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ON THE MODELING OF THE THERMOMECHANICAL FIELDS IN POROUS MATERIAL BEING UNDER RADIATION

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Summary. An approach to the complex mathematical modeling of interrelated physical mechanisms of interaction between radiation and matter is considered. The model scenario of interaction of radiation with the material includes the following elements. The essentially inhomogeneous material being under radiation is considered. During the propagation of radiation in an object, part of its energy is absorbed by the substance. This leads to the heating of the material and, consequently, the rapid development of highly inhomogeneous temperature and pressure fields in the object. The complex computational method for the study of the scenario should include the following components. Techniques of description and means of constructing a geometric model of the medium with a direct resolution of its microstructure; computational algorithms for modeling the processes of photon-electron cascade development, which leads to the energy deposit of radiation in a porous medium irradiated by ionizing radiation; mathematical models of generation and development of secondary radiation-induced thermodynamic and thermomechanical processes in the material; effective means of integration "according to data" between the specified classes of models. The geometrical model of the heterogeneous porous medium with direct view of its microstructure and statistical algorithm based on Monte Carlo method are worked out. The algorithm uses the energy and pulse probability distributions for the particles interacting with the complex chemical compound. The distributions are used for detail modeling of the scattering and absorption processes in complex heterogeneous materials. An approach for the discrete geometrical description of the realistic geometry of the heterogeneous porous material with considering its structure at the micro level is elaborated. The approach includes the algorithm of build the porous set and the detector system for statistical estimation of the radiation energy deposit in an irradiated object. Methods of integrating the results of statistical modeling of radiation transfer in porous media and the initial data for the numerical solution of the thermomechanics problems are proposed to build based on technique of multidimensional approximation. The applications of the developed simulation tool are presented in terms of results obtained with use of the hybrid computing cluster HCC K-100 (http://www.kiam.ru/MVS/resourses/k100.html).

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1 INTRODUCTION

Investigation of substance properties in extreme conditions is an actual problem. The experiments with powerful sources of radiation are rather expensive. Measuring equipment cannot provide full quantitative data for detailed description of the interaction between radiation and substance and the generation of the secondary radiation-induced effects. Therefore, the supercomputer modeling of the propagation of radiation through the matter is a powerful means for investigating the radiative, thermomechanical and electromagnetic fields in objects being under radiation [1-4].

Modern high-tech construction materials are designed to withstand loads of various nature under conditions of the complex physical effects, for instance, radiation and heat fluxes, mechanical tension etc. [5]. The protective coating of satellite being under space radiation is an example of the material in question. There is a problem of creation of the materials resistant to external influence of various nature, in particular, to radiation-induced thermomechanical effects. Promising way to solve this problem is the use of composite materials. One of the simplest variants of composite materials is gas-filled porous material. They are a solid homogeneous matrix comprising a large number of voids of a given size. The complex geometric structure of the material in conjunction with the selected chemical composition of the matrix material ensures the preservation of its properties in a multi-factor impact. Mathematical modeling is the effective tool of studying the microstructure of porous matter and allows evaluating the quality of the material. The optimal variant of the manufacturing technology of the product with the given properties could be chosen based on the analysis carried out by use of mathematical modeling.

Porous materials are widely used in mechanical engineering, heat power engineering, rocket, aviation, chemical and other industries. This is because these materials provide the required strength, thermal, hydraulic, technological properties and can operate at high temperatures and pressures. Such materials are used in thermal protection systems of rocket engines [2,5,6], they are used to create shells of gas-turbine engines [7,8].

The aim of this work is the construction of a physical-geometrical model of radiation propagation in a material with complex (composite) atomic structure, with a direct view of its structure (geometry, matrix and voids) at the micro level. The main attention is paid to the construction of a geometrical model of a porous structure object. The model includes the detector (registration) system for statistical estimation of the radiation energy deposit in an irradiated object. Corresponding algorithm of build the porous set and the detector system for evaluating the radiation energy deposit in an irradiated object is described. The physical model of the interaction of radiation with matter is based on a detailed description of the collision processes of particles with matter [9]. Supercomputing the transport processes is performed using the modeling technique elaborated by authors of this paper and implemented on the hybrid calculating cluster with application of modern technologies of parallelization (CUDA, MPI).

