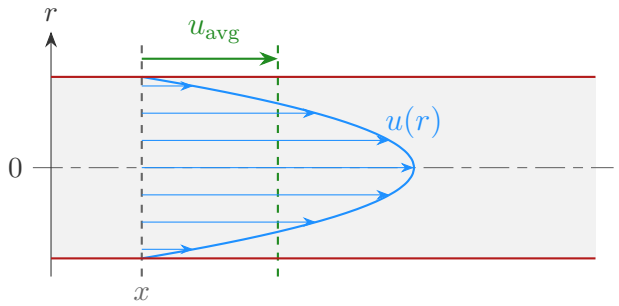


Figure 4: Velocity distribution at a point x inside a constant area duct with non-slip boundary conditions. (Continuum flow) [2]

In this work the continuum formulations will be used exclusively, with the reasons more clearly described in chapter 3.2. [3][4]

2.4. 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. [5]

2.5. 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.

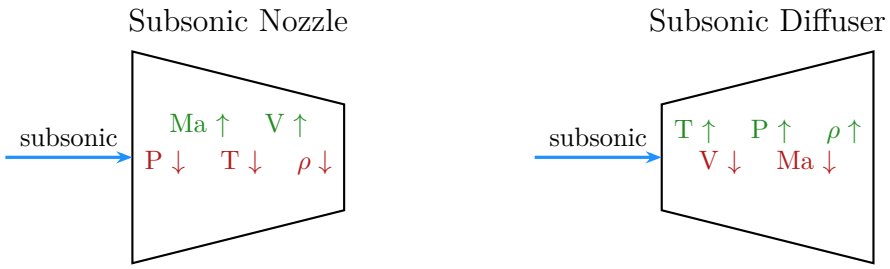


Figure 5: Change in flow properties in subsonic nozzles and diffusers [2]

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 (16) 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.

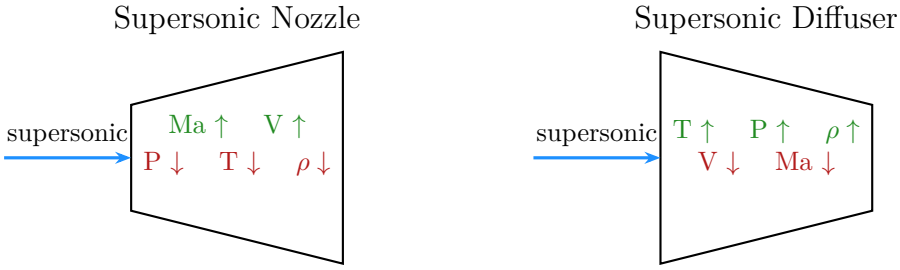


Figure 6: Change in flow properties in supersonic nozzles and diffusers [2]

3. Analytical work

Add short introduction where the content of the Chapters are introduced and the general goal and scope of the calculation is defined. Going through the main chapters and their purposes.

3.1. 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.

Reservoir

It is kept at constant pressure P_0 and constant temperature T_0, out of which the density ρ can be calculated. These values will represent the stagnation or total conditions of the system. For simplicity, it contains only one gas which is defined by its specific heat ratio γ and by its molar mass M_m. The Formulations used yield the changes in pressure, temperature and density as ratios between the local conditions and the stagnation conditions Therefore, there is no need to define stagnation conditions explicitly beforehand, since local conditions can be calculated for by multiplying chosen stagnation conditions with the calculated ratios. Therefore, only the parameters of the gas have to be defined up front, why we will define as:

$$\gamma = 1.47, \qquad M_m = 28.013 \frac{\text{g}}{\text{mol}}$$

representing nitrogen gas (N_2), since it matches relatively closely with the gases planned to use in experiments.

