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## Исследование нелинейных процессов на границе раздела газового потока и металлической стенки микроканала

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Работа посвящена исследованию влияния нелинейных процессов в пограничном слое на общий характер течений газа в микроканалах технических систем. Подобное исследование актуально для задач нанотехнологий. Одной из важных задач в этой сфере является анализ потоков газа в микроканалах в случае переходных и сверхзвуковых течений. Результаты этого анализа важны для техники газодинамического напыления и для синтеза новых наноматериалов. Из-за сложности реализации полномасштабных экспериментов на микро- и наномасштабах они чаще всего заменяются компьютерным моделированием. Эффективность компьютерного моделирования достигается как за счет использования новых многомасштабных моделей, так и за счет сочетания сеточных методов и методов частиц. В данной работе мы используем метод молекулярной динамики. Он был применен для исследования установления газового микротечения в металлическом канале. В качестве газовой среды был выбран азот. Металлические стенки микроканалов состояли из атомов никеля. В численных экспериментах были рассчитаны коэффициенты accommodations на границе между течением газа и металлической стенкой. Исследование микросистемы в пограничном слое позволило сформировать многокомпонентную макроскопическую модель граничных условий. Эта модель была интегрирована в макроскопическое описание течения на основе системы квазигазодинамических уравнений. На основе такой преобразованной газодинамической модели были проведены расчеты микротечения в реальной микросистеме. Результаты были сопоставлены с классическим расчетом течения, не учитывающим нелинейные процессы в пограничном слое. Сравнение показало необходимость использования разработанной модели граничных условий и ее интеграции с классическим газодинамическим подходом.

**Ключевые слова:** газодинамические микротечения в каналах с реальной структурой стенки, многомасштабное математическое моделирование, задача о граничных условиях, комбинация микроскопического и макроскопического подходов, параллельные вычисления

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## A study of nonlinear processes at the interface between gas flow and the metal wall of a microchannel

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The work is devoted to the study of the influence of nonlinear processes in the boundary layer on the general nature of gas flows in microchannels of technical systems. Such a study is actually concerned with nanotechnology problems. One of the important problems in this area is the analysis of gas flows in microchannels in the case of transient and supersonic flows. The results of this analysis are important for the gas-dynamic spraying technique and for the synthesis of new nanomaterials. Due to the complexity of the implementation of full-scale experiments on micro- and nanoscale, they are most often replaced by computer simulations. The efficiency of computer simulations is achieved by both the use of new multiscale models and the combination of mesh and particle methods. In this work, we use the molecular dynamics method. It is applied to study the establishment of a gas microflow in a metal channel. Nitrogen was chosen as the gaseous medium. The metal walls of the microchannels consisted of nickel atoms. In numerical experiments, the accommodation coefficients were calculated at the boundary between the gas flow and the metal wall. The study of the microsystem in the boundary layer made it possible to form a multicomponent macroscopic model of the boundary conditions. This model was integrated into the macroscopic description of the flow based on a system of quasi-gas-dynamic equations. On the basis of such a transformed gas-dynamic model, calculations of microflow in real microsystem were carried out. The results were compared with the classical calculation of the flow, which does not take into account nonlinear processes in the boundary layer. The comparison showed the need to use the developed model of boundary conditions and its integration with the classical gas-dynamic approach.

**Keywords:** gas-dynamic microflows in channels with real wall structure, multiscale mathematical modeling, boundary conditions problem, combination of microscopic and macroscopic approaches, parallel computing

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## 1. Introduction

In recent years, the development of nanotechnologies used in nanoelectronics, biomedicine and other sectors of the economy has become relevant. One of the important problems in this area is the analysis of gas flows in microchannels of technical systems in the case of transient and supersonic flows. This analysis results in various technologies of gas-dynamic spraying and installations for the synthesis of new materials. These and other considerations aroused the authors' interest in studying gas-dynamic processes in microsystems under different conditions of their occurrence and different real geometry of systems. Due to the complexity of the implementation of full-scale experiments on micro- and nanoscale, they are most often replaced by computer simulation. Within the framework of such modeling, the greatest deviations of theoretical estimates from the real situation are observed at nanoscale when taking into account the specific composition of the gaseous medium and the structure of real surfaces streamlined by gas flows. Therefore, to improve the quality of theoretical analysis, together with it, numerical approaches are used, which currently combine mesh and particle methods.

In this work, we use the molecular dynamics (MD) method [Heermann, 1990; Haile, 1992; Rapaport, 2004]. It was used to study the establishment of a microflow of gas in a metal channel. Nitrogen was chosen as the gaseous medium. The metal walls of the microchannels consisted of nickel atoms. In numerical experiments, the accommodation coefficients were calculated at the boundary between the gas flow and the metal wall. The study of the nitrogen-nickel microsystem in the boundary layer of the microchannel made it possible to form a multicomponent macroscopic model of the boundary conditions. This model was integrated into the macroscopic description of the flow based on a system of quasi-gas-dynamic (QGD) equations [Chetverushkin, 2008; Elizarova, 2009; Elizarova et al., 2014; Sheretov, 2016]. On the basis of such a transformed gas-dynamic model, calculations of microflow in the balloon-nozzle-microchannel system were carried out. The results were compared with the classical calculation of the flow, which does not take into account nonlinear processes in the boundary layer. The comparison showed the need to use the developed model of boundary conditions and its integration with the classical gas-dynamic approach.

## 2. Mathematical models

To describe the processes under study, we present the macroscopic and microscopic approaches we use. A system of quasi-gas-dynamic equations (see Section 2.1) was considered as a macroscopic description. It was used to calculate the flow in the balloon-nozzle-microchannel system (see Section 4.2) in the case of two variants of boundary conditions. The system of classical molecular dynamics equations was considered as a microscopic model (see Section 2.2). On its basis, the quasi-equilibrium state of the nitrogen-nickel system was calculated, which made it possible to form a new macroscopic model of the boundary conditions (see Section 4.1).

### 2.1. Macroscopic model

The system of QGD equations, in the case of multicomponent gas environment, in a form invariant with respect to the coordinate system for each component and the material equations closing it have the following form [Elizarova, 2009]:

$$\begin{aligned} \frac{\partial \rho_l}{\partial t} + \operatorname{div} \mathbf{W}_l^{(\rho)} = 0, \quad \mathbf{W}_l^{(\rho)} = \rho_l (\mathbf{u}_l - \mathbf{w}_l), \\ \mathbf{w}_l = \tau \left[ \frac{1}{\rho_l} \operatorname{div}(\rho_l \mathbf{u}_l) \right] \mathbf{u}_l + \mathbf{w}_l^*, \quad \mathbf{w}_l^* = \tau \left[ (\mathbf{u}_l \nabla) \mathbf{u}_l + \frac{1}{\rho_l} \nabla p_l \right]; \end{aligned} \quad (1)$$