Some results of the model calculations of thermal and mechanical fields on the hybrid calculating cluster HCC K100 (http://www.kiam.ru/MVS/resourses/k100.html) are represented.

2 MODEL OF THE RADIATION TRANSPORT IN THE POROUS MATERIAL

The developed model of the radiation transport in the medium of porous structure includes two main parts: the description of the interaction X-ray radiation and electrons with composite material and geometrical model of porous pattern involving the discrete model of the detector system for statistical estimation of the radiation energy deposit in an irradiated object.

2.1 Model of interaction between radiation and matter

The basis of the model of the propagating the radiation through the matter is the probabilistic distributions of the particle characteristics changing during the process of interaction with the atoms of the matter. These distributions are constructed by processing the verified databases on the cross-sections of the corresponding processes (http://www.nndc.bnl.gov/sigma/).

The following types of X-radiation collisional processes with the atoms are considered: coherent (Rayleigh) scattering; Compton (incoherent) scattering; photon absorption (photoionization of atoms); electron-positron pairs production.

The following processes of interaction of electrons with matter are considered: elastic scattering; excitation of the atoms; ionization collisions or shock ionization; bremsstrahlung, electron-positron annihilation.

The constructed probabilistic distributions of the collision processes are used for computing the random trajectories of the radiation particles during Monte Carlo simulation. Distributions of particle parameters that change during the simulated processes play a fundamental role in the simulation of particle transport processes. These distributions are calculated using cross-sections (differential cross sections) of the considered processes.

Let x be the values of ξ that characterizes the state of the particle. If the distribution density of this value in the current physical process (normalized by 1) $f(x)$ is known, then, the distribution of this value $F(x)$ is determined by the integral $F(x)=\int_{-\infty}^{x} f(t)\,dt$. The value $F(x)$ is equal to the probability of the value of ξ, which is less than x: $F(x)=P(\xi<x)$.

The inverse function method [10] is most often used to model a random variable ξ. This method is based on the theorem stating that, if $\gamma\in(0,1)$ is the uniformly distributed random variable, and the values x of the random variable ξ satisfy the equation $\int_{-\infty}^{x} f(t)\,dt=\gamma$, then ξ has the distribution density $f(x)$. The value x is calculated as the function, which is inverse to $F(x)$: $x=F^{-1}(\gamma)$.

Cross sections of the processes of interaction of particles with matter in most cases are presented in the form of tabular data. Therefore, tables of functions $x(\gamma)$ are constructed to simulate these processes [9].

2.2 Geometrical model of the porous medium

A porous material with isolated pores is considered. Its structure is determined by the distribution of voids by size, shape and orientation, as well as by the volume fraction of the void space of the medium. A model medium with pores of spherical shape and the same diameter is considered in this paper. The pore diameter and the average porosity of the material sample are set as parameters of the geometric structure of the medium.

The objective of the radiation transport theory is to compute the readings of detector J located in the field of radiation. The desired (measured) values are presented as the readings of some detector and are written as functional on the space of the transport equation solutions. Therefore, the register system (the set of detectors determined by the type of the required value) is an integral part of the geometric description of the medium in question.

Various algorithms can be used to construct a geometric model of the material (a specific placement of voids with specified geometric properties inside the sample). The most popular is the Lubachevsky - Stillinger algorithm [11-13]. The input data of the algorithm is the number of "particles" (pores) and their final size (diameter). Initially, it is assumed that the particles are uniformly distributed in a given volume and have a radius of zero. These particles interact between each other through a given short – range potential of the pair interaction (various kind of potentials are considered, for instance, in [14]). The evolution of the particle position is described by equations of dynamics of interacting points. The initial velocity distribution of the particles is a random value. The particle diameter increases slow during the system evolution according to a given law (for instance, linear). The size of the particles is considered in the simulating their collisions. The trajectories of the particles will generally be chaotic. As a result, the algorithm places these particles in space without intersections. An open free implementation [15] of described algorithm is used in this work.

An example of modeling the porous material microstructure using the described algorithm is represented in fig.1. The number of pores is about 4000.

