Based on kinetic theory computer models of a molecular beam in a collimator

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Abstract. The paper studies a molecular jet that is formed during a gas outflow through a circular tube from a vessel and determines geometric characteristics of the vessel that reduce the jet slope. Developed software is applicable for studying gas flow in various geometries and uses the GPU for computation.

1. Introduction
Recent years have been marked by rapid development of computing technology: clusters of multiple computers, supercomputers, GPU computing technologies. All this creates the possibility of effective use of computational methods for which there were not enough resources before.

Finite-difference methods for solving differential equations can be applied for to study physical and mathematical problems without building simplifying models. One of these methods, namely the projection method [1, 2, 3], is used in this work to solve the Boltzmann equation [4]. To speed up computations, the Nvidia CUDA technology is used for computing on video cards and video card clusters [5, 6].

The main goal of this work is to study the formation of a molecular beam at low Knudsen numbers in a collimator with a circular tube. The study researches the dependence of the shape of this beam on geometric characteristics of the collimator - the length and the radius of the tube.

2. Statement of the problem
The paper studies the outflow of gas from a vessel through a circular tube of a finite length. Scheme of the installation is shown in Figure 1.
The vessel is initially completely filled with a gas having concentration $n_0$. Outside of the vessel, the gas concentration is many orders of magnitude lower, $n_1 = n_0 \cdot 10^{-8}$.

The gas flow through the left wall of the vessel is constant, which produces a steady flow through the tube. On the remaining walls of the vessel diffuse boundary conditions are posed. The dotted lines in the figure show the planes of symmetry, that makes it possible to reduce the required computation area by a factor of 4 applying peculiar reflective boundary condition at the indicated planes.

To describe the geometric characteristics of the jet, definitions from [7] are used. Let's designate $n_{axis}(x)$ - gas concentration on the axis of symmetry, and the cutoff concentration $n_{cut}(x) = 0.5 \cdot n_{axis}(x)$.

**Definition 1.** The beam radius is the distance from the symmetry axis at which the gas concentration reaches the cutoff concentration, i.e. $n(x, y, z) = n_{cut}(x)$.

**Definition 2.** Jet slope $\alpha$ is $\tan^{-1}(dR/dx)$.

The dependence of the radius and divergence of the molecular beam on the geometric characteristics of the collimator are computed.

The jet slope is considered as the primary geometric characteristic of the jet. To calculate it, one has to find the gas concentration at all points in the computation area.

### 3. Numerical method

The Boltzmann equation is solved in Cartesian coordinates:

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + v_z \frac{\partial f}{\partial z} = I_f$$

The numerical solution is performed in two stages - solving the equation with zero right-hand side and calculating the contribution of the collision integral [8]. At the first stage, the finite-difference TVD scheme and the method of alternating directions are applied [9]. At the second one, the collision integral is taken into account using the method presented in [10].

The characteristic parameters of the gas $T_0, n_0, m_0, d_0$ are introduced: the initial temperature, the concentration of the gas in the vessel, the molecular weight of the gas and the diameter of the molecule. The characteristic values of velocity, distance and time are calculated using this parameters:

$$v_0 = \sqrt{\frac{T_0}{m_0}}, \lambda = \frac{1}{\sqrt{2 \pi n_0 d_0}^2}, \tau = \frac{\lambda}{v_0}$$

The transition to dimensionless variables is carried out.

Introducing a finite time step, grids in the space of velocities and coordinates, and a grid function, we obtain the finite-difference scheme for solving the Boltzmann equation.

$$\begin{align*}
\frac{f_{i,j,k}^{l+1/3} - f_{i,j,k}^l}{\tau} + v_x \frac{f_{i+1/2,j,k}^l - f_{i-1/2,j,k}^l}{h_x} &= 0 \\
\frac{f_{i,j,k}^{l+2/3} - f_{i,j,k}^{l+1/3}}{\tau} + v_y \frac{f_{i,j+1/2,k}^{l+1/3} - f_{i,j-1/2,k}^{l+1/3}}{h_y} &= 0 \\
\frac{f_{i,j,k}^{l+1} - f_{i,j,k}^{l+2/3}}{\tau} + v_y \frac{f_{i,j+1/2,k+1/2}^{l+1/3} - f_{i,j+1/2,k-1/2}^{l+1/3}}{h_z} &= 0
\end{align*}$$