$$\frac{\partial(\rho_l u_{l,k})}{\partial t} + \operatorname{div} \mathbf{W}_l^{(\rho u_k)} = S_{l,k}^{(\rho u)}, \quad \mathbf{W}_l^{(\rho u_k)} = \mathbf{W}_l^{(\rho)} u_{l,k} + \mathbf{e}_k p_l - \mathbf{\Pi}_{l,k}, \quad \mathbf{\Pi}_{l,k} = (\mathbf{\Pi}_{l,j,k}),$$

$$\mathbf{\Pi}_{l,j,k} = \mathbf{\Pi}_{l,k,j}^{NS} + \mathbf{\Pi}_{l,k,j}^{AD}, \quad \mathbf{\Pi}_{l,k,j}^{NS} = \mu \left( \frac{\partial u_{l,k}}{\partial j} + \frac{\partial u_{l,j}}{\partial k} + \delta_{k,j} \left( \zeta - \frac{2}{3} \right) \operatorname{div}(\mathbf{u}_l) \right), \quad (2)$$

$$\mathbf{\Pi}_{l,k,j}^{AD} = \rho_l u_{l,k} w_{l,j}^* + \delta_{k,j} \tau ((\mathbf{u}_l \nabla) p_l), \quad S_l^{(\rho u_k)} = \nu_{ll} \rho_l (u_{l,k}^* - u_{l,k}), \quad j, k = x, y, z;$$

$$\frac{\partial E_l}{\partial t} + \operatorname{div} \mathbf{W}_l^{(E)} = S_l^{(E)}, \quad \mathbf{W}_l^{(E)} = \mathbf{W}_l^{(\rho)} H_l + \mathbf{q}_l - \mathbf{\Pi}_l \mathbf{u}_l, \quad (3)$$

$$\mathbf{q}_l = -\kappa \nabla T_l - \tau \left[ (\mathbf{u}_l \nabla) \varepsilon_l + p_l (\mathbf{u}_l \nabla) \left( \frac{1}{\rho_l} \right) \right] \rho_l \mathbf{u}_l, \quad S_l^{(E)} = \nu_{ll} \rho_l (E_l^* - E_l);$$

$$n_l = \frac{\rho_l}{m_l}, \quad p_l = Z_l \rho_l \mathfrak{R}_l T_l, \quad E_l = \frac{1}{2} \rho_l |\mathbf{u}_l|^2 + \rho_l \varepsilon_l, \quad \varepsilon_l = c_{v,l} T_l, \quad H_l = \frac{E_l + p_l}{\rho_l}, \quad (4)$$

$$\gamma_l = \frac{c_{p,l}}{c_{v,l}}, \quad \operatorname{Sc}_l = \frac{\mu_l}{\rho_l D_l}, \quad \operatorname{Pr}_l = \frac{\mu_l c_{p,l}}{\kappa_l}, \quad \tau_l = \frac{\mu_l}{p_l \operatorname{Sc}_l};$$

$$\rho = \sum_l \rho_l, \quad n = \sum_l n_l, \quad \mathbf{u} = \sum_l \frac{\rho_l \mathbf{u}_l}{\rho}, \quad p = \sum_l p_l, \quad E = \sum_l E_l, \quad \varepsilon = \frac{E}{\rho} - \frac{1}{2} |\mathbf{u}|^2,$$

$$T = \sum_l \frac{n_l Z_l T_l}{n Z}, \quad m = \sum_l \frac{m_l n_l}{n Z}, \quad Z = \sum_l Z_l, \quad \mathfrak{R} = \frac{p}{\rho Z T} = \frac{k_B}{m}, \quad c_V = \frac{\varepsilon}{T}, \quad (5)$$

$$c_p = \sum_l \frac{\rho_l c_{p,l}}{\rho}, \quad \gamma = \frac{c_p}{c_v}, \quad \operatorname{Sc} = \frac{\mu}{\rho D}, \quad \operatorname{Pr} = \frac{\mu c_p}{\kappa}, \quad \tau = \frac{\mu}{p \operatorname{Sc}}.$$

Here all the variables with index  $l$  correspond to the gas of the  $l$  type (in this work, there is only nitrogen). Each component of a gas mixture is characterized by a numerical density (concentration)  $n_l$ , mass density  $\rho_l = m_l n_l$  ( $m_l$  is the mass of a gas molecule of the  $l$  type), macroscopic velocity  $\mathbf{u}_l$ , temperature  $T_l$ , and partial pressure  $p_l$ . Other parameters of the mixture components:  $E_l$ ,  $H_l$  and  $\varepsilon_l$  are the densities of the total energy, enthalpy and internal energy of the mixture components;  $D_l = D_l(T_l)$ ,  $\mu_l = \mu_l(T_l)$ ,  $\mu_{l,b} = \mu_l(T_l) \zeta_l(T_l)$ ,  $\kappa_l = \kappa_l(T_l)$  are the coefficients of diffusion, dynamic and bulk viscosities, thermal conductivity. Equations (1)–(3) contain the general parameters of the mixture  $\mu$ ,  $\zeta$ ,  $\kappa$  and  $\tau$ , which represent the coefficients of dynamic viscosity, relative bulk viscosity, thermal conductivity of the mixture, as well as the relaxation time of the mixture to a quasi-equilibrium state. These parameters are expressed in the terms of the corresponding coefficients of the mixture components  $\mu_l = \mu_l(T_l)$ ,  $\zeta_l = \zeta_l(T_l)$ ,  $\kappa_l = \kappa_l(T_l)$ ,  $\tau_l = \tau_l(T_l, \rho_l)$  and depend on the temperature. In the material equations (4)–(5), the parameters  $Z_l = Z_l(T_l, \rho_l)$ ,  $\gamma_l = \gamma_l(T_l, \rho_l)$ ,  $c_{v,l} = c_{v,l}(T_l)$ ,  $c_{p,l} = c_{p,l}(T_l)$  and  $\mathfrak{R}_l = \frac{k_B}{m_l}$  are the compressibility factors, adiabatic exponents, specific heat capacities at constant volume and constant pressure, individual gas constants ( $k_B$  is the Boltzmann constant),  $\operatorname{Pr}_l$ ,  $\operatorname{Pr}$ ,  $\operatorname{Sc}_l$ ,  $\operatorname{Sc}$  are the Prandtl and Schmidt numbers for the components and for the mixture as a whole. The vectors  $\mathbf{W}_l^{(\rho)}$ ,  $\mathbf{W}_l^{(\rho u_k)}$ ,  $\mathbf{W}_l^{(E)}$  up to sign coincide with vectors of mass, energy and momentum flux density for the mixture components. The exchange terms  $S_{l,k}^{(\rho u)}$  and  $S_l^{(E)}$  take into account the redistribution of momentum and energy due to collisions of particles of various types [Elizarova, 2009].

Equations (1)–(3) are supplemented with the necessary initial and boundary conditions (see [Elizarova, 2009]). The initial conditions for the QGD equations are taken in accordance with the equilibrium state of the gaseous medium in the absence of interaction with external factors.