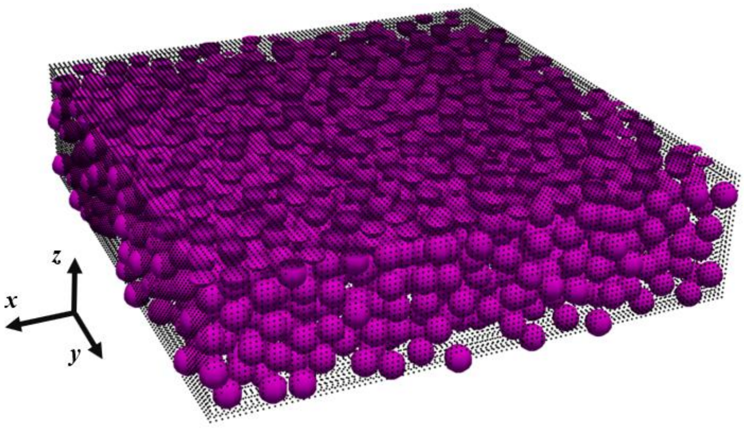


Fig. 1. Placement of voids 50 μm in the sample 1x1x0.25 mm

The registration system designed for statistical estimation of functionals on the space of solutions of the transport equation (desired values) includes a set of "detectors" – spheres. These detectors record the events of interaction of radiation quanta and electrons with matter. The scheme of the detector placement algorithm is as follows.

- The Voronoi diagram is based on the pore centers [16];
- The nodes of the constructed diagram are taken as the centers of detectors;
- The radius is selected as the maximum radius at which the detector placed in each node does not intersect with all the pores located inside Voronoi cells incident to a given node.

The constructed detectors do not intersect with voids, however, can intersect with each other. The following procedure is used to exclude such an intersection.

- Delaunay triangulation [17] is constructed at the vertices corresponding to the centers of the detectors;
- If the distance between the detectors corresponding to the vertices of a given triangulation edge exceeds the sum of the detector radii, the radius of one of the detectors is reduced so that the detectors do not intersect. If it is impossible one of the detectors is removed.

After applying this operation to all the Voronoi cells the intersections of the detectors are eliminated.

The result of this procedure for model object shown in fig.1 is represented in fig.2. The number of detectors of different size is about 3500.

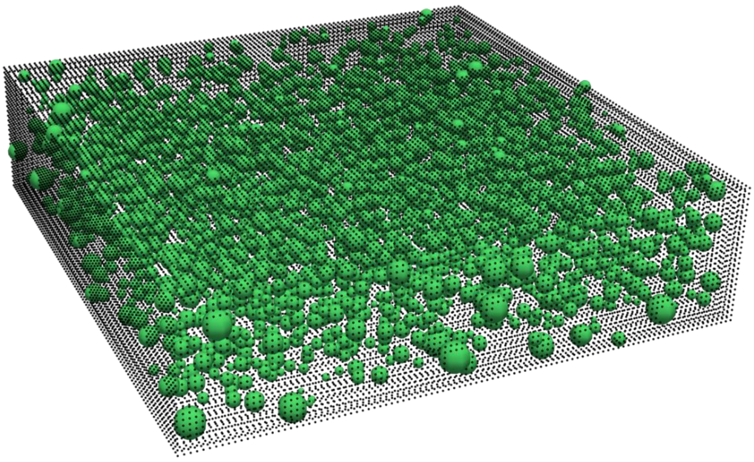


Fig. 2. Placement of detectors in the sample 1x1x0.25 mm

The mutual disposition of the pores and detectors is shown in fig. 3.

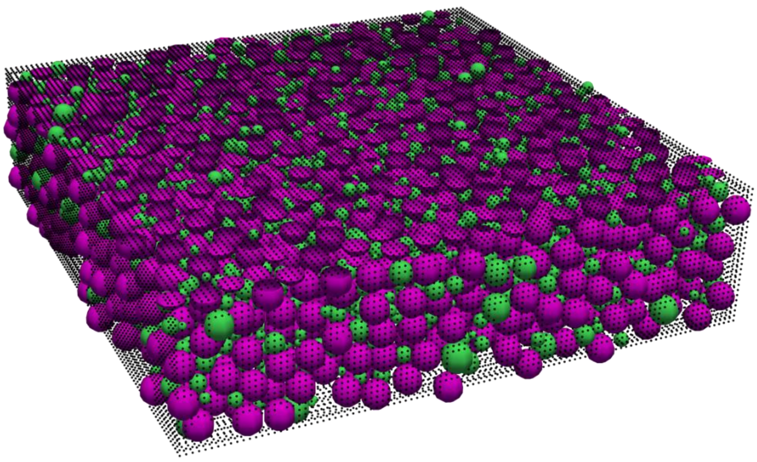


Fig. 3. Mutual arrangement of pores and detectors

The size distribution of the detectors is shown as a histogram in fig.4. The detectors do not intersect with each other and lie entirely inside the filler (do not intersect with the pores).

