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Research Article

Real-time simulation of fluid flow in porous media using the self-organized gradient percolation method

Anh Khoa Nguyen*, Thi Kim Nhung Dang

ABSTRACT

A significant reduction in the computaional time of simulations of fluid flow in porous media is showed using the (one-dimensional) Self-organised Gradient Percolation (SGP) method. The SGP method is often used for the simulations at numerical timestep instead of real time, thereby limiting comparing with benchmark from other methods (e.g., finite element methods). The aim of the current study is to convert the numerical timestep into the real time of simulations of the SGP method. In particuar, by describing the change in time of variance in the probability density function of the SGP as an ordinary differential equation. The temporal evolution of the liquid front z in a porous sample at timestep t (it is denoted by dz/dt) is described as the time-dependent capillary rise using Poiseuille's equation. The Newton's method is then applied to interrelate the numerical timestep with the real-time of simulations with the chosen initial timestep. The SGP algorithm (from our previous study) is updated these points to simulate the model outcomes at real-time. Hence, in the current study, for the correctness of the SGP algorithm, we apply the SGP model to the two case studies (with the same porous sample, but with two diferent liquids). The numerical outcomes from the SGP model are inferred at the real simulation time corresponding to specific time steps. Then, these predictions at these inferred real times from the SGP model are compared with those obtained using conventional numerical methods, in which the mass balance equation is solved with the van Genuchten and Brooks–Corey models to describe the capillary pressure curve. We present the development of self-organization gradient percolation model, considered in the case of non-reactive impregnation permits to provide simulations in real time with a reduction of the computational time by a factor of 100 (as expected from our previous study).

Key words: Percolation, self-organised, capillary rise, porous media, numerical simulations

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INTRODUCTION

The current study focuses on simulating the flow of fluid $\vec{q}$ without chemical reactions in unsaturated zone described by Richards' equation in combining with the Darcy's law[1]:

$$\Phi \frac{\partial S}{\partial t} = -\vec{\nabla}(\vec{q}) \tag{01}$$

where Φ is porosity (dimensionless) defined as

$$\Phi = V_p / V_T \tag{02}$$

and V_p is the porous volume and V_T is the bulk volume (both in m^3), and $\vec{q}$ is the flow density vector ($m.s^{-1}$).

The quantity $\vec{q}$ is related to the driving force denoted by $-\vec{\nabla} P_{cap}$, i.e., capillary force using the Darcy's law. The form as described in Equation (01) described Darcy's law under isotropic conditions:

$$\vec{q} = -k \vec{\nabla} P_{cap} \tag{03}$$

where k is permeability of the porous solid (in $m^2.Pa^{-1}.s^{-1}$) with respect to the fluid. However, in the unsaturated case, Darcy's law is written in the form[1]:

$$\vec{q} = -\psi(S) \frac{K_{int}}{\eta} \vec{\nabla} P_{cap} \tag{04}$$

where K_{int} is intrinsic permeability (m^2), P_{cap} is the capillary pressure (Pa), η is the dynamic viscosity (Pa.s), and S is the saturation (unitless) of the fluid phase:

$$S = V_f / V_p \tag{05}$$

where V_f (in m^3) and $\psi(S)$ (unitless) are the porous volume occupied by fluid and the relative permeability as a function of saturation, respectively. Herein, the driving force is described in the form:

$$-\vec{\nabla} P_{cap} = -\frac{\partial P_{cap}}{\partial S} \vec{\nabla} S \tag{06}$$

where $\frac{\partial P_{cap}}{\partial S}$ is the capillary pressure curve. Substituting Equation (06) into Equation (04) leads to

$$\vec{q} = -\psi(S) \frac{K_{int}}{\eta} \frac{\partial P_{cap}}{\partial S} \vec{\nabla} S \tag{07}$$

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Equation (07) plugged into Equation (01) leads to, also called Richards' equation in[2]:

$$\Phi \frac{\partial S}{\partial t} = \vec{\nabla} \left(\frac{K_{int}\, \psi(S)}{\eta} \frac{\partial P_{cap}}{\partial S} \vec{\nabla}(S) \right) \quad (08)$$

