# A MATHEMATICAL MODEL FOR AIR TREATMENT

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**Summary.** In this paper a mathematical model for air treatment is included and completed with numerical implementation. This work discusses technology for modeling the gas cleaning process in a sorbent filter. For this aim, the multiscale approach was applied. Proposed method is based on the quasi-gas-dynamic equations (QGD) as a model at the macroscale and as a microscale model, we use the Newtonian dynamics equations. The software implementation uses MPI and OpenMP technologies and is focused on the use of supercomputer systems with central and vector processors. Splitting method according to physical processes and domain decomposition technique were used for parallelization.

## 1 INTRODUCTION

There is a well-known and fair opinion that no product can be called absolutely safe. There is also the concept of zero risk to which we should strive, but it is unattainable. The scientific and expert community has recently began to recognize the dangers and risks to living systems that associated with the unregulated development of nano-industry and the propagation of toxic nano-production. The potentially dangerous properties of nanomaterials, and their impact on the environment are still not understood. The positive properties of a particular nano-product can be blocked by a huge damage to human health or nature.

Nanomaterials are released and get into the environment without a systematic study of their impact on nature. There are no control systems, devices of tracking and detection, methods for their safe utilization. Developers of nanotechnology and power structures rarely provide the opportunity for independent and competent experts to participate in discussions and decisions about nanotechnology. How to conduct “nanotechnology” in the world and what measures to take to make it peaceful, controlled, and safe in all respects.

One of the most striking examples of such damage is the ingress of various kinds of nanoparticles into the human lungs during breathing. In particular, great harm to health is inhaled by carbon nanoparticles formed during incomplete combustion of fuel in motor engines and at thermal power plants. A similar problem arises at metallurgical enterprises, enterprises of the chemical industry, as well as in the process of smoking. The production as a rule uses efficient cleaning systems, but there is practically no control for household emissions of nanoparticles.

Let's discuss methods of air treatment. The traditional method of gas cleaning is the use of technologies for forced ventilation of rooms with passing polluted air through mechanical, electrical and other types of filters. In open air spaces, personal protective equipment (masks, gas masks, etc.) is used. In both cases, the quality of cleaning is determined by the properties of the filter systems. The most effective gas cleaning system at the final stage uses membrane filters that capture nanoparticles with a size of 20 nm and more. However, the nanoparticles with smaller sizes freely pass through filters (if we have a low concentration of nanoparticles) or very quickly disable the membrane filter system (if we have a high concentration of nanoparticles). Therefore, the task is to replace membrane filters with alternative gas cleaning systems.

One of the ways to solve the problem is the use of special sorbents, consisting of millimeter and submillimeter non-circular granules. A feature of such sorbents is the presence of a free charge on the surface of the granules that attracts nanoparticles of almost any size. At the same time, the total surface area of the granules is much more (some orders) than in membrane systems. Also one of the advantages of sorbent filters is their relatively simple regeneration: passing an aqueous solution through a filter, that takes most of the nanoparticles into the recycling system, and then drying the filter [1, 2]. One of the ways to optimize sorbent filters is the selection of the sorbent material, and the selection of the surface shape of the granules (see Fig. 1). The specific combination of these properties can increase the efficiency of sorbent filters.

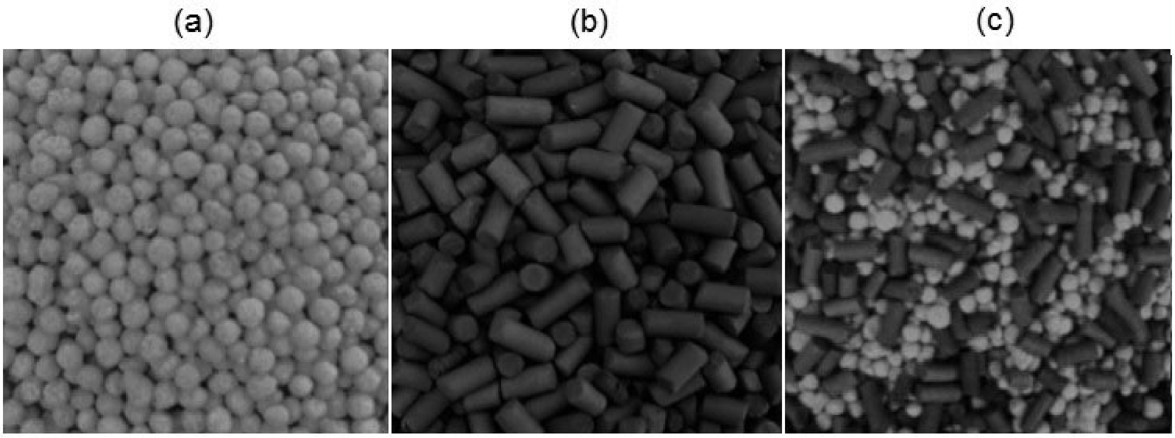


Fig. 1. Variants of sorbents differing in the form of granules

In this paper a technology for modeling the gas cleaning process in a sorbent filter is proposed. For this purpose, the multiscale approach developed by us earlier in the papers [3, 4] is used. At the first stage of this work, the direct gas cleaning problems with given parameters of the sorbent filter are solved. At the subsequent stages, the inverse problems will be considered, which allow us to optimize the gas cleaning system. In this paper, we propose a numerical method for solving the direct problem.