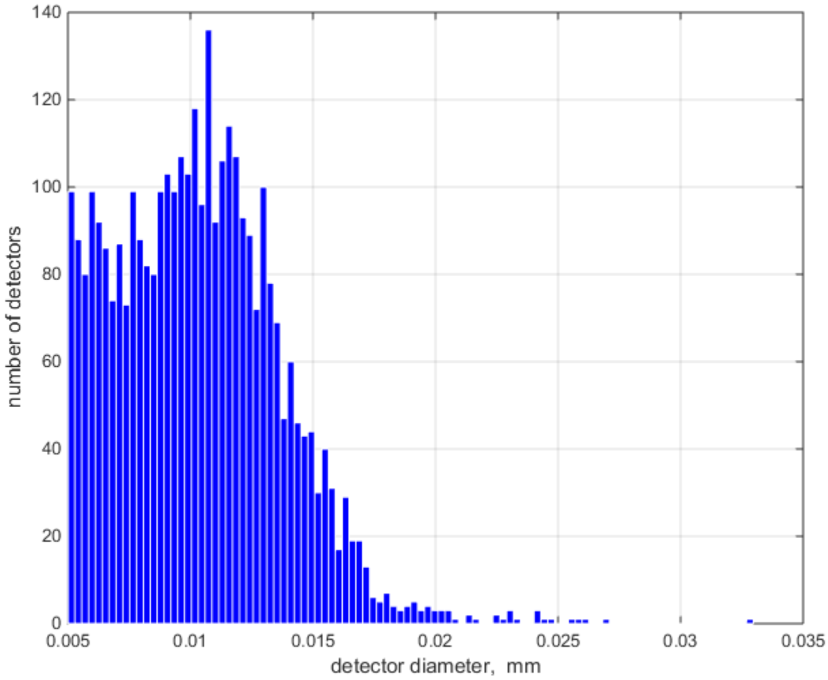


Fig. 4. Size distribution of the detectors

The process of radiation transport in the porous medium (Fig. 1) is simulated by effective modifications of the Monte Carlo method [18-20] using the constructed detection system (Fig. 2 - 4).

3 MODELING OF RADIATION TRANSPORT

Results of modeling the interaction of 10 keV X-ray radiation with a porous object (Fig. 1) presented in this section of the article.

The porous sample (Fig. 1) is irradiated by photon flux of X-ray radiation. Direction of the flux is along axis *z*. During the propagation of radiation in an object, part of photon energy is absorbed by the substance, which leads to its heating. Result of the modeling is the spatial distribution of energy deposit density. The constructed detector system (Fig. 2 - 4) is used for computing the required value (energy deposit) during simulating the radiation transport. Supercomputing the transport processes is performed using the elaborated modeling technology [18-21].

The values of energy density calculated in the centers of the detectors are shown (in relative units) in Fig.5. Required density distribution are computed by use of hybrid calculating cluster HCC K100 (http://www.kiam.ru/MVS/resourses/k100.html). The image of the surface $Q(x, y)$ at the level z=0.095 mm from the face perpendicular to which the X-ray radiation enters the object is constructed using Delaunay triangulation (Q is energy deposit density).

