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# Application of path-percolation theory and Lattice-Boltzmann method to investigate structure–property relationships in porous media

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ABSTRACT

In this study, path-percolation theory was applied to randomly generate porous media, and effective porosities of these domains were determined. A statistical approach was pursued to determine effective porosity with confidence levels of 95%, 97%, and 99%. Furthermore, the Lattice-Boltzmann method was applied to obtain the velocity distribution throughout the porous channels to evaluate effective tortuosity. Two dimensional lattices with nine velocity components were utilized for fluid flow simulations. A new effective diffusivity model for porous media was developed using the effective porosity and tortuosity determined by path-percolation and Lattice-Boltzmann theories, respectively. Diffusion behavior of gasses in porous media as a function of porosity is typically unpredictable when the porosity is below 0.6, but the developed diffusion model as a function of effective porosity is shown to be useful in all effective porosity ranges.



## 1. Introduction

Percolation theory describes a probabilistic model that includes a phase transition [1]. This theory can be used to simulate an inhomogeneous medium, which must be constituted by at least two phases. As an example, a virtual, square porous medium can be constructed with randomly assigned void and solid constituents. Let us assign the probability of generating a void (pore) as $p$, hence the solid generation probability becomes $1 - p$. Two-dimensional percolation theory dictates that the fluid particles can only move in four directions; up, down, left, and right, and they cannot move to cross nodes. The probability of an open path from the center of the porous domain to any of the sides is called the *percolation probability* and denoted by $\theta(p)$ [2]. Percolation probability becomes unity if the whole domain is void (that is, $\theta(1) = 1$). As $p$ decreases, percolation probability decreases, and below a critical point called the *percolation threshold*, $p_c$, becomes zero.

The Lattice Boltzmann Method (LBM) is a mesoscopic scale technique, which lies between microscopic and macroscopic scale analyses, and is utilized by investigating the behavior of a collection of particles as a unit [3–5]. A distribution function represents any property of these units. LBM can be used to simulate single and multiphase flows with a wide range of behaviors including condensation, cavitation, phase separation, surface interaction, etc. In this study, LBM was utilized to simulate mass and momentum flow in randomly generated porous media.

There are a few studies which combine percolation theory and Lattice-Boltzmann applications to examine flow in porous media. Nabovati and Sousa [6] simulated fluid flow in two dimensional random porous media by using the Lattice-Boltzmann method to determine the relation between permeability and porosity. They randomly placed identical rectangles with overlapping to construct the porous domains. It was found that, for the same porosity, the permeability decreased when the regularity of the porous medium was disturbed. Furthermore, permeability varied exponentially with porosity, independently from porous media organization. Koponen et al. [7] investigated the relationship between tortuosity and porosity by using a lattice-gas cellular automation method. In their simulations, the domain of interest was constructed by randomly placing rectangles of the same size with overlapping. A porosity range of 0.5–0.9 was used, while the tortuosity varied linearly with porosity. Koponen et al. [8] analyzed permeability and effective porosity of porous media by using the same methods as in their previous work [7]. A Newtonian, incompressible, two

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dimensional flow was used for the simulations, and they obtained curve fit equations for tortuosity, effective porosity, and permeability as functions of porosity. Matyka et al. [9] performed a numerical study on the relation between tortuosity and porosity in a microscopic model of a porous medium. They obtained streamlines of the flow by using Lattice-Boltzmann theory, and a new empirical model was found for tortuosity depending on system size and porosity. Grucelski and Pozorski [10] applied the Lattice Boltzmann method to perform fluid flow and heat transfer computations. The domain was constructed by uniformly placing circular particles with different diameters within a certain range. They provided free overlapping and intersection of the particles with the system boundaries. The temperature profiles and pressure drop were obtained as the results of their study.

A new alternative method called *path-percolation modeling* was developed by Jung et al. [11] to simulate the electrical property variations in a spatially disordered porous medium. This method was adapted here to determine the micro-properties related to mass transfer through a porous medium. After randomly constructing the porous domain, and performing the cluster labeling, the Lattice-Boltzmann method was utilized to solve the momentum balance equation and obtain the velocity distribution throughout the channel. The uniqueness of this study is based on the statistical modeling it pursues and the cluster labeling process, which is described in detail in the following section. Preventing the overlapping is also another novel outcome described in this study. Besides the stochastic based random diffusion media generation, the other target of the study is to develop a new effective diffusivity model suitable for all values of porosity using effective porosity, tortuosity, and diffusion ratio determined by combined path-percolation and Lattice Boltzmann methods. The results of this study can be useful to predict the mass diffusion behavior in any porous medium application.

