Numerical study of unsteady rarefied gas flow through an orifice

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ABSTRACT

Transient flow of rarefied gas through an orifice caused by various pressure ratios between the reservoirs is investigated for a wide range of the gas rarefaction, varying from the free molecular to continuum regime. The problem is studied on the basis of the numerical solution of unsteady S-model kinetic equation. It is found that the mass flow rate takes from 2.35 to 30.37 characteristic times, which is defined by orifice radius over the most probable molecular speed, to reach its steady state value. The time of steady flow establishment and the steady state distribution of the flow parameters are compared with previously reported data obtained by the Direct Simulation Monte Carlo (DSMC) method. A simple fitting expression is proposed for the approximation of the mass flow rate evolution in time.

1. Introduction

The nonequilibrium flows of gases appear in different technological domains like the vacuum equipment, high altitude aerodynamics and in a relatively new field as the microelectromechanical systems (MEMS). The deviation of a gas from its local equilibrium state can be characterized by the Knudsen number, which present the ratio between the molecular mean free path and the characteristic length of the problem. For the relatively large values of the Knudsen number the classical continuum approach fails to describe the gas behavior and the kinetic equations, like the Boltzmann equation or model kinetic equations, must be solved to simulate the gas flows.

The gas flow through a thin orifice is a problem of a large practical interest for the design of the vacuum equipment, space or the microfluidic applications. The under-expanded jets through the orifices are predominately used by particle analyzer systems to separate and isolate molecules, ions of substances for analyzing their physical and chemical properties. The time dependent characteristics of these jets are important for the investigation of the response time of the vacuum gauges developed for the measurements of the rapid pressure changes [1].

The steady state flows through the orifice, slit and short tube have been successfully studied applying the DSMC method and the kinetic equations [2–9]. However, only a few results on the transient rarefied flows through an orifice [10], a short tube [11], a long tube [12] or a slit [13] may be found in open literature. The flow conditions in [10] are limited to high and moderate Mach number owing to significant statical noise of DSMC method at low Mach number. The authors of [1] also studied experimentally and numerically the transient gas flow, but between two tanks of the fixed volumes. The rapid high amplitude pressure changings in time are examined and their characteristic time was found to be of the order of few seconds.

The aim of this work is to analyze the transient properties of gas flow through an orifice induced by various values of the pressure ratio over a broad range of gas rarefaction. The unsteady nonlinear S-model kinetic equation is solved numerically by Discrete Velocity Method (DVM) to obtain the mass flow rate and macroscopic parameters as a function of time. The time to reach the steady state conditions for the mass flow rate is also estimated. An empirical expression for evaluation of time-dependent mass flow rate is proposed.

2. Problem formulation

Consider an orifice of radius R_0 contained in an infinitesimally thin wall, which isolates two infinite reservoirs. Both the upstream and downstream reservoirs are filled with a monatomic gas but maintained at different pressures p_0 and p_1, respectively, with $p_0 > p_1$. The temperatures of the wall and of the gas in the reservoirs are equal to T_0. At time $t = 0$, the orifice is opened instantly and the gas starts to flow from the upstream reservoir to the downstream one.

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Let us introduce a cylindrical coordinate system (r',ϑ,z') with the origin positioned at the center of the orifice and the Oz' axis directed along the axis of the reservoirs (see the lateral section shown in Fig. 1). We assume that the flow is cylindrically symmetric and does not depend on the angle ϑ and therefore the problem may be considered as two dimensional in the physical space with the position vector $s' = (r',z')$.

The gas-surface interaction has a very small impact on an orifice flow [14]; consequently, this flow is governed by two principal parameters: the pressure ratio p_1/p_0 and gas rarefaction δ determined as

$$\delta = \frac{R_0 p_0}{\mu_0 v_0}, \quad v_0 = \sqrt{\frac{2kT_0}{m}}, \tag{1}$$

where μ_0 is the viscosity coefficient at the temperature T_0, v_0 is the most probable molecular speed at the same temperature; m is the molecular mass of the gas; k is the Boltzmann constant. It is to note that the gas rarefaction parameter is inversely proportional to the Knudsen number; i.e., when δ varies from 0 to ∞, the flow regime changes from the free molecular to the hydrodynamic regime.

It is convenient to define the characteristic time t_0 of the flow as follows

$$t_0 = \frac{R_0}{v_0}. \tag{2}$$

The unsteady S-model kinetic equation [15] is used to simulate the transient rarefied gas flow through the orifice. The conservative formulation of this equation [16,17] is implemented

$$\frac{\partial}{\partial t'}(r'f') + \frac{\partial}{\partial r'}(r'f'v_p\cos\varphi) - \frac{\partial}{\partial\varphi}(f'v_p\sin\varphi) + \frac{\partial}{\partial z'}(r'f'v_z)$$
$$= r'\nu'(f^{S'} - f'), \tag{3}$$