Where $f^l$ for each of the indices are defined as follows:

$$f_{i+1/2,j,k} = \begin{cases} f_{ij} + \frac{1}{2} v_x \phi(\theta_{i+1/2,j,k})(f_{i+1,j,k} - f_{i,j,k}), v_x > 0 \\ f_{i+1,j,k} - \frac{1}{2} v_x \phi(\theta_{i+1/2,j,k})(f_{i+1,j,k} - f_{i,j,k}), v_x < 0 \end{cases}$$

Then the obtained value of the distribution function is changed by including the collision integral.
The solution algorithm is described in more detail in [7].

4. Boundary conditions

Diffuse boundary conditions are imposed on the flat walls of the vessel. Taking into account the condition of no gas flow through the surface, the distribution function for reflected molecules takes the form:

\[ f_{\text{out},i,j,k}^{l+1} = \frac{\sum v_x < 0 v_x f_{\text{in},i,j,k}^{l}}{\sum v_x > 0 v_x e^{-v^2/2}} \cdot e^{-v^2/2} \]

For the left wall of the vessel and the rest of the boundaries of the counting area, the "zero boundary condition" is used. For example, on the left border:

\[ \forall v_x > 0 : f^{l+1}(x, v) = f^l(x, v) = f_0(x, v) \]

That is, the value of the distribution function on this surface does not change for velocities directed towards the interior of the computation area. This generates a constant incoming flux of particles, which allows the formation of a stationary molecular beam.

\[ F = \sum_{v_x > 0} v_x \cdot f = \sum_{v_x > 0} v_x \cdot f_0 = \text{const} \]

The boundary conditions on the side surface of the tube in the collimator are somewhat difficult to pose. In the finite-difference expression, the cells have the shape of a cube. So, the surface of a circular cylinder needs to be replaced with a different surface. In order to bring the new surface as close as possible to the cylinder, we will replace it with a polyhedron of a special shape. Its structure is shown in Figure 2.

A normal and a tangent plane are drawn in each cell near the surface of the cylinder. These planes form a polyhedron, from which the gas passing through the tube is diffusely reflected.

**Figure 2.** Circular hole approximation scheme

Diffuse boundary conditions will be applied for the values of \( \mathbf{v} \) for which the condition \((v \cdot n) > 0\) is satisfied.

The expression for the reflected distribution function takes the form:

\[ f_{\text{out},i,j,k}^{l+1} = \frac{\sum_{v \cdot n > 0} (v \cdot n)f_{\text{in},i,j,k}^{l}}{\sum_{v \cdot n < 0} (v \cdot n)e^{-v^2/2}} \cdot e^{-v^2/2} \]

For the values of \( \mathbf{v} \) that don’t satisfy the condition, a zero boundary condition is used or a difference scheme is applied.
This method requires checking that the side surface of the tube really reflects all particles falling on it and does not adsorb its inside. This can be verified by counting the total number of molecules "inside the wall" which should not rise over time.

5. Impermeability check

![Figure 3: Dependence of the number of molecules inside the wall on time step](image)

Using the least squares method, we approximate the number of molecules by a constant.

\[ N_{\text{wall}} = C = (3.3 \pm 0.3) \times 10^{-5} \]

The number of molecules inside the wall during the flow remains at the level of measurement error, which shows that the side surface of the hole fully reflects the entire incident gas flow.

