ISTECS JOURNAL
Science and Technology Policy

[Papers]

Estimation of the Properties of Heterogeneous Porous Medium Using Lattice Gas Automata Model

Dedy Kristanto[1] and Mariyamni Awang[2]

[1]Petroleum Engineering Department, Universitas Pembangunan Nasional "Veteran"
Jl. SWK 104 (Lingkar Utara), Condongcatur, Yogyakarta 55283, Indonesia
Tel/fax: +62-274-486056, e-mail : dedykris@yahoo.com
[2]Petroleum Engineering Department, University of Technology Malaysia
Skudai 81310, Johor Bahru, Malaysia. e-mail: k-mariy@utm.my
Tel: +607-5505358, Fax: +607-5581463

ABSTRACT

Most models for reservoir simulation are on the scale of meters to hundreds of meters. However, increasing resolution in geological measurements results in finer geological models. Simulations of particle movements provide an alternative to conventional reservoir simulation by allowing the study of microscopic fluid flow, which is chosen to the scale of geological models. In this work, a porous medium was modeled by lattice a gas automata model.

The FHP-II model (FHP: Frisch, Hasslacher and Pomeau) of lattice gas automata was developed to simulate microscopic flow and estimate the properties of heterogeneous porous medium. Heterogeneity simulated by places solid obstacles randomly in a two-dimensional test volume. The properties of the porous medium were estimated by the shape, size, number of the obstacles and by the distribution of the obstacles within the volume. Simulating of porous medium and rock properties were varying from 10% to 35% of porosity. Numerical correlations of the porous medium properties were found between the tortuosity, effective porosity and permeability as a function of porosity. Reasonable agreement between the lattice gas automata simulation and theoretical results were obtained.

Keywords: Lattice Gas Automata, porous medium, tortuosity, porosity, permeability

1. INTRODUCTION

Modeling fluid flow in a porous medium is of interest in petroleum engineering. Within the earth sciences alone, knowledge of flow characteristics in a porous medium strongly impacts of the production of oil and gas. In each of these instances, the permeability of the porous medium – a measure of the sease with which fluid flows through reservoir rocks – is one of the important physical properties. Due to the in oil

and gas production the permeability of reservoir rocks directly affects the economic potential of a well.

Many numerical methods have been developed to simulate the fluid flow and to estimate the physical properties of a porous medium. The conventional methods, such as finite difference and finite element have been useful for simulating fluid flow in a porous medium, and have been used extensively. Numerical methods based on the finite difference approximation of the governing equations are probably the most commonly used tools for simulating fluid flow and predicting their performance. In practice, the porous media usually represented by discrete grid blocks, and transfer of each constituent being tracked is computed across each block face for a succession of small time increments. Finite difference and finite element methods use floating-point mathematics, which require incline computation and have limited accuracy. However, lattice gas automata methods use mainly Boolean manipulation.

The lattice gas automata methods have been used to simulate fluid flow in complex media and to estimate the parameters such as porosity and permeability. Rothman [1], measured the permeability of a rock sample by using lattice gas automata. The lattice gas automata model that Rothman's used was the FHP model, (Frisch, Hasslacher and Pomeau, FHP). This model describes the individual particles motion, and the numerical calculation involved in simulating each lattice gas is just simple binary manipulation.

Lattice gas automata model is a variant of cellular automata and consists of lattices where the intersection points of the lattice can take a finite number of states. The automata evolve in discrete time steps; the state of each site at any time is estimated by its own state and the state of a set of neighboring sites at the previous time step. A lattice gas model in which the state of the fluid needs to be known only at the lattice sites and only at discrete times can run much faster on a computer than a conventional simulation method. The lattice gas model has another big advantage over molecular simulation since all the collisions occur at the same time. This is advantageous if the simulation is being run on a parallel computer. These two times saving advantages of the lattice gas model allow simulations of a significantly large scale to be performed.

Furthermore, there are three types of FHP model of lattice gas automata, i.e., FHP-I, FHP-II, and FHP-III, which have been developed, based on the particles usage (with or without rest particles) and the possible outcomes collision configurations occurred [1, 2]. The simplest of the FHP models is the FHP-I in which there are no rest particles, and gives 64 possible in-states. The FHP-II model introduces a rest particle and allows the particles to collide according to the following rules, and this gives 128 possible interactions outcomes. While, the FHP-III model is an extension of FHP-II, which allows

all collisions conserve mass and momentum at each site, and gives 76 possible collisions. This work used the FHP-II model of lattice gas automata to simulate and analyze of fluid flow in heterogeneous porous medium. The aim of this work is to use lattice gas automata to estimate the porosity, effective porosity, tortuosity and permeability, which are used to characterize transport phenomena in a porous medium. The computation involved in the lattice gas model is completely deterministic, and the behavior of each lattice gas directly influences the results of the simulation.

