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RANDOM NETWORKS IN MODELING HEAT AND MASS TRANSFER
IN POROUS MATERIALS

A detailed literature review on mathematical models of mass and heat transfer processes in porous media based on random graphs (networks) is presented. In these models, individual pores (graph nodes) are considered to be connected with a given probability by narrow channels (graph edges) through which a liquid or gas can move. A classification of the main types of random networks used in mathematical modeling of porous media is given, as well as corresponding discrete and continuous mathematical models for single-component Newtonian liquids and mixtures of immiscible liquids. In coupled heat and mass transfer problems, double random networks are usually considered, one of which corresponds to heat-mass transfer with a liquid, and another is associated with heat transfer through a solid phase. The available algorithms for constructing random graphs, mathematical models of heat and mass transfer on networks, and the results of modeling of liquid flow, several miscible or immiscible liquids of Newtonian and non-Newtonian liquids are presented. It is shown that, in addition to the possibility of the disappearance of a network edge due to the suffusion and/or aggregation of liquid/solid phase particles, it is also possible to restore the connection between neighboring nodes due to the destruction and washout of the solid phase, as well as disaggregation/disintegration of particle conglomerates. The results of the review analysis of the literature can be used to select the best random graph (network) model, discrete or continuous mathematical model, and numerical method for calculations on a specific case of a porous medium.

Key words: flows in porous media, random graphs, machine learning methods, mathematical modeling.

MS 2020 classification: 76S05, 05C80.

Introduction

Random graphs (or random networks) are mathematical objects that arise by taking n vertices (vertex set) and placing an edge (edge set) between any pair of distinct vertices with a fixed probability, independently for all pairs (Hofstad, 2016). Edges may appear or disappear during the evolution of the corresponding dynamical system (for example, due to the erosion of solid particles in a porous medium or, conversely, pore clogging); they may also be directed and weighted. This approach is referred to as neuron-like, as it corresponds to the structure of neural networks used in artificial intelligence approaches (Zhou et al., 2020). Random graphs are widely used in applied mathematics and mechanics to model fluid flow and heat transfer in porous media, multiphase systems with phase transitions, and related processes. The most well-known examples are the random graph models of Erdős-Rényi and Gilbert: $G(n, m)$, where a random graph has n vertices and m edges and all such graphs are equally likely, and $G(n, p)$, where each edge is present independently with probability p . The number of edges k incident to a vertex is called the degree of that vertex. For large n , the degree distribution of a random graph approaches the Poisson distribution $p_k = \langle k \rangle^k e^{-\langle k \rangle} / k!$, where $\langle k \rangle$ is the average over all vertices (Li et al., 2021). In the limit $n \rightarrow \infty$, with $m = [C_n^2 p]$ (where square brackets denote the integer part), the models of random graphs $G(n, m)$ and $G(n, p)$ become equivalent.

When applied to heat and mass transfer in porous media, graph models are referred to as pore-network models. Mass transfer processes may be accompanied by heat transfer. For example, evaporation of water from soil leads to a decrease in its surface temperature. Spontaneous fluid percolation may lead to local temperature jumps of several degrees due to surface chemical interaction between the fluid and the solid phase. Heat transfer occurs not only through the fluid in the pore space, but also through the solid phase. Thus, the geometry of the "thermal network" differs from that of the network associated with mass transfer, and therefore, they are usually specified separately. Both networks are treated as random, since flow stagnation with local pore blocking may occur, causing abrupt changes in both mass transfer between network nodes and convective heat transfer. Similar problems arise for flow through porous media involving immiscible fluids, where the concentrations, and even the presence of each fluid in a given pore, are random (Joekar-Niasar, & Hassanizadeh, 2012; Fyhn et al., 2021; Savani et al., 2017a).

