STATISTICAL SIMULATION OF A STEADY-STATE RAREFIED GAS FLOW VIA A PIPELINE VACUUM SYSTEM IN A MOLECULAR-VISCOUS REGIME

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A physicomathematical model of transport processes of molecules in a molecular-viscous regime is described which is consistent with the knowledge of the random motion of molecules in a molecular regime and of a laminar flow in a viscous regime. The Monte Carlo method is applied for the statistical three-dimensional simulation of a steady-state rarefied gas flow via vacuum system elements of arbitrary geometry in a molecular-viscous regime. The results of computational experiments on the determination of the conduction of long and short cylindrical pipelines are reported.

For analysis of molecular flows in complex geometry vacuum systems the method of statistical tests (the Monte Carlo method) is applied, which in the traditional form may be extended to a near-molecular regime with an account of the first intermolecular collisions. The available physicomathematical methods of simulation of transport processes and the methods of statistical tests in the modified form, i.e., the methods of direct simulation, test particles, etc., used for calculations at smaller Knudsen numbers, are based on approximate representations of the mechanism of interaction and the behavior of molecules and in the general case they distort the statistics of collisions in a rarefied gas. The absence of the integrity model of a rarefied gas flow in a molecular-viscous regime entails use of a priori assumptions [1-10]. The degree of reliability of the results obtained depends on the adequacy of intuitive assumptions in the physics of transport processes and the successful choice of a simulation method. Slow convergence of the iteration process in the Monte Carlo method does not allow practical application of the above calculation methods in a molecular-viscous regime in which trajectories of a great number of molecules are simultaneously traced.

In [11, 12] the simulation method of statistical tests (the Monte Carlo method) [10], modified in accordance with the dynamic theory of kinetic equations [4], was used to model a steady-state rarefied gas flow in a molecular-viscous regime ($0.1 < \mathrm{Kn} < 100$, $0.01 < \mathrm{Re} < 10$), which made it possible to account for the weight and geometric sizes of the molecule, intermolecular collisions, and intermolecular interaction forces.

In the present work a physicomathematical model of a rarefied gas flow is presented for the entire range of a molecular-viscous regime at Knudsen numbers from 0.01 to 100 which is consistent with the knowledge of the random migration of molecules in a molecular regime and of a laminar flow in a viscous regime. Computational and full-scale experiments have been conducted to determine conduction of cylindrical pipelines at different length-to-diameter ratios (L/D): 0.1, 2, 4, 6, 8, 10, 40. For consistency, the following have been accepted: rarefied gas is air; temperature is 293 K; the pressure ratio in the inlet and outlet sections of pipeline vacuum system components (VSC) is more than 0.5. The error does not exceed 5% in computations and is no more than 12% in full-scale experiments.

In the VSC conduction computations the following assumptions are made. A gas flow via the VSC is modeled as a set of molecules which are characterized by mass and effective diameter and move along the trajectories described by piecewise-linear functions with segments equal to a free path length.

The VSC configuration in a three-dimensional space is described by a set of connected separate surfaces represented by a single algebraic equation and a system of inequalities not higher than second order [10].

On tracking migration of a separate molecule in the VSC, in order to determine its trajectory, we assume the molecule's repulsions during collision with the VSC walls to be diffuse in accordance with the cosine law. The direction of motion of a separate molecule after an intermolecular collision is determined in terms of the dynamic theory of kinetic equa-

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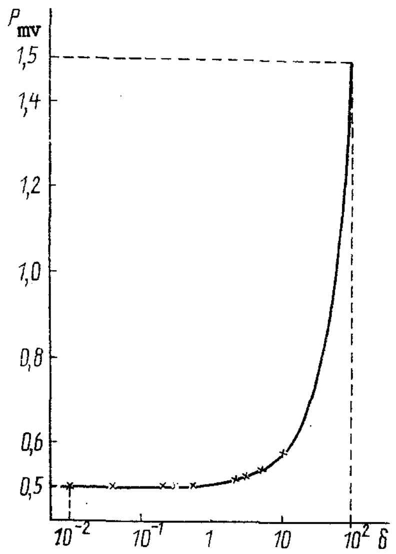

