

Rarefied gas dynamics and its applications to vacuum technology

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Abstract

Basic concepts of rarefied gas dynamics are given in a concise form. Some problems of rarefied gas flows are considered, namely, calculations of velocity slip and temperature jump coefficients, gas flow through a tube due to pressure and temperature gradients, and gas flow through a thin orifice. Results on the two last problems are given over the whole range of gas rarefaction. A methodology for modelling the Holweck pump is described. An extensive list of publications on these topics is given.

1 Brief history of rarefied gas dynamics

Rarefied gas dynamics is based on the kinetic approach to gas flows. In 1859 Maxwell [1] abandoned the idea that all gaseous molecules move with the same speed and introduced the statistical approach to gaseous medium, namely, he introduced the velocity distribution function and obtained its expression in the equilibrium state. Thus Maxwell gave the origin to the kinetic theory of gases. Then, in 1872 Boltzmann [2] deduced the kinetic equation which determines the evolution of the distribution function for gaseous systems being out of equilibrium.

In 1909 Knudsen [3], measuring a flow rate through a tube, detected a deviation from the Poiseuille formula at a low pressure. Such a deviation was explained by the fact that at a certain pressure the gas is not a continuous medium and the Poiseuille formula is not valid anymore. A description of such a flow required the development of a new approach based on the kinetic theory of gases. This can be considered as the beginning of rarefied gas dynamics.

Later, advances were made by Hilbert [4], Enskog [5] and Chapman [6] to solve the Boltzmann equation analytically via an expansion of the distribution function with respect to the Knudsen number. The main result of this solution was a relation of the transport coefficients to the intermolecular interaction potential, but no numerical calculation of rarefied gas flows could be realized at that time.

In 1954 the so-called model equations [7,8] were proposed to reduce the computational efforts in calculations of rarefied gas flows. Using these models it was possible to obtain numerical results on rarefied gas flows in the transition regime. Thus in 1960 a numerical investigation of rarefied gas flows began in its systematic form. For a long time, it was possible to solve only the model equations. Practically, all classical problems of gas dynamics (Poiseuille flow, Couette flow, heat transfer between two plates, flow past a sphere, etc.) were solved over the whole range of gas rarefaction by applying the model equations. In 1989 first results based on the exact Boltzmann equation were reported, see, for example, Ref. [9]. However, even using the powerful computers available nowadays, a numerical calculation based on the Boltzmann equation itself is still a very hard task, which requires great computational efforts. Thus, the model equations continue to be a main tool in practical calculations.

Below, the main concepts of rarefied gas dynamics and some examples of its application will be given. In the last section, the main results of rarefied gas dynamics that could be applied to vacuum technology are listed.

2 Basic concepts of rarefied gas dynamics

2.1 Knudsen number and rarefaction parameter

The principal parameter of rarefied gas dynamics is the Knudsen number (Kn) which characterizes the gas rarefaction and is defined as the ratio

$$\text{Kn} = \frac{\ell}{a}, \quad (1)$$

where ℓ is the equivalent molecular mean free path given as

$$\ell = \frac{\mu v_m}{P}, \quad v_m = \left(\frac{2k_B T}{m} \right)^{1/2}, \quad (2)$$

v_m is the most probable molecular velocity, $k_B = 1.380662 \times 10^{-23}$ J/K is the Boltzmann constant, m is the molecular mass of the gas in kg, T is the temperature of gas in K, P is its pressure in Pa, and μ is the gaseous viscosity in Pa s.

Regarding the value of the Knudsen number, we may distinguish the following three regimes of gas flow. If the Knudsen number is small ($\text{Kn} \ll 1$), the gas can be considered as a continuous medium and the hydrodynamic equations [10] can be applied. This regime is called *hydrodynamic*. If the Knudsen number is large ($\text{Kn} \gg 1$), the intermolecular collisions can be neglected. Under this condition we may consider that every molecule moves independently from each other and, usually, the test particle Monte Carlo method [11,12] is employed. This regime is called *free-molecular*. When the Knudsen number has some intermediate value, we can neither consider the gas as a continuous medium nor discount the intermolecular collisions. In this case the kinetic equation should be solved [13–21], or the DSMC method [11,12] is used. This regime is called *transitional*.

