Computer modeling of air flows purification using sorption filters

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Abstract. The problem of computer modeling the processes of air purification from nanoparticles using sorption filters is considered. The paper proposes a complex model for describing the flow of contaminated air in the sorbent layer. The model is based on a system of quasigasdynamic equations defining the main characteristics of the air medium flow containing the mixture of gases and finely dispersed pollutants. Micro- and nanoparticles of heavy metals, coal and household dust can be considered as contaminants. The model takes into account the diffusion of pollutant particles, their adsorption on the surface of the sorbent granules and absorption inside the sorbent granules. The model is implemented numerically using splitting by physical processes and the mesh method. The basic algorithm is the finite volume method on irregular grids. An important part of the model is its parallel implementation adapted to computations on hybrid supercomputer systems. The preliminary calculations confirmed the robustness of the developed modeling technology.

1. Introduction
The traditional method of gas purification is the use of forced ventilation technologies in rooms with the passage of contaminated air through mechanical, electrical and other types of filters. In open spaces, personal protective equipment (masks, gas masks, respirators, etc.) are used. In both cases, the quality of cleaning is determined by the properties of the filter systems. The most effective gas purification system at the final stage is membrane filters that capture nanoparticles with a size of 20 nm and more. However, smaller nanoparticles pass freely through the filters (if we have a low concentration of nanoparticles) or very quickly turn off the membrane filter system (if we have a high concentration of nanoparticles). Therefore, the challenge is to replace membrane filters with alternative gas purification systems.

One of the ways to solve the problem is to use special sorbents consisting of millimeter and submillimeter non-round granules. A feature of such sorbents is the presence of a free charge on the surface of the granules, which attracts nanoparticles of almost any size. Moreover, the total surface area of the granules is much (by several orders) larger than in membrane systems. Also, one of the advantages of sorption filters is their relatively simple regeneration: passing an aqueous solution through a filter, which directs most of the nanoparticles to the recirculation system, and then drying the filter. One of the ways to optimize sorbent filters is to select the sorbent material and the shape of the granule surface. A specific combination of these properties can increase the efficiency of sorbent filters [1-5]. This purification technology is relevant in connection with the development of waste-free methods that allow capturing and
recovering various types of micro- and nanoparticles of pollutants. Preliminary mathematical modeling is important when designing purification devices based on sorption filters. However, there is no software that fully implements this multistage and multiscale technology.

In this work, we have chosen the problem of mathematical modeling the processes of gas purification from nanoparticles using filter sorbents. To solve it in general case, a previously developed multiscale technology [6-7] is proposed for modeling the process of cleaning a polluted air flow passing through a sorbent layer. This technology includes two scale levels, which are the macroscopic and the microscopic levels. Within its framework, at the macroscopic level, the main characteristics of the air flow are calculated on the basis of a system of quasigasdynamic equations (QGD) [8]. These equations are complemented by the convection-diffusion equations for pollutant particles. The processes of adsorption and absorption of pollutant particles are taken into account using boundary adhesion models on the outer and inner surfaces of the sorbent granules. This complex macromodel includes specific equations of state and the dependencies of the kinetic coefficients on the thermodynamic parameters of the air. These dependencies can be partially taken from the literature (if the data can be found for the investigated thermodynamic conditions), but it is more expedient to calculate them independently at the microscopic level based on the particle models, including molecular dynamics method [9].

This paper presents the first stage of the study, taking into account the macroscopic level description of the main processes of the contaminated air mixture and the sorbent granules interaction. For its numerical implementation, splitting by physical processes and the finite volume grid method were used. The definition of the real geometry of the treatment system was carried out using the construction of irregular three-dimensional grids (tetrahedral, hexahedral and mixed). The proposed computing technology was implemented in the form of a parallel code on the K60 hybrid supercomputer system (Keldysh Institute of Applied Mathematics of RAS) with CPU and GPU. MPI and OpenMP technologies were used for parallelization on the CPU. For GPUs, the CUDA Toolkit and GPU Direct data transfer technology were used. The preliminary calculations carried out below confirmed the efficiency of the developed modeling technology.