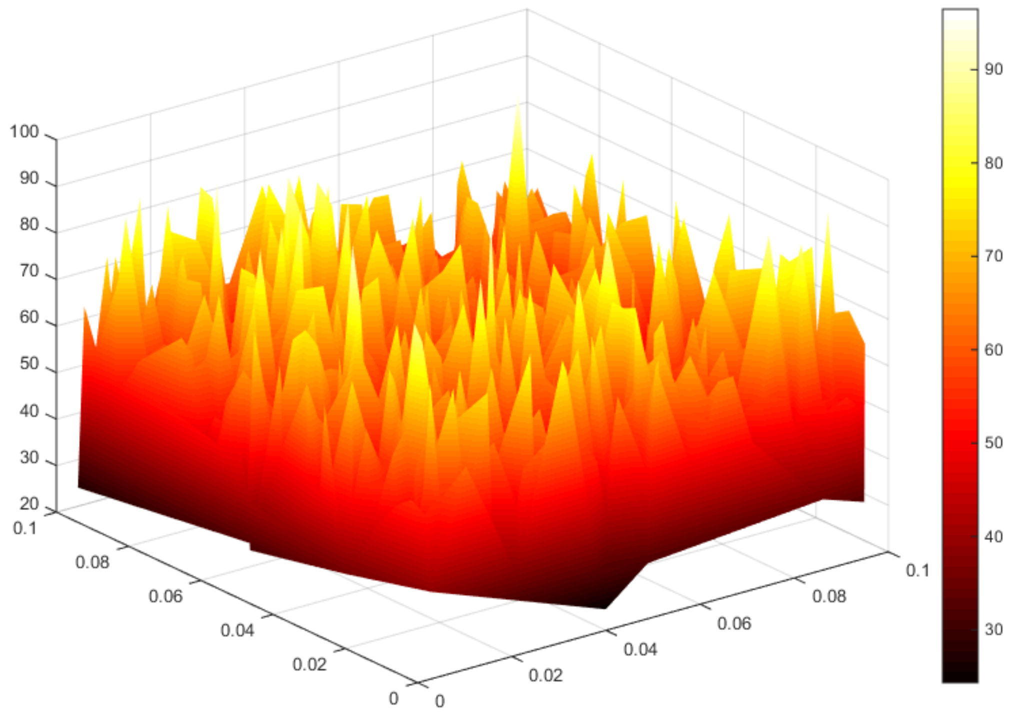


Fig. 5. Values of energy deposit density in the centers of detectors near z=0.095 mm

3D visualization of the results requires transfer computed values from the detector system on a rectangular grid.

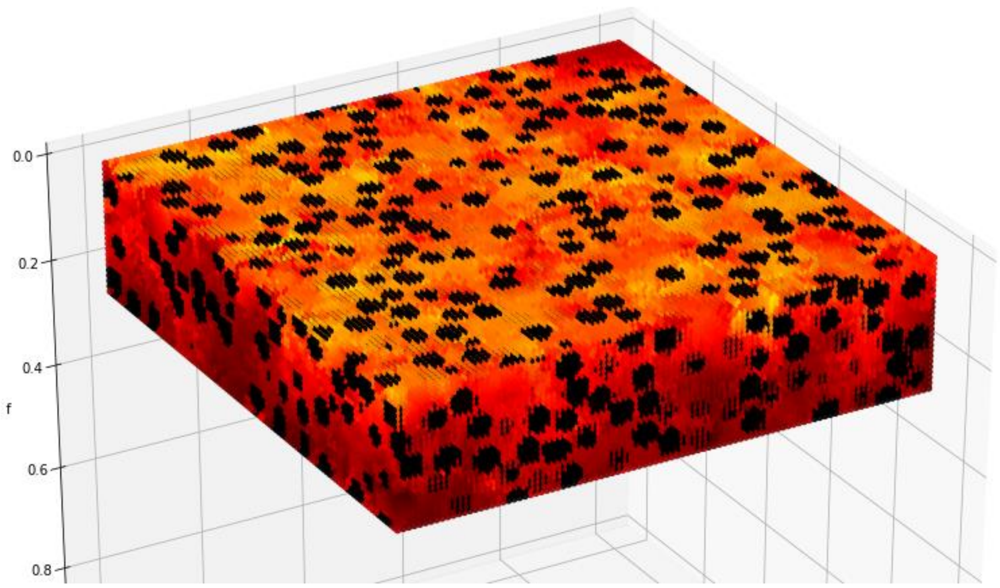


Fig. 6. The results of the approximation of energy deposit in the cells of a rectangular grid; black color shows the pores

A multi-dimensional approximation by use of nonlinear regression model [22] is performed for calculating values of energy deposit density in nodes of rectangular grid of 10x100x25 size. Fig. 6 shows the required values on this grid.

4 MODELING OF RADIATION-INDUCED THERMOMECHANICAL FIELDS

During the propagation of radiation in an object, part of its energy is absorbed by the substance. This leads to the heating of the material and, consequently, the rapid development of highly inhomogeneous temperature and pressure fields in it.

