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# Rarefied gas flow through a diverging conical pipe into vacuum

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ABSTRACT

The paper is devoted to the study of a rarefied gas flow through a finite length conical pipe into vacuum. The problem is solved in the complete geometrical setup, which included not only the pipe, but also high- and low-pressure reservoirs. The analysis is based on the direct numerical solution of the Boltzmann kinetic equation with the S-model collision integral in three space dimensions. The method of the solution is based on the recent implicit total variation diminishing (TVD) method on unstructured spatial meshes. It is conservative with respect to the collision integral and work across all flow regimes. The results are provided for various ratios of the outlet and inlet diameters, pipe's lengths and Knudsen numbers. The computed flow rates are compared with the case of the circular pipe of constant radius as well as an approximate method for very long pipes. The influence of the pipe geometry on the flow field is also examined. The presented results can be used as a benchmark for calculations by other methods and codes.



## 1. Introduction

A rarefied gas flow through a finite-length pipe or capillary into vacuum is a popular problem in the rarefied gas dynamics [1,2]. The majority of the computational studies deal with the flow through a circular pipe with the constant cross sectional area. Examples include the Direct Simulation Monte Carlo (DSMC) studies for short tubes [3] and deterministic studies for short, moderate and long pipes [4–6]. A comparison of the results from different approaches with experimental data for the short tube can be found in [7].

It is important that all cited studies analyse the problem in the complete setup, which includes not only the pipe, but also high and lower pressure reservoirs, rather than a simplified formulation, in which the reservoirs are replaced by the evaporation and/or condensation boundary conditions at the pipe's ends [8,9]. It appears that the such a setup, albeit in the planar case, was first considered in [10,11]. The influence of the geometrical setup on the flow rate for circular pipe flow was investigated in detail in [5,6].

However, there seem to be no results in the literature for the rarefied gas flow into vacuum through a conical pipe. If one is only interested in the mass flow rate and density distribution along the axial line of the pipe, an approximate method [12,13] can be used. However, it is valid for very long pipes only, for which the ratio of both inlet and outlet radii to the length is small. Moreover, the analysis presented in [4–6] shows that for small Knudsen numbers this condition along is not enough and that the product of the Knudsen number and the pipe length has to be large for the approximate method to be applicable.

The present work is devoted to the deterministic kinetic study of the rarefied gas flow into vacuum through moderate and long conical pipes and can thus be viewed as a continuation of [4–6]. The results are based on the numerical solution of the S-model kinetic equation [14–16] using the recent three-dimensional finite-volume method [17,18]. The computations are carried out for various length and outlet to inlet diameter ratios across the range of rarefaction conditions from the free-molecular to nearly continuum flow regimes. Numerical results for the mass flow rate and distribution of macroscopic macroparameters are presented in the broad range of Knudsen numbers, pipe's length and outlet to inlet radii ratios. The influence of the pipe geometry on the flow rate and distribution of macroscopic quantities is examined.

## 2. Formulation of the problem

The formulation of the problem is an extension of [3–6]. Consider a rarefied gas flow through a conical pipe of length $L$,

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connecting two infinitely large reservoirs (volumes) filled with the same monatomic gas. The inlet and outlet radii of the pipe are denoted as a$R_1$, $R_2$, respectively. The gas in the left reservoir is kept under pressure $p_1$ and temperature $T_1$, whereas in the right reservoir the pressure is $p_2$ is so low that it can be regarded as equal to zero. It is assumed that reservoirs' volumes are significantly larger than the pipe volume and the gas is in equilibrium far away from the ends of the latter. The real form and size of the reservoirs are thus of no importance. The complete accommodation of momentum and energy of molecules occurs at the pipe surface, which is kept under the same constant temperature $T_1$.

Let us introduce a Cartesian coordinate system ($x$,$y$,$z$) with the centre located in the centre of the inlet section of the pipe $x = y = z = 0$ and the $Oz$ axes directed along the tube. A steady three-dimensional state of the rarefied gas is determined by the velocity distribution function $f(\boldsymbol{x},\boldsymbol{\xi})$, where $\boldsymbol{x}=(x,y,z)$ is the spatial coordinate, $\boldsymbol{\xi}=(\xi_x,\xi_y,\xi_z)$ is the molecular velocity vector. For the rest of the paper, the non-dimensional formulation is used, in which the spatial coordinates $\boldsymbol{x}$, mean velocity $\boldsymbol{u} = (u_1,u_2,u_3) = (u_x,u_y,u_z)$, number density $n$, temperature $T$, heat flux vector $\boldsymbol{q} = (q_1,q_2,q_3)$, viscosity $\mu$ and distribution function $f$ are scaled using the following quantities:

$$R_1, \quad \beta, \quad n_1, \quad T_1, \quad mn_1\beta^3, \quad \mu_1 = \mu(T_1), \quad n_1\beta^{-3}, \tag{1}$$

where $\beta = \sqrt{2kT_1/m}$; $n_1 = p_1/kT_1$ is the number density in the left reservoir; $m$ is the mass of a molecule, $k$ is the Boltzmann constant. Below, the non-dimensional variables are denoted by the same letters as the dimensional ones.

