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# CALCULATION OF NITROGEN FLOW IN NICKEL MICRONOZZLE BASED ON NUMERICAL APPROACHES OF GAS AND MOLECULAR DYNAMICS

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**Key words:** Gas Flow, Micronozzle, Molecular Dynamics, Quasigasdynamic Equations, Nitrogen, Nickel, Macroparameters of Gas Area.

**Abstract.** The work is devoted to the modeling of gas flows in micronozzles. The complexity of studying such processes is connected both with the small sizes of technical system that makes it difficult to carry out the natural experiments and with the violation of hypothesis of continuity of the considered gas medium. An additional factor of complexity is the lack of information on the real processes taking place at the gas-metal boundary. An attempt to consider the features of gas flow in a micronozzle using a multiscale approach is made. The multiscale approach has two computational levels and uses the calculations by macroscopic quasigasdynamic model and microscopic model of molecular dynamics. In this approach the macromodel is supplemented by parameters and boundary conditions from database made in micromodel calculations. The flow of nitrogen in the nickel micronozzle is considered as an example. Previously the parameters of interacting the nitrogen molecules and atoms of the nickel surface were calculated and saved in database. In this paper they were used to form the material coefficients in the quasigasdynamic equations. The performed preliminary modeling has shown that at low flow velocities in calculations it is possible to obtain a flow with a profile of longitudinal velocity close to the Poiseuille flow profile. It shows the adequacy of the developed numerical techniques.

## 1 INTRODUCTION

Modern computer technology allows modeling very large systems and complex processes at the level of detailing that was previously not available. So relevance of studying the complex gasdynamical processes in technical micro- and nanosystems developed for the introducing nanotechnology in industry has increased. A feature of mathematical problems in this area is the simultaneous study of processes at many scales, including micro- and macrolevels. One of the modern and actively developing approaches to solving such problems is a multiscale approach that combines the methods of continuum mechanics and particle methods. This combination allows you to replace an expensive and difficult realized physical experiment with computer calculations.

In the paper, one of the aspects of modeling technical microsystems is considered. It is connected with calculating the parameters of gas microflows under technical vacuum

conditions. For a correct description of such processes, it is necessary to know the properties of real gases and to reproduce them in a numerical experiment. One way to obtain the missing information about the properties of a gas medium is molecular dynamics simulation [1, 2].

The formulation of the problem of gas flow through a micronozzle of a technical system is considered. In the practical part the calculations of the nitrogen flow moving from a chamber into a nickel micronozzle of cylindrical geometry and further into the field of a technical vacuum will be made. It is assumed that in the environment there is already a small amount of the same gas at a significantly lower pressure and at a temperature that coincides with the temperature of inhibition.

The problem was solved with the help of multiscale approach [3-5], that has two levels of detailing: macro- and microscopic. At the macrolevel of detailing, a description of the gas medium flows occurs. At the microlevel transport coefficients, parameters of the equations of state and the boundary conditions parameters are calculated. The macroscopic model of the flow is based on the quasigasdynamic (QGD) equations [6], the microscopic model – on the use of molecular dynamics (MD) methods [1, 2]. Modeling takes place at different levels in 2 basic stages: 1) calculations at the microlevel in order to accumulate a database on the flow characteristics in the temperature and pressure ranges of interest; 2) flow calculations at the macrolevel using the database obtained at the previous stage.

The main goal of this work is to perform the calculations for described problem, analyze the obtained calculated data and compare them with experiment data.

## 2 MATHEMATICAL MODELS

### 2.1 Microscopic model

In this work we consider the case of one type of the gas for the flow and one type of metal for the micronozzle. Then at the microlevel the gas-metal system is represented as a set of particles which behavior is described by Newton's equations:

$$m_{l,i}\frac{d\mathbf{v}_{l,i}}{dt}=\mathbf{F}_{l,i},\quad \mathbf{v}_{l,i}=\frac{d\mathbf{r}_{l,i}}{dt},\quad i=1,...,N_l,\quad l=a,b, \tag{1}$$

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

$$\mathbf{F}_{l,i}=-\frac{\partial U\left(\mathbf{r}_{l,1},...,\mathbf{r}_{l,N_l}\right)}{\partial\mathbf{r}_{l,i}}+\mathbf{F}_{l,i}^{ext},\quad i=1,...,N_l,\quad l=a,b, \tag{2}$$