2. Problem formulation
The process of passing the air mixture through the sorbent layer is described using a complex two-component mathematical model. The first component of the model relates to the description of the flow of the contaminated air mixture in the laboratory installation (see Fig. 1). The second component of the model relates to the processes of interaction of the air mixture with the surface of the sorbent granules.

![Figure 1. Model geometry.](image-url)
The system of QGD equations [6, 7] in a form invariant with respect to the coordinate system for each component of the air mixture and the material equations closing it have the following form:

\[
\frac{\partial \rho_l}{\partial t} + \text{div} \mathbf{W}_l^{(\rho)} = 0, \tag{1}
\]

\[
\frac{\partial (\rho_l u_l)}{\partial t} + \text{div} \mathbf{W}_l^{(\rho u)} = S_l^{(\rho u)}, \tag{2}
\]

\[
\frac{\partial E_l}{\partial t} + \text{div} \mathbf{W}_l^{(E)} = S_l^{(E)}, \tag{3}
\]

\[
\begin{cases}
E_l = \rho_l \left( \frac{1}{2} |\mathbf{u}_l|^2 + \varepsilon_l \right), & H_l = E_l + p_l, \quad p_l = Z_l \rho_l R_l T_l, \quad \varepsilon_l = c_{V,l} T_l, \\
\gamma_l = \frac{c_{p,l}}{c_{V,l}}, & \text{Pr}_l = \frac{\mu_l}{\rho_l D_l}, \quad \text{Sc}_l = \frac{\mu_l}{\rho_l} \frac{\chi_l}{\lambda_l}, \quad \text{Ma}_l = \frac{u_l}{a_l}, \quad \text{Re}_l = \frac{\rho_l |u_l| \lambda_l}{\mu_l}.
\end{cases} \tag{4}
\]

Here all variables with the index \(l\) relate to a gas of the type \(l\), each component has its own concentration \(n_l\), mass density \(\rho_l = m_n u_l\) (\(m_l\) is mass of molecule of gas \(l\)). Each gas is also characterized by its temperature \(T_l\) and macroscopic velocity \(u_l\). Other parameters of the mixture components: \(p_l\) are partial pressures of gases in the mixture; \(E_l\), \(H_l\) and \(\varepsilon_l\) are total energy densities, enthalpies, and internal energies of the mixture components; \(\mu_l = \mu_l (T_l), D_l = D_l (T_l)\) and \(\chi_l = \chi_l (T_l)\) are kinetic coefficients of mixture components, namely, coefficients of dynamic viscosity, diffusion and thermal conductivity. Variables \(Z_l = Z_l (T_l, \rho_l), \gamma_l = \gamma_l (T_l, \rho_l), c_{V,l} = c_{V,l} (T_l), c_{p,l} = c_{p,l} (T_l)\) and \(R_l = k_B / m_l\) are compressibility coefficients, adiabatic indices, specific heat capacities and individual gas constants of the mixture components (\(k_B\) is Boltzmann constant); \(\text{Pr}_l, \text{Sc}_l, \text{Ma}_l\) and \(\text{Re}_l\) are the Prandtl, Schmidt, Mach, and Reynolds numbers for the mixture components; \(\lambda_l\) are mean free paths; vectors \(\mathbf{W}_l^{(\rho)}, \mathbf{W}_l^{(\rho u)}\) and \(\mathbf{W}_l^{(E)}\) coincide, up to sign, with the fluxes of mass density, momentum density of the corresponding components, and energy density. The exchange terms \(S_l^{(\rho u)}\) and \(S_l^{(E)}\) take into account the redistribution of momentum and energy between the components of the mixture [7, 8].

Equations (1)–(4) are supplemented by equations of the convection-diffusion type for the concentrations of particles of air pollutants:

\[
\frac{\partial C_k}{\partial t} + \text{div} \mathbf{W}_k^{(C)} = - (\mathbf{u}, \nabla C_k) + \Phi_k, \quad \mathbf{W}_k^{(C)} = - D_k^{(C)} \nabla C_k, \tag{5}
\]

where \(C_k\) are the concentrations of the \(k\) type pollutant, \(\mathbf{W}_k^{(C)}\) are the corresponding fluxes, \(\mathbf{u}\) is the average flow velocity of the air mixture, \(\Phi_k\) are the functions of the \(k\) type pollution sources, \(D_k^{(C)}\) are the diffusion coefficients of the pollutant components.