Usually another quantity characterizing the gas rarefaction is used instead of the Knudsen number, *viz.* the rarefaction parameter defined as

$$\delta = \frac{a}{\ell} = \frac{1}{\text{Kn}}. \quad (3)$$

Large values of δ correspond to the hydrodynamic regime and the small values of δ are appropriate to the free molecular regime. This parameter is more convenient because many solutions are given in terms of this parameter.

2.2 Velocity distribution function

The state of a monoatomic gas is described by the one-particle velocity distribution function $f(t, \mathbf{r}, \mathbf{v})$, where t is the time, \mathbf{r} is a vector of spatial coordinates, and \mathbf{v} is a velocity of molecules. The distribution function is defined so that the quantity $f(t, \mathbf{r}, \mathbf{v}) d\mathbf{r} d\mathbf{v}$ is the number of particles in the phase volume $d\mathbf{r} d\mathbf{v}$ near the point (\mathbf{r}, \mathbf{v}) at the time t .

All macro-characteristics of gas flow can be calculated *via* the distribution function:

number density

$$n(t, \mathbf{r}) = \int f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}, \quad (4)$$

hydrodynamic (bulk) velocity

$$\mathbf{u}(t, \mathbf{r}) = \frac{1}{n} \int \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}, \quad (5)$$

pressure

$$P(t, \mathbf{r}) = \frac{m}{3} \int V^2 f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}, \quad (6)$$

stress tensor

$$P_{ij}(t, \mathbf{r}) = m \int V_i V_j f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}, \quad (7)$$

temperature

$$T(t, \mathbf{r}) = \frac{m}{3n k_B} \int V^2 f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}, \quad (8)$$

heat flow vector

$$\mathbf{q}(t, \mathbf{r}) = \frac{m}{2} \int V^2 \mathbf{V} f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}, \quad (9)$$

where \mathbf{V} is the peculiar velocity

$$\mathbf{V} = \mathbf{v} - \mathbf{u}. \quad (10)$$

2.3 Boltzmann equation

The distribution function obeys the Boltzmann equation [11–21] which in the absence of external forces reads

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} = Q(f f_*), \quad (11)$$

where $Q(f f_*)$ is the collision integral, which has a complicated expression and is omitted here. Till now, a numerical solution of Eq.(11) with the exact expression of the collision integral is a very difficult task, that is why some simplified expressions of $Q(f f_*)$ are used. These expressions are called the model kinetic equations. They maintain the main properties of the exact collision integral, but they allow us to reduce significantly the computational efforts when the kinetic equation is solved numerically.

The most usual model equation was proposed by Bhatnagar, Gross and Krook (BGK) [7] and by Welander [8]. They presented the collision integral as

$$Q_{\text{BGK}}(f f_*) = \nu \left[f^M - f(t, \mathbf{r}, \mathbf{v}) \right], \quad (12)$$

where f^M is the local Maxwellian

$$f^M = n(t, \mathbf{r}) \left[\frac{m}{2\pi k_B T(t, \mathbf{r})} \right]^{3/2} \exp \left\{ -\frac{m[\mathbf{v} - \mathbf{u}(t, \mathbf{r})]^2}{2k_B T(t, \mathbf{r})} \right\}. \quad (13)$$

The local values of the number density $n(t, \mathbf{r})$, bulk velocity $\mathbf{u}(t, \mathbf{r})$, and temperature $T(t, \mathbf{r})$ are calculated *via* the distribution function $f(t, \mathbf{r}, \mathbf{v})$ in accordance with the definitions (4), (5), and (8), respectively. The quantity ν is the collision frequency assumed to be independent of the molecular velocity and equal to $\nu = P/\mu$. However, this model does not provide the correct value of the Prandtl number.

