Numerical modeling of Knudsen’s thermal creep experiment

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Abstract. In his study of thermal creep phenomena in 1910, M. Knudsen build a construction that was composed of 10 pairs of cylindrical tubes of different diameters heated at its junctions. He observed that at some conditions the construction worked as a gas compressor and he was able to obtain the pressure ratio at the ends of the device up to 10. The aim of the present work was to model the experiment using the power of modern computers and the efficient method for solving the Boltzmann kinetic equation. The computations were made for the same set of temperatures, gas pressures and geometrical parameters of the installation as in the experiment, and for molecular hydrogen with real Lenard-Jones potential and realistic rotational energy relaxation time. The Boltzmann equation was solved by the conservative projection method. The computations were carried out with the use of specially developed by the authors program-solving environment for modeling of rarefied gas flows with arbitrary geometry and real gas parameters. The obtained results are in reasonable good agreement with the experimental data.

1. Introduction

In 1910 Martin Knudsen has studied thermal creep phenomena in a cylindrical tube with the temperature gradient applied on the walls and constructed a device operating as a pump. In contrast to classical vacuum pumps, the device worked without moving parts and doesn’t use oil, hence it was environmentally friendly. The last feature was not much considered in that time, but became very important now.

Knudsen has measured pressure difference at the ends of the device built from the capillary and large-scale cylindrical tubes connected in series [1]. The diameter of the capillary tubes was about 0.5 mm and the temperature grows linearly along the tubes from $T_1$ to $T_2 > T_1$. The diameter of the large-scale tubes was about 10 – 15 mm and the temperature decreases there from $T_2$ to $T_1$. It was noticed that under certain conditions pressure rate on the device ends rises up to 10 times, i.e. it could operate as a pump. In the beginning of the 20th century such pumps don’t obtain practical applications because the diameter of the capillary tubes limited maximal operating pressure by approximately $1.33 \cdot 10^4$ Pa.

The aim of the present work consists in modeling of the Knudsen experiment on the base of solution of the Boltzmann kinetic equation for a diatomic gas. The rotational degrees of freedom are taken into account by the application of a 2-levels relaxation model [2]. The Boltzmann...
equation is solved by a splitting scheme with three stages: transport stage, elastic relaxation and rotational-translational relaxation. The transport equation is approximated by the finite volumes method. Tetrahedral unstructured grids generated with the help of GMSH software [3] are used. The collision integral is evaluated by the conservative projection method [4]. The method ensures that the laws of conservation of mass, momentum and energy are strictly observed and the collision integral of the Maxwellian distribution function is equal to zero.

Rarefied gas flows induced by thermal creep in microchannels have been studied in [5, 6] with the help of DSMC and BGK.

Using aerogel membranes make it possible to create Knudsen pump prototypes performing operations at atmospheric pressure [7].

2. Mathematical framework
The Boltzmann equation is solved

$$\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = I(f, f)$$

$$I(f, f) = \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{b_m} (f' f_* - f f_*) \varphi db d\varphi d\xi_*$$

A spherical domain on a uniform grid with a spacing $h$ is chosen as the discrete velocity space. The maximum velocity is taken equal to $4.8 \sqrt{\frac{kT_{\text{max}}}{m}}$ because the values of the distribution function for the greater velocities are negligible small.

For convenience of data input and analysis, all values are represented in the dimensionless form. Reference quantities are selected, and all parameters are normalized to those quantities. Free path is chosen as the length unit, characteristic free time as the time unit, and thermal velocity as the velocity unit.

To ensure high efficiency of complex calculations, there was developed a problem-solving environment (PSE) [8] enabling parallel computations. The PSE is capable effectively solve a large class of rarefied gas dynamics problems. It includes solvers which enable quick calculations of 2D and 3D gas flows on rectangular structured grids and calculations of flows on non-structured tetrahedral grids allowing description of arbitrary 3D geometries. This makes the PSE a universal tool not just for academic purposes but for engineering analysis as well.

High modularity makes the PSE flexible and scalable which is important for its future development. Due to the cross-platform design of the code and the possibility to use graphic processors that are rapidly developing at present time, the problems can be solved in a wide range of architectures.

Fig.1 shows the diagram of data flow from user-supplied input parameters and computational grid generation to visualization of results with the help of third parties software. In the centre of the figure is the solver – a program that carries out all calculations required for gas modeling.

