

MULTISCALE SIMULATION OF THREE-DIMENSIONAL UNSTEADY GAS FLOWS IN MICROCHANNELS OF TECHNICAL SYSTEMS

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Abstract. *The work is devoted to modeling the gas flows in microchannels of technical systems in conditions of multiscale computational domain. As an example, the problem of nitrogen flow in nickel microchannel for three-dimensional geometry is considered. General attention is paid to the calculation of gaseous medium macroparameters considering the molecular processes that occur in the gas flow and on the walls of the microchannel. The difference in the scales of the computational domain (the length of the channel, cross section of the channel, the free path of the molecules, the thickness of the boundary layer) and near-surface interaction of the gas with the metal lead to the necessity taking into account the relief and the properties of the microchannel at the molecular level. As a result, the mathematical model of the research flow can not be fully formulated within the framework of the macroscopic approach. For decision of the problem multiscale approach combining the solution of a quasigasdynamic (QGD) equations and correction of gasdynamic parameters by molecular dynamics method (MD), is used. QGD system of equations is solved by method of finite volumes. The MD system of equations is applied within each control volume and is solved by Verlet scheme. In MD calculations particles interactions are described by the potentials determining the basic properties of the components of the considered system. Parallel implementation of the approach is based on method of splitting into physical processes and separation of areas. Algorithms are focused on the use of computer systems with central and hybrid architectures. Calculations showed that the overall numerical algorithm is resistant to the use of data for the flow correction obtained by the MD calculations. With the help of MD methods basic coefficient relations for QGD system were obtained, the transitions from MD to QGD and back were checked, three-dimensional calculation of the nitrogen flow in the nickel microchannel was produced. The results confirmed the efficiency of the developed approach.*

1 INTRODUCTION

Present paper is devoted to the description and the parallel program realization of the multiscale approach intended for modeling of nonlinear processes of gas mixture transportation via the technical systems microchannels. The physics for functioning of similar systems is usually described by whole hierarchy of mathematical models descending down to the atomic level. As a result of such association the possibility appears to make an exact predicting the properties of the modeled objects and processes. However at the same time the level of computing complexity of specific tasks significantly increases that becomes surmountable only by using powerful clusters and supercomputers.

As an example the supersonic cold gasdynamic spraying (SCGS) the nanoparticles on a substrate [1] is considered. This problem is relevant for many directions of nanotechnology, including the production of new materials in electronics and medicine. The main technological process in the SCGS installations is called a nanoimprinting, it is accelerating nanoparticles by a supersonic flow and delivering them to the substrate warmed up to the necessary temperature where sticking occurs. Among the various aspects of the problem let's distinguish a transport question that is related to the calculations of gas flow parameters in all parts of the SCGS installation. The purpose of such calculation is to determine the optimum flow conditions.

Features of a transport problem are connected with a spraying installation design. In the simplified look the SCGS installation consists of a Dewar bottle up to several tens liters in lower part of which there is the mobile work desk with a set of replaceable substrates. Over a table there is a subsystem supplying gas and nanoparticles, this subsystem is attached to the top wall of the reservoir. The free space in the reservoir is filled with either technical vacuum, or strongly rarefied gas. The subsystem giving the nanoparticles consists of ballons with pure gas mixture and gas mixture with nanoparticles, of micronozzles matrix and of microchannels on which nanoparticles are fed to a near area of a substrate. Thus a pure gas mixture is used to manage the process, and the gas mixture with nanoparticles is used to give them a start pulse.

From the mathematical point of view the transport problem consists in calculating the gas and nanoparticles motions in all parts of installation. It is necessary to consider that the simulated environment near solid surfaces is not continuous, and the equation of state for gas mixture with nanoparticles is unknown. Modeling of a transport problem in full leads to take into account the real geometry of the SCGS installation and all physical processes proceeding in it in different scales on time and space. It demands too big computing expenses.

Within this work the following combined approach is offered. It combines calculations of the gaseous medium flow in specific microchannels and calculations of interacting the streams with a substrate, and also movements of nanoparticles in a gas flow and their interaction with a substrate at contact with the deposition place. At that simulation is carried out on two scale levels – the basic level having the characteristic sizes from several tens microns to tens of millimeters, and additional level having the characteristic sizes about a micron or less. At the basic level (in macroscale) gas and nanoparticles flows in all parts of installation are calculated, and also the external factors connected with management of spraying process are taken into account. At the additional level (in microscale) the interactions are calculated for: 1) gas molecules among themselves (forming the equation of state for mixture and realizing the mixing of components), 2) gas molecules and solid surfaces atoms (describing phenomena in boundary layers), 3) gas molecules and nanoparticles atoms (describing formation of boundary layers on a surface of nanoparticles), 4) gas molecules and substrate atoms (considering processes of heat exchange with a substrate), 5) atoms of nanoparticles with the substrate atoms (processes of repulsion, sticking, implementation of nanoparticles into substrate).

The specified physical processes are complex and multistage. Therefore at this stage of researches the simplified description of a problem is used. It assumes splitting into physical processes. The main simulation loop represents alternation in time of calculations at the macro- and microlevels. In the represented embodiment of research the calculation of nitrogen - hydrogen mixture flow after leaving the nozzle and exiting to the half-open microchannel and further in free space is considered (Fig. 1).