## 2.2. Microscopic model

As a mathematical model, the molecular dynamics method [Heermann, 1990; Haile, 1992; Rapaport, 2004] was used. In the case of studying the particles of two kinds (metal and gas), the

system of equations is

$$m_l \frac{d\mathbf{v}_{l,i}}{dt} = \mathbf{F}_{l,i}, \quad \frac{d\mathbf{r}_{l,i}}{dt} = \mathbf{v}_{l,i}, \quad i = 1, \dots, N_l, \quad (6)$$

where  $i$  is the particle number,  $l$  is kind of the particle,  $N_l$  is the total number of particles of kind  $l$ ,  $m_l$  is the mass of particle of kind  $l$ ,  $\mathbf{r}_{l,i}$  and  $\mathbf{v}_{l,i}$  are the position and the velocity vectors of the  $i$ th particle of kind  $l$ , respectively,  $\mathbf{F}_{l,i}$  is the resultant force acting on the  $i$ th particle.

The forces are the sum of the forces of interaction of the  $i$ th particle with surrounding particles determined by the functional of potential energy and the forces of external action having the following form:

$$\mathbf{F}_{l,i} = -\frac{\partial U(\mathbf{r}_{l,1}, \dots, \mathbf{r}_{l,N_l})}{\partial \mathbf{r}_{l,i}} + \mathbf{F}_{l,i}^{ext}, \quad i = 1, \dots, N_l. \quad (7)$$

Here,  $U$  is the total potential energy of a system of particles,  $\mathbf{F}_{l,i}^{ext}$  is the interaction force of the  $i$ th particle of type  $l$  with the surrounding particles.

The potential energy of the system  $U$  is represented as the sum of the partial potential energies, which are calculated according to the formulas of the selected interaction potentials. In the case of modeling the gas flow inside the channel, when considering one type of gas and one type of channel material, three types of interactions (gas-gas, gas-metal, and metal-metal) should be considered, which corresponds to three interaction potentials:

$$U = U_{aa} + U_{bb} + U_{ab},$$

$$U_{aa} = \sum_{i=1, j>i}^{N_a} \varphi_{aa}(|\mathbf{r}_{a,i} - \mathbf{r}_{a,j}|), \quad U_{ab} = \frac{1}{2} \sum_{i=1}^{N_a} \sum_{j=1}^{N_b} \varphi_{ab}(|\mathbf{r}_{a,i} - \mathbf{r}_{b,j}|), \quad (8)$$

$$U_{bb} = \sum_{i=1}^{N_b} \left[ \varphi_{1,bb}(\mathbf{r}_{b,i}) + \sum_{j>i} \varphi_{2,bb}(|\mathbf{r}_{b,i} - \mathbf{r}_{b,j}|) \right],$$

where  $U_{aa}$ ,  $U_{bb}$  and  $U_{ab}$  are the potential interaction functions for gas with gas, metal with metal and gas with metal particles systems, respectively. Each type of interaction is described using the corresponding potential  $\varphi_{ll}$ . For the interaction of nitrogen molecules with each other, we used the Mie potential in the form of « $n - 6$ » [Mie, 1903] adapted in [Fokin, Kalashnikov, 2009] to calculations of a mixture of hydrogen and nitrogen. For the interaction of nickel atoms with each other, the embedded atom model (EAM) potential was used [Daw, Baskes, 1984], which takes into account not only pairwise interactions  $\varphi_{2,bb}$ , but also the influence of the environment on a specific particle  $\varphi_{1,bb}$ . The EAM potential was taken in the form proposed in [Zhou et al., 2004]. To take into account gas-metal interactions, we used the standard Lennard-Jones potential [Lennard-Jones, 1931] with parameters calculated by the Lorentz – Berthelot formulas [Lorentz, 1881; Berthelot, 1889].

To model the process of accelerating the gas flow and to reach the required temperature with gas, the Langevin thermostat was used [Heermann, 1990], and the Berendsen thermostat was used [Berendsen et al., 1984] to reach only the required temperature. Both thermostats were used in the preparatory stages and were turned off during the main calculation.

The initial conditions at the microlevel are determined by the equilibrium or quasi-equilibrium thermodynamic state of the particle system at a given temperature, pressure, and average momentum. The boundary conditions at the molecular level depend on the modeled situation. To determine the general properties of a medium, it suffices to consider the selected three-dimensional volume with periodic boundary conditions in all coordinates. When studying microsystems of real geometry, such as a microchannel, one or several directions have a finite size, and the preservation of the shape of an object is achieved by selecting a potential or fixing the system. In this case, either the mirror

boundary conditions can be used as boundary conditions, when the particles interact with their mirror reflection and do not consequently leave the boundary or the condition of the particle disappearing at the boundary and its appearance in another place of the microsystem (so that the overall equilibrium in the system is not disturbed). An input stream of particles on one side of the selected volume and a free exit of particles on the other can also be specified.

### 2.3. Combination of models

In the case of a dynamic complex calculation, the combination of the above two models is performed on the basis of the scheme of splitting by physical processes [Marchuk, 1988]. At each time step, the grid methods first solve equations (1)–(5). Then, in the boundary zones near the solid walls of the microsystem, equations (6)–(7) are solved. The calculation procedure is completed at the integration step by the correction of the macroscopic parameters of the gaseous medium.

In this work, we used the macroscopic and microscopic models separately. Using a microscopic level model, the processes of establishing equilibrium in a metal [Podryga, Polyakov, 2015; Podryga et al., 2015] and in a gas [Podryga et al., 2015] were previously investigated. In [Podryga, 2017; Podryga, Polyakov, 2016; Podryga et al., 2020], the properties of nitrogen and other gases were calculated, and the dependences of kinetic coefficients on temperature were refined.

## 3. Numerical analysis methods and software implementation

To solve the macroscopic equations (1)–(5), an explicit grid method of control volumes [Eymard et al., 2000; Li et al., 2000] was used. It was used on grids of various types: Cartesian, unstructured triangular and tetrahedral, as well as on hybrid ones, combining cells of various types. For approximations in these cases see [Polyakov, 2013; Polyakov et al., 2017a; Polyakov et al., 2017b]. This work presents the results of two-dimensional calculations obtained on Cartesian grids (see Section 4.2).

The system of equations (6)–(8) is solved using the velocity Verlet integration [Verlet, 1967]:

$$\mathbf{r}_{l,i}^{n+1} = \mathbf{r}_{l,i}^n + \mathbf{v}_{l,i}^n \Delta t + \frac{\mathbf{F}_{l,i}^n (\Delta t)^2}{2m_{l,i}}, \quad \mathbf{v}_{l,i}^{n+1} = \mathbf{v}_{l,i}^n + \frac{\mathbf{F}_{l,i}^{n+1} + \mathbf{F}_{l,i}^n}{2m_{l,i}} \Delta t, \quad i = 1, \dots, N_l. \quad (9)$$

Here,  $\Delta t$  is the integration step,  $n$  is the step number,  $\mathbf{F}_{l,i}^n$  is the force value at step  $n$ , and  $\mathbf{F}$  is the force calculation procedure. To achieve the desired parameters of gas and metal in a state of thermodynamic equilibrium, the temperature control procedure [Heermann, 1990; Berendsen et al., 1984] is added to (9).

