

2 Flow of gases

When planning a molecular beam apparatus the knowledge of the different flow regimes is important. These play a key role in the formation of molecular beams and in the design of conductance requirements in the whole vacuum system.

2.1 Flow regimes

The mean free path, λ , is defined as the average distance a particle in a gas travels before colliding with another particle. A way to obtain the mean free path is to calculate it via the viscosity, η , as [24, p.664]

$$\lambda = \frac{\eta \cdot \sqrt{\pi}}{2 \cdot p} \cdot \sqrt{\frac{2k_B T}{m}} = \frac{\eta \cdot \pi}{4 \cdot p} \cdot \bar{v}, \quad (2.1)$$

where $\bar{v}$ is the average velocity of the gas particles, given by

$$\bar{v} = \sqrt{\frac{8k_B T}{\pi m}}. \quad (2.2)$$

Three idealized regimes are distinguished depending on the pressure and the geometry of the vacuum equipment the gas is flowing through (e.g. the diameter of a tube or orifice, the length of a channel): molecular flow, continuum flow and transition flow [20, pp.25–27].

If the pressure is sufficiently low, the mean free path of the particles will be much greater than the diameter of the vacuum equipment. Therefore the majority of particles will move along straight trajectories until hitting a wall. Collisions between

the particles occur very rarely, they move independently of each other. These conditions are called molecular flow. The flow is only caused by the kinetic energy of the particles.

If the pressure is sufficiently high, the mean free path of the particles is much smaller than the diameter or length of the vacuum equipment. Therefore particles will collide very often with each other, resulting in frequent exchange of momentum and energy. The particles can be treated as a continuum and flow is caused by local pressure gradients. Thus, this regime is named continuum flow. Continuum flow can be either turbulent or laminar viscous.

Transition flow occurs when the pressure is between the limits above; neither molecular or continuum flow prevails.

To quantitatively distinguish the flow regimes the dimensionless Knudsen number, Kn , is defined as

$$Kn = \frac{\lambda}{D}, \quad (2.3)$$

where λ is the mean free path and D is the characteristic dimension of the vacuum equipment (e.g. diameter of a tube). The transition between flow regimes is continuous, but a classification by the Knudsen number is:

$$\begin{aligned} Kn > 1 & \quad \text{molecular flow,} \\ 1 > Kn > 0.01 & \quad \text{transition flow,} \\ Kn < 0.01 & \quad \text{continuum flow.} \end{aligned} \quad (2.4)$$

2.2 Conductance

In the following sections the conductance in the different flow regimes is discussed. The conductance, C , of a tubing component is generally defined as [13, p.92]

$$C = \frac{q_{pV}}{p_1 - p_2}, \quad [C] = \text{m}^3/\text{s}, \quad (2.5)$$

where q_{pV} is the throughput and $p_1 - p_2$ is the pressure difference between the entrance and the exit of the tubing component.

2.2.1 Molecular flow

Particles that enter a tube will move on a straight trajectory until they hit either the wall of the tube or make it directly to the exit of the tube. Particles that have collided with the wall will be scattered in random directions and thus go back and forth in the tube until they leave the tube either through the entrance or the exit area. Therefore the conductance in molecular flow, C_{mol} , can be described statistically by the conductance of the entrance area, C_O , and the transmission probability, P , for a particle to make it through the tubing component [13, pp.135–139]:

$$C_{\text{mol}} = C_O \cdot P. \quad (2.6)$$

Orifice

The conductance, C_O , of an ideal orifice with infinitely small wall thickness ($L = 0$) and area A is

$$C_O = \frac{\bar{v}}{4} A. \quad (2.7)$$

The transmission probability of an ideal orifice ($L = 0$) is obviously 1. Table 2.1 shows the orifice conductance per area, C_O/A , for different gases according to Eq. (2.7).

Tube

The transmission probability, P_T , for a tube with length L and diameter D is given by [13, pp.142–144]

$$P_T(L, D) = \frac{14 + 4\frac{L}{D}}{14 + 18\frac{L}{D} + 3\left(\frac{L}{D}\right)^2}. \quad (2.8)$$

Gas	$\bar{v}$ [m/s]	C_O/A [l/(s · cm ²)]
H ₂	1762	44.0
He	1246	31.1
H ₂ O	587	14.7
N ₂	471	11.8
Ar	394	9.8
Xe	218	5.4

Table 2.1: Molecular orifice conductance per area for gases at 20 °C.