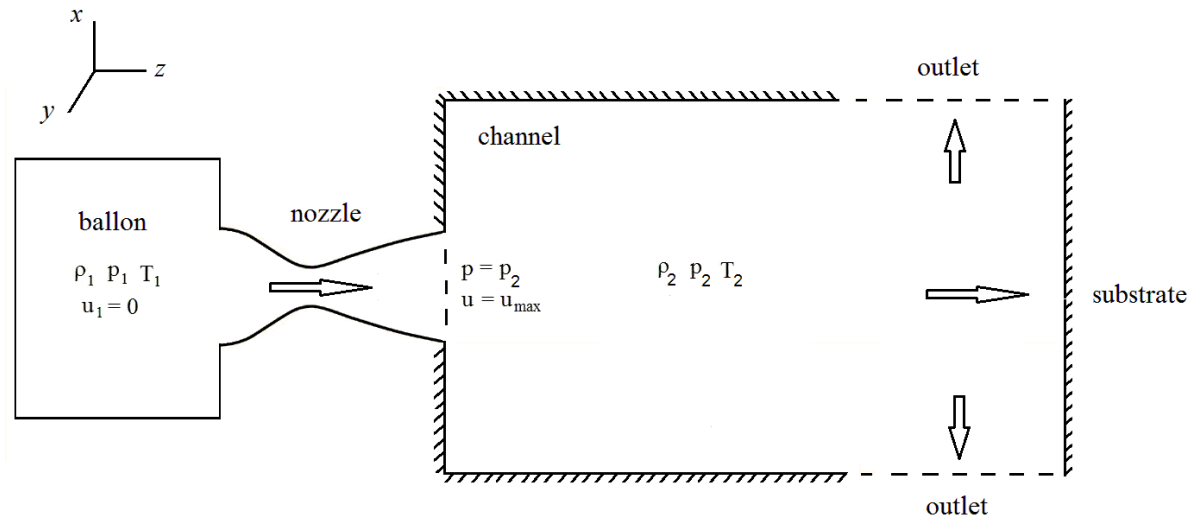


Figure 1: The geometry of a model problem for convenience presented in the form of a two-dimensional section. From a tank through a micronozzle in microchannel the gas mixture is supplied. Gas mixture is used to manage the nanoparticles trajectories for delivering them in the right places of a substrate.

Some part of research has been done in the previous works [2-6]. In particular, in [2-5] methods of thermodynamic equilibrium calculations in metal-metal, gas-gas and gas-metal systems were developed. In work [6] association micro- and macromodels of the gas environment in uniform object of research was proposed and partially approved. The main objective of this research is development of a full three-dimensional multiscale numerical method and parallel algorithm for its realization, suitable for calculating of gas mixture flow in the microchannel and near a substrate taking into account the boundary effects resolved by MD [7]. Description of the model and the algorithm details is given in the following sections.

2 MATHEMATICAL MODELS

2.1 Macroscopic model

The macroscopic model of the flow in all parts of installation is based on the quasigasdynamic (QGD) equations [8]. The choice of QGD equations is associated with two factors. Firstly, QGD equations well proved in calculating supersonic flows of the rarefied viscous and heat-conducting gases. Secondly, they are well suited to calculating the flows in microsystems as the natural parameter of a nondimensionalization in them is the mean free path. Thirdly, QGD system of the equations is applicable in the wide range of Knudsen numbers that gives the chance to model complex system of microchannels with different diameters, using the same mathematical model.

In case of gas mixture the QGD system of equations is written for each gas separately and has an identical form [8-9]. These equations in case of binary mixture in invariant concerning system of coordinates with the constraint and the equations of state have the form:

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

$$\begin{aligned} \frac{\partial}{\partial t} \rho_l u_{l,k} + \operatorname{div} \mathbf{W}_l^{(\rho u_k)} &= S_l^{(\rho u_k)}, \\ \mathbf{W}_l^{(\rho u_k)} &= \rho_l \mathbf{u}_l u_{l,k} + \mathbf{e}_k \left(p_l + \frac{2}{3} \mu_l \operatorname{div} \mathbf{u}_l \right) - \\ &\quad - \mu_l (\nabla u_{l,k} + (\nabla, \mathbf{e}_k) \mathbf{u}_l) - (\rho_l \mathbf{w}_{l,k} \mathbf{u}_l + \rho_l \mathbf{w}_l u_{l,k}), \\ S_l^{(\rho u_k)} &= v_{ll'} \rho_l (u_{l',k}^* - u_{l,k}), \quad l = a, b, \quad l' = b, a, \quad k = x, y, z; \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{\partial}{\partial t} E_l + \operatorname{div} \mathbf{W}_l^{(E)} &= S_l^{(E)}, \\ \mathbf{W}_l^{(E)} &= (\rho_l \mathbf{u}_l - \rho_l \mathbf{w}_l) H_l - \chi_l \nabla T_l + \left(\frac{2}{3} \mu_l \operatorname{div} \mathbf{u}_l \right) \mathbf{u}_l - \\ &\quad - \sum_{k=x,y,z} \mu_l (\nabla u_{l,k} + (\nabla, \mathbf{e}_k) \mathbf{u}_l) + (\rho_l \mathbf{w}_l, \mathbf{u}_l) \mathbf{u}_l, \\ S_l^{(E)} &= v_{ll'} \rho_l (E_{l'}^* - E_l), \quad l = a, b, \quad l' = b, a, \\ E_l &= \frac{1}{2} \rho_l |\mathbf{u}_l|^2 + \rho_l \varepsilon_l, \quad H_l = \frac{E_l + p_l}{\rho_l}, \\ p_l &= Z_l \rho_l \Re_l T_l, \quad \varepsilon_l = c_{V,l} T_l, \quad l = a, b. \end{aligned} \quad (3)$$

$$\begin{aligned} E_l &= \frac{1}{2} \rho_l |\mathbf{u}_l|^2 + \rho_l \varepsilon_l, \quad H_l = \frac{E_l + p_l}{\rho_l}, \\ p_l &= Z_l \rho_l \Re_l T_l, \quad \varepsilon_l = c_{V,l} T_l, \quad l = a, b. \end{aligned} \quad (4)$$

Here we assume that gas mixture consists of a and b gases with numerical densities (concentrations) n_a and n_b and mass densities $\rho_a = m_a n_a$ and $\rho_b = m_b n_b$, where m_a and m_b – masses of gas molecules a and b . Each gas is characterized by its temperature T_l and macroscopic velocity \mathbf{u}_l . Other parameters of mixture components: p_l – partial pressures, E_l – total energy densities, ε_l – specific internal energies, H_l – total enthalpies, $\mu_l = \mu_l(T_l)$ and $\chi_l = \chi_l(T_l)$ – coefficients of viscosity and heat conduction, $Z_l = Z_l(T_l)$ – compressibility coefficients, $c_{V,l} = c_{V,l}(T_l)$ – specific heat capacities at constant volume, $\Re_l = k_B / m_l$ – gas constants (k_B – Boltzmann constant). Vectors $\mathbf{W}_l^{(\rho)}$, $\mathbf{W}_l^{(\rho u_k)}$, $\mathbf{W}_l^{(E)}$ up to a sign are identical to the density flux of the corresponding components of the momentum density and energy density, $\rho_l \mathbf{w}_l$ – QGD correction vectors to the density flux, that are proportional to the Maxwell relaxation time τ for gas mixtures, \mathbf{e}_k – unit vectors.