2. MODEL OF FLUID FLOW IN HETEROGENEOUS POROUS MEDIUM

In the FHP-II model, at each site of two-dimensional hexagonal lattice particle can move into any of six directions. The sketch of two-dimensional simulation model is shown in Figure 1. The longitudinal direction is the "y" direction, where W is the number of sites in that direction and the transverse direction is the "x" direction, with L sites. The particles of unit mass and unit velocity move along the lattice links of unit length (Figure 1). The cells are associated with the unit velocity vectors connecting the node to six nearest neighbors, [2, 3],

$$c_i = \{\cos(\pi i/3), \sin(\pi i/3)\} \quad i = 1, 2, ..., 6 \tag{1}$$

At a given time t_n, the state of the lattice x_{ij} is defined by

$$n(x_{ij}, t_n) = \{n_i(x_{ij}, t_n)\} \quad i = 1, 2, ..., 6 \tag{2}$$

where $n_i(x_{ij}, t_n)$ is a Boolean variable; $n_i(x_{ij}, t_n) = 1$ if the i-th cell is occupied and 0 if it is vacant. Collision and propagation produce the microscopic motion with progression of time. Evolution of the system is specified by the assumed collision and propagation rules for particles. One time step refers to one set of collision and propagation steps.

The one-particle distribution function at the each node of 6-bit state, $f_i(x, t)$ gives probability of finding a particle with velocity c_i at position x and time t. The updating of f includes two processes, i.e., collision is given by Equation (3), and propagation is given by Equation (4), respectively, where Δ_i signify the particle velocity change due to collision.

$$f_i(x, t) = f_i(x, t) + \Delta_i(f(x)) \tag{3}$$

$$f_i(x, t) = \quad f(x + c_i, t + 1) \tag{4}$$

The collision rules are Boolean expressions, which define the relationship between the input and output states of a site and updated according to Equation (5),

$$n_i(x_{ij}, t_n{}^+) = n_i(x_{ij}, t_n{}^-) + \Delta_i\{n(x_{ij}, t_n{}^-)\} \tag{5}$$

$$
\begin{aligned}
\Delta_i = {}& \xi n_{i+1} n_{i+4}(1 - n_{i+6})(1 - n_{i+2})(1 - n_{i+3})(1 - n_{i+5}) \\
& + (1 - \xi) n_{i+2} n_{i+5}(1 - n_{i+6})(1 - n_{i+1})(1 - n_{i+3})(1 - n_{i+4}) \\
& - n_{i+6} n_{i+3}(1 - n_{i+1})(1 - n_{i+2})(1 - n_{i+4})(1 - n_{i+5}) \\
& + n_{i+1} n_{i+3} n_{i+5}(1 - n_{i+6})(1 - n_{i+2})(1 - n_{i+4}) \\
& - n_{i+6} n_{i+2} n_{i+4}(1 - n_{i+1})(1 - n_{i+3})(1 - n_{i+5})
\end{aligned} \tag{6}
$$

where Δ_i is the collision function which takes the value of 1 or 0, and ξ is the random variable ($\xi = 1$). Here $t_n{}^-$ and $t_n{}^+$ stand for the time of pre- and post collision. The collision phase of each time step is the process of transformation between the input and output states of the lattice sites under a set of collision rules.
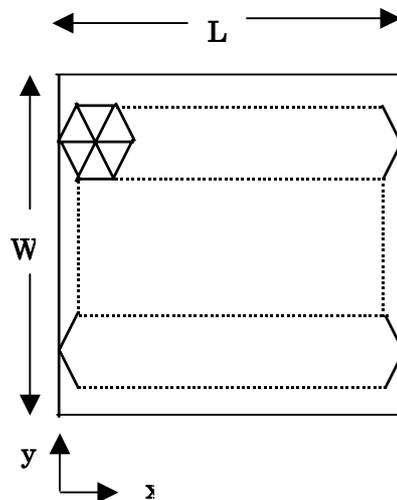
Figure 1. Sketch of the two-dimensional hexagonal lattice model studied.