The general algorithm certainly depends on the problem being solved. If we are talking about determining the properties of a gaseous medium or a solid wall, then we only use the well-known procedure for balancing a system of particles with given thermodynamic parameters. If it is necessary to consider the evolution of a complex system, then at the beginning it needs to be prepared. We show this by considering the interaction of gas with a metal plate. In this case, the algorithm consists of the following steps:

- calculation of the thermodynamic equilibrium state of the gas volume;
- calculation of the thermodynamic equilibrium of the metal plate;
- calculation of the quasi-equilibrium in a gas-metal system;
- calculation of the acceleration of gas flow with the help of the Langevin's thermostat;
- calculation of the quasi-equilibrium in a gas-metal system with the fixed velocity.

Parallel implementation of the above numerical techniques was presented in [Podryga et al., 2020; Polyakov et al., 2016]. In this work, we used these algorithms and a set of programs oriented on supercomputer with central node architecture. The software implementation was based on the parallel interfaces MPI and OpenMP.

## 4. Results of modeling

In this work, two problems were considered. The first one concerned the direct modeling of the gas flow in a metal microchannel based on the molecular dynamics model. In this case, the real atomic structure of the metal surface and intermolecular interactions in the gas-metal system were taken into account. The second problem was associated with the formation of a macroscopic model of conditions at the gas-metal interface and its introduction into the macroscopic gas-dynamic description. The results of these studies are presented below.

### 4.1. Results of MD simulation

To achieve the first aim of our research, we considered the nitrogen flow inside a nickel microchannel with a length of 1 to 3  $\mu\text{m}$  and a thickness of about 600 nm was considered. The calculated geometry contained two nickel plates (bottom and top) with layers of adsorbed nitrogen adhering to them and a free nitrogen layer between them (see Fig. 1). In this case, the real structure of the nickel base of the microchannel, the effect of the initial adsorption of nitrogen molecules on the walls of the microchannel, and also the release of the energy of the walls of the microchannel into the environment were taken into account. The calculations were carried out in the framework of the NVT model (fixed Number of particles, Volume and Temperature). At the beginning, the gaseous medium was stationary and balanced using the Langevin thermostat with parameters corresponding to normal conditions ( $T = 273,15 \text{ K}$ ,  $P = 101\,325 \text{ Pa}$ ,  $v = 0$ ). Then the gas medium in the middle section was accelerated to a predetermined average velocity using the Langevin thermostat. Next, the thermostats turned off.

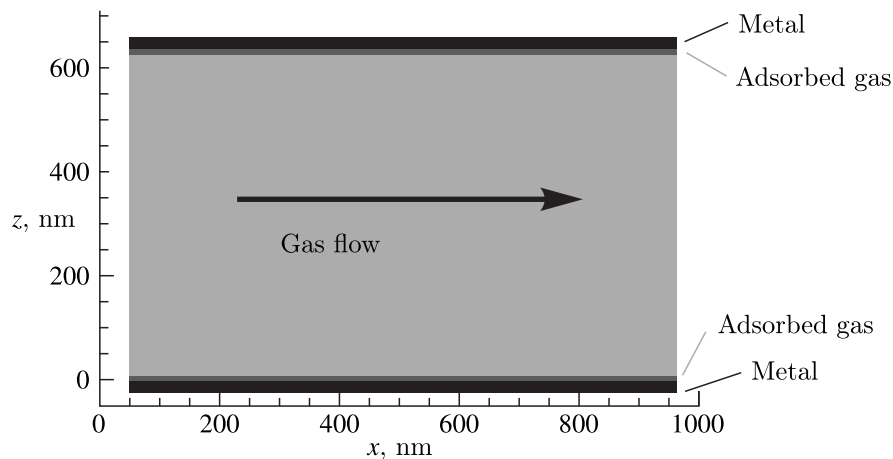


Figure 1. Computational geometry

The calculations were carried out for several widths of a nitrogen flow and several values of velocity, both exceeding the speed of sound in nitrogen, and having significantly lower values. To speed up the calculations in the second direction ( $y$ ), a thin layer and periodic boundary conditions were taken. The parameters of the three microsystems under consideration were the following:

1. Sizes of the lower and upper nickel plates in nanometers were  $1017n \times 101,7 \times 8,5$ .

2. Sizes of the gaseous medium between the plates in nanometers were  $1017n \times 101,7 \times 614,5$ .
3. The number of nickel atoms in both plates was  $162,57n$  millions.
4. The number of nitrogen molecules on the plates and between them was  $42,38n$  millions ( $n = 1, 2, 3$ ).

Our previous calculations [Podryga, Polyakov, 2021] demonstrate that, in the subsonic regime, the transverse profile of the longitudinal velocity component acquires a smooth, almost parabolic shape, the center of which will shift to one or the other side relative to the channel walls. This develops over time into a regime of large-scale turbulence.

In a supersonic flow regime, the profile of the longitudinal velocity component acquires a sharper hyper-Gaussian shape, the center of which practically does not change its position. However, in the boundary layer, small-scale beatings of the gas flow against the channel walls are observed. Over time, this picture can develop into small-scale turbulence, but without leaving the boundary layer.

The calculations show (see Fig. 2) the dynamics of the values of the main gas-dynamic parameters in several sections on coordinate  $z$ :

- In the gas layer adsorbed on a metal ( $z = 11,12$  nm).
- In the moving layer closest to it ( $z = 12,18$  nm).
- In the middle section of the Knudsen layer ( $z = 25,43$  nm  $\sim \frac{1}{3}$  of the mean free path in nitrogen under normal conditions).
- In the center of the channel ( $z = 305,11$  nm).

A detailed analysis of the calculated data leads us to the gas flow structure shown in Fig. 3. It consists of four layers between which there is an exchange of mass, momentum, and energy. Given this structure, we can say that under the conditions of the adsorption effect, the main gas flow actually interacts not with the metal wall, but with the buffer gas and gas adsorbed on the surface.

In the main gas layer, the equations of gas dynamics are valid. In the buffer gas layer, the equations of multiphase hydrodynamics should be solved. In the adsorbed gas layer, it suffices to confine to the two-dimensional convection-diffusion equation. On a solid wall, it is necessary to consider the processes of thermal conductivity and scattering of the normal component of the momentum. At the boundary of the layers, the conditions of continuity of the corresponding flows of mass, momentum, and energy are set. The formulation of these equations and boundary conditions is the subject of future analysis.

Next, it is necessary to decide which model of the boundary layer to obtain. When it comes to applying this model in macroscopic tasks, it is usually limited to calculating the accommodation coefficients by mass, momentum, and energy (temperature). If we are talking about multiscale modeling based on a combination of macro- and microscopic models, then the best, albeit computationally intensive, calculation option is to select boundary layers and carry out molecular calculations in them, followed by matching solutions at the interface. In our works, we used both approaches [Podryga, 2016; Polyakov, Podryga, 2018; Kudryashova et al., 2018].