The main unknown is the molecular velocity distribution function $f'(t',s',v)$, $v = (v_p\cos\varphi, v_p\sin\varphi, v_z)$ is the molecular velocity vector representing the molecular velocity space. The polar coordinates are introduced in a plane (v_r, v_ϑ) and v_p, φ are the magnitude and orientation of the molecular velocity vector in this (v_r, v_ϑ) plane. The molecular collision frequency ν' is supposed to be independent on the molecular velocity and can be evaluated [15] by

$$\nu' = \frac{p'}{\mu'}. \tag{4}$$

The equilibrium distribution function $f^{S'}$ [15] in eq. (3) is defined in as

$$f^{S'} = f^{M'}\left[1 + \frac{2m\boldsymbol{V}\boldsymbol{q}'}{15n'(kT')^2}\left(\frac{mV^2}{2kT'} - \frac{5}{2}\right)\right],$$
$$f^{M'} = n'\left(\frac{m}{2\pi kT'}\right)^{3/2}\exp\left(-\frac{mV^2}{2kT'}\right), \tag{5}$$

where $f^{M'}$ is the local Maxwellian distribution function, $\boldsymbol{V} = v - \boldsymbol{u}'$ is the peculiar velocity vector, $\boldsymbol{u}' = (u_r', 0, u_z')$ is the bulk velocity vector, $\boldsymbol{q}' = (q_r', 0, q_z')$ is the heat flux vector, n' is the gas numerical density.

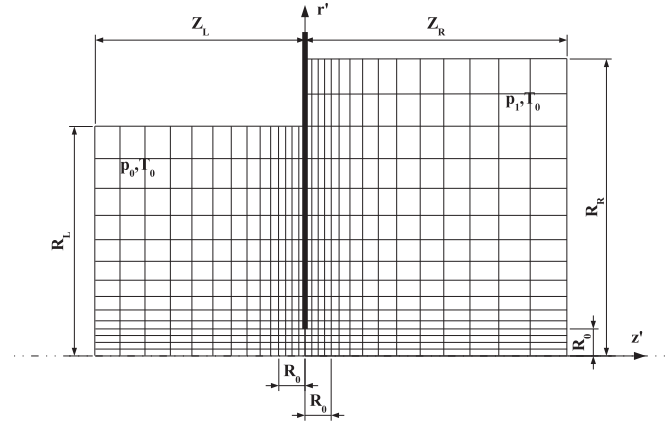**Fig. 1.** Lateral section and computational domain of the flow configuration.

It is useful to define the dimensionless variables as follows

$$t = \frac{t'}{t_0}, \boldsymbol{s} = \frac{s'}{R_0}, \boldsymbol{c} = \frac{v}{v_0}, \boldsymbol{u} = \frac{\boldsymbol{u}'}{v_0}, n = \frac{n'}{n_0},$$
$$T = \frac{T'}{T_0}, p = \frac{p'}{p_0}, \boldsymbol{q} = \frac{\boldsymbol{q}'}{p_0 v_0}, \mu = \frac{\mu'}{\mu_0}, f = \frac{f'v_0^3}{n_0}, \tag{6}$$

with the help of the state equation $p_0 = n_0 kT_0$. In relations (6), the dimensionless molecular velocity vector $\boldsymbol{c}$ is equal to $(c_p\cos\varphi, c_p\sin\varphi, c_z)$.

In this study, the inverse power law potential is employed as the molecular interaction potential; therefore, viscosity can be calculated by power law temperature dependence as

$$\mu = T^\omega, \tag{7}$$

where ω is the viscosity index, which is equal to 0.5 for Hard Sphere model and 1 for the Maxwell model [18].

Incorporating dimensionless quantities (6) into S-model kinetic equation (3), the dimensionless conservative form of governing equation is obtained

$$\frac{\partial}{\partial t}(rf) + \frac{\partial}{\partial r}(rfc_p\cos\varphi) - \frac{\partial}{\partial\varphi}(fc_p\sin\varphi) + \frac{\partial}{\partial z}(rfc_z)$$
$$= r\delta n T^{1-\omega}(f^S - f). \tag{8}$$

The above equation is subjected to the following boundary conditions. The distribution function of outgoing from the axis molecules f^+ is calculated from the distribution function of incoming to the axis molecules f^- taking into account the axisymmetric condition as

$$f_{r=0}^+(t, z, r, \varphi, c_p, c_z) = f_{r=0}^-(t, z, r, \pi - \varphi, c_p, c_z), \tag{9}$$

where the superscripts $+$ and $-$ refer to the outgoing and incoming molecules, respectively. It is supposed that the computational domain is large enough for obtaining the equilibrium far-field. Hence, we assume that the molecules entering the computational

Table 1
Numerical grid parameters.

Phase space	Reservoir	Total number of points
Physical space z,r	Left	$N_O = 40$ $N_{zl} \times N_{rl} = 96 \times 96$
	Right	$N_{zr} \times N_{rr} = 101 \times 101$
Molecular velocity space φ, c_p, c_z	Left & right	$N_\varphi \times N_{cp} \times N_{cz} = 40 \times 16 \times 16$