There are two kinds of boundary conditions in our model: no-slip boundary and constant pressure boundary conditions. No-slip boundary conditions are introduced at a boundary by forcing any particle colliding with the boundary to return along the link on which it approached, or boundary collision rules that exactly reverse the velocities of all particles, so that the particles in a layer close to the boundary have zero average

momentum. The constant pressure boundary condition simulated by maintaining a constant increment of the momentum. While, the total mass conserved by circulating the probability values of the particles, [2, 4, 5].

The microscopic Boolean states of all the particles are averaged to obtain the density and velocity using the following equations,

$$N_i\left(x_{ij}, t_n\right) = \left\langle n_i\left(x_{ij}, t_n\right)\right\rangle \tag{7}$$

$$\rho = \sum_{i=0}^{6} N_i\left(x_{ij}, t_n\right) \tag{8}$$

$$\rho \, \mathrm{u} = \sum_{i=0}^{6} c_i N_i\left(x_{ij}, t_n\right) \tag{9}$$

The pressure is given by,

$$p = \frac{3}{7}\rho \tag{10}$$

Viscosity of fluid is given by,

$$v = \frac{1}{28}\frac{1}{d(1-d)^3}\frac{1}{1-4d/7} - \frac{1}{8} \tag{11}$$

where d is the mean density per link ($= \rho/7$).

In one dimension of single-phase flow through a porous medium is generally described by Darcy's law, which linearly relates fluid velocity to pressure gradient. Darcy's law is given by Equation (12), [1, 6].

$$q = -\frac{k}{\mu}\frac{dp}{dx} \tag{12}$$

where q is the volumetric rate of flow per unit area, μ is the viscosity of the fluid, k is the permeability of the medium, and dp/dx is the applied pressure gradient.

A simple model of fluid flow that satisfies Darcy's law is flow between two parallel

plates (plane Poiseuille flow), as shown in Figure 2. This figure shows that if the pressure gradient along this two-dimension channel is uniform, then the velocity (u) of the fluid will be parallel to the channel walls. Thus, for the system shown, $u_y = 0$. The x component of velocity is strongly influenced by the interaction of the fluid with the walls of the channel. Particularly, in porous medium the velocity of viscous fluids at a solid boundary is assumed to be zero (no-slip boundary condition), [1].
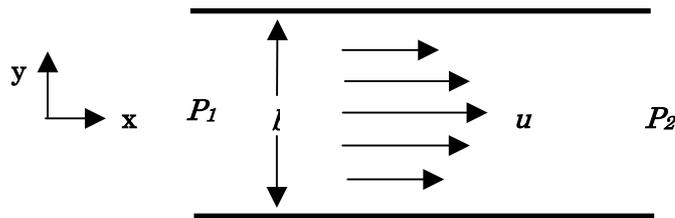
Figure 2. The geometry of channel flow between two parallel plates, [1].

The permeability coefficient (k) is a measure of fluid conductivity through the porous medium. The permeability is given by Carman-Kozeny equation, [6],

$$k = \frac{\phi_{eff}^{3}}{c\tau^{2}S^{2}} \tag{13}$$

where c is the Kozeny coefficient. The porosity of the porous medium is given by,

$$\phi = \left(1 - \frac{V_0}{V}\right) \tag{14}$$

where V_0 is the volume of the obstacles, and V is volume in two-dimensional space. The tortuosity (τ) of the porous medium is,

$$\tau = 0.8(1 - \phi) + 1 \tag{15}$$

The specific surface area (S) is given by,

$$S = -\frac{z}{R_0}\phi \ln\phi \tag{16}$$

where z is two-dimensional space ($z = 2$), and R_0 is the hydraulic radius of the obstacles.

3. RESULTS AND DISCUSSION

3.1. Comparison of the Developed Simulator

The fluid flow simulator developed on the 400x300 lattice units at 2000 time steps to describe a fluid flow in a porous medium was compared with the results of previous researchers, i.e., Frisch et al. [2] for a plate and Rothman [1] for a rectangular shaped. The simulation results are shown in Figure 3 and Figure 4, respectively. From those figures are shows that the porous media and streamlines of the fluid flow simulated by the developed simulator has the same features with the Frisch's and Rothman's work.

