Simulation of non-equilibrium gas kinetic processes in the multitube Knudsen pump on the basis of the Boltzmann equation

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A periodic system of multitube micropumps with pumping down based on the Knudsen effect is simulated in this work. The simulation is performed on an unstructured mesh. The Boltzmann equation is solved, and the advection and relaxation processes are simulated separately. The differential equation for advection is approximated with the first-order discrete difference scheme, and the collision integral is calculated with the projection method. The dependences of pump-down on the Knudsen number and temperature gradient were obtained from supercomputer computations. Data on the pumping rate were also obtained.

Introduction

The Knudsen pump [1,2] is one of the systems that implements a non-equilibrium gas flow. Such flows are not described by continuum mechanics; the statistical gas distribution function shall be used for their description. The following two approaches are widely used for simulation of such flows: the Monte Carlo method [3], and numerical solution of the Boltzmann equation. The Monte Carlo method is ill-suited to the study of slow processes due to the high statistical noise $O(N^{1/2})$. In this work the non-equilibrium gas flow is simulated with the conservative projection method of solving the Boltzmann equation on an unstructured spatial mesh. Promising materials are described in the papers [4-8], relaxation processes in such materials are of particular interest [9-12] and surface effects [13-14].

Since the distribution function depends on six variables – three coordinates and three velocities – simulation of such problems requires much memory and takes much time. Therefore, parallel computations were performed on a supercomputer using the OpenMPI library. Various Knudsen pumps have been studied with these methods before [15, 16]. The previously used simulation methods were summarized in this work, and computations for a more advanced pump model were carried out for the larger range of parameters.
1. System schematic

![Figure 1](image)

**Figure 1.** Side view and wall temperature (a) and front view (b)

The object of computations is a periodic system of multitube micropumps described in [17]. A quarter of one pump is shown in Figure 1. Each pump comprises two vessels connected by 18 thin tubes. On the side of the right vessel, the tubes combine into a large tube that goes to the vessel. The tube wall temperature depends on the coordinate and changes from $T_1$ to $T_2$ as shown in Figure 1. An important parameter of the system is the $T_2/T_1$ ratio. The pumped gas is argon.

The value that allows assessing operation of the pump is pump-down defined as the ratio between the mean pressures in the vessels

$$k = \frac{p_1}{p_2}$$

2. Kinetic theory

There is solved the Boltzmann equation

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \int_0^{2\pi} \int_0^1 \left( f' f'_1 - f f_1 \right) gb db d\phi d_3 \xi_1$$

For simulation of the flow, it is convenient to pass on to dimensionless variables

$$b^* = \frac{b}{\sigma_{\text{eff}}}, \quad x^* = \frac{x}{\lambda}, \quad t^* = \frac{t}{t_0}, \quad \xi^* = \frac{\xi}{\xi_0}, \quad f^* = \frac{f}{n_0 \xi_0^{-3}},$$

where

$$\xi_0 = \sqrt{\frac{kT_1}{m_0}}, \quad t_0 = \frac{\lambda}{\xi_0}$$

The free path length is taken as the unit of the system linear dimension

$$\lambda = \frac{1}{\sqrt{2\pi} \sigma_{\text{eff}} n_0}$$

(1)

The equation becomes

$$\frac{\partial f^*}{\partial t^*} + \xi^* \frac{\partial f^*}{\partial x^*} = \frac{1}{\sqrt{2\pi}} f^*(f^*)$$

For this form, parameters are set, and the equation is solved on a computer cluster. An important dimensionless parameter that defines the gas behavior is the Knudsen number...
The Knudsen number can be changed either by changing \( n_0 \) and thus \( \lambda \), or by scaling the system. The both approaches were applied.

3. Mesh space

Projection of the distribution function on the velocity mesh and coordinate mesh spaces is used for its numerical representation at every instant.

![Coordinate mesh](image)

**Figure 2.** Coordinate mesh

The coordinate mesh is irregular and in general case may consist of arbitrary polyhedrons. The mesh is generated with the GMSH software [19] according to the specified geometrical model and algorithm. The resulting mesh consists of tetrahedrons inside the vessels and triangular prisms inside the tubes.