In the work [Podryga, Polyakov, 2021], the numerical technique for the instantaneous and equilibrium (which are achieved by averaging over time) accommodation coefficients calculation was developed. These results can be used to model stationary or moderately nonequilibrium gas-dynamic processes, when the near-boundary high-frequency oscillations of the gas flow parameters do not affect the overall course of the process. In the opposite situation, for a more accurate description of the processes occurring in the boundary layers, it is proposed to solve its own problem in each layer highlighted above:



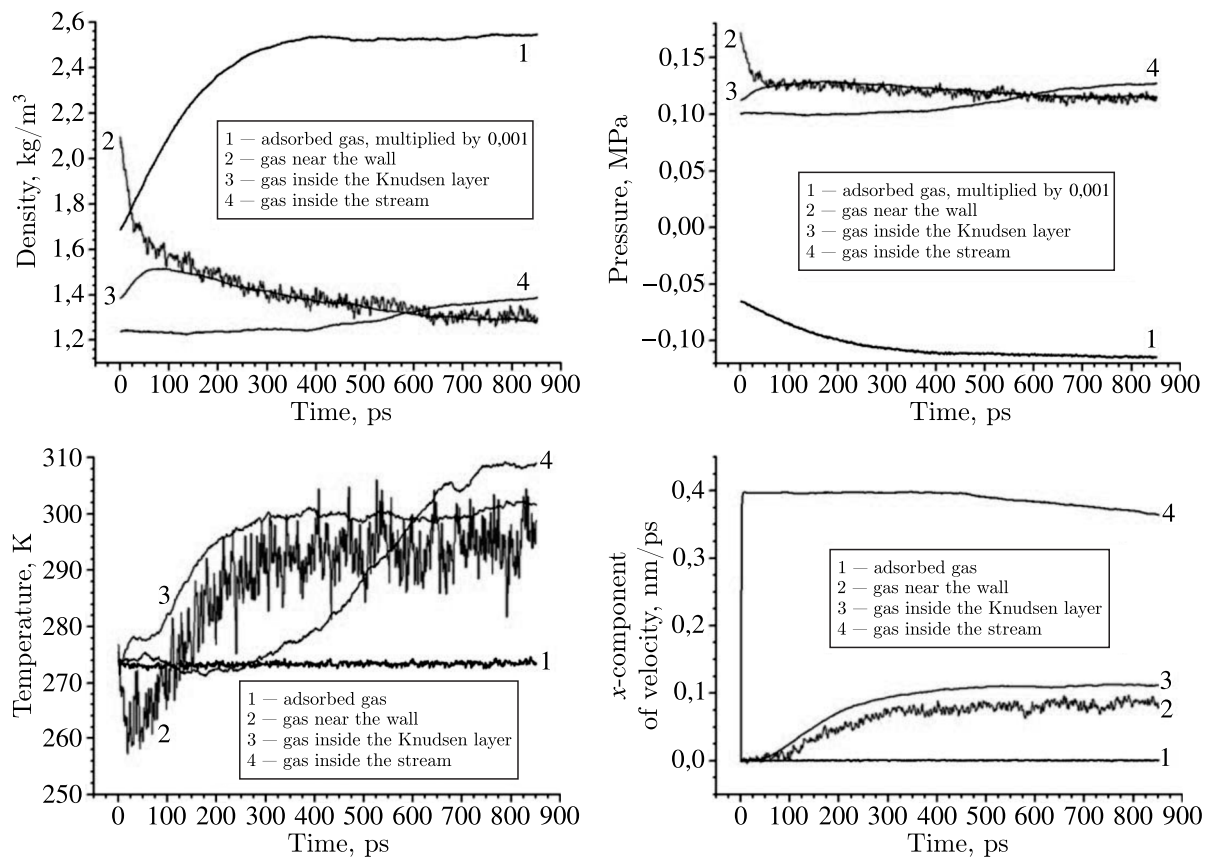


Figure 2. Dynamics of flow parameters averaged over the  $x, y$  coordinates in different sections over  $z$ . Digit 1 corresponds to the layer of gas adsorbed on the metal. Digit 2 corresponds to the layer of free-moving gas nearest to it. Digit 3 corresponds to the Knudsen gas layer. Digit 4 corresponds to the central layer of gas (center of the channel). Curves 1 of density and pressure are multiplied by the value of 0,001

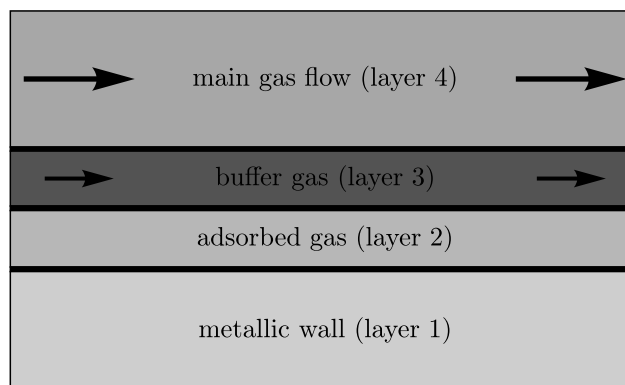


Figure 3. Structure of gas flow near the solid surface

- single-phase gas dynamics (in Navier–Stokes or QGD forms) is considered in the main flow;
- in the buffer gas layer, a calculation is performed based on a multiphase gas-dynamic model, where atoms of the metal surface of the channel, knocked out by the gas flow in the case of a supersonic or hypersonic flow, are considered as the second phase;

- in the adsorbed gas layer on the metal surface, the movement of gas molecules over the surface and heat exchange with the metal surface and the buffer gas are calculated;
- in the metal, the heat propagation is calculated and the mechanical impulse of pressure is released from the gas phase.

To interface the layers with each other, it is proposed to use balance equations that ensure the correct conservation of mass, momentum, and energy in the medium:

$$\begin{aligned} \frac{\partial \rho_{mg}}{\partial n} &= \eta_1(\rho_{bg} - \rho_{mg}), & \frac{\partial \rho_{bg}}{\partial n} &= \eta_2(\rho_{ag} - \rho_{bg}), & \frac{\partial \rho_{ag}}{\partial n} &= \eta_3(\rho_{ag} - \rho_{ag}^*); \\ W_{n,mg}^{(I,-)} &= W_{n,bg}^{(I,+)}, & W_{n,bg}^{(I,-)} &= W_{n,ag}^{(I,+)}, & W_{n,ag}^{(I,-)} &= W_{n,w}^{(I,+)}; \\ W_{n,mg}^{(E,-)} &= W_{n,bg}^{(E,+)}, & W_{n,bg}^{(E,-)} &= W_{n,ag}^{(E,+)}, & W_{n,ag}^{(E,-)} &= W_{n,w}^{(E,+)}. \end{aligned} \quad (10)$$

Here, the letters  $\rho$  denote the gas densities in the corresponding layers, the layers themselves are marked by the indices «mg» (main gas flow), «bg» (buffer gas), «ag» (adsorbed gas), «w» (metal wall),  $\rho_{ag}^*$  is the maximum possible density of the adsorbed gas, determined by the number of vacancies on the metal surface,  $\mathbf{n}$  is the normal to the surface of the layers,  $\eta_k$  is the corresponding mass transfer coefficients,  $W_n^{(I)}$  and  $W_n^{(E)}$  are the normal components of the momentum and energy fluxes density, and the subscripts «-» and «+» denote the left and right limiting values of boundaries of separation of layers.