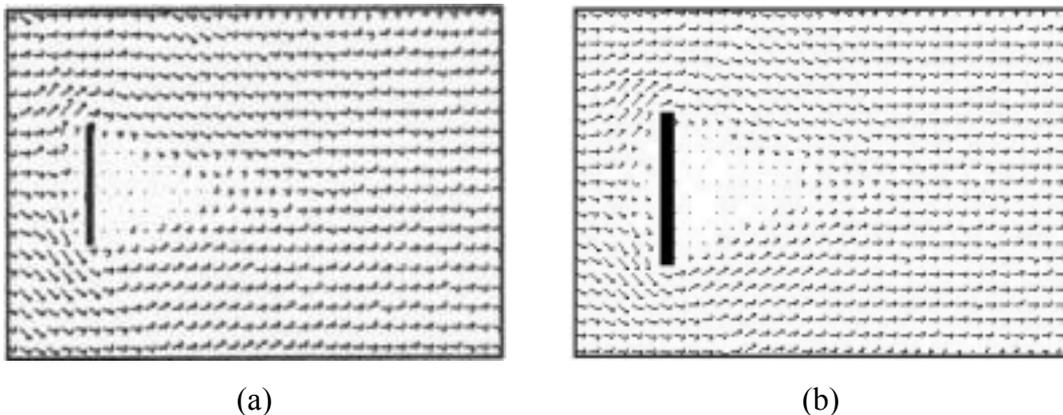(a)   (b)

Figure 3. Comparison of the fluid flow simulated for plate medium shape of obstacle: (a) Frisch et al. [2], and (b) Result of this simulation

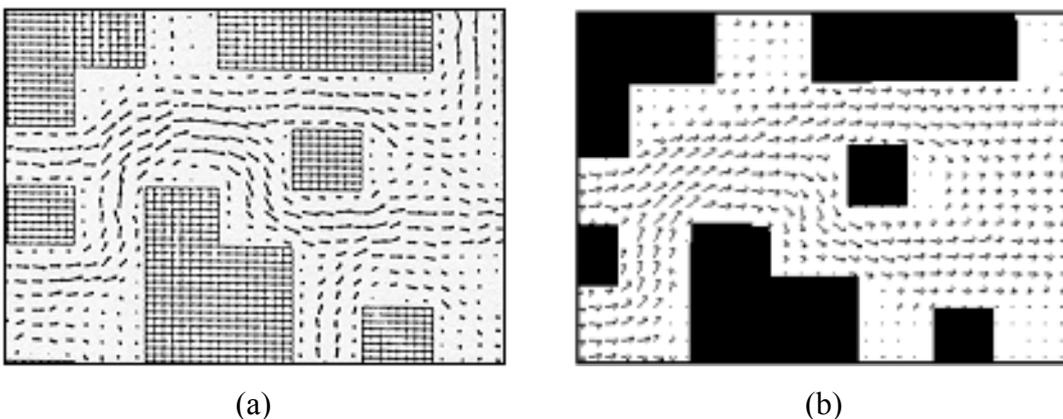(a)   (b)

Figure 4. Comparison of the fluid flow simulated for rectangular shape of obstacle: (a) Rothman [1], and (b) Result of this simulation

Based on the results on Figure 3 and Figure 4, it is concluded that developed simulator shown qualitatively matches the same results from a two-dimensional flow approach. The fluid flow in porous medium can be described and simulated well by FHP-II model of the lattice gas automata.

3.2. Simulation to Construct Heterogeneous Porous Medium

The simulation program was written in Borland Delphi-5. The condition of the cells on the hexagonal lattice were identified by 8 bit strings, where 6 bit strings were used to represent the presence or absence of particles with their own velocity direction. The 7-th bit represents the existence of rest particles and the 8-th bit represents the presence of obstacles components at the corresponding places. The number of fluid particles per lattice site was 1.54 to 2.25, which provided the good approximation for the solution of the linearized Navier-Stokes equation within the lattice gas automata method (ranging from 1.5 to 3.5, [7]). The fluid was forced to move in the positive "x" direction (from left side to right side of the porous medium model) by applying a force on the particles. The no-slip boundary conditions imposed by reflecting particles back along the link they traveled carried the particles to interact with the site on a solid surface.

The porous medium properties were estimated using 800x600 lattice units, where in the estimations, the velocity field was first allowed to saturate for 8000 time steps for each configuration. The number of spherical obstacles varied from 44 to 96, corresponding to porosities of porous medium ranging from 10% to 35%. The two-dimensional simulations to construct the velocity field of the fluid flow in heterogeneous porous medium are shown in Figure 5 to Figure 10, respectively.
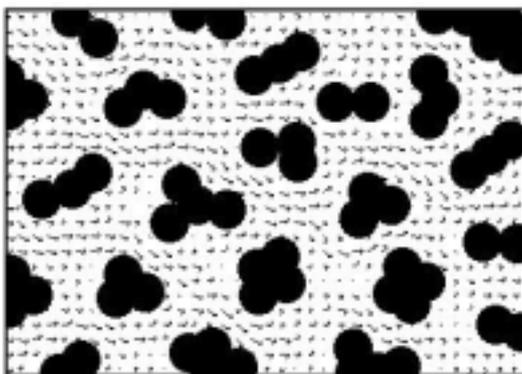