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:

$$U = U_{aa} + U_{bb} + U_{ab}, \tag{3}$$

$$U_{aa} = \sum_{i=1,\, j>i}^{N_a} \varphi_{aa}\left(\left|\mathbf{r}_{a,i} - \mathbf{r}_{a,j}\right|\right), \tag{4}$$

$$U_{bb} = \sum_{i=1}^{N_b}\left[\varphi_{1,bb}\left(\mathbf{r}_{b,i}\right) + \sum_{j>i}\varphi_{2,bb}\left(\left|\mathbf{r}_{b,i} - \mathbf{r}_{b,j}\right|\right)\right], \tag{5}$$

$$U_{ab} = \frac{1}{2}\sum_{i=1}^{N_a}\sum_{j=1}^{N_b}\varphi_{ab}\left(\left|\mathbf{r}_{a,i} - \mathbf{r}_{b,j}\right|\right). \tag{6}$$

Each type of interaction is described by the corresponding potential $\varphi_{ll'}$. For nitrogen molecules it was used Mi's potential in the form of "n-6" [7] adapted in work [8]. For interaction of nickel atoms among themselves it was used the form of EAM [9] potential which considers not only pair interactions $\varphi_{2,bb}$, but also the impact of the environment on a particular particle $\varphi_{1,bb}$. To account the gas-metal interactions a standard potential Lennard-Jones [10] was used.

The initial conditions at the microlevel include starting distribution of particle coordinates and velocities and 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 [11-14].

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 if which the periodic continuation medium unlimited distances in all three spatial directions is assumed. In this case, periodic boundary conditions are used.

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 maintained 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 [15, 16].

The system of equations (1) is solved using Velocity Verlet Integration [17]:

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \mathbf{v}^n \Delta t + \frac{\mathbf{F}^n}{m} \frac{(\Delta t)^2}{2}, \quad \mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\mathbf{F}^{n+1} + \mathbf{F}^n}{2m} \Delta t \ , \tag{7}$$

here $\Delta t$ – the integration step, $n$ – the step number, $\mathbf{F}^{n+1}$ – the force value on the current step.

### 2.2 Macroscopic model

QGD equations in case of one type of the gas in invariant concerning system of coordinates with the constraint and the equations of state have the form:

$$\frac{\partial \rho_l}{\partial t} + \operatorname{div} \mathbf{W}_l^{(\rho)} = 0, \tag{8}$$

$$\frac{\partial \left( \rho_l u_{l,k} \right)}{\partial t} + \operatorname{div} \mathbf{W}_l^{(\rho u_k)} = 0, \ k = x, y, z, \tag{9}$$

$$\frac{\partial E_l}{\partial t} + \operatorname{div} \mathbf{W}_l^{(E)} = 0, \tag{10}$$

$$E_l = \frac{1}{2} \rho_l \left| \mathbf{u}_l \right|^2 + \rho_l \varepsilon_l, \quad \varepsilon_l = c_{V,l} T_l, \quad H_l = \frac{E_l + p_l}{\rho_l}, \quad p_l = Z_l \rho_l \Re_l T_l. \tag{11}$$

Here $l = a$, gas has numerical density (concentration) $n_a$ and mass density $\rho_a = m_a n_a$, where $m_a$ – mass of gas molecules $a$. Gas is characterized by its temperature $T_l$ and macroscopic velocity $\mathbf{u}_l$. Other parameters: $p_l$ – partial pressures, $E_l$ – total energy densities, $\varepsilon_l$ – specific internal energies, $H_l$ – total enthalpies, $Z_l = Z_l \left( T_l \right)$ – compressibility coefficients, $c_{V,l} = c_{V,l} \left( T_l \right)$ – 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.

In [13] on the example of nitrogen molecule system the technique of specifying the equations of state was considered. In [18] three methods for determining the kinetic coefficients were presented, comparing methods were produced and examples of calculating the coefficients of nitrogen molecule system were given.