Inlet Nozzle

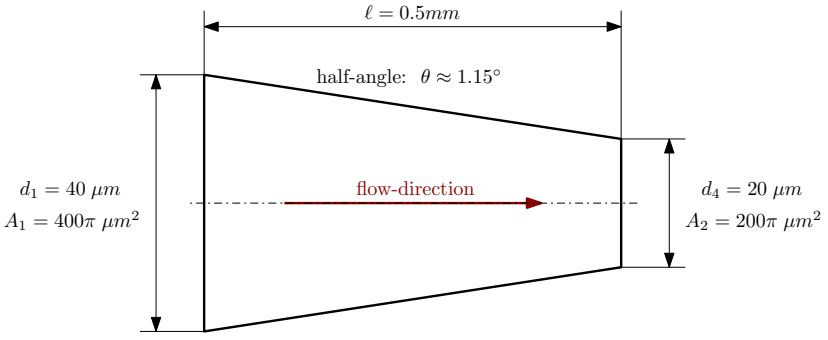


Figure 7: Non-technical drawing of the inlet nozzle geometry (not in proportion)

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

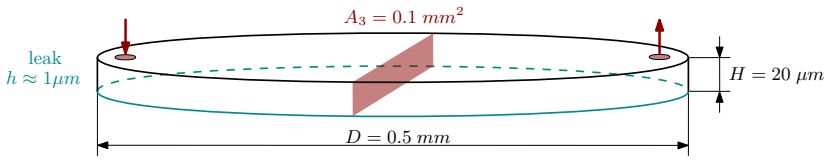


Figure 8: Non-technical drawing of the reactor geometry (not in proportion)

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

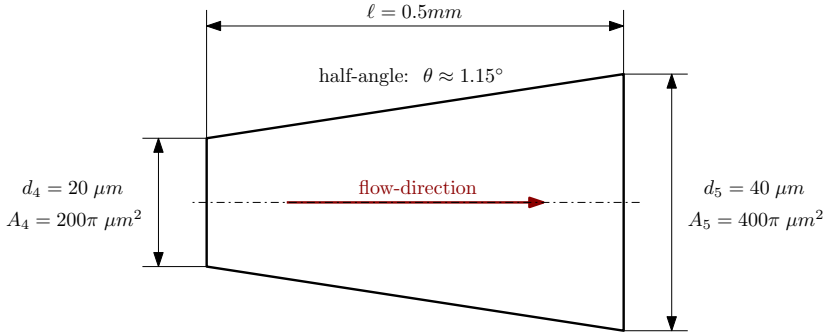


Figure 9: Non-technical drawing of the outlet nozzle geometry (not in proportion)

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 chamber does not influence the gas flow inside the assembly since the large pressure ratio between reactor and vacuum will force the flow to be chocked, and thus the back pressure looses its influence.

3.2. Expected Flow Regimes

Continuum Regime

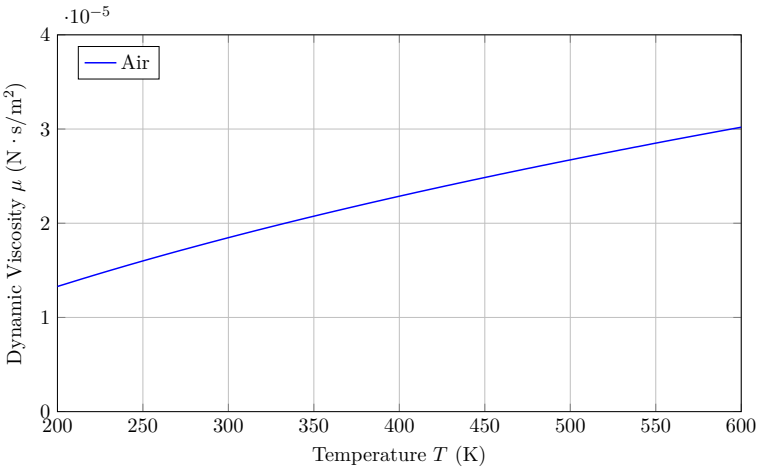
The whole Theory relies heavily on the continuum model. For every location of the flow, but the vacuum, it will suffice to approximate the state variables at certain locations using a simple continuum model and use these state variables to calculate the Knudsen number.