In the macroscopic representation of the density, the momentum and energy fluxes in the gas phase are determined by the expressions

$$W_n^{(I)} = \rho u_n^2 + p_n, \quad W_n^{(E)} = \rho u_n \left( \frac{|\mathbf{u}|^2}{2} + \varepsilon + \frac{p}{\rho} \right). \quad (11)$$

Here  $\mathbf{u}$  is the velocity vector of the gaseous medium,  $u_n$  is its normal component,  $p_n$  is the normal pressure,  $p$  is the total pressure in the volume, and  $\varepsilon = c_V T$  is the internal energy.

In solid phase, we have the expressions

$$W_n^{(I)} = \sigma_n = (\boldsymbol{\sigma} \mathbf{n}), \quad W_n^{(E)} = -\kappa_w \frac{\partial T_w}{\partial n}. \quad (12)$$

Here  $\boldsymbol{\sigma}$  is the stress tensor at the channel wall boundary,  $T_w$  is the wall temperature, and  $\kappa_w$  is the wall thermal conductivity coefficient.

Expressions (11)–(12) are used in the corresponding boundary equations (10). The unknown parameters of these equations are determined using molecular dynamics calculations. Let us give an example of the refinement of these equations. In continuation of the calculations [Podryga, Polyakov, 2021], in this work, the quasi-equilibrium values of the thermodynamic parameters of the layers indicated in Fig. 3 were calculated by the MD method. For example, for a channel length of  $l = 1000$  nm (variant geometry  $n = 1$ ), the width of the incident flow  $w = 500$  nm,  $Mach = 1,15$ , the following data were obtained:

$$\begin{aligned} \rho_{mg} &\approx 1,289 \text{ kg} \cdot \text{m}^{-3}, & p_{mg} &\approx 0,11396 \text{ МПа}, & T_{mg} &\approx 292,98 \text{ К}, & v_{mg,x} &\approx 383,275 \text{ m} \cdot \text{s}^{-1}; \\ \rho_{bg} &\approx 1,312 \text{ kg} \cdot \text{m}^{-3}, & p_{bg} &\approx 0,11801 \text{ МПа}, & T_{bg} &\approx 292,05 \text{ К}, & v_{bg,x} &\approx 72,912 \text{ m} \cdot \text{s}^{-1}; \\ \rho_{ag} &\approx 185,53 \text{ kg} \cdot \text{m}^{-3}, & p_{ag} &\approx -109,38 \text{ МПа}, & T_{ag} &\approx 273,41 \text{ К}, & v_{ag,x} &\approx 0,32148 \text{ m} \cdot \text{s}^{-1}; \\ \rho_w &\approx 137,14 \text{ kg} \cdot \text{m}^{-3}, & p_w &\approx -134,76 \text{ МПа}, & T_w &\approx 273,23 \text{ К}, & v_{w,x} &\approx 0,00092 \text{ m} \cdot \text{s}^{-1}; \\ \rho_w^* &\approx 8874,61 \text{ kg} \cdot \text{m}^{-3}, & p_w^* &= 0 \text{ МПа}, & T_w^* &\approx 273,15 \text{ К}, & v_{w,x}^* &= 0 \text{ m} \cdot \text{s}^{-1}. \end{aligned} \quad (13)$$

These data show how strongly the gas-dynamic parameters differ in the above layers. Also for comparison, here are given the parameters of nickel in volume (values with the «\*» index). They demonstrate that the density of nickel in the layer of contact with the gas turns out to be significantly lower than its volumetric value. This effect is due to the fact that the gas «stretches» the surface layer of nickel due to the adsorption effect. This is evidenced by negative values of pressure in the adsorbed gas layer and on the metal surface.

The above data make it possible to estimate the unknown constants in the boundary equations (10) for specific thermodynamic parameters of the gas flow. In particular, the methods of calculating the accommodation coefficients [Podryga, Polyakov, 2021] can be used to calculate the coefficients  $\eta_k$  and other unknown constants included in the momentum and energy fluxes densities. By performing a cycle of similar MD calculations, it is also possible to restore the dependence of these constants on temperature and pressure in the required range. After refining all the dependencies, it is possible to carry out calculations at the macroscopic level using the equations of gas dynamics and boundary equations (10) without the use of molecular dynamics methods.

#### 4.2. Results of QGD simulation

To achieve the second aim of our research, we considered the macroscopic description of the problem and used it for microsystem shown in Fig. 4. System sizes are for balloon area –  $L_B = 6 \mu\text{m}$ ,  $R_B = 0,6 \mu\text{m}$ ; for the nozzle –  $L_N = 0,3 \mu\text{m}$ ,  $R_N = 0,1 \mu\text{m}$ ; for the channel –  $L_C = 18 \mu\text{m}$ ,  $R_C = 0,3 \mu\text{m}$ . At start time, the temperature of gas and metal was  $T = 273,15 \text{ K}$ , the velocity was approximately 0, the pressure in balloon was 16 atm. For introducing the equations (10) into QGD system, we integrated (1)–(3) over the cross section of the boundary layer and substitute the corresponding fluxes. As a result, we obtained a spatially one-dimensional approximation of the QGD system for the buffer gas. For the adsorbed gas, we obtained the one-dimensional diffusion convection equation.

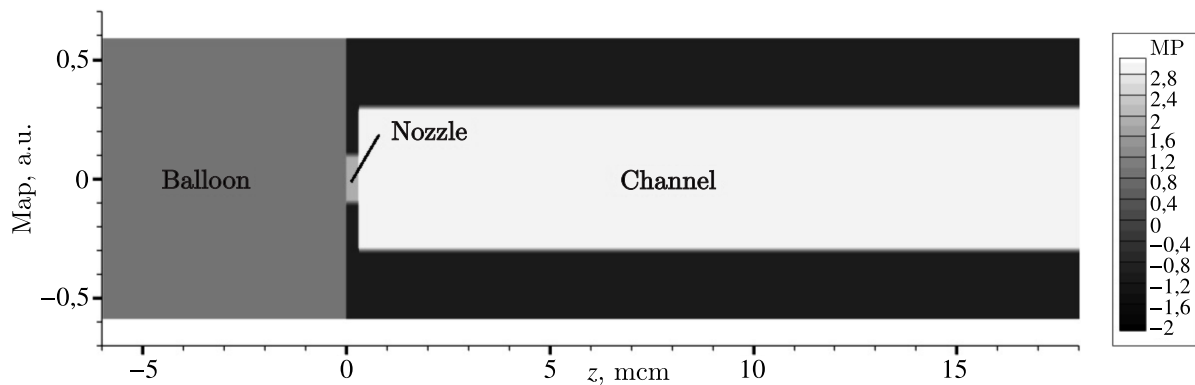


Figure 4. Geometry of microsystem

Figures 5 and 6 consist of the steady state distributions of density, pressure, temperature and longitudinal velocity. These profiles were obtained within the framework of the classical model of boundary conditions. Extension of this model using the integrated conditions (10)–(12) and numerical parameters (13) leads to strong distortions of the flow parameters near the walls (according to our estimates for selected task parameters, up to 15–20% of the average values). The final form of these profiles has not yet been accurately determined, since the process in the boundary layer turns out to be unsteady. In this case, it takes a long time for the entire system to reach a regular flow regime. It can also be noted that, in subsonic flows with low Mach numbers (of the order of 0,1), the differences in the boundary flow regime insignificantly affect the average profile of the longitudinal velocity.