Equations (1)–(3) and (5) are supplemented with the necessary initial and boundary conditions. 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. For equations (5), it is assumed that the purification system does not initially contain contamination, that is, the concentration fields \(C_k\) correspond to some equilibrium values \(C_k^*\), that do not exceed the maximum permissible limits.

The boundary conditions for the QGD equations at the inlet, outlet, and walls of the treatment system are set in the traditional way. At the entrance to the system, the Paussail flow is specified, at the exit from the system, the so-called "soft" boundary conditions [7] are specified. On the solid walls of the channel, the impermeability conditions are set for the density of the air medium, the no-slip conditions and the conditions of the third kind are set for the
momentum and energy, respectively. For the concentration of contaminants on the channel walls, the impermeability condition is implemented (the normal component of the concentration flux is set to zero).

On the surface of the granules for the density of air with impurities, the conditions of partial flow are set, and for the momentum and energy, the conditions of the third kind are specified, which describe the process of partial absorption by the granule surface of part of the energy and momentum of the medium. In this case, the boundary conditions for the concentrations are set in the flux form. In particular, the following nonlinear condition of limited absorption is realized:

\[
W^{(C)}_{k}(n) = A_k (C_k - C^*_{k}) (1 - C_k/\bar{C}^{**}_{k}).
\]  

(6)

Here \(n\) is the outer normal to the surface of the granule (or the boundary layer surrounding the granule), \(C^*_{k}\) is the maximum concentration of the \(k\)-th component of the pollutant retained by the element of the surface of the sorbent granule, \(A_k\) is the intensity of the capture of nanoparticles of the \(k\)-th component of the pollutant on the surface of the sorbent granule (may depend on the total number of vacancies on the surface of the granule, free of all nanoparticles of all types of pollutant). Parameters \(A_k, \bar{C}^{**}_{k}\) are calculated in advance by the molecular dynamics method, in case of using microscopic level calculations.

3. Algorithm and its parallel realization

The parallel implementation of the algorithm is based on the domain decomposition method and is adapted for computations on hybrid supercomputers. The division of the region is performed by a geometric way, in which all cells of the computational grid fall into one or another macrodomain processed by one of the supercomputer nodes (see Fig. 2).

![Figure 2](image_url)

**Figure 2.** Computational domain decomposition options.

Inside the macrodomain, the computational domain is again divided into microdomains in accordance with the number of central processing unit (CPU) threads or the number of graphics accelerators (GPU) and multiprocessors in each GPU. Thus, a two-stage division of the region (grid) into calculated macro- and microdomains is performed.
The general block diagram of the algorithm is shown in Fig. 3.

![Diagram](image)

**Figure 3.** Computational domain decomposition options.

With parallel implementation of the algorithm, it turned out that the optimal combination of computations with the help of the CPU and the GPU is achieved when the cycle in time is performed with the help of CPU threads, and the computations that make it up are fully implemented on the GPU. As a toolkit for parallel implementation, we used MPI tools (for parallelization across nodes and head threads of a supercomputer, which have access to a specific GPU). To increase the speed of computations on the CPU using the OpenMP technology, free CPU threads were used. The GPU computing was implemented using the CUDA Toolkit and GPUDirect data transfer technology.

4. Numerical experiments

Numerical experiments were carried out on a model problem with the following parameters: length of the computational domain was \( L = 60 \text{ cm} \), the radius was \( R = 5 \text{ cm} \), the radius of spherical sorbent granules was \( R_g = 0.75 \text{ cm} \), the number of granules was \( N_g = 210 \), granules were located in the central part of the system (Fig. 4).