The finite element method (F.E.M) and theta-method are often applied to solve Richards' equation[3–6]. In recent years, Self-organised Gradient Percolation (SGP) has been used to calculate the local saturation without solving Richards' equation with less computational time[2]. In this SGP method, the mathematics interrelated with physical issue of the non-reactive impregnation phenomenon is addressed using the initial conditions of the algorithm given by an analytic solution of the Richards' equation. Briefly, in our previous work[2], the influence of the model input parameters on the model outcomes was also pointed out using local sensitivity analysis. The sorption curve, $\frac{\partial P_{cap}}{\partial S}$ at steady state of liquid saturation, is essential to solve Equation (08), represented by capillary pressure curve, such as van Genuchten's model or Brook's model or others. Furthermore, the convolution operator was applied to setup the spatial continuity of the wetting fluid and to respect the boundary conditions of the problem. The comparisons with the F.E.M and measured data confirm the reduction of the computational cost of the SGP method and that there are no spurious oscillations. However, the model outcomes from the SGP method were provided at each time steps, which were not converted into real time, thus limiting the model brenchmarks at specific time[7]. Hence, it is not trivial to overcome this disadvantage, and more especially identifying the real time of the model outcomes. Therefore, in this work, we propose describing the time-step iterations in the SGP algorithm as ordinary differential equation, thereby enabling a direct correspondence between the time steps and real time.

MATERIALS AND METHODS

Datasets

The two datasets in our current study were originated from our previous studies where a porous media is hung upon the lipid interface (i.e., glycerine for test 1 and oil for test 2), as described in our previous studies[2,7,8]. In particular, the database used in the current study (i.e., Table 1, and Figure 1) was acquired in our previous study[7]. Brifely, the first dataset was acquired from the tested refractory material of cylindrical alumina 99% (with dimensions (i.e., height×diameter) of (40 mm × 35 mm)). When Equation (08) was applied to the first test, van Genuchten model was employed to describe $\frac{\partial P_{cap}}{\partial S}$, thus allowing us to calculate the numerical solutions[2,7,9].

The second dataset was acquired the tested refractory material of alumina 99% (with dimensions (i.e., height×diameter) of (40 mm × 35 mm))[2,7,8]. Similarly, when Equation (08) was applied to the second test, Brooks and Corey model was employed to describe $\frac{\partial P_{cap}}{\partial S}$, thus allowing us to calculate the numerical solutions[2,7,9].

The parameters of van Genuchten model and Brooks and Corey model were clarified in our previous studies[2,7,9]. The clarification of integrating these models into the SGP model is not the key point of this study, thus we do not focus on provide a further detailed explaination.

The two datasets were used as baseline for the model outcomes calculated from the SGP model vs the finite element model in previous studies[2,8].

SGP model of non-reactive fluid flow in porous media

Model assumptions

The sorption curve at initial time step is described as the Probability Density Function (PDF) from Gaussian distribution (Figure 1 left), so the equation of the sorption curve is expressed by

$$S = S_{max} exp\left(-\frac{h^2}{2\sigma^2}\right) \quad (09)$$

where h is height, S_{max} is maximum saturation, and σ is variance.

At each iterations of time-steps, the sorption curve is increased automatically to meet a pure physics point of view. The sorption curve equation at a time-step is described as such equation in the previous time-step combining an incremental increase in variance. The incremental increase in variance is related to the driving force with more details in our previous study[2].

Algorithm of the SGP model

In Figure 1 left, a square represents a local average saturation denoted by $X_{i,j}$. The value of $X_{i,j}$ is derived from a Normal distribution. The saturation inside a square is written in the form:

$$S_{i,j} = X_{i,j} * f(i,j) \quad (10)$$

The calculation using equation Equation (10) is developed from our previous studies[2,7], thus we do not clarifiy further in the current study. Briefly, in our previous study[7], to make the simulated porous model by the SGP method be continuous, we employed a convolution operator (denoted by $\langle * \rangle$) with function *f (i, j)*. Also, the convolution operator allows to describe de boundary conditions with more details in our previous study[2].

