THE APPROACH TO THE MODELING OF THE RADIATION TRANSPORT IN THE POROUS MATERIAL

V. Egorova, R. Uskov*, M. Zhukovskiy

Keldysh Institute of Applied Mathematics of RAS, Miusskaya sq. 4, 125047, Moscow, Russia

*Corresponding Author: roman.uskov@gmail.com

ABSTRACT

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 taking into account 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. The applications of the developed simulation tool are presented in terms of results obtained with use of the hybrid computing cluster K-100 (http://www.kiam.ru/MVS/resourses/k100.html).

KEYWORDS: Radiation transport, Porous material, Statistical algorithm

1. INTRODUCTION

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. 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. One of the promising ways to solve this problem is the use of composite materials. One of the simplest variants of composite materials are gas-filled porous materials. 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.

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 are able to operate at high temperatures and pressures. Such materials are used in thermal protection systems of rocket engines [1], they are used to create shells of gas-turbine engines [2, 3].

Non-destructive testing (NDT) is an effective tool of studying the structure of porous materials. Radiographic inspection of their microstructure allows evaluating the quality of the material. Supercomputer modeling of the interaction between radiation and matter is a powerful means for radiography. It is useful for investigating the efficiency and reliability of x-ray equipment at the design stage [4] and for developing complex experimental methods [5]. The optimal variant of the manufacturing technology of the product with the given properties is chosen on the basis of the analysis carried out by use of mathematical modeling.

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.

Some results of the model calculations 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 physical model of the interaction of radiation with matter is based on a detailed description of the collision processes of particles with matter [6]. The basis of this model 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 \( \xi \) 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 \( \xi \), which is less than \( x \): \( F(x) = P(\xi < x) \).

The inverse function method [11] is most often used to model a random variable \( \xi \). 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 \( \xi \) satisfy the equation

\[
\int_{-\infty}^{x} f(t) \, dt = \gamma,
\]

then \( \xi \) 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 [6].

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 [7 - 9]. 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 (in the simplest case-the potential of the "solid wall"). 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 [10] 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.](image)

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 [12];
- 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 [13] 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 size distribution of the detectors is shown as a histogram in Fig. 3. The detectors do not intersect with each other and lie entirely inside the filler (do not intersect with the pores).

The process of radiation transport in the porous medium (Fig. 1) under consideration by the Monte Carlo method [14,15] is simulated using the constructed detection system (Fig. 2, 3).

3. EXAMPLE OF 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, 3) 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 [14,15].

The values of energy density in relative units calculated in the centers of the detectors are shown in Fig. 4. Required density distribution are obtained by use of hybrid calculating cluster HCC K100 (http://www.kiam.ru/MVS/resources/k100.html). The image at the level \( z = 0.0095 \) cm from the face perpendicular to which the X-ray radiation enters the object is constructed using Delaunay triangulation.

![Image 1](image1.png)

**Fig. 4** Values of energy deposit density in the centers of detectors near \( z = 0.0095 \) cm.

3D visualization of the results requires transfer computed values from the detector system on a rectangular grid. A multidimensional approximation by use of nonlinear regression technology [16] is performed foe calculating values of energy deposit density in nodes of rectangular grid of 10x100x25 size. Fig. 5 shows the required values on this grid.

![Image 2](image2.png)

**Fig. 5** The results of the approximation of energy deposit in the cells of a rectangular grid; black color shows the pores.
5. CONCLUSION

A model of radiation transport in matter of heterogeneous porous material is developed. The geometric part of the model contains an algorithm for the formation 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 results of calculations showed the efficiency of the developed model for supercomputer modeling of radiation transport in matter of heterogeneous porous materials.

ACKNOWLEDGMENT

The work was financially supported by the Program #56 of RAS Presidium

REFERENCES