The exchange members $S_l^{(\rho u_k)}$ and $S_l^{(E)}$ take into account the redistribution of momentum and energy between the mixture components. They contain components of velocity \mathbf{u}_l^* and energy E_l^* , calculated at the molecular level (see Section 2.2), as well as $v_{ll'}$ – frequency of mutual collisions between molecules of variety l with molecules of variety l' , which are calculated via v_l – frequency of mutual collisions between the molecules of one type:

$$v_{ab} = v_a \left(\frac{d_{ab}}{d_a} \right)^2 \sqrt{\frac{m_a + m_b}{2m_b} \frac{n_b}{n_a}}, \quad v_{ba} = v_{ab} \frac{n_a}{n_b} = v_b \left(\frac{d_{ab}}{d_b} \right)^2 \sqrt{\frac{m_a + m_b}{2m_a} \frac{n_a}{n_b}},$$

$$d_{ab} = \frac{d_a + d_b}{2}, \quad v_l = \frac{p_l}{\mu_l} \Omega_l, \quad l = a, b.$$

where d_l – molecules diameters of variety l , Ω_l – dimensionless parameters characterizing the collision molecules of type l [10].

Coefficients of viscosity μ_l , heat conduction χ_l and compressibility Z_l , and the specific heats $c_{v,l}$ and the mean free path λ_l for the mixture components are determined from a database of molecular calculations or by direct MD computations (see Section 2.2). The local sound velocities for the mixture components are calculated according to the formulas:

$$a_l = \sqrt{\gamma_l Z_l \Re_l T_l}, \quad \gamma_l = 1 + \frac{\Re_l}{c_{v,l}}, \quad l = a, b,$$

where $\gamma_l = \gamma_l(T_l)$ – adiabatic indexes.

The parameters of the gas mixture at macrolevel are defined as follows:

$$\rho = \rho_a + \rho_b, \quad \mathbf{u} = \frac{\rho_a \mathbf{u}_a + \rho_b \mathbf{u}_b}{\rho}, \quad p = p_a + p_b, \quad E = E_a + E_b, \quad n = n_a + n_b,$$

$$T = \frac{n_a Z_a T_a + n_b Z_b T_b}{nZ}, \quad m = \frac{m_a n_a + m_b n_b}{n}, \quad Z = Z_a + Z_b, \quad \Re = \frac{p}{\rho Z T} = \frac{k_B}{m}, \quad \tau = \frac{\mu}{p}.$$

To determine the viscosity of the mixture we use the Buddenberg-Wilke formula [11]:

$$\mu = \mu_a \left(1 + G_{ab} \frac{\rho_b}{\rho_a} \frac{M_a}{M_b} \right)^{-1} + \mu_b \left(1 + G_{ba} \frac{\rho_a}{\rho_b} \frac{M_b}{M_a} \right)^{-1},$$

$$G_{ab} = \left(1 + \sqrt{\frac{\mu_a}{\mu_b}} \sqrt{\frac{M_b}{M_a}} \right)^2 \left(2 \sqrt{2 \left(1 + \frac{M_a}{M_b} \right)} \right)^{-1}.$$

Here M_a and M_b – molar masses of gases a and b . Value G_{ba} is calculated similarly by cyclic substitution of the indexes. The average local sound velocity, and the mean free path, the Mach number and the Reynolds number for the mixture are equal to:

$$a = \frac{m_a a_a + m_b a_b}{m_a + m_b}, \quad \lambda = \frac{m_a \lambda_a + m_b \lambda_b}{m_a + m_b}, \quad Ma = \frac{|\mathbf{u}|}{a}, \quad Re = \frac{\rho |\mathbf{u}| \lambda}{\mu}.$$

The system of equations (1)-(3) is closed initial and boundary conditions. The initial conditions correspond to the equilibrium gas environment in the absence of interaction with external factors:

$$\rho_l = \rho_{l,0}, \quad \mathbf{u}_l = 0, \quad p_l = p_{l,0}, \quad T_l = T_0, \quad l = a, b.$$

Here $\rho_{l,0}$, $p_{l,0}$ – the initial densities and pressures of gas components, T_0 – initial temperature.

The area of a nozzle and a tank with gas mixture were not included into calculation. It was assumed that in an initial time the partition between the nozzle and the area of the microchannel opened, and gas from area of a high pressure began to come to the area of low

pressure. The nozzle was considered as an ideal adiabatic Laval nozzle. Parameters of the gas environment at the exit from a nozzle (that is on an entrance to the medium) were calculated according to the known formulas:

$$\begin{aligned} (\mathbf{u}_l, \mathbf{n}) &= u_{in,l}, \quad \rho_l = \rho_{in,l}, \quad T_l = T_{in,l}, \quad l = a, b; \\ p_{in,l} \left(m_l Z_l(T_{in,l}) \Re_l T_{in,l} / p_{in,l} \right)^{\gamma_l(T_{in,l})} &= p_{bal,l} \left(m_l Z_l(T_{bal,l}) \Re_l T_{bal,l} / p_{bal,l} \right)^{\gamma_l(T_{bal,l})}, \\ u_{in,l} &= \sqrt{2(H_{bal,l} - H_{in,l})}, \quad \rho_{in,l} = p_{in,l} / Z_l(T_{in,l}) \Re_l T_{in,l}, \\ H_{bal,l} &= (c_{v,l}(T_{bal,l}) + Z_l(T_{bal,l}) \Re_l) T_{bal,l}, \quad H_{in,l} = (c_{v,l}(T_{in,l}) + Z_l(T_{in,l}) \Re_l) T_{in,l}. \end{aligned} \quad (11)$$

Here the parameters with index *bal* correspond to the values of parameters in the tank, and the parameters with index *in* – the respective parameters on the entrance to the environment.