The velocity mesh is uniform cubic with the step size \( \Delta \xi \). The velocity space is infinite, hence its mesh approximation contains only those velocities that are less than certain velocity \( \xi_{\text{max}} \). The following parameters were used in the computations:

\[
\Delta \xi = 0.24 \xi_{\text{max}}, \quad \xi_{\text{max}} = 4.8\sqrt{kT_1/m_0}
\]

4. Initial conditions

Initially, gas molecules have Maxwellian velocity distribution, the concentration is constant and equals \( n_0 \), and the gas temperature is \( T_1 \)

\[
f(x, \xi, 0) = \left( \frac{m_0}{2\pi k T_1} \right)^{\frac{3}{2}} n_0 \exp\left( -\frac{m_0 \xi^2}{2k T_1} \right)
\]

In the discrete approximation, the distribution is normalized with a different factor so that the total concentration remains equal to \( n_0 \)
\[ f(x_i, \xi_j, 0) = \frac{n_i}{S} \exp\left( -\frac{m_b \xi_j^2}{2kT_i} \right) \]

\[ S = \sum_k \exp\left( -\frac{m_b \xi_k^2}{2T_i} \right) \]

5. Boundary conditions
Two boundary conditions were implemented: diffuse boundary condition with total accommodation, and boundary condition of complete mirror reflection.

5.1. Diffuse boundary condition
A diffuse boundary condition simulates the vessel wall with a specified temperature. It is assumed that upon collision with boundary molecules come to thermodynamic equilibrium with the wall and exit having the Maxwellian distribution

\[ f^+(\xi_j) = \frac{n_i}{S_j} \exp\left( -\frac{m \xi_j^2}{2kT_w} \right) (\xi_j, \mathbf{n}_w) \]

\[ n_j = \sum_k f^-(\xi_k), \quad S_j = \sum_k \exp\left( -\frac{m \xi_k^2}{2kT_w} \right) (\xi_k, \mathbf{n}_w) \]

Here \( f^- \) and \( f^+ \) are distribution functions of particles interacting with the wall before and after the interaction, respectively, \( T_w \) is the wall temperature, and \( \mathbf{n}_w \) is a unit normal vector directed into the gas-filled space.

5.2. Mirror boundary condition.
The mirror boundary condition simulates the symmetry plane of the system, which allows reducing the computation volume and the number of cells. In this case, a quarter of one micropump is modelled, but in view of the symmetry planes the model represents an infinite periodic system of pumps.

\[ f^+(\xi_j) = f^- \left( \xi_j - 2(\mathbf{n}_w, \xi_j)\mathbf{n}_w \right) \]

The notations are similar to those used in (3).

6. Numerical solution
The Boltzmann equation represents a non-linear equation for the distribution function, which depends on seven variables – three coordinates, three velocities, and time. It proves convenient to separate the solution of the equation on advection and relaxation [20], since the advection process can be reduced to solution of a set of transport equations for each velocity node, and the collision integral can be calculated independently for each spatial node.

6.1. Difference scheme
Figure 3. The explicit difference scheme of the first order

The explicit difference scheme of the first order of accuracy for coordinate and time is used. Values of the function in given cell at time $t + \tau$ are defined by its values at time $t$ in the same cell and neighboring ones

$$f_{i,j}^{+\tau} = f_{i,j} + \frac{\tau}{V_i} \sum_j (\xi, n_{ik}) S_{ij} f_{i,j}^*$$

$$f_{i,j}^* = \begin{cases} f_{i,j}^\xi & (\xi, n_{ik}) > 0 \\ f_{i,j}^\eta & (\xi, n_{ik}) < 0 \end{cases}$$

The maximum time step $\tau$ is determined by the Courant condition for the unstructured mesh

$$\tau_{\text{max}} = \min_i \left\{ \frac{V_i}{\max_{j,\gamma} \{S_{ij}(\xi, n_{ik})\}} \right\}$$