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:

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

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.

Refine this argument!

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. [6, 7, 8]

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. [9]
Therefore the flow will stay laminar as long as it is contained inside the assembly and therefore mixing will be most likely diffusion mediated. [10]

Dimension of the Flow

Nozzle flow - 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.

Flow through the chamber - 3D

Free jet into vacuum - 2D *Refine sections above. They are not good!* [5]

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.

3.3. 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. [5] 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.

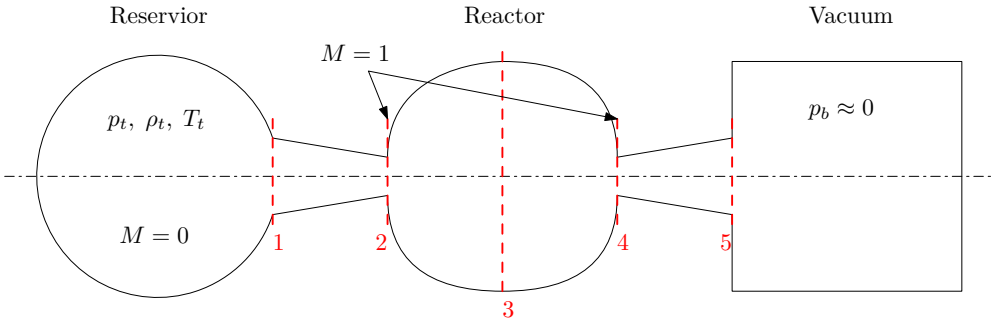


Figure 10: A descriptive caption for the figure.

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). [11, 12]

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.

$$\frac{A}{A^*} = \frac{1}{M}\left[\frac{2}{\gamma+1}\left(1 + \frac{\gamma-1}{2}M^2\right)\right]^{\frac{\gamma+1}{2(\gamma-1)}} \qquad (12)$$

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. [13]

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

$$\frac{p}{p_t} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{\gamma}{\gamma - 1}} \tag{17}$$

$$\frac{\rho}{\rho_t} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-\frac{1}{\gamma - 1}} \tag{18}$$

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 is conserved along the flow and can be calculated using following equation, which derives from the equation for mass-flow in a steady one-dimensional flow (3.6), the isentropic relations [(16) - (**??**)] and the ideal gas law (**??**). [14]

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

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. [15] Now knowing the approximate way state variables change inside the system, the assumption taken regarding the Reynolds and Knudsen number from chapter 3.2 can be tested, for a stagnation pressure p_t somewhere around ambient pressure and the stagnation temperature being relatively high since the gas will be preheated:

$$p_t = 1.5 \text{ bar} \qquad T_t = 500 \text{ K}$$

Additionally the lowest pressure at the same temperature where continuum flow formulations still hold, will be presented in the following table:

Interpretation

Go more into the solutions. Especially into the non physicality of the high mach numbers inside. Also mention non isentropic processes. This is a idealized situation this will always lead to maximum massflow in comparison to other formulation.

3.4. 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. [16]

Phenomenon of Slip

Slip, in comparison to non-slip, refers to the fact that the tangential velocity close to a surface is non-zero. 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 the second order slip boundary condition used in continuum analysis:

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

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.

Determining the TMAC for a specific application is one of the most critical aspects when dealing with slip conditions, as it directly influences the velocity slip at the gas-wall interface and, consequently, the overall behavior of rarefied gas flows. This is usually achieved through empirical studies or simulations like direct simulation Monte Carlo which will be discussed in more detail in the next section.