This section presents the results of mathematical three-dimensional modeling of radiation-induced thermomechanical effects in a porous object, the structure of which is described in section 2. The values of the energy deposit density in the cells of the thermodynamic difference grid (fig. 6), obtained using the 3D approximation of the results of statistical modeling of the interaction of radiation with the matter of the object, are used as a source of energy, initiating thermomechanical processes.

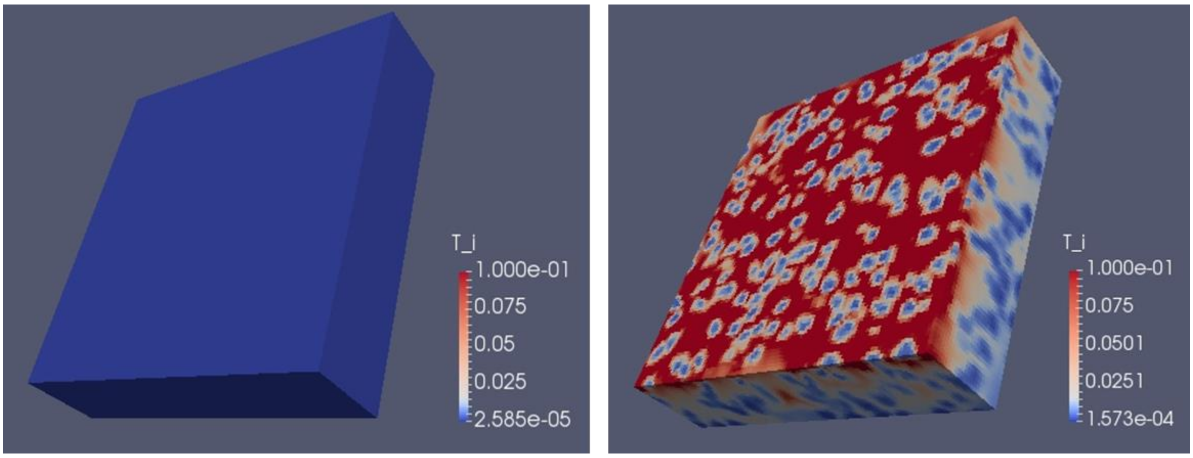
The basis for the calculation of thermodynamic processes is the ideal hydrodynamic Eulerian model of the dynamics of a compressible one-component medium in a conservative form, supplemented by the equation of state in the form of Mie-Gruneisen [23]. The conservative difference scheme of the increased order of accuracy is used for the numerical solution of the system of the ideal hydrodynamics equations [24-26]. Time integration is carried out within the framework of the predictor-corrector scheme, which provides a second order of approximation in time. An explicit scheme with a time step restriction according to the Courant condition is applied at each stage. The stage of the corrector in this scheme serves not only to increase the order of approximation in time, but also is an additional stabilizing procedure, ensuring the absence of numerical antidiffusion that occurs during the usual explicit time approximation and leads to the twisting of the solution profiles in the schemes of increased order of accuracy in space.

The modeling of thermomechanical effects in the porous structure of epoxy resin induced by the flux of x-ray photons is performed. Epoxy resin has the following parameters: density-1.13 g/cm^3, speed of sound-2.6 km/s, sublimation heat – 2 kJ/g, circumferential strength – 0.33 GPA, Gruneisen coefficient – 0.8. Photon energy fluence is about 100 J/cm^2.

The calculations are performed in a Cartesian coordinate system, in a rectangular parallelepiped 0 mm $\leq x \leq$ 1 mm, 0 mm $\leq y \leq$ 1 mm, 0 cm $\leq z \leq$ 0.25 mm (fig. 6). The plane $z = 0$ corresponds to the surface of the sample on which the x-ray radiation falls. The direction of the photon flux coincides with the z-axis. A uniform coordinate calculation grid with a step h = 0.01 mm (section 3, fig. 6) was constructed in the region, on which the results of the statistical calculation of the radiation energy deposit were approximated. The gas of low density (10^{-7} g/cm^3) is added at the initial time to carry out end-to-end calculation in pores.

The results of modeling are presented in fig. 7, 8.