Table 1: The porous material and liquid properties in tests 1 and 2, previously given in[7]

Properties of the porous and liquid samples	Values (given from [2,7])		Units (given from [2,7])
	Test 1	Test 2	
Fluid viscosity (already defined in [7]), η	1.02	0.355	$Pa \cdot s$
Fluid mass density (already defined in [7]), ρw	1260	892	$kg \cdot m^{-3}$
Intrinsic permeability, K_{int}	$9.5 \cdot 10^{-12}$	$1.87 \cdot 10^{-7}$	m^2
Initial porosity (Φ)	0.2	0.19	Unitless

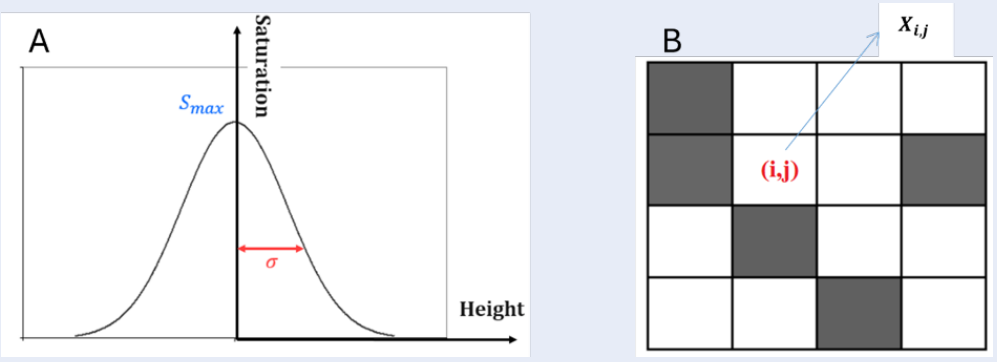

Figure 1: A, the probability density function derived from Normal distribution. B, a porous sample is represented by a site square lattice: each square at i^{th} row and j^{th} colum has its own value of local average saturation denoted by $X_{i,j}$. This figure is reproduced from our previous study by our group research (Nguyen at al.)[7].

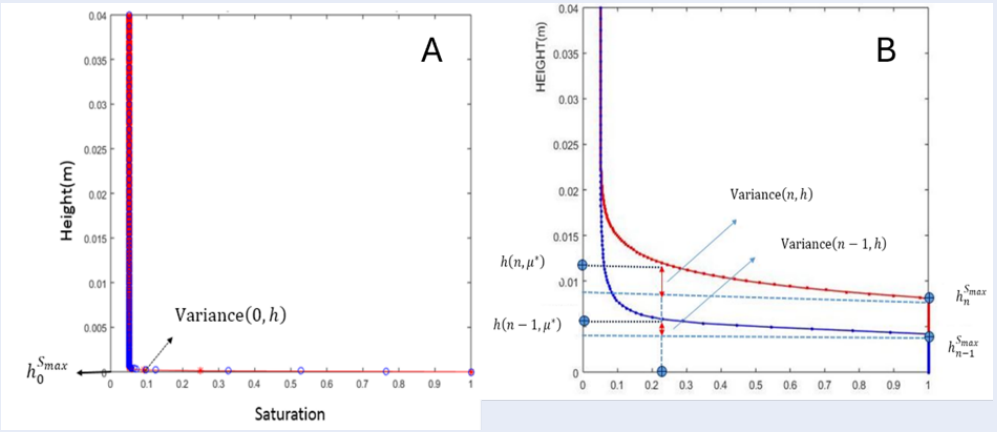

Figure 2: The sorption curve at initial time-step (A) and at general step-time (B) in which variance is denoted by in this study. This figure is reproduced from our previous study by our group research (Nguyen at al.)[7].

The algorithm of the SGP model (as depicted in Figure 3) was developed in our previous work[2,7], in which the liquid front at fully saturation is denoted by $h_n^{S_{max}}$ and timestep n. For the initial time-step (Figure 2, left), the μ-function is expressed (developed in our previous work[7]):

$$\mu(0,h) = S_{max} exp\left(-\frac{|h-c|^m}{2[\sigma(0,h)]^m}\right) \quad (11)$$

For the second time-step, the μ-function is its function in the initial time-step combining an incremental increase in variance (developed in our previous work[7]):

$$\mu(1,h) = S_{max} exp\left(-\frac{\left|h-h_1^{S_{max}}\right|^m}{2[\sigma(0,h)+c(0,h)]^m}\right) \quad (12)$$

By computation, function *c(0, h)* depends on K_{int}, ρw, g (gravity), η, and Φ are given in Table 1, and the fixed value of the μ - function (denoted by μ^*), and maximum saturation (denoted by S_{max}), already given from our previous study[7]:

$$c(0,h) = \left(\frac{\mu(0,h)}{\mu^*}\right)^{(m-1)/m} \left(\frac{K_{int}\rho wg}{\eta\Phi\left(1+[2ln(\mu^*/S_{max})]^{1/m}\right)}\right) \quad (13)$$