## 2. Path-percolation theory

There are three steps in this adaptation of statistical based path-percolation theory. The first step is determination of the system characteristics, specifically; total node numbers, trials and porosity. To accomplish this; a confidence-level study must be performed. After determining the system characteristics, a random porous media domain generation is done as. Pores or solid phases are assigned to each node in the porous medium depending on the specified porosity. A cluster labeling process is followed to eliminate the unconnected (orphan) pores, since they have no ability to transport through porous media. The physical counterpart of the percolation probability is the effective porosity, which is a micro-property of the porous domain. The effective porosity is distinct from the porosity, and obtained after the cluster labeling process.

### 2.1. Confidence level studies

The confidence level [12] expresses the reliability of any estimate and values of 95%, 97%, and 99% confidence levels were analyzed for our model.

$$Pr\left\{\left|\frac{k}{n}-p\right| \leqslant \varepsilon\right\} = CL \tag{1}$$

In Eq. (1), $p$ stands for the probability of an event to occur, which is the probability of a pore to occur in a node in our analysis. Total trial number is represented by $n$ whereas $k$ stands for the number of cases of $Pr\ \{void\} = p$ in $n$ trials. Error is represented by $\varepsilon$ and shows the difference between the true and estimated probabilities of an event. Finally, $Pr$ and $CL$ represent the probability of the event in the brackets and confidence level, respectively.

Eq. (2) is obtained after applying the law of large numbers [12]:

$$Pr\left\{\left|\frac{k}{n}-p\right| \leqslant \varepsilon\right\} = 2\mathbb{G}\left(\varepsilon\sqrt{\frac{n}{pq}}\right) - 1 = CL \tag{2}$$

where $q = 1 - p$ is the probability of generating a solid, and $\mathbb{G}$ is the Gaussian function which is related to error function as follows:

$$\mathbb{G}(z) - \frac{1}{2} = \text{erf}(z) \tag{3}$$

after combining Eqs. (2) and (3), the following relation is obtained:

$$\text{erf}\left(\varepsilon\sqrt{\frac{n}{pq}}\right) = \frac{CL}{2} \tag{4}$$

Error, $\varepsilon$, is accepted as $3 \times 10^{-4}$ for this study. Although a wide porosity range was investigated in this study, confidence level studies for three cases with $\Phi = 0.60$, $\Phi = 0.75$, and $\Phi = 0.90$ were analyzed in detail, and the related $p$ values are 0.60, 0.75, and 0.90, respectively. Hence, the $q$ values $(1 - p)$ become 0.40, 0.25, and 0.10. The total number of histories were calculated by using Eq. (4) and an error function table [12]. Mathematically, the number of the history is the trial number multiplied by the total nodes. The calculations and the results are shown in Table 1.

### 2.2. Random porous media generation with cluster labeling

After determining the trial numbers needed and the total node numbers, porous media generation with cluster labeling is initiated. It should be emphasized that the porous media generated here are considered as gas diffusion channels, and the lower and upper boundaries are accepted as inflow and outflow boundaries, respectively, while the side walls are impervious boundaries, and thus reflective.

An in-house program was developed to construct a porous medium by randomly assigning numbers between 1 and 100 to each node. After the random number assignment, the nodes with the values greater than 60 were accepted as solid and the remaining nodes became pores for a 60% porous medium simulation. Fig. 1(a–c) show a sample procedure for 60% porous media with low, medium, and high effective porosities, respectively. In this simple demonstration, 100 by 100 nodes were used. At this point, it is noted that, since the transport of molecules is the basic consideration in this study; low, medium, and high effective porosities are therefore referred as worst, medium, and best cases, respectively. Hence, Fig. 1(a–c) show the worst, medium, and best cases for transport, respectively.

The next step is cluster labeling. The connected pores are grouped into clusters. Clusters that are connected to neither inflow nor outflow boundaries are eliminated and considered as orphaned and isolated, and are therefore equivalent to a solid. After cluster

**Table 1**
History calculations for path-percolation model.

| Confidence level | $\text{erf}\left(\varepsilon\sqrt{\frac{n}{pq}}\right)$ | $\varepsilon\sqrt{\frac{n}{pq}}$ | $\phi$ | $n$ | Trials | Nodes |
|---|---|---|---|---|---|---|
| 95% | 0.475 | 1.9604 | 0.90 | 3,843,168 | 384 | 100 × 100 |
| | | | 0.75 | 8,006,600 | 801 | |
| | | | 0.60 | 10,248,448 | 1025 | |
| 97% | 0.485 | 2.1707 | 0.90 | 4,711,938 | 209 | 150 × 150 |
| | | | 0.75 | 9,816,539 | 436 | |
| | | | 0.60 | 12,565,169 | 558 | |
| 99% | 0.495 | 2.5767 | 0.90 | 6,639,383 | 166 | 200 × 200 |
| | | | 0.75 | 13,832,048 | 346 | |
| | | | 0.60 | 17,705,021 | 443 | |