Pore-network models consist of pore bodies (nodes) and connections between them (edges). Pore bodies are relatively large cavities of the pore space, whereas edges represent local constrictions separating these cavities. This approach is known as the watershed algorithm (Koch et al., 2021). Modern percolation theory on random graphs belongs to the class of models describing the geometrical properties of random media (Li et al., 2021). In statistical physics, percolation theory is often accompanied by scaling laws, fractal properties (self-similarity), self-organization criticality, and renormalization, which

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are all of immense importance theoretically in many diverse fields of physics. The term percolation, as well as the geometrical and probabilistic concepts of transport processes in porous media, first appeared as mathematical formulations in the work (Broadbent, & Hammersley, 1957). According to this concept, the connection of any two adjacent pores is probabilistic, supposing the probability is p . If most pores are connected into a single large cluster, the fluid can reach the center of this cluster from the surface of the porous medium. The percolation problem reduces to determining whether there exists a connected path of pores from the surface to the center of the medium for a given probability p . Such problems have most often been studied on square lattices. It can be shown that for $p > 0.6$, large clusters appear in the pore space that connect the surface of the medium with its center. This ensures percolation throughout most of the medium (Li et al., 2021).

Random graph models are also used to describe resource consumption and the eventual resource depletion during fluid flow in porous media. Directed edges forming shortest paths that connect pairs of nodes in the direction of fluid flow are removed if the flow rate through them falls below a certain threshold. As a result of this edge-removal procedure, together with the elimination of disconnected nodes, the graph becomes disconnected, i.e., it undergoes a percolation transition. In (Kim, & Radicchi, 2024), it was shown that under limited flow capacity, this transition is identical to that of standard percolation, where a single giant cluster shrinks as edges are removed from the graph. However, for an infinite flow budget, the transition becomes sharper than in standard percolation and is accompanied by an abrupt fragmentation of the graph into a set of clusters of equal size.

The object of this study is various types of random graphs used to model heat and mass transfer processes in porous media. The aim of this work is to identify the most promising combinations of random network type, mathematical model, and numerical algorithms for simulating transport processes in porous, fractured, and porous-fractured media.

1. Classification of models

1.1. Geometry of random networks

1.1.1. Regular lattices with random edges

In two-dimensional problems, regular triangular, square (Fig. 1a), rhombic, hexagonal, or bi-hexagonal lattices (Ewing, & Gupta, 1993) can be used. Connections (edges) between certain pairs of neighboring nodes are randomly removed (with a given probability), or their conductance (hydraulic permeability) is reduced. In three-dimensional cases, tetrahedral or cubic lattices are most commonly used. Tree-like graphs are also employed in the form of binary trees or Bethe lattices (Fig. 1 b). These are infinite connected graphs without cycles (infinite trees) in which all vertices have the same degree (Li et al., 2021).

1.1.2. Fully random networks

These networks have edges assigned with a given probability according to the Gilbert model $G(n, p)$, the Erdős-Rényi model $G(n, m)$, and several others, while the degree distribution of the vertices follows a Poisson distribution (Fig. 1 c, d).

1.1.3. Small-world graphs

A small-world network is a graph in which two arbitrary vertices a and b are not adjacent with high probability. However, one can reach b from a in a small number of steps via other vertices. As a result, such a graph is characterized by a path length (i.e., the number of steps) between two vertices $L \sim \log(n)$. In such graphs, clusters arise – relatively small subsets of vertices that are connected to their hub (i.e., a node with a degree significantly higher than the average in the graph) by short paths of length $L \sim 2 - 4$ (Fig. 1e). Such properties are exhibited by various porous media, including fractured soils.

1.1.4. Scale-free networks

Scale-free networks are networks in which the degree distribution follows a power-law, at least asymptotically. That is, the fraction $P(k)$ of nodes in the network that have k connections to other nodes depends on k as $P(k) \sim k^{-q}$, $2 < q < 3$ (Fig. 1 f). These models are based on observational data on the number of citations of scientific publications, the topology of the Internet, and others, which have shown that some nodes (hubs) have significantly more connections than others, and that the network as a whole exhibits a power-law distribution of node degrees. Similar properties are observed in some porous media.