By computation for the next timestep, the liquid front is expressed as in our previous work[7]:

$$h_1^{S_{max}} = h_0^{S_{max}} + c(0,h)\left(\frac{\mu(0,h)}{\mu^*}\right)^{(1-m)/m} (2\ln(\mu^*/S_{max}))^{1/m} \quad (14)$$

In general, the μ-function is expressed as in developed in our previous work[7]:

$$\mu(n,h) = S_{max} exp\left(-\frac{\left|h-h_n^{S_{max}}\right|^m}{2[\sigma(n-1,h)+c(n-1,h)]^m}\right) \quad (15)$$

Hence, the general form of function c at timestep n and liquid height h is expressed (also developed in our previous work[7]:

$$c(n-1,h) = \left(\frac{\mu(n-1,h)}{\mu^*}\right)^{(m-1)/m} \left(\frac{K_{int}\rho wg}{\eta\Phi\left(1+[2ln(\mu^*/S_{max})]^{1/m}\right)}\right) \quad (16)$$

and

$$h_n^{S_{max}} = h_{n-1}^{S_{max}} + c(n-1,h)\left(\frac{\mu(n-1,h)}{\mu^*}\right)^{(m-1)/m} (2\ln(\mu^*/S_{max}))^{1/m} \quad (17)$$

Time evolution

The present approach accounts for the physical processes occurring at the local microscale of the pores, where each pore can be approximated as a capillary. To establish a link between self-organised gradient percolation and local-scale physics, the temporal evolution of the liquid height z with the timestep t (it is denoted by dz/dt) is represented through the evolution of the standard deviation. Poiseuille's equation[10] also describes the time-dependent capillary rise. Accordingly, the variation of the liquid height zover time is governed by the following ordinary differential equation:

$$\frac{dz}{dt} = A\left(\frac{P_{cap}}{P_h^t} - 1\right) \quad (18)$$

where A = $\gamma D^2/32\eta$ depends on capillary diameter D and liquid properties (more precisely, γ is the surface tension and η is the dynamic viscosity), $P_{total}^t \left(= P_{cap} + p_h^t\right)$ and P_h^t are total and hydrostatic pressure at timestep n, respectively.

In Equation (18), the variable λ represents the variance shown in Figure 2. The Newton's method is then applied to approximate the solution of Equation (18), yielding the following expression with more details in Chapter 2 in[11]:

$$\lambda^{(1+k)} = \lambda^{(k)} + hA\left(\frac{P_{cap}^{(k)}}{P_h^{t,(k)}} - 1\right) \quad (19)$$

Where the subscripts *(k)* and *(k+1)* denote the approximate values at time steps *(k)* and *(k+1),* respectively, while h represents the time step size. By discretising the time domain with step size h using the Newton's method in[11], the real-time value at time step k is expressed as:

$$t^{(k)} = t^{(0)} + hk \quad (20)$$

The time evolution (i.e.,Equations (18) and (19), and Equation (20) is taken into account the algorithm of the SGP model (as depicted in Figure 3)[2,7].

Numerical simulations

Simulation with the 1D SGP model were conducted using Matlab (version 2025b) to solve the systems of equations Equation (10) to Equation (20). The simulations were run on the same PC having 2.60 GHz, x64- based processor with 32 GB of RAM. The typical simulation duration was less than 30 s for 1D SGP model on Matlab.