The system of equations (8)-(10) is closed by initial and boundary conditions. The initial conditions correspond to the equilibrium gas environment in the absence of interaction with external factors. The boundary conditions can be determined in the form of third-type boundary conditions describing an exchange of mass, momentum and energy components between the gas flow and the metal walls. In [14, 19] interaction of a gas flow with microchannel walls on the example of nitrogen-nickel system was considered. In [20] on an example of the same system the accommodation coefficients were obtained. These calculations represent a technique of obtaining the boundary conditions by direct MD computation.

For calculating the macroparameters on QGD equations the grid numerical method having a finite-volume method [21-23] in the basis is used. For this in the computational domain $D$ the spatial grid $\Omega_D$ with cells $C_m$ ($m = 1,...,M$) and time grid $\omega_t$ with variable step $\Delta t$ was introduced. Grid $\Omega_D$ 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 [24]. The computing scheme on time was obvious.

## 3 NUMERICAL EXPERIMENTS

In this section, the results of calculating the nitrogen flow after exit from chamber to the nozzle and further into the free space are presented. The problem was chosen in connection with the existence of experimental data presented in the paper [25]. The geometry of the chosen model statement of the problem practically coincides with that described in [25] (see Figure 1). The cylindrical micronozzle has a diameter $D_0 \approx 310\,\mu m$, length $L_0 = 6D_0 \approx 1860\,\mu m$. It connects the chamber of nitrogen and the open space of the vacuum area, which was initially filled with the same highly diluted gas. The dimensions of the computational domain were chosen as follows. The diameters of the computational parts in the chamber and in the vacuum space were equal $D_1 = D_2 = 6D_0$. The length of the calculated part in the chamber was $L_1 = 10L_0$; the length of the considered part of the vacuum space was $L_2 = 50L_0$. At the initial time the gas does not move: $u_1 = u_2 = 0$. In this case, it is in the cylinder under standard normal conditions: $T_1 = 295.15\,K$, $p_1 = 101325\,Pa$; in the nozzle and the vacuum space it is at the same temperature, but at lower pressures: $T_2 = 295.15\,K$, $p_2 = \delta_0 p_1$, $\delta_0 \sim 10^{-3} \div 10^{-5}$ – pumping parameter. The nozzle on the left is blocked by a partition, which opens instantly at the beginning of the calculation.

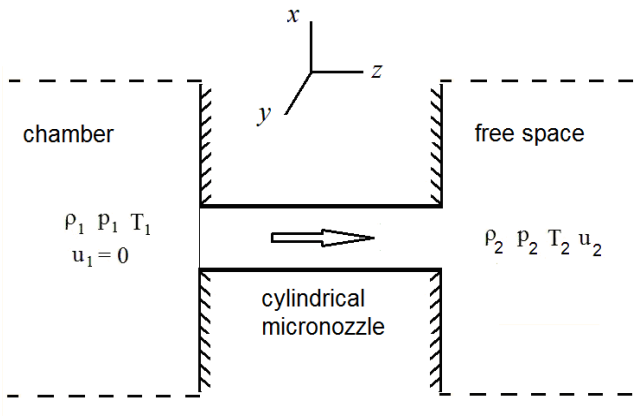


**Figure 1**: Geometry of a model problem for convenience presented in the form of a two-dimensional section

### 3.1 Calculations at microlevel

Calculations within this level consist of setting the initial state of the gas microsystem and carrying out a cycle of calculations according to the Verlet scheme (7). The initial calculation data assumes the assignment of the calculation area and its volume, the initial number of particles and their distribution on the volume, the velocity distributions on absolute values and directions, the parameters of the interaction potentials, the parameters of the final equilibrium state (for example, temperature and average momentum), parameters of the numerical integration scheme.

During calculating the properties of gas mixtures, the basic gas macroparameters were determined. These macroparameters are compressibility factor, heat capacities at constant volume and pressure, shear and bulk viscosities, thermal conductivity, diffusion coefficients. The motivation for choosing these macroparameters is determined by the fact that for a given temperature, pressure, and velocity vector, the base macroparameters make it possible to determine all other macroparameters of the gas.