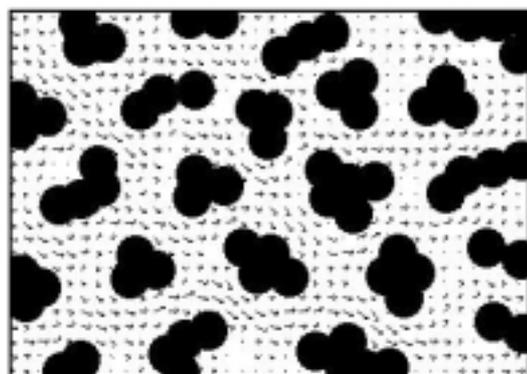**Figure 5**. The simulated fluid flow in porous medium for 34.843% porosity.

Figure 6. The simulated fluid flow in porous medium for 29.837% porosity.
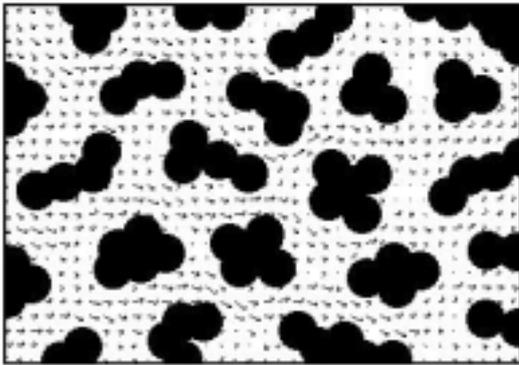
Figure 7. The simulated fluid flow in porous medium for 24.810% porosity.
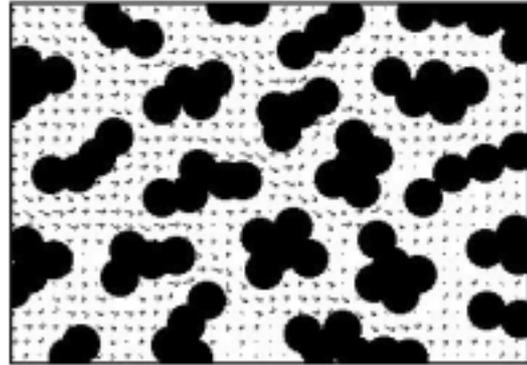

Figure 8. The simulated fluid flow in porous medium for 19.822% porosity.
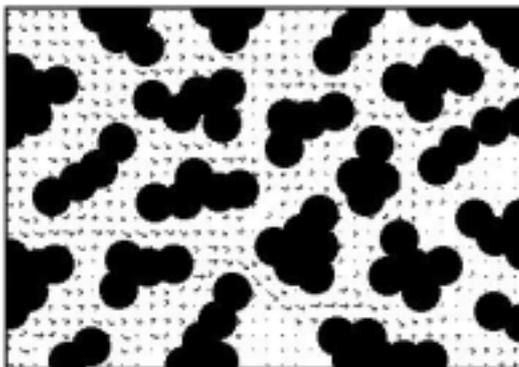
Figure 9. The simulated fluid flow in porous medium for 14.643% porosity.
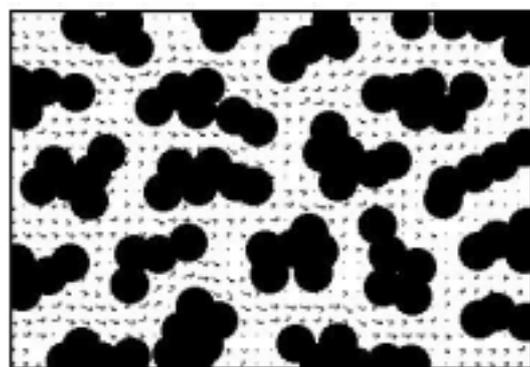
Figure 10. The simulated fluid flow in porous medium for 9.778% porosity.