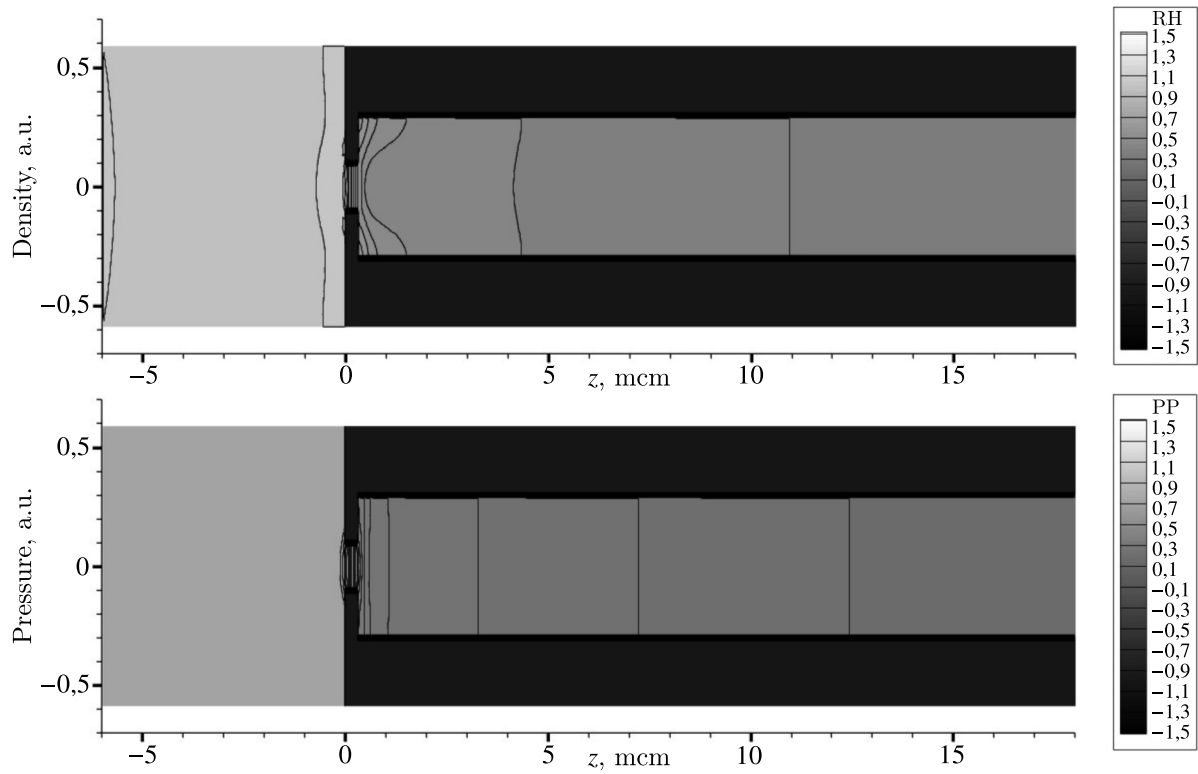


Figure 5. Density and pressure distributions, a.u.

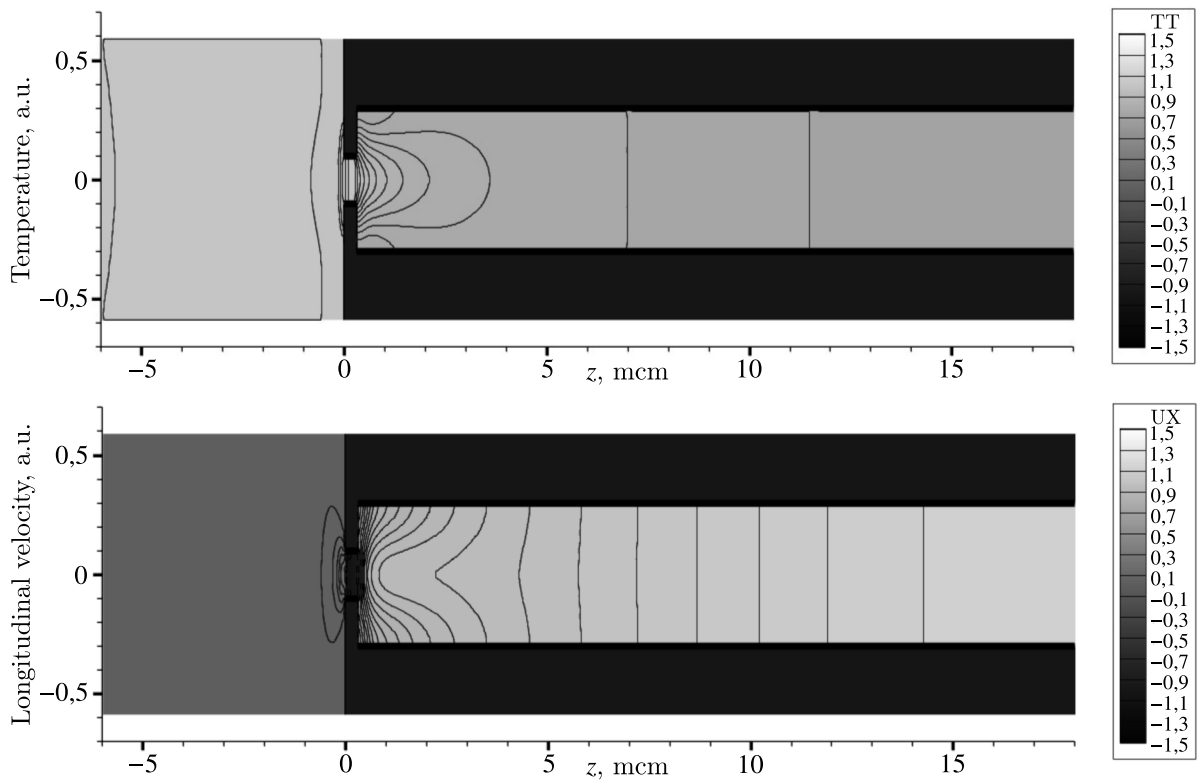


Figure 6. Temperature and longitudinal velocity distributions, a.u.

Summarizing the results of this work, we note that the proposed introduction of molecular modeling data into the macroscopic model makes it possible to more accurately describe both the flow as a whole and the processes in the boundary layer.