Fig. 1

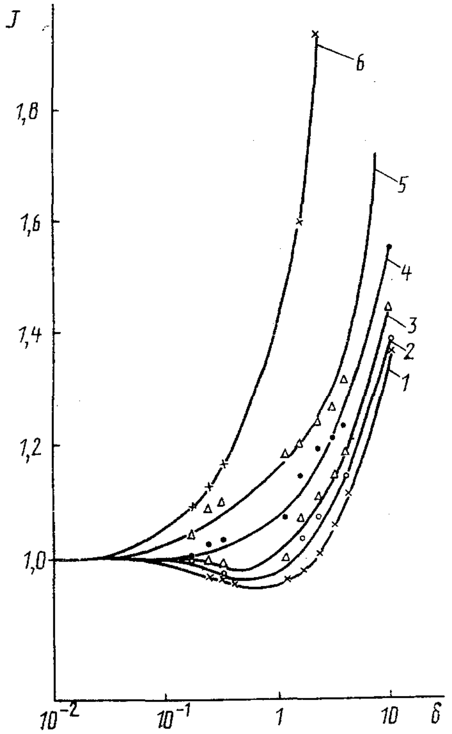

Fig. 2

Fig. 1. Statistical dependence $P_{mv}(\delta)$ of the probability of trajectory directivity of molecule motion over a rarefied gas flow in a molecular-viscous regime.

Fig. 2. Results of computational experiments on conduction determination in a molecular-viscous regime ($0.1 < Kn < 100$; $0.01 < Re < 10$) of arbitrary-length cylindrical pipelines at L/D: 1) 40; 2) 10; 3) 8; 4) 4; 5) 2; 6) 0.1.

tions. In the case of a rarefied gas flowing in a molecular-viscous regime, molecules weakly interact. The mean kinetic energy of thermal motion of molecules is considerably higher than the interaction energy. Interaction forces exert a comparable, in value, influence on the further direction of molecular motion only in the case of an intermolecular collision. As a consequence of a molecule concentration difference over a rarefied gas flow, the preferential direction is developed, along which an influence of the resultant of pair functions of interaction between molecules $\bar{\Phi}$ may remain even at distances exceeding the mean free path length. A molecule under the $\bar{\Phi}$ action acquires additional momentum along the concentration gradient of molecules in a gas flow

$$m\bar{V}_1 = \bar{\Phi}t,$$

where m is the molecule mass, and $\bar{V}_1$ is the velocity vector due to $\bar{\Phi}$ directed along the gas flow. In correspondence with the superposition principle the direction of a separate molecule after an intermolecular collision is formed by adding the vectors $\bar{V}_1$ and $\bar{V}_2$, where $\bar{V}_2$ is the velocity vector of thermal motion of the molecule, acquired as a result of an intermolecular pair collision directed equiprobably in a spheriod angle. Write the trajectory of molecule motion after the intermolecular collision in a local Cartesian coordinate system as

$$t = \frac{x_2}{\cos\alpha} = \frac{y_2}{\cos\beta} = \frac{z_2}{\cos\varepsilon},$$

where $x_2 = x_2' + x_2''$; $y_2 = y_2' + y_2''$; $z_2 = z_2' + z_2''$; $\bar{r}_2'(x_2'; y_2'; z_2')$ and $\bar{r}_2''(x_2''; y_2''; z_2'')$ are the current coordinates of possible molecule displacement at V_1 and V_2/b, respectively; b is the coefficient of kinetic energy redistribution for pair intermolecular collision obtained when fitting the computational to full-scale experiments; $\bar{r}_2(x_2;\ y_2;\ z_2)$ are the current coordinates of real displacement of the molecule; α, β, ε are the angles directing the motion trajectory:

$$\cos\alpha = \frac{x_2}{\sqrt{x_2^2 + y_2^2 + z_2^2}}\ ;\ \cos\beta = \frac{y_2}{\sqrt{x_2^2 + y_2^2 + z_2^2}}\ ;$$

$$\cos\varepsilon = \frac{z_2}{\sqrt{x_2^2 + y_2^2 + z_2^2}}\ .$$

Determine a gas flow passing through the VSC

$$Q_2 = Q_1 P,$$

herein Q_1 is the gas flow entering the VSC via the inlet section, P is the probability of molecule passage via the VSC.