## 2 PROBLEM FORMULATION

The process of passing the air flow air flow by polluted nanoparticles air flow through the sorbent can be described in many ways. In the first approximation, when the size of nanoparticles can be neglected (that is, they are considered as material points), we use a two-scale model in which the first (macroscopic) scale is associated with the size of the sorption layer, and the second (microscopic) scale is associated with processes on the surface of the sorbent granules.

In this paper, we apply the system of QGD equations [5, 6, 7] as a model at the macroscale. It is complemented by the real state equation, the dependences of the kinetic coefficients of the gaseous medium on the concentration of nanoparticles, and the convection-diffusion equation for the concentration of nanoparticles.

As a microscale model, we use the Newtonian dynamics model of nanoparticles around the surface of the granules. We take into account the processes of sticking nanoparticles to the surface of the granules, as well as other important features of the interaction of nanoparticles in the boundary layers.

## 3 PARALLEL NUMERICAL APPROACH

The numerical implementation of the combined two-scale model is based on the splitting method according to physical processes and on the method of separating the boundary layers. In this case, calculations of quasi-gas-dynamic equations and convection-diffusion equations are carried out by the grid method of control volumes on irregular grids. Suitable sets of Vorono polyhedra are used as grids [8]. On the boundary of the region and on the surfaces of the granules, special boundary layers are constructed in which the equations of Newtonian dynamics are solved. The conjugation of the main region and boundary layers is carried out at each time step on the basis of recalculating the macroparameters of the medium and the particle distributions. The general numerical algorithm at each time step is an explicit predictor-corrector scheme.

A parallel implementation of the proposed algorithm is based on the application of the domain decomposition method and dynamic load balancing of the calculators. The software implementation uses MPI and OpenMP technologies and is focused on the use of supercomputer systems with central and vector processors. Testing of parallel code confirmed the effectiveness of the developed mathematical approach.

## 4 CONCLUSIONS

- A new two-scale model of the transit of the gaseous medium through the sorbent is proposed.
- A numerical algorithm of solution and its parallel software were implemented.

- Preliminary tests of the developed code have demonstrated the viability of the proposed approach.

## REFERENCES


[1] Lutz Mädler, Sheldon K. Friedlander. Transport of Nanoparticles in Gases: Overview and Recent Advances. *Aerosol and Air Quality Research*, Vol. 7, **3**, pp. 304-342, (2007).

[2] T. Kudryashova, S. Polyakov, and V Podryga. *Numerical Approach to Simulation of Nanoprinting Processes.* Proc. of the Eleventh International Conference on Advances in Computer-Human Interactions. (ACHI 2018) March 25 – 29, Italy, 128-131. IARIA XPS Press, Wilmington, USA, 2018. (2018).

[3] T. Kudryashova, V. Podryga, and S. Polyakov, *HPC-simulation of gasdynamic flows on macroscopic and molecular levels*, in Nonlinearity. Problems, Solutions and Applications, Vol. I, **26**, L. A. Uvarova, A. B. Nadykto, and A. V. Latyshev, Eds. New York: Nova Science Publishers, 543–556, (2017).

[4] V. O. Podryga, Yu. N. Karamzin, T. A. Kudryashova, and S. V. Polyakov, *Multiscale Simulation of Three-Dimensional Unsteady Gas Flows in Microchannels of Technical Systems*, Proc. of the Seventh European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2016), June 2016, Vol. 2, 2331-2345. (2016)

[5] T. G. Elizarova, *Quasi-Gas Dynamic Equations*. Berlin, Heidelberg, New York: Springer-Verlag, (2009).

[6] Yu. Karamzin, T. Kudryashova, V. Podryga, and S. Polyakov, *Numerical Simulation of the Gas Mixture Flows Using Hybrid Computer Systems,* Proc. of the Ninth International Conference on Engineering Computational Technology (ECT 2014), Stirlingshire, UK: Civil-Comp Press, Sept. 2014, 28. doi:10.4203/ccp.105.28. (2014).

[7] B. N. Chetverushkin, *Kinetic Schemes and Quasi-Gasdynamic System of Equations*. Barcelona: CIMNE, (2008).

[8] N. N. Medvedev. Vorono-Delaunay method in the study of the structure of non-crystalline systems. Novosibirsk. RAS. (2000).

[9] Official documentation and manuals on MPI. URL: http://www.mcs.anl.gov/ research/projects/mpi/

[10] Official documentation and manuals on OpenMP. URL: http://www.openmp.org/resources/openmp-books