The S-model proposed by Shakhov [22] is a modification of the BGK model giving the correct Prandtl number. The collision integral of this model is written down as

$$Q_S(f f_*) = \frac{P}{\mu} \left\{ f^M \left[1 + \frac{2m}{15n(k_B T)^2} \mathbf{q} \cdot \mathbf{V} \left(\frac{mV^2}{2k_B T} - \frac{5}{2} \right) \right] - f(t, \mathbf{r}, \mathbf{v}) \right\}. \quad (14)$$

This model has another shortcoming: the H-theorem can be proved only for the linearized S-model. In the non-linear form one can neither prove nor disprove the theorem. This property sometimes leads to non-physical results. However, the linearized S-model works very well for non-isothermal flows.

A critical analysis and comparison of results based on the exact Boltzmann equation, BGK model, and S-model are given in the review paper [20]. From this analysis we may conclude that the model equations significantly reduce the computational efforts. However, to obtain reliable results one should apply an appropriate model equation. If a gas flow is isothermal and the heat transfer is not important the BGK equation is the most suitable model equation. If a gas flow is non-isothermal it is better to apply the S-model.

3 Methods of computation in the transition regime

The discrete velocity method is the most used one. A set of values of the velocity \mathbf{v}_i is chosen. The collision integral is expressed *via* the values $f_i(t, \mathbf{r}) = f(t, \mathbf{r}, \mathbf{v}_i)$. Thus, the integro-differential Boltzmann equation is replaced by a system of differential equations for the functions $f_i(t, \mathbf{r})$. The differential equations can be solved numerically by a finite difference method. Then, the distribution function moments are calculated using some quadrature. Details of the method are given by Kogan [15] (Section 3.13) and elsewhere [20,23].

The Direct Simulation Monte Carlo (DSMC) method is also widely used. The region of the gas flow is divided into a network of cells. The dimensions of the cells must be such that the change in flow properties across each cell is small. The time is advanced in discrete steps of magnitude Δt , such that Δt is small compared with the mean time between two successive collisions. The molecular motion and intermolecular collision are uncoupled over the small time interval Δt by the repetition of the following procedures:

- The molecules are moved through the distance determined by their velocities and Δt . If the trajectory passes the boundary a simulation of the gas–surface interaction is performed in accordance with a given law. New molecules are generated at boundaries across which there is an inward flux.
- A representative number of collisions appropriate to Δt and the number of molecules in the cell is computed. The pre-collision velocities of the molecules involved in the collision are replaced by the post-collision values in accordance with a given law of the intermolecular interaction.

After a sufficient number of repetitions we may calculate any moment of the distribution function. Details of the method are given in the books by Bird [11,12].

4 Typical problems of rarefied gas dynamics

4.1 Velocity slip and temperature jump coefficients

A moderate gas rarefaction can be taken into account via the so-called velocity slip and temperature jump boundary conditions. It means that the bulk velocity is not equal to zero on the wall, but its tangential component u_y near the wall is proportional to its normal gradient

$$u_y = \sigma_p \ell \frac{\partial u_y}{\partial x} , \quad \text{at } x=0 , \quad (15)$$

where σ_p is the viscous slip coefficient, x, y are a reference frame with the origin at the surface, x is the normal coordinate, while y is the tangential one.

A gas flow also can be induced by a tangential temperature gradient. In this case the tangential velocity is proportional to the temperature gradient

$$u_y = \sigma_t \frac{\mu}{\varrho} \frac{\partial \ln T}{\partial y} , \quad \text{at } x=0 , \quad (16)$$

where σ_t is the thermal slip coefficient and ϱ is the local mass density.