For a short tube with $L \ll D$ the transmission probability P_T becomes

$$P_{T,\text{short}} = 1 - \frac{L}{D}, \quad (2.9)$$

and for a long tube with $L \gg D$

$$P_{T,\text{long}} = \frac{4D}{3L}. \quad (2.10)$$

Figure 2.1 shows the transmission probability, P_T , according to Eq. (2.8). The conductance of a tube, C_T , is then given by Eq. (2.6).

$$C_T = C_{O,T} P_T, \quad (2.11)$$

where $C_{O,T}$ is the orifice conductance of the entrance area of the tube.

Tube with annular cross section

Several formulas for the conductance of a tube with an annular (ring-like) cross section can be found in the literature, see Appendix B.1, Page 93. The formula, which will be used in this work to calculate the conductance, C_{ann} , of an annular tube (important for the pumping speeds in the pumping stages of the MB, see Section 4.4.6, Page 68) with outer diameter D_o , inner diameter D_i and length L is

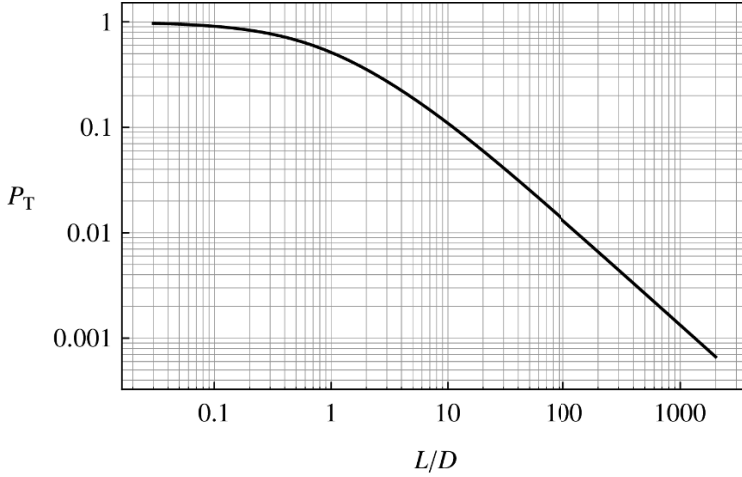


Figure 2.1: Transmission probability, P_T , for a tube as a function of the relative length, L/D , according to Eq. (2.8).

given by

$$C_{\text{ann}} = 3.81 \sqrt{\frac{T}{M}} \frac{(D_o - D_i)^2 (D_o + D_i)}{L + 1.33(D_o - D_i)}, \quad (2.12)$$

where M is the relative molecular mass; dimensions are in cm and C_{ann} in l/s. Figure 2.2 shows the transmission probability, P_{ann} , obtained from Eq. (2.12).

Tubing components in series

The simplest way to calculate the conductance of composite systems is the electric circuit analogy [13, pp.91–94]. If n elements are connected parallel, the conductances, C_i , add up to give

$$C = C_1 + C_2 + \dots + C_n. \quad (2.13)$$

and if connected in series, the inverse conductances add up to give

$$\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2} + \dots + \frac{1}{C_n}. \quad (2.14)$$

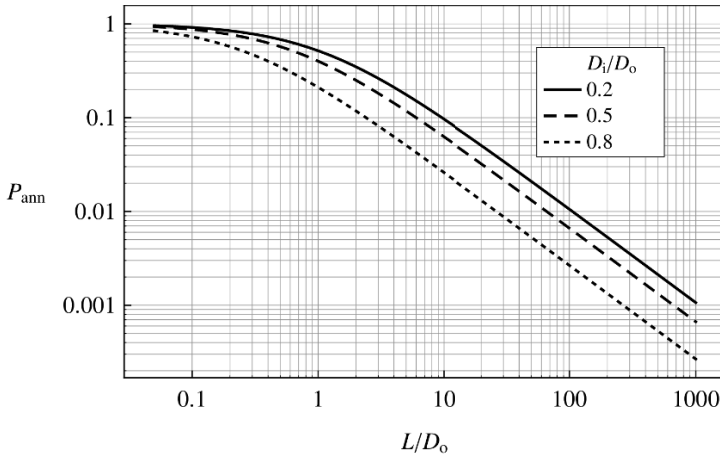


Figure 2.2: Transmission probability for annular tubes, P_{ann} , with different inner to outer diameter ratio, D_i/D_o , as a function of the relative length, L/D_o , obtained from Eq. (2.12). The transmission probability was obtained by dividing the conductance, C_{ann} , by the orifice conductance of the annular cross section.