A method of constructing a model of heterogeneous porous medium is to place solid obstacles randomly in a two-dimensional test volume. The properties of the porous medium are estimated by the shape, size, number of the obstacles and by the distribution of the obstacles within the volume. The velocity field in each position is displayed by black arrow. At each location, the length of the arrow represents the amplitude of the velocity and the direction of the arrow points to the direction of the flow. Black dot indicates solid obstacles formed. The obstacles can have irregular shapes by overlapping of the obstacles. It is shown that complex geometry of porous medium was successfully formed by the lattice gas automata method (FHP-II model). The physical models of heterogeneities that can be constructed are heterogeneous isotropic distribution of permeability and anisotropic distribution of heterogeneous permeability.

After the porous medium with the desired value of porosity was constructed, the fluid was then forced from the left side to the right side of a model. This step was done continuously for each porosity value. Visualizations of the fluid flow were analyzed, and the time steps were recorded. Visualization for each arrow was the average results of 10x10 lattice sites. The minimum time steps needed for the fluid to flow and reach the steady state conditions depended on the pores structure or geometry. In this case, the minimum average time step of 4000 is taken. The more complex the obstacles arrangement, were the more difficult for the fluid particles to flow to the right side of the porous medium. The fluid flow was forced to flow to the right side of porous medium, while at the left side of the porous medium the fluid continuously flowed at a constant rate, and thus meaning a pressure gradient.

When fluid particles hit the obstacles the velocity of fluid flow seemed to be slower, because when fluid particles collided with solid obstacles (the black color), these particles must followed the collisions rules, i.e., moved with the opposite direction of the flow (no-slip boundary conditions or bounce-back boundary conditions). The collisions between fluid particles with solid obstacles or with the particles itself are analogies a viscosity, i.e., the occurrence of the frictional force on the flowing fluid. This frictional force itself will resist the fluid flow rate. As can be seen from the figures, the majority of the flow follows several winding paths there are some dead regions where flow is very slow. The flow velocity increases at the locations where the size of pores decreases.

3.3. Estimation of Rock Properties

In order to effectively compare the model of heterogeneous porous medium properties theoretically with results of lattice gas automata simulations, it is beneficial to express the Equation (13) as explicit functions of porosity (ϕ) alone. To do this, we have to find the dependence of the porosity (ϕ) on the tortuosity (τ), effective porosity (ϕ_{eff}) and the permeability (k).

3.3.1. Tortuosity

The tortuosity (τ) for the two-dimensional heterogeneous porous medium simulated with the lattice gas automata and prediction theoretically as a function of porosity (ϕ) is shown in Figure 11. As a physical quantity, the most intuitive and straightforward definition of tortuosity is the ratio of the average length of true flow paths to the length

of the system in the direction of macroscopic flux [6, 8]. By this definition, tortuosity depends not only on the microscopic geometry of the pores, but also on the transport mechanism under consideration. For flow in heterogeneous porous medium, one can replace the tube length (*Le*) by the average length of the flow paths of the fluid particle through the sample (system). At least two possible alternatives for taking this average can be considered. One may average over the actual lengths of the flow lines themselves, disregarding thereby the fact that fluid particles move along these flow lines at different velocities. Another way of averaging is over the lengths of the flow lines of all fluid particles passing through a given cross-section during a given period of time. This leads to flux weighted averaging. The first alternative is suitable at least for piston-like flows and the latter alternative appears more natural when fluid flow in a porous medium is considered.
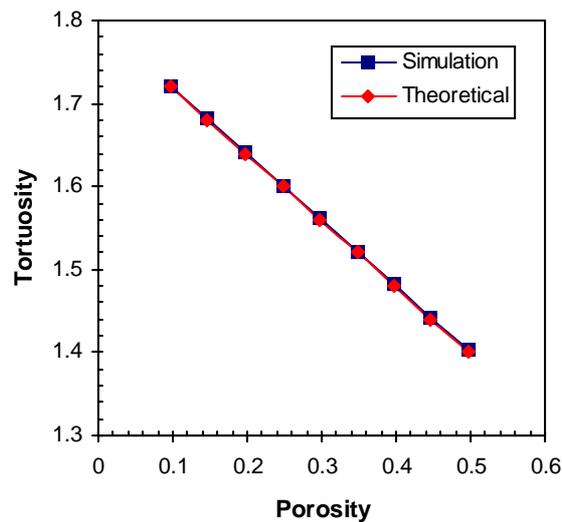
Figure 11. The simulated tortuosity (τ) of the porous system as a function of porosity (ϕ).