The temperature jump condition on a solid surface reads as

$$T_g = T_w + \zeta_t \ell \frac{\partial T_g}{\partial x} , \quad \text{at } x=0 , \quad (17)$$

where T_g is the gas temperature near the surface and ζ_t is the temperature jump coefficient. Physically, Eq.(17) means that the temperature of the gas is not equal to that of the wall, but there is a discontinuity (jump) of the temperature.

The detailed technique of calculations of the slip and jump coefficients on the basis of the kinetic equation and their numerical values can be found in Refs. [20,24–27]. The values recommended in practical calculations are as follows

$$\sigma_p = 1.018 , \quad \sigma_t = 1.175 , \quad \zeta_t = 1.954 . \quad (18)$$

These values were obtained under an assumption of the diffuse scattering of gaseous particles on the surface. In most practical situations this assumption is fulfilled. Only in some special situations can the deviation from the diffuse scattering be significant, see, for example, Ref. [28].

Numerical data of the velocity slip and temperature jump coefficients for gaseous mixtures can be found in Refs. [29–32].

4.2 Gas flow through long capillaries

Consider a monoatomic rarefied gas flowing through a long tube due to small longitudinal gradients of pressure P and temperature T denoted as

$$\xi_p = \frac{a}{P} \frac{dP}{dx} , \quad \xi_t = \frac{a}{T} \frac{dT}{dx} , \quad (19)$$

respectively. Here, x is the longitudinal coordinate coinciding with the tube axis, a is the tube radius. We assume that the tube is so long that the end effects can be neglected and the flow is considered to be one-dimensional.

The mass flow rate \dot{M} through the tube can be calculated as

$$\dot{M} = \frac{\pi a^2 P}{v_m} (-G_p \xi_p + G_t \xi_t) , \quad (20)$$

where G_p and G_t are reduced flow rates calculated on the basis of the kinetic equation. They are determined by the rarefaction parameter δ . Note that a temperature gradient causes a gas flow of rarefied gas, i.e., the gas flows from a cold region to a hot one. This phenomenon is called *thermal*

creep. The details of calculations of the coefficients G_p and G_T and recommended data can be found in Ref. [20]. Here, just the main results corresponding to diffuse scattering will be given.

In the free molecular regime, i.e., at $\delta=0$, the coefficients G_p and G_T can be calculated analytically

$$G_p = \frac{8}{3\sqrt{\pi}} , \quad G_T = \frac{1}{2}G_p . \quad (21)$$

Applying the Navier–Stokes equation with the slip boundary conditions (15) and (16) the coefficients G_p and G_T are obtained as

$$G_p = \frac{\delta}{4} + \sigma_p , \quad G_T = \frac{\sigma_T}{\delta} . \quad (22)$$

These expressions are valid near the hydrodynamic regime, i.e. $\delta \gg 1$.

Table 1: Reduced flow rates G_p and G_T vs δ , Ref. [33]

δ	G_p	G_T	δ	G_p	G_T
0.001	1.5008	0.7486	1.0	1.4758	0.3959
0.01	1.4800	0.7243	1.4	1.5550	0.3514
0.02	1.4636	0.7042	2.0	1.6799	0.3016
0.05	1.4339	0.6637	5.0	2.3666	0.1752
0.1	1.4101	0.6210	10.0	3.5749	0.1014
0.2	1.3911	0.5675	20.0	6.0492	0.05426
0.5	1.4011	0.4779	50.0	13.495	0.02212

In the transition regime the kinetic equation (11) with the S-model (14) is applied. The coefficients G_p and G_T for some intermediate values of δ obtained in Ref. [33] are given in Table 1.

If the drops of pressure and temperature are large, then the technique elaborated in the works [33–35] must be used. The data on the coefficients G_p and G_T for a rectangular channel are given in Refs. [36,37]. The method of calculations of mass flow rate through a tube of variable diameter is given in Ref. [38]. A methodology of calculation of gaseous mixtures flowing through long tubes and channels is described in Refs. [39–43].