Surface Roughness

Sudden expansion or contraction

3.5. Further simplifications and impact of the leak

In section 3.3 the flow is assumed to be fully isentropic and one-dimensional. This led to the simplification of the reactor being a variable area duct, which leads to a change in state-variables along the path of the gas flowing from the inlet to the outlet. Since this change is based on the variable area duct formulation, it won't represent an accurate solution for the given geometry. The leak is located at the perimeter of the reactor, which is not an actual location in this formulation. To be able to include the influence of the leak analytically, without using numerical tools, further simplification is needed.

Thus, this section will explore a formulation of the system, where both the inlet reservoir and the reactor are assumed to be reservoirs, with stagnation conditions associated with them. In turn disconnecting the two reservoirs and resulting in two independent problems, describing gas from a reservoir flowing into a discharge region with a given back pressure. Representing a change in stagnation conditions which can be attributed to non-isentropic processes happening when the gas enters or leaves the reactor.

Now proper assumptions have to be taken to connect both reservoirs again, first without inclusion of the leak. Stagnation conditions for the reactor are chosen, resulting in a mass-flow at the outlet. Which in turn have to be compensated by the inlet, thus mach number and the conditions inside the reservoir can be derived. Afterward two possible formulations including the leak will be presented.

Formulations without including the leak

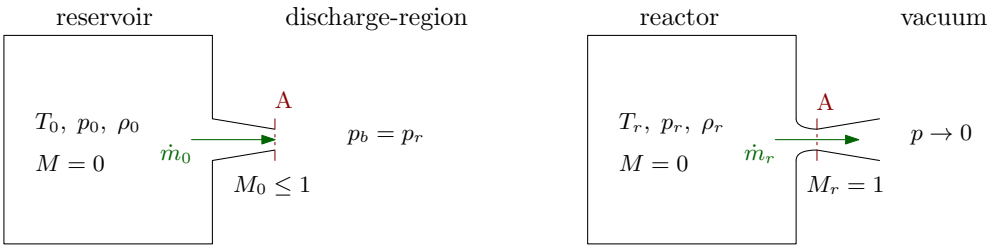


Figure 11: A descriptive caption for the figure.

Assumptions

Since this still constitutes a closed system, mass flow must be conserved, thus:

$$\dot{m}_0 = \dot{m}_r = const.$$

The reactor still discharges into vacuum, this therefore must lead to chocked flow:

$$M_r = 1$$

From the geometry it is given that:

$$A_0 = A_r = A$$

Lastly, to be able to reduce this problem to one unknown, the stagnation conditions of the reservoir and the reactor have to be related, thus reducing the unknowns to just M_0. One obvious possibility is to use the isentropic relations (equations (16) - (18)), for both Temperature and Pressure:

$$T_b = T_r \quad \rightarrow \quad T_0 = T_r \left(1 + \frac{\gamma - 1}{2} M_0^2\right)$$

and

$$p_b = p_r \quad \rightarrow \quad p_0 = p_r \left(1 + \frac{\gamma - 1}{2} M_0^2\right)^{\frac{\gamma}{\gamma - 1}}$$

Disconnecting the inlet and outlet gives the ability to define non-isentropic relations between the two reservoirs. Thus, as the second approach Temperature will be held constant between both reservoirs.

$$T_r = T_0 = T$$

This approach is going contrary to isentropic formulation, but still seems somehow plausible due to the fact that the gas in the reservoir just like the whole assembly will be preheated to a certain temperature. Since for small cavities the surface area of its walls is much larger in proportion to its internal volume, heat transfer from the walls will be significant even without high mixing due to low Reynolds numbers present in microfluidics.