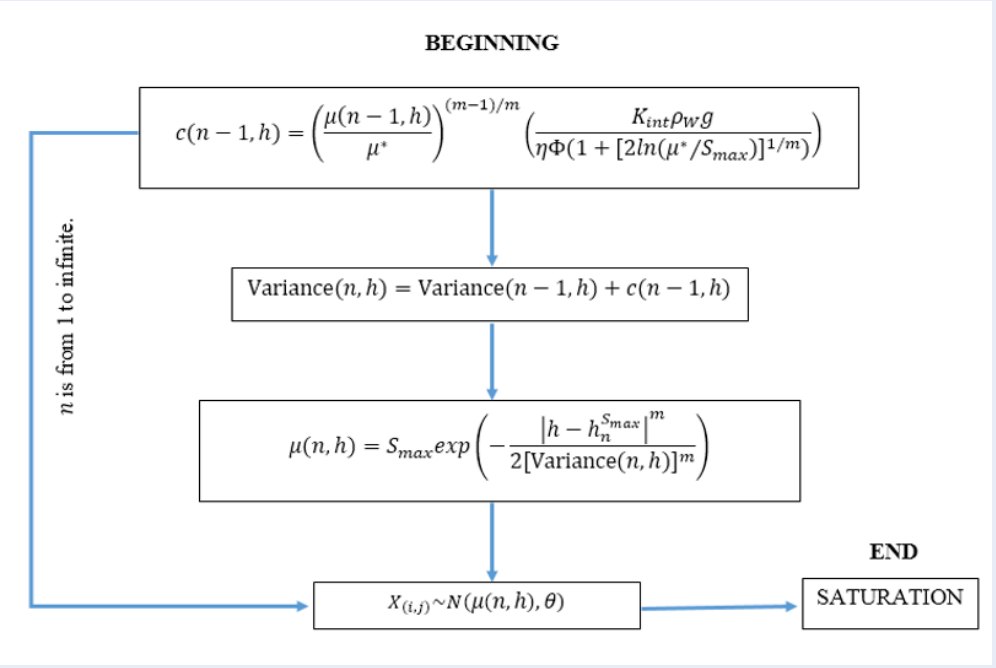

Figure 3: The algorithm of the SGP model. The SGP model algorithm begins with an analy ticalsolution of Richards' equation expressed as a probability density function (PDF) dependent on variance. In this study, we denote "variance" by σ. As the variance increases, the PDF correspondingly broadens. This PDF is then used to generate a two-dimensional site lattice percolation, whose mean value reproduces the simulated sorption curve. This figure is reproduced from our previous study by our group research (Nguyen at al.)[7].

RESULTS AND DISCUSSION

The first test

In the SGP model applied to the first test (section 2.1), we used $m = 2$ (in Equations (10), (11), (12), (13), (14), (15), (16) and (17)), then the results obtained from the SGP model is validated by compared to the numerical outcomes calculated from the FEM model (in Figure 4).

In this test (i.e., test 1 in section 2.1), the Newton's method was applied with a chosen time step size of 27.0270 and an initial time $t_0 = 0$ to simulate the model outcomes using the SGP approach (represented by red starred lines in Figure 4). According to Equation (20), steps 1, 37, and 260 correspond to real times of 1, 1000, and 7000 seconds (i.e., Figure 4 A,B,C), respectively. At these steps, the SGP model results are in good agreement with those obtained from the FEM model, confirming the accuracy of the SGP in real-time simulation.

At step 3200 in the SGP model, the corresponding real time (based on Equation (20)) is 86,400 seconds. However, at this point, the system has already reached its steady state (i.e., $\triangle P = 0$). Consequently, beyond this step, the model outputs remain unchanged. This explains why the results at step 3200 are still similar to those obtained from the FEM model at 300,000 seconds (i.e, Figure 4 D).

The second test

In the SGP model applied to the second test (described in section 2.1), we used $m = 1$ (in equations Equations (10), (11), (12), (13), (14), (15), (16) and (17)), then the results obtained from the SGP model (i.e., starred read lines, Figure 5) is validated by compared to the numerical outcomes calculated from the FEM model (i.e., open blue circles, in Figure 5).

In this test (i.e., test 2 in section 2.1), the Newton's method was employed with a time step size of 7.1429×10^2 and an initial time $t_0 = 0$ to simulate the model outcomes using the SGP approach (represented by red starred lines in Figure 5). According to Equation (20), steps 1, 7, and 17 correspond to real times of 1, 5000, and 120,000 seconds (i.e., Figure 5 A, B, and C), respectively. At these steps, the SGP model results show good agreement with those obtained from the FEM model, thereby confirming the accuracy of the SGP for real-time simulation.