The distribution function $f$ is assumed to satisfy the S-model kinetic equation [14–16], which in the non-dimensional variables takes the form

$$\begin{gathered}
\xi_x\frac{\partial f}{\partial x}+\xi_y\frac{\partial f}{\partial y}+\xi_z\frac{\partial f}{\partial z} = \nu\left(f^{(S)}-f\right), \quad \nu = \frac{nT}{\mu}\delta_1, \quad \delta_1 = \frac{R_1 p_1}{\mu_1\beta}, \\
f^{(S)} = f_M\left[1+\frac{4}{5}(1-\mathrm{Pr})S_\alpha c_\alpha\left(c^2-\frac{5}{2}\right)\right], \quad f_M = \frac{n}{(\pi T)^{3/2}}\exp\left(-c^2\right), \\
v_i = \xi_i - u_i, \quad c_i = \frac{v_i}{\sqrt{T}}, \quad S_i = \frac{2q_i}{nT^{3/2}}, \quad c^2 = c_\alpha c_\alpha.
\end{gathered} \tag{2}$$

Here $\delta_1$ is the so-called rarefaction parameter, which is inversely proportional to the Knudsen number. Summation over repeated Greek indices is assumed. For a monatomic gas the Prandtl number $Pr = 2/3$. The non-dimensional macroscopic quantities are defined as the integrals of the velocity distribution function with respect to the molecular velocity:

$$\begin{gathered}
\left(n, n\boldsymbol{u}, n\left(\tfrac{3}{2}T+u^2\right), \boldsymbol{q}\right) = \int\left(1,\boldsymbol{\xi},\xi^2,\frac{1}{2}\boldsymbol{v}v^2\right)f d\boldsymbol{\xi}, \\
u^2 = u_\alpha u_\alpha, \quad v^2 = v_\alpha v_\alpha, \quad \xi^2 = \xi_\alpha\xi_\alpha, \quad p = nT.
\end{gathered} \tag{3}$$

The kinetic equation (2) has to be augmented with the boundary conditions on the pipe and reservoir walls. Let $\boldsymbol{n} = (n_x,n_y,n_y)$ be the unit normal vector to a boundary surface, pointing inside the flow domain. The condition of diffuse molecular scattering on the pipe surface with complete thermal accommodation to the non-dimensional surface temperature $T_1 \equiv 1$ is given by:

$$f(\boldsymbol{x},\boldsymbol{\xi}) = f_w = \frac{n_w}{(\pi)^{3/2}}\exp\left(-\xi^2\right), \quad \xi_n = (\boldsymbol{\xi},\mathbf{n}) > 0. \tag{4}$$

The density of reflected molecules $n_w$ is found from the impermeability condition stating that the mass flux through the walls is equal to zero:

$$n_w = N_i/N_r, \quad N_i = -\int\limits_{\xi_n<0}\xi_n f d\boldsymbol{\xi}, \quad N_r = \int\limits_{\xi_n>0}\xi_n\frac{1}{(\pi)^{3/2}}\exp\left(-\xi^2\right)d\boldsymbol{\xi}. \tag{5}$$

The same condition (5) is used for the parts of the reservoir walls directly adjacent to the pipe; these are located at $z = 0,L$. At the rest of the reservoir wall the distribution function of the incoming molecules $\xi_n > 0$ is specified as

$$\begin{gathered}
f = f_1 = \frac{n_1}{(\pi)^{3/2}}\exp\left(-\xi^2\right), \quad z \le 0, \\
f = 0, z \ge L.
\end{gathered} \tag{6}$$

The boundary condition (6) is essentially an evaporation boundary condition for the molecules entering the flow domain and is meant to model the indefinitely large reservoirs.

The main computed characteristic of the flow is the mass flow rate $M$, which in the non-dimensional variables is given by an integral over the cross section:

$$\dot{M} = \int\limits_{A(z)}\rho(x,y,z)u_z(x,y,z)dxdy. \tag{7}$$

Here $A(z)$ is the cross-sectional area at the position $z$ along the pipe. Note, that mass flow rate $\dot{M}$ is constant along the pipe.

## 3. Details of the calculations

### 3.1. Method of solution

The formulated problem possesses the cylindrical symmetry and can thus be solved in the cylindrical coordinate system. However, our experience suggests that the direct three-dimensional solution methods are more accurate and efficient than the approaches based on the axisymmetrical formulations. In the present work the steady-state solution of the problem is found by means of an implicit time-marching algorithm for the kinetic equation (2) in the non-stationary form. The numerical method consists of the high-order accurate advection scheme applicable to hybrid unstructured meshes, conservative procedure for the calculation of the model collision integral and one-step implicit time evolution for fast steady-state convergence. As a result, it allows efficient calculation of rarefied flows in the wide range of degrees of rarefaction in arbitrary geometries.

A summary of the numerical method can be found in [18], see also [17,19] and references therein. The infinite domain of integration in the molecular velocity space is replaced by a finite computational domain. The velocity distribution function is then defined in centres of the resulting velocity mesh. The kinetic equation (2) is replaced by a system of time-dependent advection equations; each equation corresponds to a specific point from the velocity mesh. The macroscopic quantities at any spatial location are computed in such a way as to satisfy not only conservation laws, but also correct relaxation of the heat flux vector. Assuming the model collision integral is known, the equations are solved using an implicit TVD method, which is second-order accurate in space. An LU-SGS type time evolution procedure on unstructured meshes [20] is used to allow for faster steady-state convergence.

For large-scale problems such as the ones reported here the calculations are carried out on modern high-performance clusters using Message Passing Interface (MPI). In the present work the HPC "Lomonosov" of Lomonosov Moscow State University, Russia, was utilized. The runs were performed on up to 160 cores of the