3.3.2. Effective Porosity

The effective porosity for two-dimensional heterogeneous porous medium simulated using lattice gas automata predictions as a function of porosity (ϕ) is shown in Figure 12. The effective porosity for the case was estimated with the equation proposed by Koponen et al. [9],

$$\phi_{eff} = ax^3 - (2a + \phi_C)x^2 + (a + 1 - \phi_C)x \qquad (17)$$

where

$$x = \frac{(\phi - \phi_C)}{(1 - \phi_C)} \tag{18}$$

a is constant ($a = 0.3$), and ϕ_C is a critical porosity or percolation threshold, respectively. Equation (17) is simply the most general third order polynomial in which the natural constraints, $\phi_{eff} = \frac{d\phi_{eff}}{d\phi} = 1$ at $\phi = 1$ and $\phi_{eff} = 0$ at $\phi = \phi_C = 0.05$, had been used. With the given values of ϕ_C and a, this expressions also fulfills the condition that $\phi_{eff} \leq \phi$ for all $\phi \leq 1$.
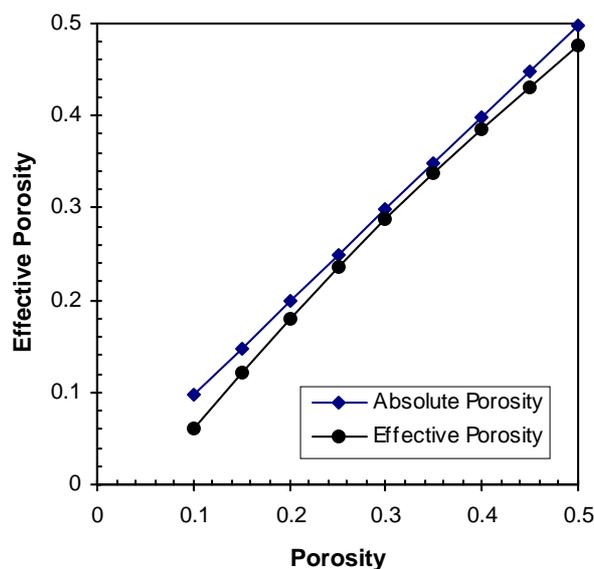

Figure 12. The simulated effective porosity (ϕ_{eff}) as a function of porosity (ϕ).

In materials with high porosity, all of the void spaces usually contribute to the flow through it. The effective porosity of the medium is then equal to porosity. In contrast with this, for low porosity materials, a large part of the total void spaces may be non-conducting. For such medium the effective porosity may therefore be significantly smaller than the geometrical porosity. At the percolation threshold, the medium becomes completely blocked, thus both permeability and porosity may be equal to zero.

While considering flow through heterogeneous porous medium [10, 11], only the interconnected pores are of interest, as the occluded pores (pores not connected to the

main void space) do not contribute to the flow. The dead-end pores are another type of pores that contributed very little to the flow. These pores belong to the interconnected pores, but, owing to their geometry, no global pathlines intersect them. The occluded pores and the dead-end pores form the non-conducting pore space of the medium. The effective porosity of the porous medium can then be defined as the ratio of the volume of the conducting pores to the total volume of the medium.

3.3.3. Permeability

The permeability for the two-dimensional heterogeneous porous medium simulated with the lattice gas automata and theoretical prediction as a function of porosity (ϕ) is shown in Figure 14. The permeability is made dimensionless by dividing with the hydraulic radius (*Ro*). To make a comparison, the permeability was also calculated by Carman-Kozeny equations,

$$k = \frac{\phi^3}{cS^2} \tag{19}$$

where *c* is the Kozeny coefficient that depends on the cross-section of the capillaries. To include the effect of tortuosity (τ) in the model, the Equation (19) becomes

$$k = \frac{\phi^3}{c\tau^2 S^2} \tag{20}$$

Equations (19) and (20) are perhaps the most widely used expressions for the permeability of porous medium. Many porous medium conform to them quite well, although quantitative agreement should not generally be expected. For porous medium which the percolation threshold appears at a finite porosity (ϕ_C), the Kozeny equation as given by Equations (19) and (20) is gave high value. The modified Equations (19) and (20) to include the effect of non-conducting pores is to replace the porosity (ϕ)

with the effective porosity (ϕ_{eff}). This will give

$$k = \frac{\phi_{eff}^3}{cS^2} \tag{21}$$

and as given in Equation (13) which has been used in this research, where all three quantities ϕ_{eff}, τ and S are function of porosity (ϕ) of the system. The simulation results given by Equations (19), (20), (21) and (13) are then compared in Figure 13.