At the microchannel walls and on the substrate following boundary conditions are imposed:

$$\begin{aligned} (\mathbf{W}_l^{(\rho)}, \mathbf{n}) &= -\alpha_l (\rho_l - \rho_l^{(w)}), \quad (\mathbf{W}_l^{(\rho u_k)}, \mathbf{n}) = -\beta_{l,k} (\rho_l u_{l,k} - \rho_{l,w} u_{l,k}^{(w)}), \quad k = x, y, z, \\ (\mathbf{W}_l^{(E)}, \mathbf{n}) &= -\eta_l (E_l - E_l^{(w)}), \quad l = a, b. \end{aligned} \quad (12)$$

Generally the gas molecules can get into a metal wall, or be reflected from it at some corner. Interaction with a wall can be elastic or inelastic, thermal or isothermal. It is convenient near a wall to enter the special microsystem consisting of gas molecules and metal atoms. In this microsystem gas components have densities of masses $\rho_l^{(w)}$, moments $\rho_l^{(w)} \mathbf{u}_l^{(w)}$ and total energy $E_l^{(w)}$. Boundary conditions on a wall can be written down in the form of third-type boundary conditions describing an exchange of mass, momentum and energy components between the gas mixture in the flow and near the walls. Coefficients α_l , $\beta_{l,k}$ and η_l , associated with accommodation coefficients [12], The coefficients associated with the coefficients accommodation are priori unknown but can be determined from either physical quantities tables (which is possible only to a limited range of temperatures and pressures), or can be calculated using molecular dynamics. The second approach seems the most justified as it is universal and will help to coordinate the interaction processes on micro- and macrolevels.

On the free surfaces a "soft" boundary conditions are given [8]:

$$\frac{\partial \rho_l}{\partial n} = 0, \quad \frac{\partial (\rho_l \mathbf{u}_l)}{\partial n} = 0, \quad \frac{\partial p_l}{\partial n} = 0, \quad l = a, b. \quad (13)$$

In the case of pumping the mixture out of the system in (13) the minimum pressure is given instead of the last condition: $p_l = p_{\min}$.

2.2 Microscopic model

The microscopic model can be used for various purposes. First, it can help to clarify the equation of state (both on pressure, and on energy) and kinetic coefficients (viscosity, heat conduction, diffusion, etc.) used in QGD equations. Secondly, the microscopic model can be used to calculate the exchange members in the equations for momentum and energy. Thirdly, the microscopic model is especially demanded in calculation of the wall interactions of gas molecules with walls atoms. In this work all listed above situations are considered.

In a case when at the macrolevel the flow of the binary gas mixture without nanoparticles is calculated, at the microlevel it is also possible to be limited to consideration the molecules of two types *a* and *b*. However it is only valid far from the walls of the microchannel. Near

the walls it is necessary to add to consideration the particles of type c , making a material of walls. In the presence of nanoparticles it is necessary to add to consideration the particles of other types.

In this work we consider the case of pure binary mixture and one type of metal particles. Then at the microlevel the gas-metal system is represented as a set of particles which behavior is described by Newton's equations [7]:

$$m_{l,i} \frac{d\mathbf{v}_{l,i}}{dt} = \mathbf{F}_{l,i}, \quad \mathbf{v}_{l,i} = \frac{d\mathbf{r}_{l,i}}{dt}, \quad i=1, \dots, N_l, \quad l=a, b, c, \quad (14)$$

where i – particle number, $l=a, b, c$ – particle type (a – molecules of first gas, b – molecules of second gas, c – metal atoms), N_l – total particles number of type l , $m_{l,i}$ – particle mass of type l with number i , $\mathbf{r}_{l,i} = (r_{x,l,i}, r_{y,l,i}, r_{z,l,i})$ and $\mathbf{v}_{l,i} = (v_{x,l,i}, v_{y,l,i}, v_{z,l,i})$ – position vector and velocity vector of the i -th particle of type l , $\mathbf{F}_{l,i} = (F_{x,l,i}, F_{y,l,i}, F_{z,l,i})$ – the total force acting on a this particle.

The forces are the sum of the component of i -th particle interaction with the surrounding particles and the component responsible for external action:

$$\mathbf{F}_{l,i} = -\frac{\partial U(\mathbf{r}_{l,1}, \dots, \mathbf{r}_{l,N_l})}{\partial \mathbf{r}_{l,i}} + \mathbf{F}_{l,i}^{ext}, \quad i=1, \dots, N_l, \quad l=a, b, c, \quad (15)$$

where U – total potential energy, $\mathbf{F}_{l,i}^{ext}$ – force of interaction with the environment.

Potential energy of the system depends on particles coordinates and describes the interaction between them. The choice of interaction potential is based on comparison of mechanical properties of potential model and real material. For the solution of an objective it is necessary to consider interactions gas-gas, metal-metal and gas-metal:

$$\begin{aligned} U &= U_{aa} + U_{bb} + U_{cc} + U_{ab} + U_{ac} + U_{bc}, \\ U_{aa} &= \sum_{i=1, j>i}^{N_a} \varphi_{aa}(|\mathbf{r}_{a,i} - \mathbf{r}_{a,j}|), \quad U_{bb} = \sum_{i=1, j>i}^{N_b} \varphi_{bb}(|\mathbf{r}_{b,i} - \mathbf{r}_{b,j}|), \\ U_{cc} &= \sum_{i=1}^{N_c} \left[\varphi_{1,cc}(\mathbf{r}_{c,i}) + \sum_{j>i} \varphi_{2,cc}(|\mathbf{r}_{c,i} - \mathbf{r}_{c,j}|) \right], \quad U_{ab} = \frac{1}{2} \sum_{i=1}^{N_a} \sum_{j=1}^{N_b} \varphi_{ab}(|\mathbf{r}_{a,i} - \mathbf{r}_{b,j}|), \\ U_{ac} &= \frac{1}{2} \sum_{i=1}^{N_a} \sum_{j=1}^{N_c} \varphi_{ac}(|\mathbf{r}_{a,i} - \mathbf{r}_{c,j}|), \quad U_{bc} = \frac{1}{2} \sum_{i=1}^{N_b} \sum_{j=1}^{N_c} \varphi_{bc}(|\mathbf{r}_{b,i} - \mathbf{r}_{c,j}|). \end{aligned} \quad (16)$$

Each type of interaction is described by a corresponding potential $\varphi_{ll'}$. For hydrogen-nitrogen mixture it was used Mi's potential in the form of "n-6" [13] adapted in work [14] to calculations of hydrogen and nitrogen mixture depending on their volume ratio in the allocated microvolume. For interaction of nickel atoms among themselves it was used the form of EAM [15] potential which considers not only pair interactions $\varphi_{2,cc}$, but also the impact of the environment on a particular particle $\varphi_{1,cc}$. To account the gas-metal interactions a standard potential Lennard-Jones [16] and Morse potential [17] were used.