Series of MD calculations of gas characteristics were performed in the temperature range from 80 to 400 K under pressure $p_0 = 101325\ Pa$. The obtained data were approximated by a set of dependencies and are shown in Figures 2-5 in comparison with the known experimental and theoretical data from. For the convenience of analysis the coefficients of shear viscosity $\mu_{N_2}$, bulk viscosity $\mu_{b,N_2}$, thermal conductivity $\kappa_{N_2}$, diffusion $D_{N_2}$ are normalized to their values $\mu^0_{N_2} = 1.667 \cdot 10^{-5}\ Pa \cdot s$, $\mu^0_{b,N_2} = 1.288 \cdot 10^{-5}\ Pa \cdot s$, $\kappa^0_{N_2} = 2.419 \cdot 10^{-2}\ W/m \cdot K$, $D^0_{N_2} = 1.850 \cdot 10^{-5}\ m^2/s$ at a temperature $T_0 = 273.15\ K$.

As can be seen from the figures, the constructed approximations are generally agree well with the experiment data. An exception is the dependence of the specific heat in the low-temperature region (less than 100 K), where the nitrogen gradually passes into the liquid phase. For this zone, one must take into account the dependence of the specific heats $c_{V,N_2}$ and $c_{p,N_2}$ from the density (pressure). There is also some discrepancy in the curves of dynamic and bulk viscosities, which is also observed in the literature in connection with the difficulty in determining these quantities in theory and in experiments. The obtained data were used below in the calculation of the selected model problems.