1.1.5. Other types of networks

In addition, the following types of random networks are distinguished: fully connected, star-shaped (centroid), ring, bus, hybrid, partial, and incomplete networks (Xiong, Baychev, & Jivkov, 2016).

1.1.6. Multiscale random networks

In real porous media, there exist large (mesoscale), small (microscale), and nanoscale pores, as well as corresponding fractures at different scales. To model heat and mass transfer processes in such complex media, multiscale random networks with different types and degrees of connectivity have been deployed (Rabbani, Babaei, & Javadpour, 2020).

1.2. Percolation models on random networks

1.2.1. Percolation on regular lattices with prescribed random conductivity

In this model, nodes and/or edges are randomly considered either occupied (with probability p) or unoccupied (with probability $1 - p$). For convenience, each unoccupied node/connection with probability $p = 0$ can often be removed. However, in models with deformation and erosion of the solid phase, such connections may reappear (with probability $p \neq 0$), and therefore they must be retained to allow for switching. In the case of flow of a mixture of immiscible fluids through a cross-section of a porous medium (Savani et al., 2017a), channels (graph edges) through which a given fluid flows at a given time are selected randomly (Fig. 2a). This is because such flow most often occurs in the form of intermittent motion of fluid slugs (Fig. 2b) with different probabilities, i.e., with different hydraulic conductivities of the edges (Fig. 2c). Monte Carlo methods are also used to model percolation on random graphs (Savani et al., 2017b; Gjennestad, Winkler, & Hansen, 2020).

1.2.2. Discrete percolation models

Discrete percolation models are typically studied using probability theory. One of the simplest examples is the Bernoulli lattice, where each cell of the lattice is open with probability p or closed with probability $1 - p$. The study of percolation on such a lattice makes it possible to determine the values of p at which large clusters of open cells appear, forming pathways for the percolation of a fluid or gas.

One of the key problems in percolation theory is the determination of the percolation threshold p_c , which indicates the critical probability at which the transition from fragmented clusters to large connected clusters capable of transmitting a fluid or gas through the entire material begins.

At the same time, there exist discrete models designed, for example, to evaluate the efficiency of filters, in which the clogging process is described by a deterministic sequence of channels becoming blocked (Goldsztein, 2009).