The calculation of the compressibility factor and heat capacity is described in detail in [4]. The coefficients of viscosity and heat conduction were calculated according to the formulas [18]:

$$\begin{aligned}
\mu_l &= \frac{1}{k_B T_l V} \int_0^\infty \langle (p_{\alpha\beta,l}(t_0+t) \cdot p_{\alpha\beta,l}(t_0)) \rangle dt, \quad \alpha\beta = xy, yz, zx, \quad l = a, b, \\
p_{\alpha\beta,l} &= \sum_i m_{l,i} \cdot v_{\alpha,l,i} \cdot v_{\beta,l,i} + \sum_i \sum_{j>i} (r_{\alpha,l,i} - r_{\alpha,l,j}) \cdot (F_{\beta,l,i} - F_{\beta,l,j}), \quad i, j = 1 \dots N_l, \\
\chi_l &= \frac{1}{k_B T_l^2 V} \int_0^\infty \langle q_{\alpha,l}(t_0+t) \cdot q_{\alpha,l}(t_0) \rangle dt, \quad \alpha = x, y, z, \\
q_{\alpha,l} &= \frac{d\delta\varepsilon_{\alpha,l}}{dt}, \quad \delta\varepsilon_{\alpha,l} = \sum_i r_{\alpha,l,i} (\varepsilon_{l,i} - \langle \varepsilon_{l,i} \rangle), \quad \varepsilon_{l,i} = \frac{m_l v_{l,i}^2}{2} + \frac{1}{2} \sum_{j \neq i}^N \varphi_{ll}(|\mathbf{r}_{l,i} - \mathbf{r}_{l,j}|),
\end{aligned} \tag{17}$$

where V – volume of the investigated system, $\varepsilon_{l,i}$ – instantaneous total energy of molecule i of type l , t_0 – initial time in calculating the coefficients.

The mean free path is calculated according to the formulas [19]:

$$\lambda_a = \frac{1}{n_a \pi d_a^2 \sqrt{2} + n_b \pi d_{ab}^2 \sqrt{1 + \frac{m_a}{m_b}}}, \quad \lambda_b = \frac{1}{n_b \pi d_b^2 \sqrt{2} + n_a \pi d_{ab}^2 \sqrt{1 + \frac{m_b}{m_a}}}, \tag{18}$$

where σ_l – effective interaction radius of molecules of type l [14].

The initial conditions at the microlevel are defined by an equilibrium thermodynamic state of particles system. Calculations of gas environment usually start with normal conditions or at first it is reduced to thermodynamic equilibrium at a given temperature and pressure. Metal parts of a microsystem must have at the start the lattice structure according to metal at given temperature. They should be no excessive stress. For more information about calculating the equilibrium state in metal-metal, gas-gas and gas-metal microsystems see the works [2-5].

The boundary conditions at the molecular level are selected depending on the simulated situation. In particular, when calculations are aimed on determining the properties of the medium, a certain allocated three-dimensional its volume is considered, out of which the periodic continuation medium unlimited distances in all three spatial directions is assumed. In this case, periodic boundary conditions are used [7].

If the calculations are made of real geometry microsystem, the one or more directions have a finite size. In this case as boundary conditions can be used or mirror boundary conditions (when particles interact with the specular reflection and don't leave thereof abroad), or a free exit of particles on one side of the allocated volume and an entrance of a particles flow – on another. For metal microsystems it is also characterized total absence of boundary conditions which are complied in a view of the forces of a mutual attraction of atoms in a metal lattice.

In this work both periodic, and mirror boundary conditions, and also an entrance of a particles flow in environment and a free exit of particles from it were used. In addition separate parts of Microsystems were thermostatted [20, 21].

3 REALIZATION

Realization of the developed multiscale approach relied on the numerical algorithm based on splitting into physical processes and using grid approximations of QGD equations (1)-(3) and subgrid calculations on the Newtonian dynamics equations (14)-(16).

The algorithm is as follows. In an initial time on the chosen grid the equilibrium condition of a macrosystem is given (10). If it is necessary near the borders of computational area equilibrium condition of gas and metal microsystems is also given.

Further on each time step predictor calculation of gas components macroparameters on grid analogs of QGD equations (1)-(3) without exchange members is made at first (QGD program block). As a result of calculation new gas components macroparameters in each control volume of a spatial grid are defined.

Then the subgrid MD computation in order to calculate the exchange members and kinetic coefficients is performed (MD program block). It is carried out independently in each control volume (cell) of a grid and produced with significantly smaller time step connected with evolution of a molecular subsystem. Criterion for stopping the MD calculation is or to achieve characteristic evolution time of molecular system, or change (for 1-2%) one or several macroparameters of molecular system (averages momentum, kinetic or potential energy). If strong changes of macroparameters don't happen, then the calculation is performed to achieve some predetermined points in time proportional to the Maxwellization time of MD system. Also in MD block the return to macroscopic level is carried out and correction of momentum densities and total energy densities is calculated by means of the computed exchange members. Correction is performed in each point of a grid. MD calculation process is finalized by calculations of kinetic coefficients and the equation of state. Thus, communication of macro- and microlevels in grid spatial and temporal areas is carried out by alternately recalculation of macroparameters on QGD and MD equations.

In case of nanoparticles presence in the flow the third block of calculations (NP program block) is used. In NP block it is decided or the convection-diffusion equations for concentration of nanoparticles of each type (this situation is considered for a case of small nanoparticles), or Newton's equations for the ballistic transport of nanoparticles (in the case of large nanoparticles). In this paper, that part of calculations is not considered.

The described part of algorithm is completed with check the criterion of the calculations end and transition to the following step on time in case of non-performance of criterion.