In practice, this estimate often turns out to be too high, hence a somewhat lower value is taken

$$\tau = C\tau_{\text{max}}, \quad C < 1 \quad (4)$$

Projection method
The applied method was first described in [21] and further developed in [22, 23]. The projection of the collision integral on the velocity mesh is used

$$I(\xi) = \sum_f I_f \delta(\xi - \xi_f)$$

Making use of the integral symmetry, the values of $I_f$ can be written as

$$I_f = \frac{1}{4} \int \int \int \Phi(\xi_f) (f' f_i - f f_i') g b d\phi d^3\xi d^3\xi_i$$

$$\Phi(\xi_f) = \delta(\xi - \xi_f) + \delta(\xi_i - \xi_f) - \delta(\xi' - \xi_f) - \delta(\xi_i' - \xi_f)$$

$$f_{i,j}^{+\tau} = f_{i,j} + \frac{\tau}{V_i} \sum_j (\xi, n_{ik}) S_{ij} f_{i,j}^*$$

$$f_{i,j}^* = \begin{cases} f_{i,j}^\xi & (\xi, n_{ik}) > 0 \\ f_{i,j}^\eta & (\xi, n_{ik}) < 0 \end{cases}$$

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$$\Phi(\xi_f) = \delta(\xi - \xi_f) + \delta(\xi_i - \xi_f) - \delta(\xi' - \xi_f) - \delta(\xi_i' - \xi_f)$$
Post-collision velocities $\xi'$ and $\xi''$ can be calculated using values of the spreading angle, angle of the collision $\gamma$ and initial velocities. The spreading angle is calculated by numerical integration of the motion equation in the center-of-mass reference system and by finding asymptotic of $(d^2r/dt^2)_{\gamma=\infty}$.

$$\mu \frac{d^2r}{dt^2} = -\nabla U(r)$$

The Lennard-Jones potential is used as interaction potential

$$U(r) = 4\varepsilon \left( \frac{\sigma^{12}}{r^{12}} - \frac{\sigma^6}{r^6} \right)$$

Parameter $\sigma_{eff}$ in the expression (1) for the free path length is defined by the formula $\sigma_{eff} = \sigma \sqrt{\Omega^{(2,2)}}$, where $\Omega^{(2,2)}$ depends only on the ratio $kT/\varepsilon$ and is tabulated in [24]. Parameter $\varepsilon$ depends on the specific gas and is found by experiment. Its values for different gases are also provided in [24]. For argon at 300K $\Omega^{(2,2)} = 1.093$.

The integral (5) is calculated with application of the Korobov integration grid. The grid is constructed in the 8-dimensional space on nodes $\left\{\xi_a, \xi_b, \xi_c, \xi_d\right\}$, with nodes $\xi_a$ and $\xi_b$ lying on the grid $\{\xi\}$.

For calculation of the integral (5), it is necessary to approximate the values $\delta (\xi' - \xi')$ and $\delta (\xi'' - \xi'')$, since the post-collision velocities $\xi'$ and $\xi''$ do not lie on the grid $\{\xi_a, \xi_b\}$. The laws of conservation of mass, momentum and energy shall also be observed. The approximation is performed using two pairs of the nearest nodes of the grid; $\xi_d$ is the displacement vector.

$$\delta (\xi' - \xi') = r \delta (\xi_a - \xi_a) + (1-r) \delta (\xi_{a+d} - \xi_a)$$
$$\delta (\xi'' - \xi'') = r \delta (\xi_b - \xi_b) + (1-r) \delta (\xi_{b-d} - \xi_b)$$

(6)

The laws of conservation of mass and momentum hold for the approximation (6). Factor $r$ is found from the energy conservation condition

$$\xi'^2 + \xi''^2 = r \left( \xi_a^2 + \xi_b^2 \right) + (1-r) \left( \xi_{a+d}^2 + \xi_{b-d}^2 \right)$$

It is also necessary to calculate $f'f''$. The exponential interpolation below retains the Maxwellian distribution for the case of thermal equilibrium.

$$f'f'' = (f_a f_b)^r \left( f_{a+d} f_{b-d} \right)^{(1-r)}$$

7. Software implementation

The mesh is generated in the GMSH software wherein sizes of different regions are specified. Distribution on clusters for computation in several processes is also done there. The special software then breaks the mesh data down into files, each of which, along with cell data, contains information on boundaries of each cell supplemented by information on boundary conditions from a separate file [25-30]. The program outputs VTK text files containing values of macro-quantities for each cell. The file data can be processed with any program supporting this format; in our case the ParaView platform was used.