Modeling was performed for the flow of air environment with the following parameters: 

- initial density \( \rho_0 = 1.225 \times 10^{-3} \text{ g/cm}^3 \),
- initial pressure \( p_0 = 101325 \text{ Pa} \),
- temperature \( T_0 = 273.15 \text{ K} \),
- kinematic viscosity \( \mu_0 = 1.7894 \times 10^{-5} \text{ g/cm} \cdot \text{s} \),
- inlet velocity \( v_0 = 1.0956 \text{ cm/s} \) (Re=150).

The air mixture contained 79% nitrogen, 21% oxygen. The pollutant was coal powder \((k=1)\) with a density of \( \rho_p = 0.5 \text{ g/cm}^3 \) and a particle diameter of \( d_p = 0.002 \text{ cm} \) the weight of one particle is approximately \( m_g = 2.09 \times 10^{-9} \text{ g} \).

Diffusion coefficient of impurity was \( D_{1(C)} = 1.095 \text{ cm}^2/\text{s} \), capture coefficient was \( A_1 = D_{1(C)}/d_p \).

Concentrations were \( C_1^0 = C_1^{**} = 10^{-7} \text{ g/cm}^3 \), \( C_1^* = 0 \). To speed up the calculations, the mixture flow was calculated once at the start of the program.

In the computational domain, a tetrahedral mesh was built with the number of nodes 319316 and the number of cells 1780727. The number of boundary cells was the following: on the side walls of the system – 51324 (the number of pollutant particles near the walls at the beginning of the process was 5625), on the surface of the granules – 42798 (the number of particles pollutant near the granules at the beginning of the process was 4600).

The times for calculating the solution (calculating the starting flow and calculating the concentration evolution) are given in Table 1. The Intel Xeon Gold 6142 v4 was used as the CPU.
Figure 4. Model computational domain and distribution of the velocity modulus in the volume.

Table 1. Times of calculation of individual stages and the task as a whole.

| CPU thread number | GPU number | Time 1, s | Time 2, s | Time 3, s |
|-------------------|------------|-----------|-----------|-----------|
| 28                | 0          | 22.47     | 7350.21   | –         |
| 28                | 1          | 22.47     | 7350.21   | 242.71    |
| 28                | 2          | 22.47     | 7350.21   | 164.25    |
| 28                | 4          | 22.47     | 7350.21   | 95.37     |
| 56                | 8          | 12.56     | 3792.34   | 63.21     |
| 128               | 16         | 6.93      | 1954.53   | 38.14     |
| 256               | 32         | 3.82      | 991.74    | 23.56     |

The NVidia Volta GV100GL was used as the GPU. The time 1 was connected with preliminary computation of starting flow on CPU. The time 2 was connected with main computations for 50000 steps on CPU. The time 3 was connected with main computations for 50000 steps on both CPU and GPU.

As can be seen from Table 1, the full cycle of the algorithm associated with calculations at the macrolevel can be implemented both on the CPU and on the GPU. In this case, the use of a GPU is preferred. The limitation for using GPUs is the total amount of their RAM and the need to transfer data between the nodes of the supercomputer.

We note that from the point of view of the physics of the process, we have demonstrated the effect of cleaning the air environment where the concentration of pollution at the outlet from the system has decreased to 30% of the input value (see Fig. 5).

To bring the resulting concentration to the maximum permissible, it is necessary to increase the number of sorbent granules. In this sense, the developed program can be used to optimize the design of purification systems.

5. Conclusion

We have considered the problem of computer modeling of air purification processes from polluting solid impurities. This problem is especially important in the case when the particles of pollutants have micro- and nanosizes. Membrane or sorbent filters are usually used to clean the air from...
such particles.

In this work, the sorbent filters were considered for which we made the following:
- proposed a two-scale mathematical model of cleaning processes in a sorbent filters;
- developed a parallel numerical algorithm and a corresponding computer program;
- tested the proposed method on one of the model problems.

A feature of our approach is the reliance on supercomputer computing and ab initio calculations of material coefficients and constants based on molecular dynamics methods. Our future developments will be devoted to the extension of the proposed approach and the accumulation of a database of material coefficients.

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