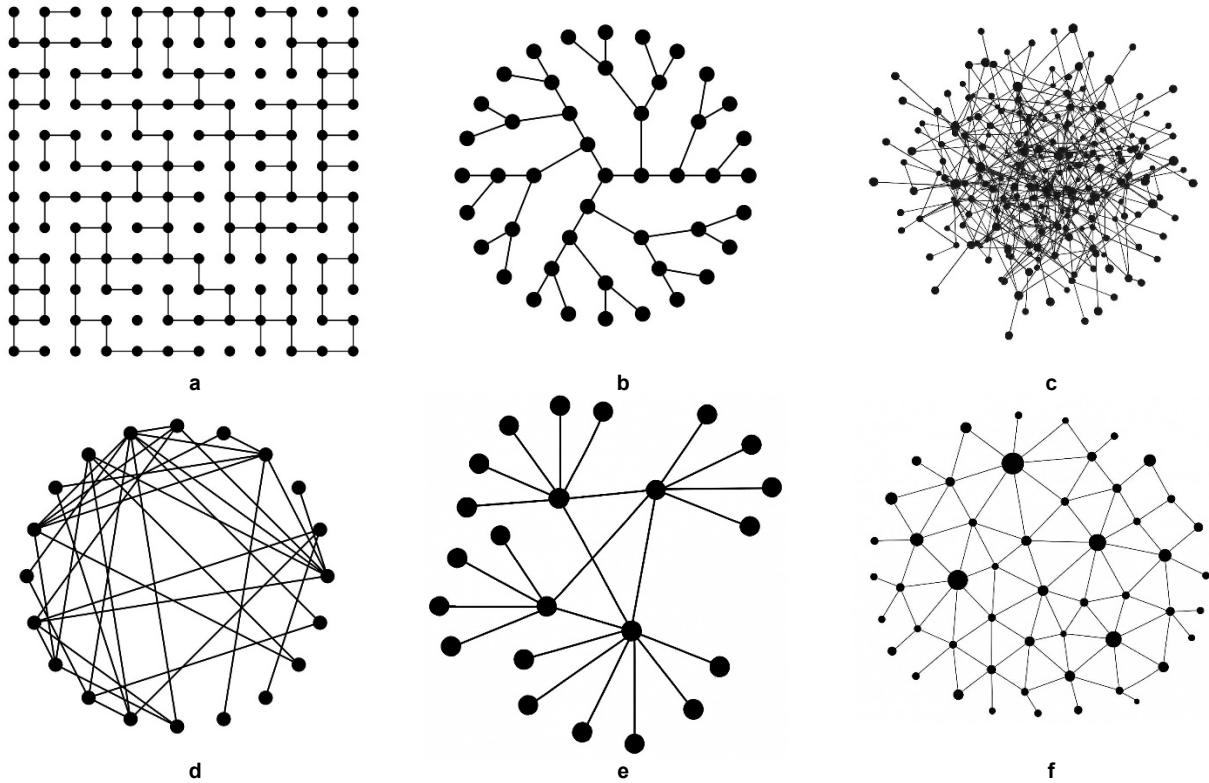


Fig. 1. Pore-network geometries: regular lattice (a), Bethe lattice (b), 3D random network with $p = 0.5$ (c), 2D random network with $p = 0.2$ (d), small-world network (e), and scale-free network (f)

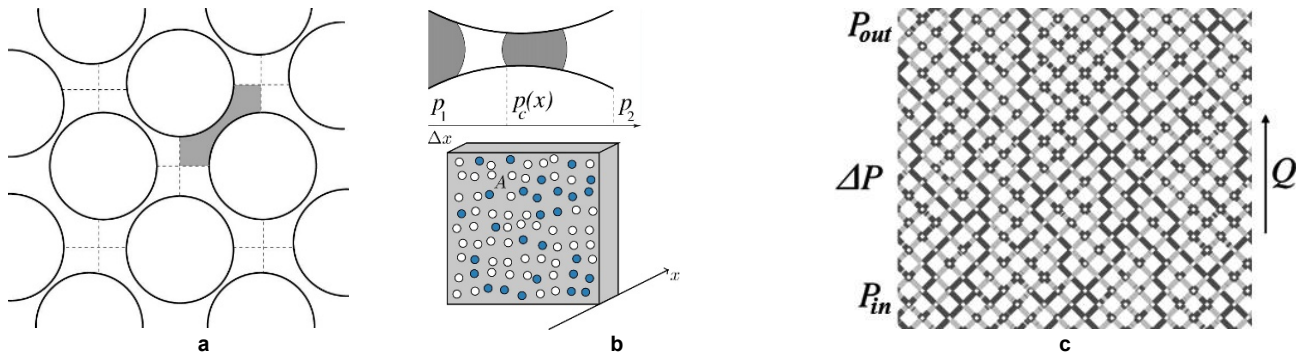


Fig. 2. Pore-space geometry: (a) Kozeny model, with the link between two vertices shown in gray; (b) a single link with two immiscible fluids flowing through the pore space; (c) a random rhomboidal network of nodes and channels with different randomly assigned hydraulic conductances, indicated by color