4.3 Orifice flow

Consider an orifice in an infinitely thin partition that separates two semi-infinite reservoirs. One of them contains a monoatomic gas at a pressure P_0 . The other reservoir is maintained at a smaller pressure $P_1 < P_0$. The mass flow rate \dot{M} through the orifice is determined by the rarefaction parameter δ with reference to the pressure P_0 and by the pressure ratio P_1/P_0 . It is usual to use the reduced flow rate defined as

$$W = \frac{\dot{M}}{\dot{M}_0} , \quad \dot{M}_0 = \frac{\sqrt{\pi}a^2}{v_m} P_0 , \quad (23)$$

where \dot{M}_0 corresponds to the mass flow rate into vacuum, i.e., at $P_1 = 0$, in the free molecular regime, i.e., at $\delta = 0$. If $P_1 \neq 0$ then there are two opposite flows through the orifice in the free molecular regime. Since they are independent the total flow rate is given as

$$W = 1 - \frac{P_0}{P_1} . \quad (24)$$

The papers [44,45] report numerical data on the flow rate W , where the problem was solved by the DSMC method. The number of particles fluctuates during the calculations, but it was maintained in the interval from 5×10^6 to 15×10^6 . The number of samples was sufficient to guarantee the statistical scattering of the flow rate with 1%.

The dependences of the reduced flow rate W on the rarefaction parameter δ for $P_1/P_0 = 0; 0.1; 0.5$ and 0.9 are represented in Fig. 1. It can be seen that the numerical results are in a good agreement with the corresponding experimental data [46,47]. For $\delta > 100$ the variation of the flow rate is within the numerical accuracy for all pressure ratios considered here. Therefore the data presented here cover the whole range of the gas rarefaction δ . In the free-molecular regime ($\delta = 0$), the numerical value of W tends to its theoretical expression (24). In many practical applications it is necessary to know the correction to this limit value related to the intermolecular collisions. Near the free-molecular regime the flow rate W can be written as

$$W = \left(1 - \frac{P_1}{P_0}\right)(1 + A\delta) \quad \text{at } \delta < 1 . \quad (25)$$