At the 20th time step in the SGP model, the corresponding real time (based on Equation (20)) is

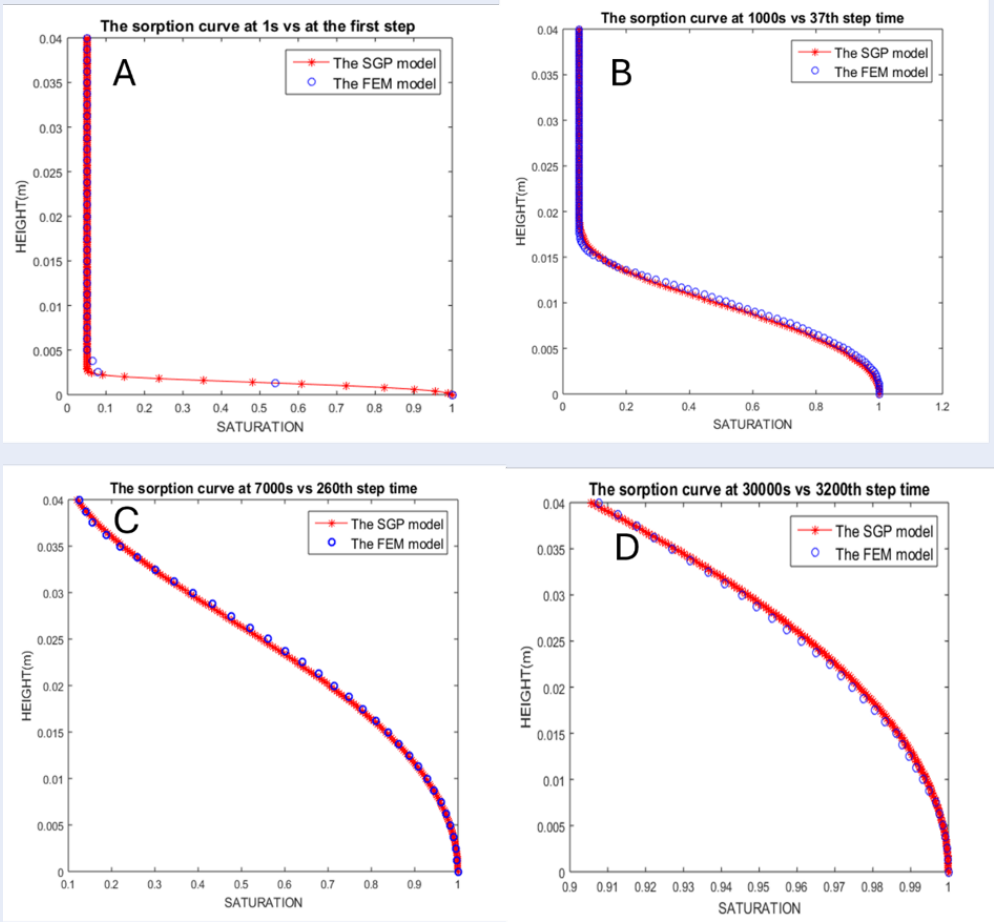

Figure 4: Comparisons between the model outcomes from the SGP (red starred and lines) vs from the FEM model (open bluecircles) at different time steps (i.e., at 1s (A), 1000s (B), 7000s (C), and 30000s (D)) . This figure is reproduced by Matlab (version 2025b) by our research group (Nguyen et al)[7].

140,000 seconds. However, at this point, the system has reached its steady state (i.e., $\triangle P = 0$). Consequently, beyond this step, the model outputs remain unchanged. This explains why the results at the 20th step are still similar to those obtained from the FEM model at 272,800 seconds (i.e., Figure 5D).

CONCLUSIONS

In our current study, we developed a novel model by solving the time evolution in the self-organised gradient percolation (SGP) framework using the Newton's method. This approach enables us to infer the real simulation time corresponding to specific time steps.We then compared the predictions at these inferred real times from the SGP model with those obtained using conventional numerical methods, in which the mass balance equation is solved with the van Genuchten and Brooks–Corey models to describe the capillary pressure curve. The results demonstrate that the real-time evolution predicted by the SGP model closely matches that obtained from the FEM approach.We also observe that once the system reaches a steady state, the model outputs no longer change. Therefore, beyond the inferred steady-state time in the SGP model, the results from both approaches remain consistent.

LIST OF ABBREVIATIONS

1D - One-dimensional
SGP – Self-organised Percolation
F.E.M – Finite element method
PDF – Probability density function

COMPETING INTERESTS

The authors declare that: in this research, there is no conflict of interests.