1.2.3. Continuum percolation models on random networks

In the case of two immiscible fluids with relative concentrations φ and $1 - \varphi$, the average flow velocity $\bar{v} = \varphi \bar{v}_1 + (1 - \varphi) \bar{v}_2$ is determined by the pressure difference at the inlet (P_{in}) and outlet (P_{out}) nodes of the network (Fig. 2c), where $\bar{v}_1$ and $\bar{v}_2$ are the velocities of fluids 1 and 2 (e. g., hydrophilic and hydrophobic), which satisfy Darcy's law:

$$\bar{v}_1 = -\frac{K_1(p, \varphi)}{\mu_1} \bar{\nabla} P_1, \quad \bar{v}_2 = -\frac{K_2(p, \varphi)}{\mu_2} \bar{\nabla} P_2, \quad (1)$$

where μ_1 , μ_2 are the fluid viscosities, and K_1 , K_2 are the permeabilities of the network edges corresponding to each fluid and dependent on the probability p . The local hydrostatic pressures P_1 , P_2 are related through the capillary pressure $P_c = P_1 - P_2$ (Savani et al., 2017a).

Darcy's law establishes a linear relationship between the pressure gradient and the filtration velocity of a fluid through a porous medium. This linear relationship holds only for slow flows with Reynolds number $Re < 10$. The filtration velocity at which Darcy's law ceases to be valid is referred to as the critical filtration velocity. The pore size distribution significantly affects the critical characteristics of the percolation process. Variability in material properties (network heterogeneity) also influences the velocity parameters of filtration.

For the systematic study of traditional problems within the framework of the hydrodynamic theory of filtration, the stochastic theory of filtration processes is employed.

2. Machine learning in percolation models

2.1. Machine learning methods

2.1.1. Supervised learning

Machine learning methods have rapidly become pervasive instruments due to better fitting quality and predictive quality in comparison with traditional models in terms of phase transitions and critical phenomena. Usually, machine learning can be divided into supervised and unsupervised learning. In the former, the machine receives a set of inputs and labels. Supervised learning models are trained with high accuracy to predict labels.

For the analysis of a two-dimensional percolation model, we use datasets obtained via Monte Carlo simulations and a convolutional neural network (CNN). The CNN architecture consists of four layers, including two convolutional layers and two fully connected layers (Fig. 3). Percolation configurations X are used as input data:

$$X = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,N} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{M,1} & a_{M,2} & \cdots & a_{M,N} \end{pmatrix} \quad (2)$$

The CNN receives the permeability p as an output.

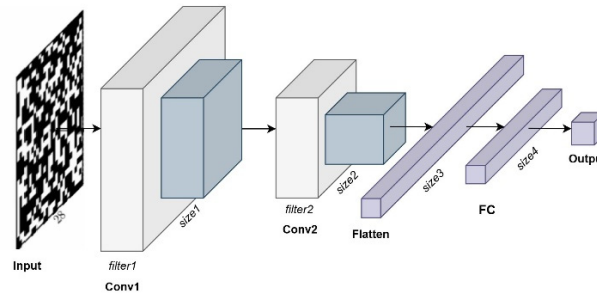


Fig. 3. The structure of the CNN with four layers, including "Conv1", "Conv2", "FC" та "Output"

2.1.2. Unsupervised learning

On the other hand, in unsupervised learning models, there are no labels. Unsupervised learning can be used as a meaningful analysis tool, such as sample generation, feature extraction, and cluster analysis.

The following unsupervised models are used to generate new initial configurations: a variational autoencoder (VAE) and a convolutional variational autoencoder (cVAE). A VAE is an architecture introduced by Diederik P. Kingma and Max Welling and belongs to the class of variational Bayesian methods (Kingma, & Welling, 2014). The VAE is composed of an encoder and a decoder. The VAE uses two different CNNs as two probability density distributions. The encoder in the VAE, called the inference network $P_{encoder}(Z|X)$, can generate the latent variables Z . The decoder in the VAE, called the generative network $P_{decoder}(\hat{X}|Z)$, reconstructs the raw configuration X .

To better reconstruct the raw two-dimensional configuration X , the fully connected layer in the VAE is replaced by the convolutional layer. Now we have got the cVAE. The architecture of the cVAE is shown in Fig. 4. Usually, the performance of the cVAE is better than the VAE due to the configuration X with spatial attribute (Cheng et al., 2021).