## 5. Conclusions

In this work, the problem of modeling the gas flows in microchannels with real geometry and properties of its walls was considered. A multiscale approach was proposed that combined the macroscopic model of a gaseous medium with descriptions of boundary processes at the microlevel using the equations of molecular dynamics. This combination allowed us to describe the processes in the boundary layer more accurately. As an illustration of the developed approach, the nitrogen flow in the nickel microchannel was calculated. The obtained parameters of the gaseous medium near the walls of the microchannel confirm the adequacy of the approach.

## References

- Berendsen H. J. C., Postma J. P. M., Van Gunsteren W. F., DiNola A., Haak J. R.* Molecular dynamics with coupling to an external bath // *J. Chem. Phys.* — 1984. — Vol. 81, No. 8. — P. 3684–3690.
- Berthelot D.* Sur le melange des gaz // *Comptes Rendus de L'Academie des Sciences.* — 1889. — Vol. 126. — P. 1703–1706.
- Chetverushkin B. N.* Kinetic schemes and quasi-gas dynamic system of equations. — Barcelona: CIMNE, 2008.
- Daw M. S., Baskes M. I.* Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals // *Phys. Rev. B.* — 1984. — Vol. 29, No. 12. — P. 6443–6450.
- Elizarova T. G.* Quasi-gas dynamic equations. — Berlin: Springer-Verlag, 2009.
- Elizarova T. G., Zlotnik A. A., Chetverushkin B. N.* On quasi-gas-dynamic and quasi-hydrodynamic equations for binary gas mixtures // *Dokl. Math.* — 2014. — Vol. 90, No. 3. — P. 719–723.
- Eymard R., Gallouet T. R., Herbin R.* The finite volume method // *Handbook of Numerical Analysis.* — Amsterdam: North Holland Publishing Company, 2000. — Vol. 7. — P. 713–1020.
- Fokin L. R., Kalashnikov A. N.* The transport properties of an N<sub>2</sub>–H<sub>2</sub> mixture of rarefied gases in the EPIDIF database // *High Temp.* — 2009. — Vol. 47, No. 5. — P. 643–655.
- Haile J. M.* Molecular dynamics simulation. — New York: Wiley, 1992.
- Heermann D.* Computer simulation methods in theoretical physics. — 2nd ed. — Berlin: Springer-Verlag, 1990.
- Kudryashova T., Karamzin Yu., Podryga V., Polyakov S.* Two-scale computation of N<sub>2</sub>–H<sub>2</sub> jet flow based on QGD and MMD on heterogeneous multi-core hardware // *Adv. Eng. Softw.* — 2018. — Vol. 120. — P. 79–87.
- Lennard-Jones J. E.* Cohesion // *Proc. Phys. Soc.* — 1931. — Vol. 43, No. 5. — P. 461–482.
- Li R., Chen Zh., Wu W.* Generalized difference methods for differential equations. Numerical analysis of finite volume methods. — New York: Marcel Dekker Inc., 2000.
- Lorentz H. A.* Uber die Anwendung des satzes vom virial in der kinetischen theorie der gase // *Ann. Phys.* — 1881. — Vol. 248. — P. 127–136.
- Marchuk G. I.* Metody rasshchepeniia. — Moscow: Nauka, 1988.
- Mie G.* Zur kinetischen theorie der einatomigen korper // *Ann. Phys.* — 1903. — Vol. 11, No. 8. — P. 657–697.
- Podryga V. O.* Calculation of kinetic coefficients for real gases on example of nitrogen // Dimov I., Faragó I., Vulkov L. (eds.) Numerical Analysis and Its Applications. NAA 2016. LNSC. — Cham: Springer, 2017. — Vol. 10 187. — P. 542–549.

- Podryga V. O.* Computational technology of multiscale modeling the gas flows in microchannels // IOP Conf. Ser.: Mater. Sci. Eng. — 2016. — Vol. 158. — P. 012 078. — DOI: 10.1088/1757-899X/158/1/012078
- Podryga V. O., Polyakov S. V.* Molecular dynamics simulation of thermodynamic equilibrium establishment in nickel // Math. Models Comput. Simul. — 2015. — Vol. 7, No. 5. — P. 456–466.
- Podryga V. O., Polyakov S. V.* Molecular dynamic calculation of gas macroparameters in the stream and on the boundary // KIAM Preprints. — 2016. — No. 80.
- Podryga V. O., Polyakov S. V.* Correction of boundary conditions in micromodels by molecular dynamic method // Favorskaya M. N., Favorskaya A. V., Petrov I. B., Jain L. C. (eds.) Smart Modelling for Engineering Systems. Proc. Int. Conf. CMCM 2021, vol 2, Smart Innovation, Systems and Technologies, 2021. — Vol. 215. — P. 9–24. — DOI: 10.1007/978-981-33-4619-2\_2
- Podryga V. O., Polyakov S. V., Puzyrkov D. V.* Supercomputer molecular modeling of thermodynamic equilibrium in gas-metal microsystems // Vychislitel'nye metody i programmirovaniye. — 2015. — Vol. 16, No. 1. — P. 123–138.
- Podryga V. O., Vikhrov E. V., Polyakov S. V.* Molecular dynamic calculation of macroparameters of technical gases by the example of argon, nitrogen, hydrogen, and methane // Math. Models Comput. Simul. — 2020. — Vol. 12, No. 2. — P. 210–220.
- Polyakov S. V.* Exponential difference schemes with double integral transformation for solving convection-diffusion equations // Math. Models Comput. Simul. — 2013. — Vol. 5, No. 4. — P. 338–340.
- Polyakov S. V., Karamzin Yu. N., Kudryashova T. A., Podryga V. O.* New grid approach for solution of boundary problems for convection-diffusion equations // Dimov I., Faragó I., Vulkov L. (eds.). Numerical Analysis and Its Applications. NAA 2016. LNCS. — Cham: Springer, 2017a. — Vol. 10 187. — P. 550–558.
- Polyakov S. V., Karamzin Yu. N., Kudryashova T. A., Tsybulin I. V.* Exponential difference schemes for solving boundary-value problems for diffusion-convection-type equations // Math. Models Comput. Simul. — 2017b. — Vol. 9, No. 1. — P. 71–82.
- Polyakov S., Podryga V., Puzyrkov D., Kudryashova T.* Parallel software for simulation of nonlinear processes in technical microsystems // Voevodin V., Sobolev S. (eds.) Supercomputing. RuSCDays 2016. CCIS. — Cham: Springer, 2016. — Vol. 687. — P. 185–198.
- Polyakov S., Podryga V.* Multiscale multilevel approach to solution of nanotechnology problems // EPJ Web Conf. — 2018. — Vol. 173. — P. 01010. — DOI: 10.1051/epjconf/201817301010
- Rapaport D. C.* The art of molecular dynamics simulation. — Cambridge: Cambridge University Press, 2004.
- Sheretov Yu. V.* Regularized hydrodynamic equations. — Tver: Tver State University, 2016.
- Verlet L.* Computer «experiments» on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules // Phys. Rev. — 1967. — Vol. 159. P. 98–103.
- Zhou X. W., Johnson R. A., Wadley H. N. G.* Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers // Phys. Rev. B. — 2004. — Vol. 69. — P. 144 113. — DOI: 10.1103/PhysRevB.69.144113