6. Reaching steady flow regime

In order to measure the geometric characteristics of the jet, it is required to continue the computation until a steady flow regime is formed. For this, the dependence of the gas flow through the plane perpendicular to the x axis is calculated:

\[ F(x) = \int dy \int_{y_v} d^3 v \cdot f(x, y, z, v) \]

In finite-difference expression, this value takes the form:

\[ F_i = \sum_{j,k} \sum_{|v| < v_{\text{cut}}} m \cdot \Delta v \cdot f_{i,j,k,m,n,p} \]

The flow is considered steady if the above value changes within the measurement error in 10 time steps. The natural metric on the function space is applied:

\[ \rho(x, y) = \max_j |y_j - x_j| \]

Let us introduce the value \( \rho(x, y) = \max_j |y_j - x_j| \) that is the distance between \( F(t) \) and \( F(t - \Delta t) \) in the sense of the above metric, \( \Delta t = 10 \). If the value is equal to zero within the measurement error, then it is accepted that the stationary flow has been established.

7. Simulation results

The simulation was carried out on a grid with the following parameters:

\( \tau = 0.1 \) is time step.
\( h = h_x = h_y = h_z = 1 \) is a step in coordinate space.
\( \Delta v = \Delta v_x = \Delta v_y = \Delta v_z = 0.48 \) is a step through the space of velocities.
$|v_{cut}| = 4.8$ is maximum molecular velocity.

$\Omega = [0; 100] \times [0; 25] \times [0; 25]$ is the size of the computation area.

$x_w = 25$ is location of the right side of the vessel.

$(y_h, z_h) = (12, 12)$ is location of the center of the tube.

Additional parameters are determined for different configurations of tube radius and wall thickness.

Additional parameters are determined for different configurations of tube radius and wall thickness.

| Table 1. Configurations of the problem |
|---------------------------------------|
| Configuration | a | b | c | d | e |
| Tube radius $r_h$ | 4 | 4 | 4 | 2 | 6 |
| Wall thickness $d_w$ | 2 | 5 | 10 | 4 | 4 |

For each configuration, values $\rho(t)$ were obtained to determine when the flow becomes stationary. They are shown in Figure 4.

One can see that for all configurations at $t > 500$, a steady flow is established.

The concentration distributions for different configurations in the longitudinal and cross sections are shown in Figure 5.
The dependencies of the jet radius on the coordinate are shown in Figure 6.

**Figure 5.** Distributions of concentration for stationary flow

The R (x) dependence for each configuration is approximated by a straight line. For the approximation, not all points of R (x) are used, but only those for which the Knudsen number is not too large. This is explained by the fact that for a flow close to free molecular (that is, at high Knudsen numbers) a “ray effect” arises [11], which leads to distortion of the concentration values.

The dependence of the Knudsen number at the axis of symmetry on the x coordinate is shown in Figure 7.
Figure 7. Jet radius (blue) and Knudsen number (red) versus distance from the jet exit.

It is calculated that the value of the derivative changes sharply at $Kn \sim 10^2$. However, on the graph of the Knudsen number, there is no sharp change of the derivative at all.

The jet slope is calculated for each configuration, which is presented in Table 2.

Table 2. Jet slope values

| Configuration | $k = \tan\alpha$ | $\alpha$ – jet slope |
|---------------|-----------------|----------------------|
| a             | $0.414 \pm 0.01$| $22.5^\circ \pm 0.5^\circ$ |
| b             | $0.355 \pm 0.006$| $20.3^\circ \pm 0.4^\circ$ |
| c             | $0.240 \pm 0.004$| $13.5^\circ \pm 0.3^\circ$ |
| d             | $0.33 \pm 0.01$  | $18.8^\circ \pm 0.6^\circ$ |
| e             | $0.34 \pm 0.01$  | $19.2^\circ \pm 0.6^\circ$ |

*a The parameters of each configuration are shown in the table 1.

8. Conclusions

The article presents simulation of gas outflow from a vessel through a circular tube. It is shown that an increase in the length of the tube significantly affects the geometry of the molecular beam and decreases its slope. The radius of the exit hole have small effect on the beam geometry.

A method for modeling curved reflective surfaces is developed at an example of a circular tube.

The developed application uses computing technologies on GPUs, which can significantly speed up finite-difference solution of the Boltzmann equation.

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