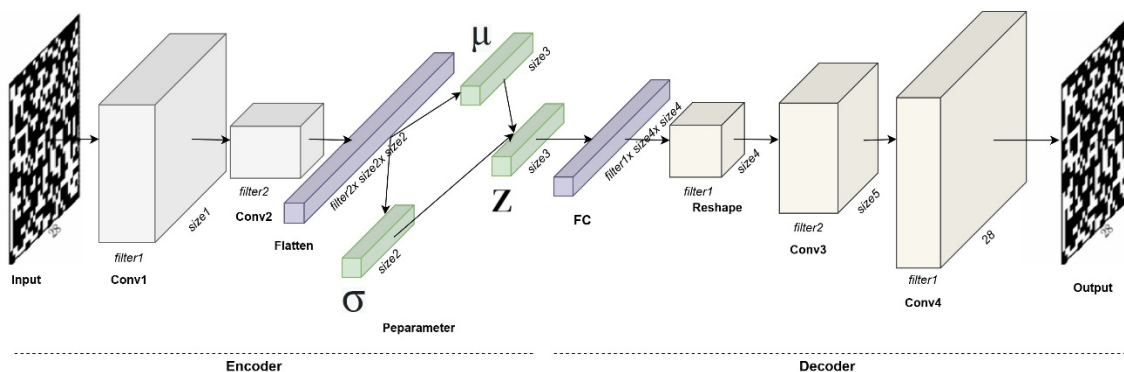


Fig. 4. The structure of the cVAE with an encoder and a decoder. The left part refers to the encoder with three layers, including the input layer, two convolutional layers, a flatten layer, and a fully connected layer with mean value " μ " and the standard deviation " σ ". The right part is a decoder with four layers, including the layer " Z ", a fully connected layer "FC", a reshape layer, two transposed convolutional layers, and an output layer

2.1.3. Training and optimization

For training, we make use of the TensorFlow library to perform the CNN with four layers. Let the first two layers of this CNN consist of two convolutional layers ("Conv1" and "Conv2"), both of which possess "filter1"=32 and "filter2"=64 filters of size 3x3, and a stride of 1. Each convolutional layer is followed by a max-pooling layer of size 2x2. The final convolutional layer ("Conv2") is strongly interlinked to a fully connected layer "FC" with 128 variables. The output layer ("Output"), followed by "FC", is a fully connected layer. For the two convolution layers and the fully connected layer "FC", a rectified linear unit (ReLU) $a = \max(0, x)$ is chosen as activation function due to its reliability and validity (Agarap, 2018). However, the output layer has no activation function.

After determining the framework of CNN, here we mention how to train CNN for deducing p . First, we carry out the Adam algorithm (Kingma, & Ba, 2014) as an optimizer to update parameters, i.e., weights and biases. Then, a mini batch size of 256 and a learning rate of 10^{-4} are selected for its timesaving. Following this treatment, CNN is trained for 1000 epochs on 40000 uncorrelated and shuffled configurations, respectively. Before training, we split X configurations (2) into a 32 000 training set and an 8000 testing set.

While training, we monitor using the loss function, i.e., mean squared error (MSE) (3) for training and testing sets (Cheng et al., 2021). y_i^{raw} and y_i^{pred} denote the true and predicted values of p in Eq. (3).

$$MSE = \frac{1}{M} \sum_{i=1}^M (y_i^{pred} - y_i^{raw})^2. \quad (3)$$

If the loss function on the test set reaches a minimum, the optimal CNN is obtained. As the number of epochs increases, the MSE continues to decrease until it reaches a plateau. Another performance metric of the CNN is the difference between the initial permeability p and its predicted value $\hat{p}$. The dark gray points in Fig. 5 indicate a strong positive correlation between the actual permeability p and its predicted value $\hat{p}$. Additional statistical tests show that most deviations between p and $\hat{p}$ are less than 0.1. An additional optimization step, principal component analysis (PCA) can be used to reduce the dimensionality of the input data before training, facilitating data analysis, noise reduction, and the analysis of latent variables (Yu, & Lyu, 2020).