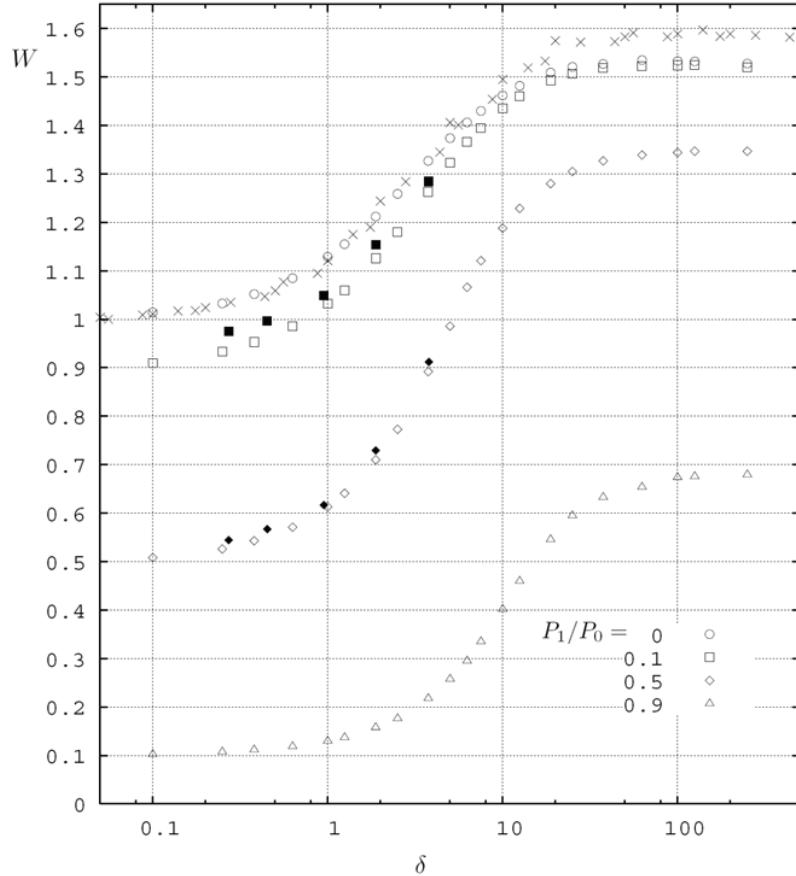


Fig. 1: Reduced flow rate W vs rarefaction parameter δ : open symbol—DSMC simulation [44,45]; filled symbols—experimental data from Ref. [46]; crosses—experimental data from Ref. [47]

The values of the constant A are 0.13; 0.15; 0.23; and 0.31 for the pressure ratio $P_1/P_0 = 0$; 0.1; 0.5; and 0.9, respectively. These values were obtained by the least-squares method on the basis of the numerical results.

5 Modelling of Holweck pump

A Holweck pump is composed of two coaxial cylinders. One of them has grooves in a spiral form and the other is smooth. A rotation of the smooth cylinder causes the gas flow, i.e., the pumping effect. So, in the general case the gas flow through such a pump is three-dimensional. To reduce the computational efforts we consider a two-dimensional flow, i.e., we shall neglect the groove curvature and the end effects. More exactly, we consider a plane surface having several grooves regularly distributed over it as shown in Fig. 2(a). Another surface, which is smooth, moves in the direction ξ over the grooved surface and causes a gas flow in the direction η . The cross-section of one groove, i.e., AA, is presented in Fig. 2(b).

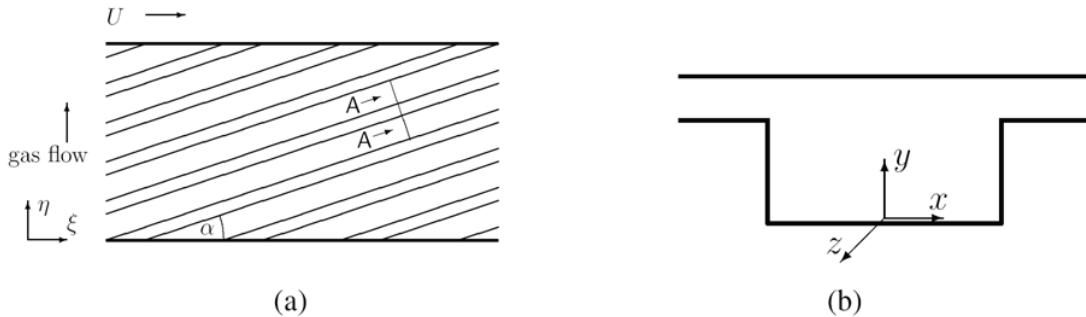


Fig. 2: Scheme of pump and cross-section of groove AA

The solution of the problems is divided into two stages. In the first stage we solve four independent problems over the whole range of the gas rarefaction:

- i) longitudinal Couette flow, i.e., the gas flow due to a surface motion along the axis z . The coordinate system (x, y, z) is shown in Fig. 2(b);
- ii) longitudinal Poiseuille flow, i.e., the gas flow caused by a pressure gradient along the axis z ;
- iii) transversal Couette flow, i.e., the gas flow due to a surface motion along the axis x ;
- iv) transversal Poiseuille flow, i.e., the gas flow caused by a pressure drop in the direction x through a pair of grooves and ridges. The solution of these four problems is determined by the groove and ridge sizes and by the rarefaction parameter δ .

In the second stage a linear superposition of the four solutions obtained previously is realized in accordance with the methodology described in Refs. [33–37]. This stage does not require much computational effort and allows us easily to change many parameters such as groove inclination, fore vacuum and high vacuum pressures, angular velocity of rotating cylinder, species of gas, temperature of the gas, etc.