The latter case also applies to the calculation of the effective pumping speed at a certain point in a vacuum system. It is given by the pumping speed, S_p , provided by the vacuum pump and the conductance, C , of the tubing connecting said point to the pump. The effective pumping speed, S_{eff} , is then given by

$$\frac{1}{S_{\text{eff}}} = \frac{1}{S_p} + \frac{1}{C}. \quad (2.15)$$

However, two conditions must be met for the circuit analogy to hold: the rate of flow of gas through a single tube must be proportional to the pressure difference between its ends, and the conductivity of a tube must be independent of the components to which its ends are connected. The latter is in general not true, as Eq. (2.14) gives a rather poor approximation with errors up to 40 % for two tubes with identical radii connected in series [19]. A better expression for the

transmission probability, P , for the connected tubes is given by

$$\frac{1}{P} = \frac{1}{P_1} + \frac{1}{P_2} - 1, \quad (2.16)$$

where P_1 and P_2 are the transmission probabilities of the respective tubes.

An advanced version of Eq. (2.16) is also considering changes of cross sections and gives the transmission probability, P_{1n} , of n components as [20, p.47]

$$\frac{1}{A_1} \left(\frac{1}{P_{1n}} - 1 \right) = \sum_{i=1}^n \frac{1}{A_i} \cdot \left(\frac{1}{P_i} - 1 \right) + \sum_{i=1}^{n-1} \left(\frac{1}{A_{i+1}} - \frac{1}{A_i} \right) \cdot \delta_{i,i+1}, \quad (2.17)$$

where

- P_i transmission probability of the i -th component,
- A_i cross section of the i -th component,
- $\delta_{i,i+1} = 1$, if $A_{i+1} < A_i$ (reduction of cross section),
 $= 0$, if $A_{i+1} \geq A_i$ (no reduction of cross section).

The conductance of n components, C_{1n} , is then calculated by multiplying the transmission probability, P_{1n} , with the orifice conductance of the cross section of the first component, C_{O,A_1} , giving

$$C_{1n} = C_{O,A_1} P_{1n}. \quad (2.18)$$

2.2.2 Continuum flow

In continuum flow the conductance is pressure dependent [13, pp.96–103]. For a converging nozzle the throughput, q_{pV} , follows from the conservation of the mass flowing from the upstream to the downstream side:

$$q_{pV} = A_{\min} \cdot \sqrt{\frac{\pi}{4}} \cdot p_1 \cdot \bar{v} \cdot \psi \left(\frac{p_2}{p_1} \right), \quad (2.19)$$

Gas species	Isentropic exponent κ [13, p.97]	Critical pressure ratio p^*/p_1	Maximum value of flow function ψ_{critical}
Inert gases	≈ 1.667	0.487	0.513
Diatom gases	$= 1.4$	0.528	0.484
Complicated molecules (e.g. oil vapours)	≈ 1.1	0.585	0.444

Table 2.2: Isentropic exponent, critical pressure ratio, and maximum value of the flow function for various gas species.