Calculation

The mass flow rates from the reactor into vacuum, can be calculated using the isentropic mass flow equation:

Reservoir → Reactor

$$\dot{m}_0 = A\, p_0 \sqrt{\frac{\gamma}{RT}}\, M_0 \left(1 + \frac{\gamma - 1}{2}\, M_0^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

Reactor → Vacuum

$$\dot{m}_r = A\, p_r \sqrt{\frac{\gamma}{RT}} \left(1 + \frac{\gamma - 1}{2}\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

Thus from ($\dot{m}_r = \dot{m}_0 = const.$)

$$A\, p_r \sqrt{\frac{\gamma}{RT}} \left(1 + \frac{\gamma - 1}{2}\right)^{-\frac{\gamma+1}{2(\gamma-1)}} = A\, p_0 \sqrt{\frac{\gamma}{RT}}\, M_0 \left(1 + \frac{\gamma - 1}{2}\, M_0^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

Which constitutes the general conservation of mass equation for the system without connecting the state variables of the reservoirs in any way. This will be the starting point for both of the following approaches.

Isentropic approach

Using the isentropic relations to express T_0 and p_0 in terms of T_r and P_r the previously defined conservation of mass equation yields:

$$\begin{aligned} &A\, p_r \sqrt{\frac{\gamma}{RT_r}} \left(1 + \frac{\gamma - 1}{2}\right)^{-\frac{\gamma+1}{2(\gamma-1)}} \\ &= A\, p_r \left(1 + \frac{\gamma - 1}{2} M_0^2\right)^{\frac{\gamma}{\gamma-1}} \sqrt{\frac{\gamma}{RT_r}} \left(1 + \frac{\gamma - 1}{2} M_0\right)^{-\frac{1}{2}} M_0 \left(1 + \frac{\gamma - 1}{2}\, M_0^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}} \end{aligned}$$

Canceling out variables present on both sides and combining the potential expressions on the right side it results a function of M_0 only dependent on γ, since the summing the exponents equals zero.

$$M_0 = (1 + \frac{\gamma - 1}{2})^{-\frac{\gamma+1}{2(\gamma-1)}} \quad \text{with} \quad \gamma = 1.47 \quad \rightarrow \quad M_0 = 0.57$$

Thus resulting in following ratios between the conditions in the reactor and the reservoir.

$$\frac{T_r}{T_0} = ..., \quad \frac{p_r}{T_0} = ..., \quad \frac{\rho_r}{\rho_0} = ...$$

Constant temperature approach

Starting from the general conservation of mass equation, but choosing the temperatures to be equal yields:

$$p_r \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} = p_0 M_0 \left(1 + \frac{\gamma-1}{2} M_0^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

Again using the isentropic relation (17) for p_0

$$p_r \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} = p_r \left(1 + \frac{\gamma-1}{2} M_0^2\right)^{\frac{\gamma}{\gamma-1}} M_0 \left(1 + \frac{\gamma-1}{2} M_0^2\right)^{-\frac{\gamma+1}{2(\gamma-1)}}$$

Rearranging leads to an equation only dependent on γ and the mach number M_0 at the inlet.

$$\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} = M_0 \left(1 + \frac{\gamma-1}{2} M_0^2\right)^{\frac{1}{2}}$$

Which can be solved analytically, since by squaring both sides and rearranging it resembles a simple quadratic equation:

$$M_0^4 + \frac{2}{\gamma-1} M_0^2 - \frac{2}{\gamma-1}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}} = 0$$

Now substituting $M_0^2 = f \quad \rightarrow \quad M_0 = \sqrt{f}$

$$f = -\frac{1}{\gamma-1} \pm \sqrt{\frac{1}{(\gamma-1)^2} + \frac{2}{\gamma-1}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}}$$