Results of the computational experiments are represented in Figs. 1 and 2, where $J(L/D;\ \delta)$ is the ratio of experimental conduction to that calculated in the molecular regime [10]; $\delta = 1/\mathrm{Kn}$. The real mechanism of molecular interaction may be represented by the function $P_{mv}(\delta)$ (Fig. 1), statistically obtained when fitting computational to full-scale experiments, where

$$P_{mv}(\delta) = \frac{2\pi - \gamma(|\bar{\Phi}(\delta)|)}{2\pi}\ ;$$

herein γ is the angle to the gradient vector of molecule concentration in a gas flow, prescribed in the local spherical coordinate system [10]; $\gamma(\ |\ \bar{\Phi}(\delta)\ |\ )$ is the value of a real region of angle distribution γ.

The dependence $P_{mv}(\delta)$ reflects the distribution after intermolecular collision of the angle γ directing the molecule motion trajectory as a function of the Knudsen number. The values of P_{mv} express the probability of trajectory directivity of molecules along the gas flow after intermolecular collision as a function of the degree of vacuum in a molecular-viscous regime. The dependence $P_{mv}(\delta)$ reflects the intermolecular interaction mechanism on its statistical level as applied to the great number of molecules and the process of forming the motion directivity when a laminar flow develops.

The results of the computational experiments show (Figs. 1 and 2) that the first intermolecular collisions are observed at $\delta \approx 0.01$. The direction of the molecule motion trajectory after intermolecular collision remains equiprobably in a spherical angle of 4π steradian at $\delta < 0.5$ ($\gamma \in [0,\ 2\pi)$, $\gamma(\ |\ \bar{\Phi}(\delta)\ |\ ) = 2\pi$, $P_{mv}(\delta) = 0$). At $\delta > 0.5$ the direction of molecular motion is additionally affected by the force field of intermolecular interaction $\bar{\Phi}$ of a group of surrounding molecules, and at $\delta \approx 100$ the molecule motion is directed along the rarefied gas flow ($\gamma \in [0;\ 0]$; $\gamma(\ |\ \bar{\Phi}(\delta)\ |\ ) = 0$; $P_{mv}(\delta) = 1$). Analyzing experimental data (Fig. 2), it is worth noting that the minimum conduction value flattens with decreasing the length-to-diameter ratio (L/D) and shifts towards higher Knudsen numbers. At $L/D < 6$ the dependence $J = J(L/D;\ \delta)$ has no minimum. The presence of a minimum conduction value may be explained by the fact that the considerably increasing number of additional intermolecular pair collisions and the practically zero value of $\bar{\Phi}$ at $\delta < 0.6$ (see Fig. 1) entail additional difficulties when molecules move along a pipeline and, consequently, decrease the probability of passing through the VSC, which is not compensated by increasing the inlet section conduction.

Results of computational and full-scale experiments are in fair agreement within an accuracy of 15%. Findings of the present work confirm the necessity of revising the existing knowledge on the physics of a rarefied gas flow in a molecular-viscous regime.

Based on the data obtained in computational experiments, we have obtained, by the least-square method with an accuracy of 15%, the analytical expression for conduction calculations in automatic control and design systems of vacuum units [13, 14], valid at $\mathrm{Kn} > 0.1$:

$$J = \frac{1 + 202G + 2653G^2}{1 + 236G}\ ,$$

where

$$J = \frac{U}{U_m}\ ;\ G = \frac{4{,}7\cdot 10^{-3}}{\mathrm{Kn}}\left(1 + \frac{0{,}21D}{L}\right).$$

NOTATION

Kn, Knudsen number; Re, Reynolds number; U, conduction in a molecular-viscous regime; U_m, conduction in a molecular regime; L and D, pipeline length and diameter, respectively.

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