where p_1 and p_2 are the pressures at the upstream and downstream side, respectively and $A_{\min}$ is the narrowest cross section of the nozzle. The *flow function* ψ describes the dependence on the pressure ratio and is given by

$$\psi\left(\frac{p_2}{p_1}\right) = \sqrt{\frac{\kappa}{\kappa-1} \cdot \left(\left(\frac{p_2}{p_1}\right)^{\frac{2}{\kappa}} - \left(\frac{p_2}{p_1}\right)^{\frac{1+\kappa}{\kappa}} \right)}, \quad (2.20)$$

where κ is the isentropic exponent¹ of the gas. Figure 2.3a shows that ψ has a maximum, ψ_{critical} , at the critical pressure, p^* , when the gas flow reaches the speed of sound between $p_2 = 0.45p_1$ and $0.6p_1$ (depending on κ). A further lowering of the downstream pressure would decrease the mass flow again, according to Eq. (2.20). However, in reality the flow function takes on its maximum value, ψ_{critical} , once the gas flow reaches the speed of sound as no further interaction with the molecules upstream is possible, see Fig. 2.3b; the flow condition is called choked flow. Table 2.2 shows the isentropic coefficient, the critical pressure ratio and the maximum value of the flow function for various gas species. The expressions for ψ_{critical} and p^*/p_1 are given in Eqs. (2.21) and (2.22), respectively.

$$\psi_{\text{critical}} = \psi\left(\frac{p^*}{p_1}\right) = \left(\frac{2}{\kappa+1}\right)^{\frac{1}{\kappa-1}} \cdot \sqrt{\frac{\kappa}{\kappa+1}}. \quad (2.21)$$

$$\frac{p^*}{p_1} = \left(\frac{2}{\kappa+1}\right)^{\frac{\kappa}{\kappa-1}} \quad (2.22)$$

¹ the ratio of the heat capacity at constant pressure to the heat capacity at constant volume

Orifice

For a thin walled orifice with cross section A_O the expression for the throughput of the converging nozzle, Eq. (2.19), has to be corrected for the sudden contraction of the flow at the orifice opening. Depending on the pressure ratio, the following correction for $A_{\min}$ is applied [13, p.103]:

$$A_{\min} = \begin{cases} 0.60 \cdot A_O & \text{if } p_2 \approx p_1 \\ 0.86 \cdot A_O & \text{if } p_2 < p^* \quad (\text{choked flow}). \end{cases} \quad (2.23)$$

Therefore the conductance of an orifice in continuum flow under choked flow conditions is given by

$$C_{O,\text{cont}} = 0.86 \cdot A_O \cdot \sqrt{\frac{\pi}{4}} \cdot \bar{v} \cdot \psi_{\text{critical}}. \quad (2.24)$$

Note that the conductance of the orifice in choked flow is independent of the pressure, as in molecular flow.

Tube

The type of continuum flow in a tube is characterised by the Reynolds number [13, pp.116–119]:

$$Re = \frac{32}{\pi^2} \cdot \frac{q_{pV}}{\eta \cdot \bar{v} \cdot D} \begin{cases} < 2300 & \text{laminar viscous flow} \\ > 4000 & \text{turbulent flow}. \end{cases} \quad (2.25)$$

For a tube connecting two vessels with pressures p_1 and p_2 , the conductance in laminar viscous flow, $C_{T,\text{lam}}$, is given by

$$C_{T,\text{lam}} = \frac{\pi}{256} \cdot \frac{1}{\eta} \cdot \frac{D^4}{L} \cdot (p_1 + p_2), \quad (2.26)$$