The efficient paralleling, on the one hand, allowed a substantial reduction in the computation time (from weeks to hours), and, on the other hand, enabled precision calculations on fine grids that require large memory. Today solvers use two paralleling technologies – the MPI (Message Parallel Interface) that is used for computations on clusters of ordinary processors, and the Nvidia CUDA (Computer Unified Device Architecture) designed for general purposes computations on the GPUs.

3. Modeling results
Fig. 2 shows the design of $i$-th cascade of the Knudsen pump. Capillar and large-scale tubes with the same length $L$ are connected successively.
In the first series of experiments Knudsen takes $T_1 = 373K$ and $T_2 = 623K$. In the present paper Lenard-Jones potential for Hydrogen molecules was used with parameters $\varepsilon = 38K$ and $\sigma = 2.915 \text{ Å}$. The ratio of rotational and translational relaxation times was taken equal to 100.
and rotational energy accommodation coefficient at the wall was taken equal to 0.5.

Tetrahedral mesh for one cascade of the device is shown in Fig. 3. The edges of tetrahedrons near the symmetry line were taken much larger than the edges near the walls.

![Figure 3. Tetrahedral mesh](image)

Boundary conditions of perfect accommodation with outgoing Maxwellian function were posed at the walls and external flanks of the tubes. The computation was continued until the achievement of a steady distribution of gas parameters in the system.

Fig. 4 presents a plot of pressure ratio $a = \frac{p_2}{p_1}$ versus Knudsen number $Kn$ for $l/r = 10$.

Table 1 shows pressure ratio on the ends of the tube for various ratios $l/r$.

| $Kn$ | $l/r = 1$ | $l/r = 5$ | $l/r = 10$ | $l/r = 50$ | $l/r = 100$ |
|------|-----------|-----------|------------|------------|------------|
| 0.1  | 1.037     | 1.035     | 1.035      | 1.036      | 1.035      |
| 0.5  | 1.099     | 1.130     | 1.135      | 1.134      | 1.135      |
| 1.0  | 1.115     | 1.165     | 1.183      | 1.186      | 1.184      |
| 2.5  | 1.127     | 1.203     | 1.219      | 1.220      | 1.221      |
| 5.0  | 1.136     | 1.216     | 1.235      | 1.236      | 1.237      |
| 10.0 | 1.150     | 1.227     | 1.248      | 1.248      | 1.249      |

One could make a conclusion based on the data provided that the steady-state pressure ratio $a = \frac{p_2}{p_1}$ does not depend on the tube length if the condition $\frac{l}{\chi} > 5$ is met, where $\chi = min(r, \lambda)$, $\lambda$ being the molecular mean free path.

The results of the numerical modeling are compared with the experimental data of Knudsen [1] in Table 2.

Fig. 5, 6, 7 show steady-state distribution of temperature, density and pressure for one-cascade Knudsen pump with $\frac{p_1 + p_2}{2} = 34.931$ Pa. The values on the plot were normalized by the following reference values: $373 K$ for temperature, $28.7$ Pa for pressure and $5.76 \cdot 10^{23} m^{-3}$ for density.

4. Conclusion

Numerical modeling of the Knudsen pump was carried out. The Boltzmann equation was solved by the conservative projection method. The rotational degrees of freedom were taken into
Figure 4. Pressure ratio versus Knudsen number

Table 2. The numerical results compared with the experimental data

| Data source              | $p_2$ | $p_1$ | $\frac{p_1+p_2}{2}$ | $p_2 - p_1$ | $\frac{p_2}{p_1}$ |
|--------------------------|-------|-------|----------------------|-------------|-------------------|
| Experimental data        | 2.973 | 2.813 | 2.893                | 0.160       | 1.057             |
| Numerical modeling       | 2.973 | 2.813 | 2.893                | 0.160       | 1.057             |
| Experimental data        | 37.597| 32.131| 34.931               | 5.466       | 1.170             |
| Numerical modeling       | 37.264| 32.597| 34.931               | 4.666       | 1.170             |
| Experimental data        | 189.851| 175.319| 182.652              | 14.532      | 1.083             |
| Numerical modeling       | 189.051| 176.252| 182.652              | 12.799      | 1.075             |
| Experimental data        | 702.342| 689.943| 696.609              | 12.399      | 1.018             |
| Numerical modeling       | 703.542| 689.677| 696.609              | 13.866      | 1.018             |

account by the application of the 2-levels relaxation model. The obtained results are in good agreement with the experimental data of Knudsen.
**Figure 5.** Steady-state distribution of temperature

**Figure 6.** Steady-state distribution of density

**Figure 7.** Steady-state distribution of pressure

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