3.1 Finite volume scheme for QGD equations

The grid numerical method having a finite-volume method in the basis is used for calculation the macroparameters on QGD equations [22-24]. For this in the computational domain D the spatial grid Ω_D with cells C_m ($m=1, \dots, M$) and time grid ω_t with variable step Δt was introduced. Grid Ω_D in general is a hybrid, that is, it includes several element types: tetrahedrons, pentahedrons, hexahedrons, octahedrons and heptahedrons.

All parameters of gas components (density, pressure, temperatures, velocity vector components, etc.) have been carried to the centers of mass of grid elements, that is to the centers of cells. Stream variables have been set in the centers of cells sides. Spatial approximations of the main members have been executed by the technique presented in work [25]. The computing scheme on time was obvious. The resulting grid equations at a predictor stage have an appearance:

$$\begin{aligned}\hat{\rho}_{l,m} &= \rho_{l,m} + \frac{\Delta t}{|V_m|} \sum_{p=1}^{M_m} W_{l,n,m,p}^{(\rho)} |S_{m,p}|, \quad W_{l,n,m,p}^{(\rho)} = (\mathbf{W}_{l,m,p}^{(\rho)}, \mathbf{n}_{m,p}), \\ \hat{\rho}_{l,m} \hat{u}_{l,k,m} &= \rho_{l,m} u_{l,k,m} + \frac{\Delta t}{|V_m|} \sum_{p=1}^{M_m} W_{l,n,m,p,k}^{(\rho u)} |S_{m,p}|, \quad W_{l,n,m,p,k}^{(\rho u)} = (\mathbf{W}_{l,m,p}^{(\rho u_k)}, \mathbf{n}_{m,p}), \quad k = x, y, z, \quad (19) \\ \hat{E}_{l,m} &= E_{l,m} + \frac{\Delta t}{|V_m|} \sum_{p=1}^{M_m} W_{l,n,m,p}^{(E)} |S_{m,p}|, \quad W_{l,n,m,p}^{(E)} = (\mathbf{W}_{l,m,p}^{(E)}, \mathbf{n}_{m,p}), \quad m = 1, \dots, M, \quad l = a, b.\end{aligned}$$

Here f_m, \hat{f}_m – values of the corresponding functions on the lower and upper layers in time in the center of the control volume V_m (coinciding into effect of the selected approximation with grid cell C_m), $|V_m|$ – value of the control volume V_m , $|S_{m,p}|$ – faces squares $S_{m,p}$ of the control volume V_m , M_m – faces number of the control volume V_m , $W_{n,m,p}^{(\alpha)}$ – scalar multiplication of flux $\mathbf{W}_{m,p}^{(\alpha)}$ via face $S_{m,p}$ on the external normal $\mathbf{n}_{m,p}$ to this face ($\alpha = \rho, \rho u_x, \rho u_y, \rho u_z, E$). Fluxes approximations $\mathbf{W}_{m,p}^{(\alpha)}$ are similar to the proposals in [25], but do not use artificial viscosity.

Obtained predictor variables $\hat{\rho}_l, \hat{\rho}_l \hat{\mathbf{u}}_l, \hat{E}_l$ are transmitted in MD block. Modified parameters $\hat{\rho}_l \hat{\mathbf{u}}_l^*$ and \hat{E}_l^* are calculated in the result of its work. According to it the final values of momentum $\hat{\rho}_l \hat{\mathbf{u}}_l^{**}$ and energies \hat{E}_l^{**} densities are calculated:

$$\begin{aligned} \hat{\rho}_{l,m} \hat{\mathbf{u}}_{l,k,m}^{**} &= \hat{\rho}_l \hat{\mathbf{u}}_{l,k,m}^* + \Delta t \mathbf{v}_{ll'} \hat{\rho}_{l,m} (\hat{\mathbf{u}}_{l,k,m} - \hat{\mathbf{u}}_{l,k,m}^*), \quad k = x, y, z, \\ \hat{E}_{l,m}^{**} &= \hat{E}_{l,m}^* + \Delta t \mathbf{v}_{ll'} \hat{\rho}_{l,m} (\hat{E}_{l,m} - \hat{E}_{l,m}^*), \quad m = 1, \dots, M, \quad l = a, b, \quad l' = b, a. \end{aligned} \quad (20)$$

By the received in MD block macroparameters all the kinetic coefficients (μ_l, χ_l), the mean free path λ_l and the parameters in the equations of state $Z_l, c_{v,l}$ are calculated.

3.2 Algorithm for solving Newton's equations

The equation system (15) - (17) is solved by the Velocity Verlet algorithm [26]:

$$\begin{aligned} 0) \quad \mathbf{F}_{l,i}^0 &= \mathbf{F}(\mathbf{r}_{a,1}^0, \dots, \mathbf{r}_{a,N_a}^0; \mathbf{r}_{b,1}^0, \dots, \mathbf{r}_{b,N_b}^0; \mathbf{r}_{c,1}^0, \dots, \mathbf{r}_{c,N_c}^0), \quad i = 1, \dots, N_l, \quad l = a, b, c; \\ \forall n &= 0, 1, 2, \dots; \\ 1) \quad \mathbf{r}_{l,i}^{n+1} &= \mathbf{r}_{l,i}^n + \mathbf{v}_{l,i}^n \Delta t + \frac{\mathbf{F}_{l,i}^n (\Delta t)^2}{2m_l}, \quad i = 1, \dots, N_l, \quad l = a, b, c; \\ 2) \quad \mathbf{F}_{l,i}^{n+1} &= \mathbf{F}(\mathbf{r}_{a,1}^{n+1}, \dots, \mathbf{r}_{a,N_a}^{n+1}; \mathbf{r}_{b,1}^{n+1}, \dots, \mathbf{r}_{b,N_b}^{n+1}; \mathbf{r}_{c,1}^{n+1}, \dots, \mathbf{r}_{c,N_c}^{n+1}), \quad i = 1, \dots, N_l, \quad l = a, b, c; \\ 3) \quad \mathbf{v}_{l,i}^{n+1} &= \mathbf{v}_{l,i}^n + \frac{\mathbf{F}_{l,i}^{n+1} + \mathbf{F}_{l,i}^n}{2m_l} \Delta t, \quad i = 1, \dots, N_l, \quad l = a, b, c. \end{aligned} \quad (21)$$

Here Δt – integration step, n – step number, $\mathbf{F}_{l,i}^n$ – force value on step n , \mathbf{F} – procedure for calculating the forces based on formulas (15), (16).