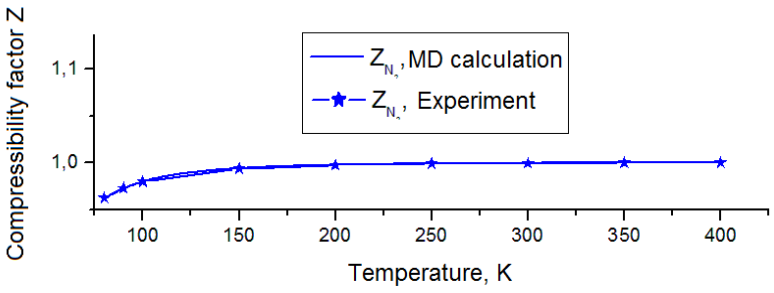


**Figure 2**: Compressibility factor $Z_{N_2}$ of nitrogen as a function of temperature

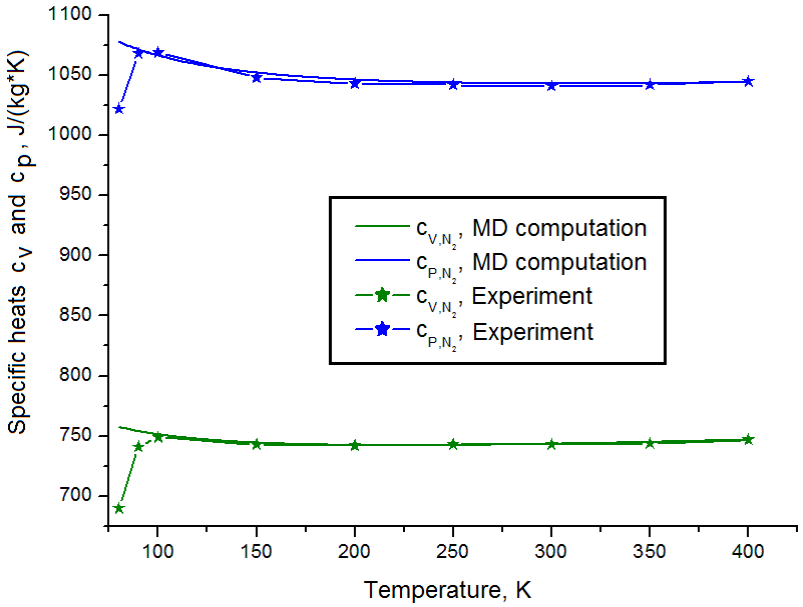


**Figure 3**: Dependences of the specific heats $c_{V,N_2}$ and $c_{p,N_2}$ of nitrogen on temperature

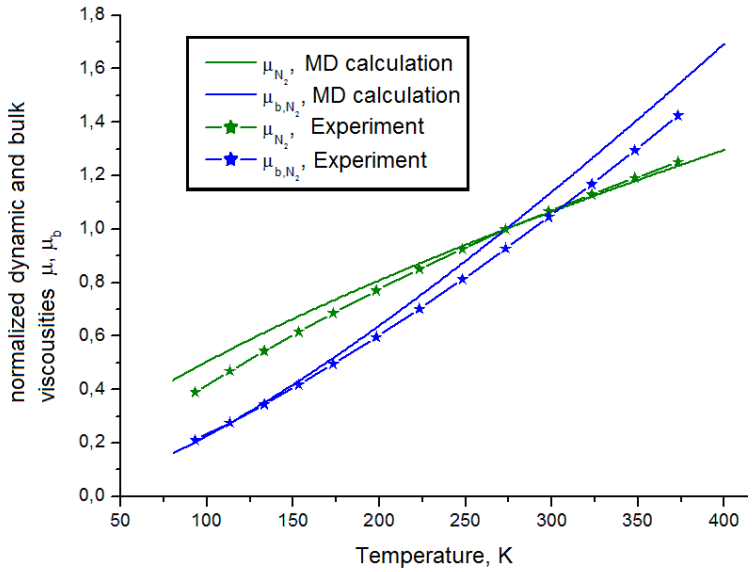


**Figure 4**: Coefficients of normalized dynamic $\mu_{N_2} / \mu^0_{N_2}$ and relative bulk $\mu_{b,N_2} / \mu^0_{b,N_2}$ viscosities of nitrogen as a function of temperature

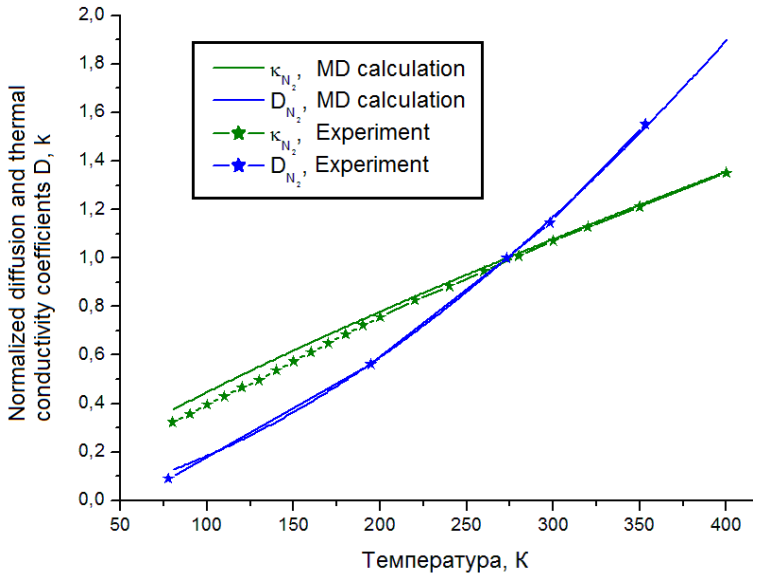


**Figure 5**: Normalized coefficients of thermal conductivity $\kappa_{N_2} / \kappa^0_{N_2}$ and diffusion $D_{N_2} / D^0_{N_2}$ of nitrogen as a function of temperature

### 3.2 Calculations at macrolevel

Calculations were carried out under conditions of two- and three-dimensional geometry. On Figure 6 two-dimensional distributions of the concentration of nitrogen molecules normalized by the value $10^{24} m^{-3}$, and the longitudinal velocity component are presented at different times.