The code is written in C++ using the OpenMPI library for implementation of distributed computing.
8. Results of computations

All computations were performed in 128 processes. The spatial mesh included 38,819 elements, and the velocity mesh – from 6000 to 17,000 elements. The Korobov grid consisted of about 50,000 nodes. Parameter \( C \) in (4) equals 0.5. The ratio \( \tau / t_0 \) ranges from 0.002 to 0.004. The mesh size and time step change due to the change in the maximum mesh velocity in (2), which, after passing on to dimensionless variables, is proportional to \( \sqrt{T_2/T_1} \).

Inside the vessels the pressure is nearly uniform. In the vessel being pumped down, the concentration decreases, which results in a slight increase of the Knudsen number.

\[
k^+(t) = k_{\infty} - Ae^{-t/t_{ch}}
\]  

Figure 5 shows the pump-down versus time, and the approximation obtained by using the formula (7). The experimental curve includes two parts. In the first part, macro parameters of gas in the tubes are stabilized. Since the size of the tubes is less than the size of the system as a whole, the gas in the tubes comes into a quasi-stationary state rather quickly, during about 300\(t_0\). Next, in the second part of the curve, a lower process of attaining equilibrium between the vessels proceeds.

Parameters \( k_{\infty}, A \) and \( t_{ch} \) are selected with the least squares methods to ensure the best fit to the second part of the curve. The curve fit is quite good; the mean-square difference between the accurate value and the approximate one in the second part is about \(10^{-5}\). This allows finding parameters \( k_{\infty} \) and \( t_{ch} \) of interest with good accuracy without the need to calculate the entire dependence. Parameter \( k_{\infty} \) is the value of
function \( k^*(t) \) in the limit \( t \to \infty \), i.e. the steady-state pump-down, and \( t_{ch} \) is the characteristic pump-down time.

**Figure 6.** Parameter \( k_\infty \) versus Knudsen number for different \( T_2/T_1 \).

Determination of parameter \( k_\infty \) with the least square method allows calculating the steady-state pump-down more accurately without waiting for the establishment of the system equilibrium. The dependence in Figure 6 was obtained for various Knudsen numbers and various temperatures after computing the parameter \( k_\infty \). A rather smooth maximum is observed with the Knudsen numbers ranging from 0.3 to 0.4. For investigation of the dependence of the Knudsen number on the temperature ratio, it might be established that the maximum pump-down value \( k_{\text{max}} \) is always observed at \( Kn = 0.36 \).

**Figure 7.** Parameter \( k_{\text{max}} \) versus \( T_2/T_1 \).

The dependence of the maximum pump-down versus the temperature ratio is shown in Figure 7. The dependence is monotonous and almost linear, with the slope decreasing with \( T_2/T_1 \). It should be noted that of main interest is the low-temperature region where the pump-down can be approximated by a linear dependence.

\[
k_{\text{max}} \approx 1 + 0.17 \left( \frac{T_2}{T_1} - 1 \right)
\]

Figure 8 presents the characteristic pump-down time versus Knudsen number.
Figure 8. Parameter $t_{ch}$ versus Knudsen number for $T_2/T_1 = 1.7$.

Conclusion
The numerical solution of the Boltzmann equation is rather resource-intensive, but with the use of modern technologies in the field of distributed computing the characteristics of systems of interest can be computed rather accurately. The use of unstructured meshes and software that generates them makes this method of solution applicable to problems with slow non-equilibrium flows.

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