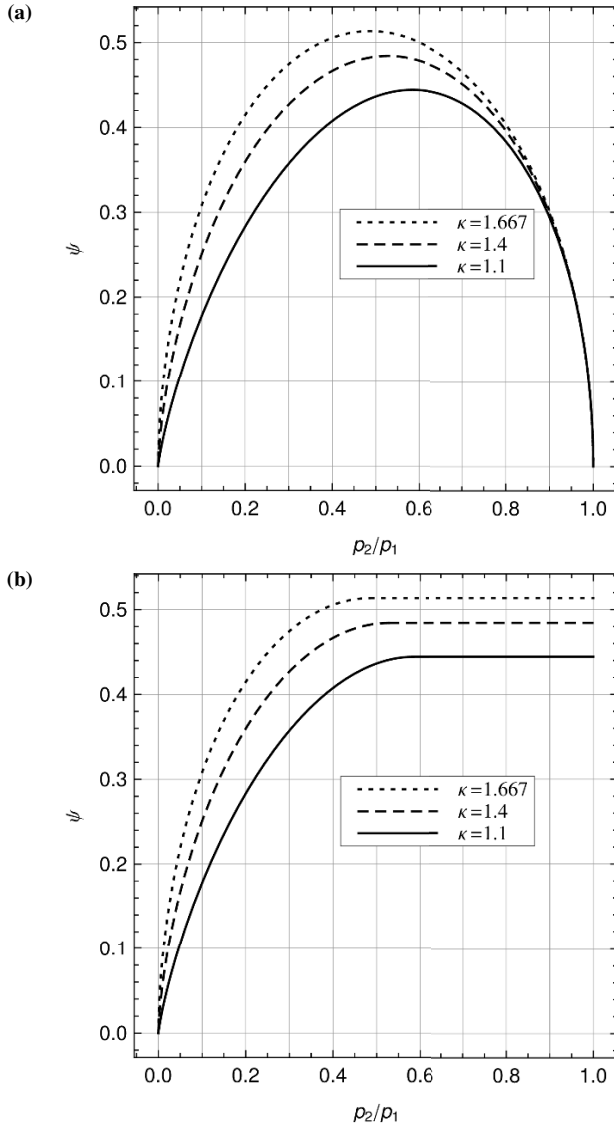


Figure 2.3: (a) Theoretical behaviour of the flow function, ψ , according to Eq. (2.20). (b) Real behaviour of ψ according to Eqs. (2.20) and (2.21). As the critical pressure is reached, the flow function stays on its critical value, ψ_{critical} .

and in turbulent flow, $C_{T,turb}$, by

$$C_{T,turb} = 1.015 \cdot D^{\frac{19}{7}} \cdot \left(\frac{\bar{v}^6}{\eta} \right)^{\frac{1}{7}} \cdot \left(\frac{p_1 + p_2}{L} \right)^{\frac{4}{7}} \cdot (p_1 - p_2)^{-\frac{3}{7}}, \quad (2.27)$$

where η is the viscosity of the gas.

2.2.3 Transition flow and conductance over the whole pressure range

When conditions change from molecular to continuum flow, both types of flow occur at the same time. The resulting flow is called transition flow, which is difficult to describe exactly, but good experimental data and approximations are available.

Orifice

The conductance of an orifice is given by Eqs. (2.7) and (2.24) for molecular and continuum flow, respectively. If in continuum flow one assumes choked flow and $\psi_{critical} = 0.484$ (for air) then the ratio of the conductance in the continuum limit, $C_{O,cont}$, to the molecular conductance, C_O , is

$$\frac{C_{O,cont}}{C_O} = 0.86 \cdot \psi_{critical} \cdot 2\sqrt{\pi} = 1.48. \quad (2.28)$$

Therefore the conductance of the orifice increases by a factor of 1.48 when changing from molecular to continuum flow.

Figure 2.4 shows the measured conductance, C , of an orifice, normalized to its molecular conductance, over a wide range of the inverse Knudsen number. In the continuum limit (i.e. $Kn^{-1} \approx 10000$) the experimental data is in good agreement with Eq. (2.28). The observed maximum at $Kn^{-1} \approx 100$ is explained by the not yet fully developed clogging of the flow at the downstream side of the orifice [12].

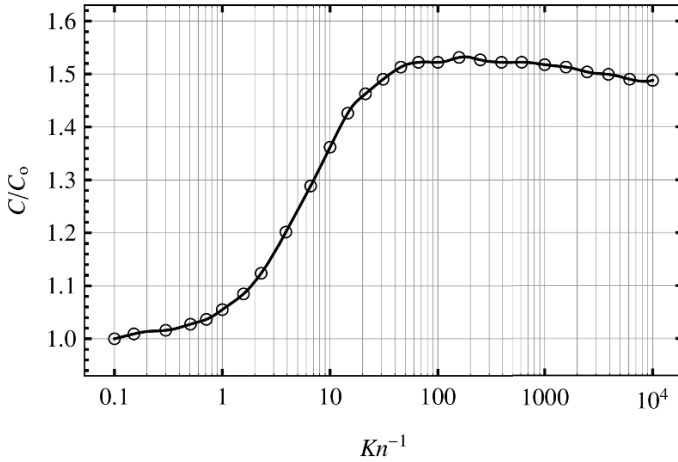


Figure 2.4: Interpolation (line) of the experimental data (circles) for the ratio C/C_0 as a function of the inverse Knudsen number from [12, Fig.2]. Values for the interpolation are listed in Table B.3, Page 99.