Applying the present approach, the compression ratio and pumping speed were calculated. The results related to the compression ratio are shown in Fig. 3, from which it can be seen that the numerical results are in good agreement with the experimental data. The details of the numerical calculations and the measurements can be found in Ref. [48].

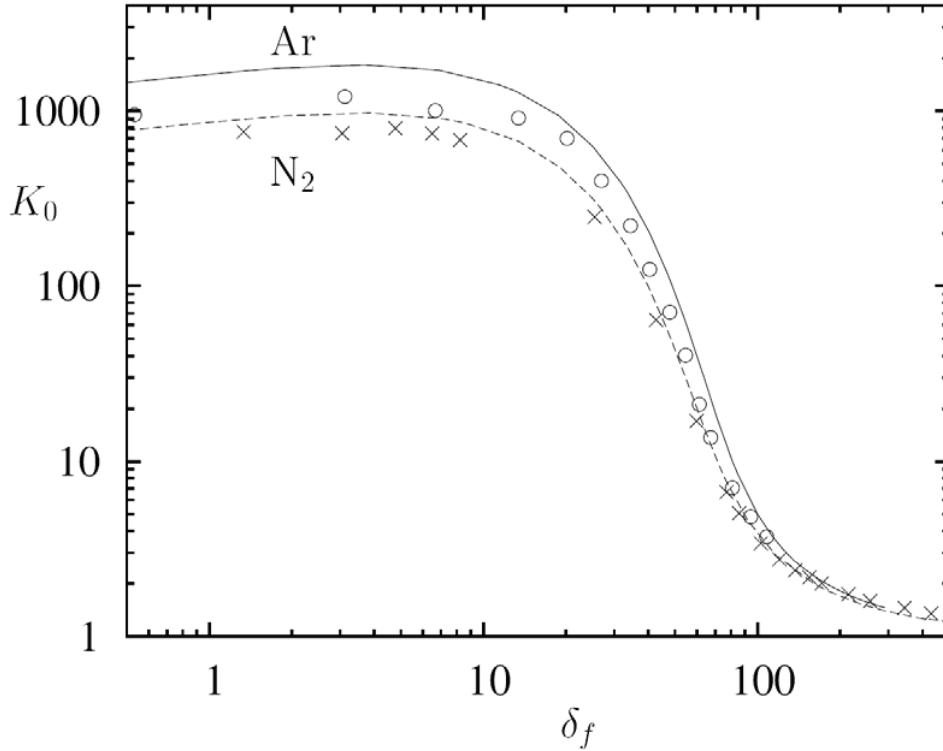


Fig. 3: Limit compression pressure ratio K_0 vs fore vacuum rarefaction δ_f : lines—*theoretical results*; symbols—*experimental data*

6 Summary of recent theoretical results

- Velocity slip coefficients for a single gas Refs. [20,27,49–51].
- Velocity slip coefficients for gaseous mixtures Refs. [29–31,52,53].
- Temperature jump coefficient for a single gas Refs. [27,54–56].
- Temperature jump coefficient for gaseous mixtures Refs. [32,57–59].
- Single gas flows through long tubes and channels over the whole range of the gas rarefaction Refs. [20,36–38,60–64].
- Mixture gas flows through long tubes and channels over the whole range of the gas rarefaction Refs. [39–43,65].
- Gas flow through orifices and slits Refs. [44,45,66–68].
- Couette flow of a single gas over the whole range of the gas rarefaction Refs. [69–74].
- Couette flow of mixtures over the whole range of the gas rarefaction Refs. [75–77].
- Modelling of vacuum pumps over the whole range of the gas rarefaction Refs. [48].

Some numerical calculations of the mass flow rate \dot{M} through tubes, channels and orifices can be carried out on-line on the site <http://fisica.ufpr.br/sharipov>.

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