As can be seen from the figures, better results are obtained when the tortuosity and effective porosity are both included (Equation 13). The fitted value of the Kozeny coefficient (*c*) is 5.8 for Equation (13), 8.2 for Equation (19), 6.5 for Equation (20), and 10.4 for Equation (21), respectively. This is in good agreement with various models and measurements found in the literature, where typically values for the Kozeny coefficient (*c*) are reported in the range from 2 to 12, [9]. It is evident that the permeability of two-dimensional heterogeneous porous medium is very much affected by restrictions on flow caused by narrow passages and dead-end pores.
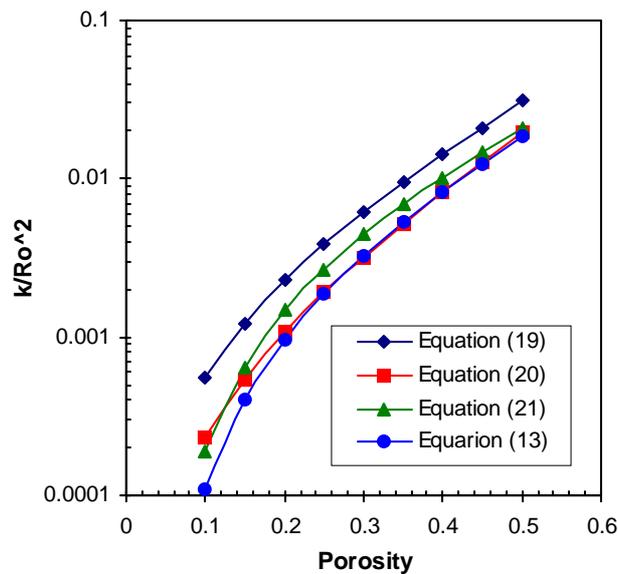

Figure 13. The simulated dimensionless permeability (k/Ro^2) of the porous system as a function of porosity (ϕ).

It has been recognized, that applications of lattice gas automata methods to flow through porous medium must carefully evaluate the sensitivity of results to the resolution of the underlying lattice [1]. It is now know, that the bounce-back boundary condition typically employed at solid-fluid boundaries does not necessarily create zero flow at the solid wall [4]. Any error due to bounce-back boundary condition would decrease as the system size increases, since larger-scale flows should depend less on flow through very narrow tubes or throats. A pore-space that contains very narrow channels, on the order of one to two lattice units in radius, may produce significant

errors in estimated permeability if the bulk flow is dominated by narrow passageway. For certain choice of model parameters, and with certain wall orientations, the ideal location of the zero, halfway between the wall site and the nearest interior site, can be achieved exactly for know flow (e.g., Poiseuille flows). However, this result does not hold in general and small deviations from the ideal zero point are possible. This problem is for practical purposes inconsequential for flows through tubes of large radii, however, if the radius of a tube is a small, for example just one or two lattice units, then the effect of resulting permeability can be substantial due to the quadratic dependence of permeability on radius [12]. The accuracy of the results is in the neighborhood of 10% to 25%, with errors decreasing as the sample size increases.

4. CONCLUSION

The model of fluid flow simulations in a porous medium had been developed and the complex geometry or heterogeneous of a porous medium can be simulated by FHP-II model of lattice gas automata, where for heterogeneous system in which the obstacles are placed randomly, heterogeneity can increase the permeability.

The shape, size, and number of the obstacles and the distribution of the obstacles within the volume estimate the properties of the porous medium. Numerical correlations were also found between the tortuosity, effective porosity and permeability of heterogeneous porous medium as a function of porosity. Furthermore, the effective porosity and permeability of the lattice gas automata simulation results gave a reasonably good approximation.

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Profiles

Dedy Kristanto is Lecturer at Petroleum Engineering Department, Universitas Pembangunan Nasional "Veteran" Yogyakarta, Indonesia. Graduated with a B.S in Petroleum Engineering from Universitas Pembangunan Nasional "Veteran" Yogyakarta, Indonesia, M.Sc in Petroleum Engineering from Bandung Institute of Technology, Indonesia. Since 2000, he enrolled at the University of Technology Malaysia, Johor Bahru, Malaysia in pursuit of a Doctoral degree in Petroleum Engineering. He conducts research in reservoir engineering, simulation and enhanced oil recovery.

Mariyamni Awang is associate Professor at Petroleum Engineering Department, University of Technology Malaysia. Graduated with a BS from the University of Queensland in Chemical Engineering, M.S from Pennsylvania State University in Petroleum and Natural Gas Engineering and a PhD in Petroleum Engineering from Stanford University. She teaches and conducts research in reservoir engineering, simulation and enhanced oil recovery.