Therefore the ratio of the orifice conductance, C_{orifice} , to the molecular orifice conductance, C_0 , over the whole pressure range can be expressed by

$$\gamma(Kn) = \frac{C_{\text{orifice}}}{C_0} = \begin{cases} 1 & \text{if } Kn^{-1} < 0.1, \\ \epsilon & \text{if } 0.1 < Kn^{-1} < 10000, \\ 1.48 & \text{if } Kn^{-1} > 10000, \end{cases} \quad (2.29)$$

where ϵ is the interpolated ratio from Fig. 2.4.

The conductance of an orifice, C_{orifice} , for air over the whole pressure range is therefore given by

$$C_{\text{orifice}} = \gamma(Kn)C_0. \quad (2.30)$$

Tube

A long tube can be approximated by two parallel tubes of which one is considered to be in molecular and the other in laminar viscous flow [13, pp.159–162]:

$$C_T \approx C_{T,\text{mol}} + C_{T,\text{lam}}. \quad (2.31)$$

This equation correctly describes the conductances in the molecular and continuum limit and is an approximation in transition flow. By adding the respective conductances from Eqs. (2.10) and (2.26) one obtains

$$C_T = \frac{\pi}{12} \left(\frac{3}{32} \cdot \frac{\bar{p} \cdot D}{\eta \cdot \bar{v}} + Z \right) \cdot \frac{D^3}{L} \cdot \bar{v}, \quad (2.32)$$

where $\bar{p}$ is the average of the pressures at the entrance and the exit of the tube. According to the addition, Z equals 1. However, *Knudsen* found a semi empirical expression for the dimensionless correction factor given by

$$Z = \frac{1 + \frac{1.28}{Kn}}{1 + \frac{1.58}{Kn}}, \quad (2.33)$$

where the Knudsen number is to be calculated at the average pressure $\bar{p}$. The dimensionless bracket term in Eq. (2.32) is called the *conductance function*, f , and is only dependent on the Knudsen number:

$$f = \frac{3}{32} \cdot \frac{\bar{p} \cdot D}{\eta \cdot \bar{v}} + Z = \frac{3 \cdot \pi}{128} \cdot \frac{1}{Kn} + Z. \quad (2.34)$$

Figure 2.5 shows f as a function of the inverse Knudsen number. It is 1 in the molecular region, decreases with increasing pressure to a minimum at $Kn^{-1} \approx 0.6$ and then increases rapidly. The conductance, C_T , of a tube with diameter D and length L over the whole pressure range is therefore expressed by

$$C_T = \frac{\pi}{12} \cdot f \cdot \frac{D^3}{L} \cdot \bar{v}. \quad (2.35)$$

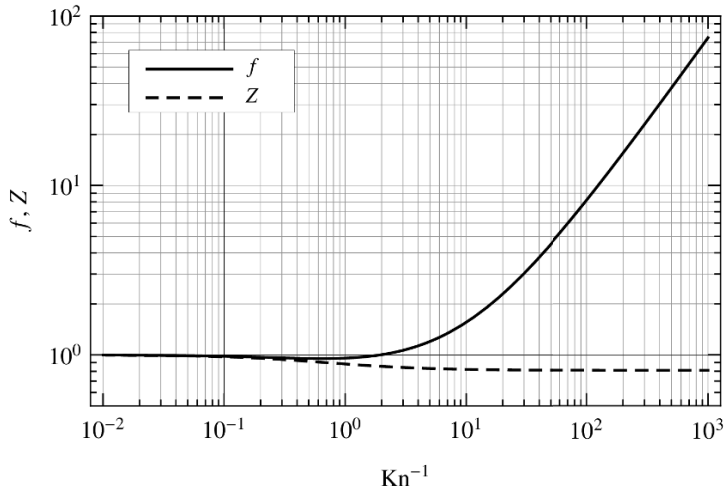


Figure 2.5: Conductance function, f , and correction factor, Z , from Eqs. (2.33) and (2.34) as a function of the inverse Knudsen number.

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