Berendsen thermostat [20] is used to achieve the desired temperatures of gas and metal. Langevin thermostat [21] is used to achieve the desired temperature and momentum of gas.

3.3 Parallel realization

Parallel realization of algorithm assumes using the cluster (or a supercomputer) with the central or hybrid architecture having on each node several multicore central processing units (CPU), and also several vector or graphic processing units (VPU or GPU). Parallelization of algorithm is made on the principles of geometrical parallelism and separating the areas. The main gasdynamic calculation is performed on discrete QGD equations on the grid distributed between cluster nodes by using technique "domain decomposition" [27]. Inside the QGD node

the computations are distributed between CPU threads. Subgrid MD computations are assigned to the CPU or VPU, or GPU, in its presence. Distribution of QGD calculations between CPU threads is also made geometrically. Parallelization of MD computations is made by partition of entire particles set relating to one cell of a grid on groups of identical power (explicitly these calculations were represented in [5]). Each unit of CPU or VPU, or GPU threads processes one or several molecular groups relating to one or several grid nodes. Program implementation of algorithm is executed on the hybrid technology [28] using MPI [29], OpenMP [30] and CUDA [31].

4 NUMERICAL EXPERIMENTS

For approbation of the developed approach the following preliminary testing was held. As computational domain the microchannel of rectangular section with sizes $15 \times 15 \times 90 \mu\text{m}^3$ and with rectangular hole for nozzle of the diffuser with sizes $3 \times 3 \mu\text{m}^2$ was selected (see Fig. 2). The channel ended with an output in the free space, however in it the flow wasn't calculated any more. Pure nitrogen was considered as gas. Nickel was considered as the walls material.

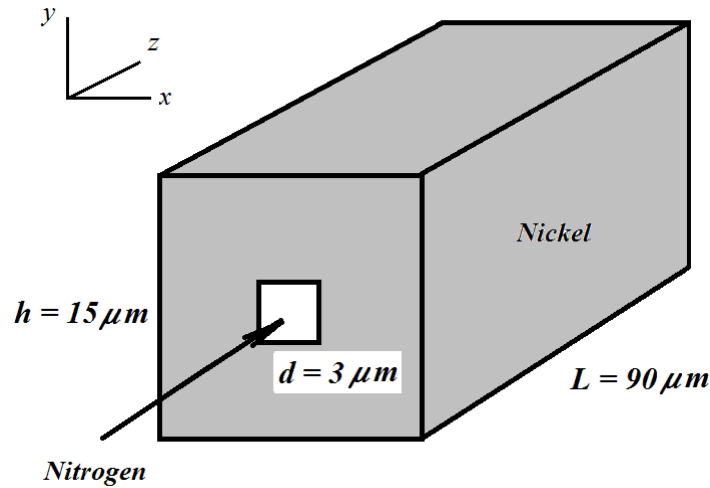


Figure 2: The model calculated area.

In a given computational domain uniform Cartesian grid, consisting of a cubic cells was constructed. The starting grid $\Omega^{(0)}$ had $M_v^{(0)} = 15 \times 15 \times 90 = 20250$ cells of linear size $a^{(0)} = 1 \mu\text{m}$. Subsequent grid was obtained by grinding the cells of previous grid on 8 parts (by 2 times in each direction). As a result, grid $\Omega^{(k)}$ had $M_v^{(k)} = M_v^{(0)} 8^k$ cells. The volume of each cell in such grid is equal to $|V_m^{(k)}| = (a^{(k)})^3 \mu\text{m}^3$. The number of cells abutting to the side surface of calculated area excluding the input and output holes for grid $\Omega^{(k)}$ amounts to $M_s^{(k)} = 5400 \times 4^k + 216 \times 2^k$. Values $M_v^{(k)}$ and $M_s^{(k)}$ define the computing capacity of the developed algorithm. What they are bigger the more computing capacity of QGD block and less computing capacity of MD program block it is needed. We show this by example.

If the metal surface of the channel is described by a single repulsive potential without regard to its actual structure, we can restrict the following arguments. In each cell $C_m^{(0)}$ of starting grid $\Omega^{(0)}$ (having the volume $|V_m^{(0)}| = 1 \mu\text{m}^3$) at normal conditions ($p = 101325 \text{ Pa}$,

$T = 273.15\text{ K}$) there is a number of nitrogen molecules that is equal to $N_{part}^{(0)} = N_A |V_m^{(0)}| V_\mu^{-1} \approx 2.6867811 \times 10^7$ ($N_A \approx 6.022140857 \times 10^{23} \frac{1}{mol}$ – Avogadro's number,

$V_\mu \approx 22.413962 \times 10^{15} \frac{\mu m^3}{mol}$ – mole volume gas at normal conditions). This amount is suffi-

cient to obtain a representative statistics at MD calculations, however, too much for the actual calculations. Therefore, in the long-term calculations it is better to use a more detailed grid containing a larger number of cells, but with a smaller volume of single cell and comprising a smaller number of particles in it (see Table 1). The analysis shows that the optimal ratio of grid cells and particles in one cell of the grid is achieved for the grid $\Omega^{(3)}$. If the initial pressure in the channel is 0.001 atm, the starting number of gas molecules in the cell decreases to 52. This amount is insufficient for correct usage of local MD calculations within a single cell. Therefore, in areas of low pressure it is necessary to increase linear size of the cell the expense of neighboring cells. The particles number is calculated on the basis of densities values in the considered and the neighboring cells:

$$\bar{N}_{l,i,j,k} = \sum_{i',j',k'=-m,\dots,+m} \frac{\rho_{l,i+i',j+j',k+k'}}{m_l} |V_{i+i',j+j',k+k'}|, \quad |\bar{V}_{i,j,k}| = \sum_{i',j',k'=-m,\dots,+m} |V_{i+i',j+j',k+k'}|, \quad l = a, b, \quad (22)$$

where $m = 0, 1, 2, \dots$ – the number of neighboring cells for each positive direction, which should be considered in the MD calculations.

| k | $M_V^{(k)}$ | $M_S^{(k)}$ | $a^{(k)}, \mu m$ | $ V_m^{(k)} , \mu m^3$ | $N_{part}^{(k)}$ |
|-----|-------------|-------------|------------------|------------------------|------------------|
| 0 | 20 250 | 5 616 | 1 | 1 | 26 867 811 |
| 1 | 162 000 | 22 032 | 0.5 | 0.125 | 3 358 476 |
| 2 | 1 296 000 | 87 264 | 0.25 | 0.015625 | 419 810 |
| 3 | 10 368 000 | 347 328 | 0.125 | 0.001953125 | 52 476 |
| 4 | 82 944 000 | 1 385 856 | 0.0625 | 0.000244140625 | 6 560 |

Table 1: Parameters of grids and amount of nitrogen particles in each cell.