There is only one real solution for this equation using the positive square root. For $\gamma = 1.47$ we get the solution:

$$f \approx 0.31 \quad \rightarrow \quad M_0 \approx 0.55$$

Formulations including the leak

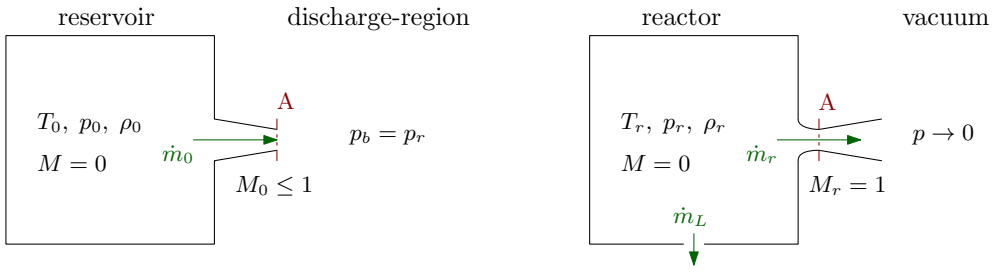


Figure 12: A descriptive caption for the figure.

3.6. 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 called Prandl-Meyer fans and occur when super-sonic flow has to turn around a sharp edge. *Prandtl–Meyer angle and maximum angle. More information about connection with characteristic lines, also explanation on the process of rarefication and transition regime.*

Method of characteristics

Ideal 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.

Determining flow field for free expansion Some text here!
[17] [18]

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. [4] [19]

Discussion

Intro Go through the analytical part in words. Mention things not done. Create red line.

Conclusion

Symbols and Notation

Primary Symbols and Definitions

a speed of sound
A cross-sectional area of a duct
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 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)
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
Ideal gas law

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

1D Euler equation

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

Control Volume Analysis

Continuity Equation:

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

In case if one-dimensional flow $\frac{\partial}{\partial t} = 0$ for a given inlet/outlet:

$$\int \rho(\vec{V}\cdot\hat{n})dA = \rho\vec{V}\cdot\hat{n}\int dA = \rho VA \tag{5}$$

Thus for steady one-dimensional flow:

$$0 = \sum \rho VA \tag{6}$$

Momentum Equation:

$$\frac{d}{dt}\int_V \rho V\, dV + \int_S \rho V(V\cdot dA) = -\int_S p\, dA + \int_V \rho g\, dV \tag{7}$$

Energy Equation:

$$\frac{d}{dt}\int_V \rho e\, dV + \int_S \rho hV \cdot dA = \dot{Q} - \int_S pV \cdot dA \tag{8}$$

Continuous one-dimensional flow

Speed of Sound:

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\gamma\left(\frac{\partial p}{\partial \rho}\right)_T} \tag{9}$$

$$a = \sqrt{\gamma\frac{p}{\rho}} = \sqrt{\gamma RT} \quad \texttt{[therm perf]} \tag{10}$$

Mach Number:

$$M = \frac{V}{a} \tag{11}$$

Area-ratio in terms of mach number:

$$\frac{A}{A^*} = \frac{1}{M}\left[\frac{2}{\gamma+1}\left(1+\frac{\gamma-1}{2}M^2\right)\right]^{\frac{\gamma+1}{2(\gamma-1)}} \quad \texttt{[isen, perf]} \tag{12}$$

Isentropic Relations:

$$\frac{p}{\rho^\gamma} = \text{constant} = \frac{p_t}{\rho_t^\gamma} \quad \texttt{[isen, perf]} \tag{13}$$

From this:

$$\frac{p}{p_t} = \left(\frac{\rho}{\rho_t}\right)^\gamma = \left(\frac{T}{T_t}\right)^{\frac{\gamma}{\gamma-1}} = \left(\frac{a}{a_t}\right)^{\frac{2\gamma}{\gamma-1}} \quad \texttt{[isen, perf]} \tag{14}$$

Bernoulli's Equation for Compressible Flow

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

Stagnation Relations

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

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

$$\frac{\rho}{\rho_t} = \left(1+\frac{\gamma-1}{2}M^2\right)^{-\frac{1}{\gamma-1}} \quad \texttt{[isen, perf]} \tag{18}$$

$$\frac{a}{a_t} = \left(1+\frac{\gamma-1}{2}M^2\right)^{-\frac{1}{2}} \quad \texttt{[adiab, perf]} \tag{19}$$

List of Figures

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