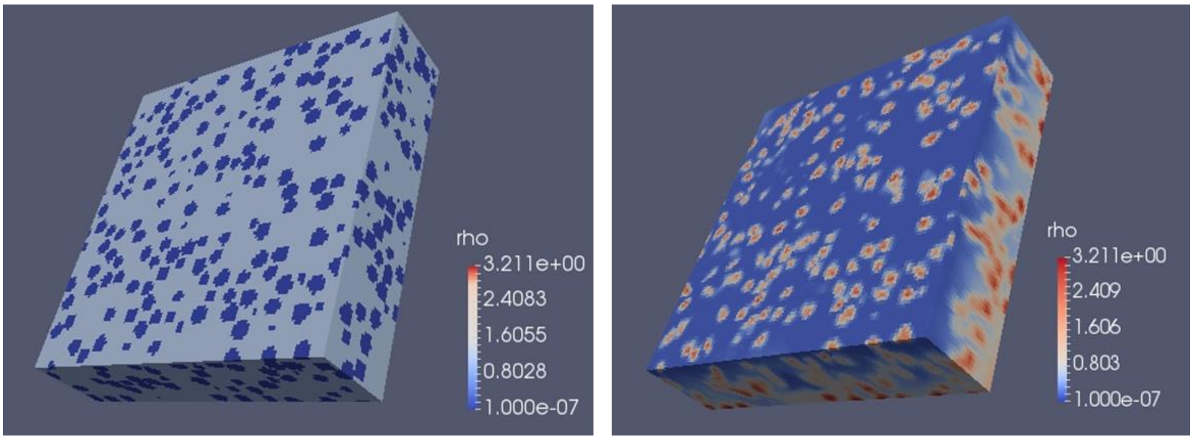
The irradiated object is in thermal equilibrium at the initial time (fig. 7a).



a) initial time b) after exposure to radiation

Fig.7. Temperature distributions in the object, keV

The results of the calculation of the density distribution in the object is shown in fig. 8.



a) initial time b) after exposure to radiation

Fig.8. Density distributions in the object, g/cm^3

Fig. 8 shows that the voids in the object are filled with the substance after irradiation of the object. As a result, the pores become the centers of concentration of the substance, which reduces the mechanical impulse of the shock wave propagating deep into the epoxy resin. The dependence of the average density of the substance in the pores on time is presented in fig. 9.

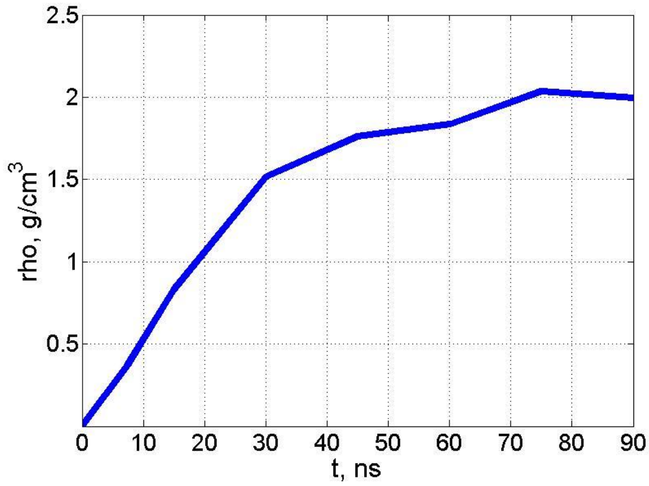


Fig. 9. The time dependence of the average density of the substance in the pores

5 CONCLUSION

The technology of the complex modeling of the radiation transport and the radiation-induced thermomechanical fields in heterogeneous matter of porous type is worked out. The technology includes the statistical method of modeling of the radiation particles flux propagation in porous substance, the method of the numerical solution of the thermodynamic equations and the means of data integration between results of radiation transport simulation and energy sources density in equations describing the development of thermomechanical effects.

The geometric part of the model contains an algorithm for the construction of a realistic geometric model of a porous medium with a direct account of the material structure at the micro level. The algorithm includes a procedure for constructing a detection system for statistical evaluation of radiation energy deposit during its propagation in the object. The detection system is constructed as a set of non-intersecting spherical detectors, which also do not intersect with the pores. The data integration method based on the algorithm of the multidimensional approximation developed by use of the nonlinear regression model.

The results of model calculations show the efficiency of the elaborated technology for supercomputer modeling of the generation and developing the complex radiation effects in matter of heterogeneous porous materials.

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