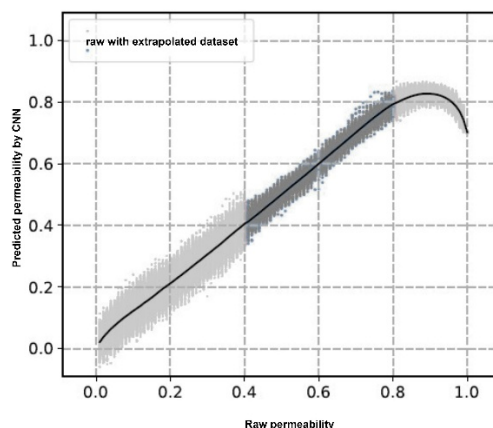


Fig. 5. Correlation between raw permeability and CNN-predicted permeability. Dark gray points denote data from the training range of the original dataset (0.4–0.8). Light gray points denote data from the extrapolated ranges (0–0.4 and 0.8–1.0). The black curve shows the mean predicted permeability for raw permeability values ranging from 0.01 to 1.0 with a step size of 0.01

Discussion and conclusions

As machine learning approaches are becoming increasingly popular and effective, they can be used to study percolation in porous-media models. In this paper, a CNN was used to model the permeability of porous media. VAE and cVAE were applied to generate new configurations – the generated variants preserve the main structural features but differ from the initial configurations, which confirms the robustness and generalization ability of the CNN. In addition, PCA was used for optimization in order to reduce the dimensionality of the initial configurations.

Neural networks provide fairly accurate predictions but require further cross-validation. The machine learning methods considered here are effective for studying physical characteristics in the percolation model. However, it should be acknowledged that they are based on a two-dimensional percolation model and therefore have certain limitations.

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ВИПАДКОВІ МЕРЕЖІ У МОДЕЛЮВАННІ ТЕПЛОМАСОПЕРЕНОСУ В ПОРИСТИХ МАТЕРІАЛАХ

Представлено детальний огляд літератури з математичних моделей процесів тепломасоперееносу в пористих середовищах на основі випадкових графів (випадкових мереж). У цих моделях окремі пори (вузли графа) вважаються з даною ймовірністю зв'язаними між собою вузькими каналами (ребрами графа), крізь які рухається рідина або газ. Наведено класифікацію головних типів випадкових мереж, що використовуються в математичному моделюванні пористих середовищ, а також відповідних дискретних і континуальних математичних моделей для однокомпонентних ньютоновських і неньютоновських рідин. У зв'язаних задачах теплоперееносу розглянуто подвійні випадкові мережі, з яких одна відповідає тепломасоперееносу з рідиною, а друга – перееносу крізь тверду фазу. Наведено наявні алгоритми побудови випадкових графів, математичні моделі тепломасоперееносу на мережах і результати моделювання фільтрації рідини, кількох змішуваних або незмішуваних ньютоновських і неньютоновських рідин. Крім можливого зникнення ребер мережі внаслідок суфозії та/або агрегації частинок рідини / твердої фази, можливим також є відновлення зв'язків між сусідніми порами шляхом руйнування і вимивання твердої фази, а також дезагрегації / розпаду конгломератів частинок. Результати оглядового аналізу літератури можуть бути використані для вибору найкращої для конкретного випадку пористого середовища моделі випадкового графа (мережі), дискретної або континуальної математичної моделі, а також чисельного методу розрахунків. Розглянуто застосування методів машинного навчання для дослідження фізичних характеристик пористого середовища в моделі перколяції.

Ключові слова: течії в пористих середовищах, випадкові графи, методи машинного навчання, математичне моделювання.

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