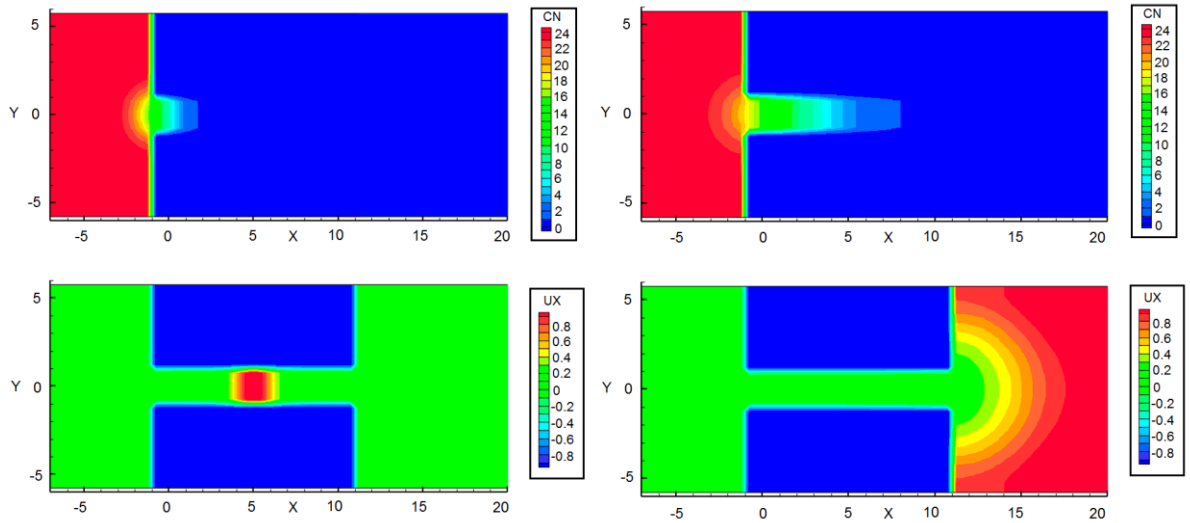


**Figure 6**: Distributions of the normalized concentration of nitrogen molecules (from above) and the longitudinal velocity component (from below) at time points $t = 0.0553, 0.553\ \mu s$

Normalization parameter on space is equal to $0.5D_0$. In dimensionless variables, the length of the region is $L_x = 732$, diameter is $D_y = D_z = 12$. In the two-dimensional case, the calculations were carried out in a rectangle $L_x \times D_y$, in the three-dimensional case, the calculations were carried out in a cylinder of square cross section with common dimensions $L_x \times D_y \times D_z$.

An analysis of the obtained data shows that the passage of gas into the micronozzle is implemented symmetrically and corresponds to the physics of the process.

Three-dimensional calculations confirmed the results obtained in the two-dimensional case, namely, the dynamics of distributions of the main gasdynamic parameters. The difference between the three-dimensional calculations and the two-dimensional ones was expressed in the difference in the times when specific distributions were formed. In particular, the times of thermal wave output from the micronozzle differed approximately by 1.3 times that can be connected with the chosen square form of a micronozzle.

Figure 7 shows the profiles of normalized nitrogen concentration on the axis of the vacuum space. As can be seen from the figure, the main behavior of the concentration coincides with the experimental data. Thus, with the help of the developed algorithms, it is possible to obtain information about real physical processes.

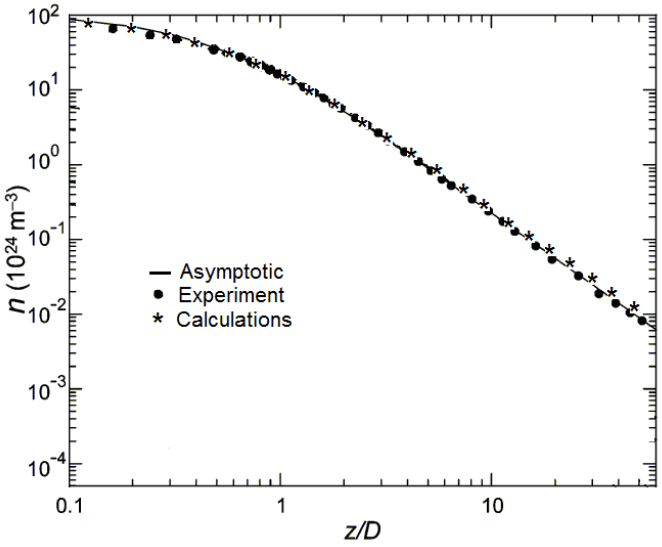


**Figure 7**: Established profiles of the normalized nitrogen concentration obtained in the natural experiment [25] and in the numerical calculation

Direct MD calculations of nitrogen flow in a thin channel with a thickness about 500 nm were also carried out. They showed that for flow velocities of the order of 1 nm/ns or less, at the exit from the microchannel the velocity profile is formed close to the Poiseuille profile. However, the final conclusion about the parameters of such flow requires additional investigation.

## 4 CONCLUSIONS

- Multiscale numerical approach to three-dimensional modeling of nonlinear interaction of gas with metal in microsystems was performed.
- Parallel realization of the approach using hybrid parallel computing technology was developed.
- Verification of numerical approach and validation of parallel software were fulfilled.
- Proposed numerical approach allows simulating qualitatively the behavior of gas - metal complex microsystems under the real conditions.

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