If the metal surface is viewed at the atomic level, then in MD block computing it becomes necessary accounting nickel crystal lattice structure. However, in this paper, this case is not considered.

Testing of the developed approach was carried out on supercomputer MVS-10P (JSCC RAS). The calculations were performed on the central processors Intel Xeon E5-2690 and vector processors Intel Xeon Phi 7110X. The number of CPU cores ranged from 16 to 2048. The number of VPU cores ranged from 60 to 7680. Calculations were carried out on grids $\Omega^{(k)}$ for $k=2,3,4$. The results of a computation speedup testing are shown in Figure 3. It demonstrates a good parallel solution used in the constructed software.

The preliminary computation of steady state flow on grid $\Omega^{(3)}$ shows the following. A zone of gas condensation with a high pressure appears near the nozzle. It prevents a further acceleration of gas and acts as a stabilizer of a flow. A similar density distribution is given in the experimental paper [32]. A comparison of these data shows a good enough qualitative agreement of our calculations with the measurements (see Figure 4). On the other hand, in [32] the nozzle parameters are not specified and moreover, the measured temperature distribution

is given for two-temperature approximation that is not used in our predictions. Therefore, it is not possible to conduct a quantitative comparison of flow parameters for this experiment.

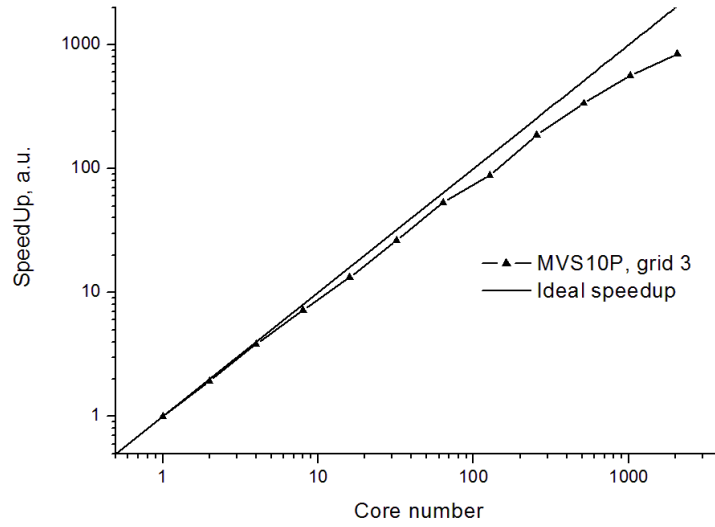


Figure 3: The speedup computations for grid $\Omega^{(3)}$.

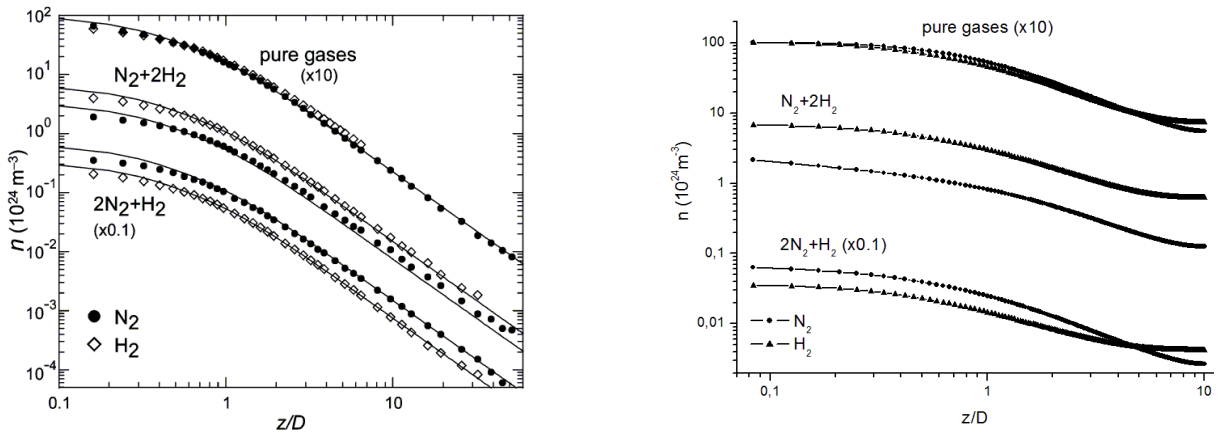


Figure 4: The distributions of the number density in experiments [32] (on the left side) and the data from our computations (on the right side).

5 CONCLUSIONS

- The problem of modeling the gas flows in microchannels of technical systems in the conditions of many scales of computational domain is considered. For a solution the two-scale approach combining the solution of QGD equations and correction of gasdynamic parameters by MD method is offered.
- The general numerical algorithm is based on solving the QGD equations system by a grid finite-volume method. The system of MD equations is used independently in each cell of a grid and is solved by means of Verlet scheme.
- The parallel implementation of approach is based on the methods of splitting into physical processes and domain decomposition. The parallel program is focused on the use of modern computing systems with the central and hybrid architectures. The program is realized by means of MPI, OpenMP and CUDA technologies.

- The research of proposed approach showed the following. The developed parallel algorithm is quite effective and steady to using the data of MD computations correcting the flow. By means of the developed program it is possible to calculate dependences of kinetic coefficients of QGD system on temperature and other factors. Transition from macrolevel to microlevel and back is carried out correctly.
- Comparing the calculated macroparameters of a three-dimensional flow agrees well with the results of natural experiments.

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