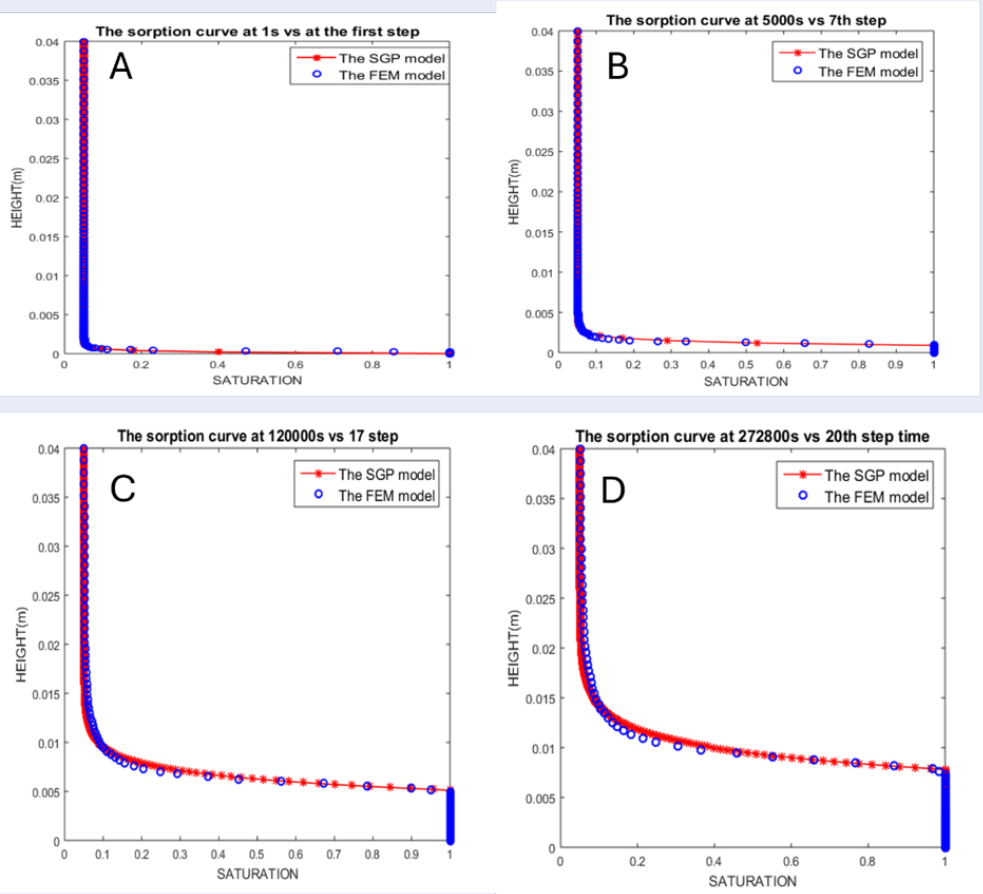

Figure 5: Comparisons between the model outcomes from the SGP model (red starred lines) vs from the FEM model (open vblue circles) at different time steps (i.e., at 1s (A), 5000s (B), 120000s (C), and 272800s (D)). This figure is reproduced by Matlab (version 2025b) by our research group (Nguyen at al) [7] .

AUTHOR'S CONTRIBUTION

Anh Khoa Nguyen: Conceptualization, Methodology, Software, Investigation, Formal analysis, Validation, Visualization, Writing-original draft.

Thi Kim Nhung Dang: Conceptualization, Writing-review& editing.

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TÓM TẮT

Sự giảm đáng kể về thời gian mô phỏng của dòng chảy chất lỏng trong vật liệu có cấu trúc rỗng đã được làm rõ bằng phương pháp gradient percolation tự tổ chức (SGP) trong một chiều. Phương pháp SGP thường được sử dụng cho các mô phỏng tại các bước thời gian số thay vì thời gian thực, do đó giới hạn việc so sánh với các kết quả đối sánh với các phương pháp số khác (ví dụ, phương pháp phần tử hữu hạn). Mục đích của nghiên cứu này là chuyển đổi các bước thời gian số thành thời gian thực của các mô phỏng bằng phương pháp SGP. Cụ thể, bằng việc diễn tả sự thay đổi theo thời gian của phương sai của hàm mật độ xác suất của phương pháp SGP thành các phương trình sai phân thường. Sự thay đổi theo không gian của mặt phân cách của chất lỏng z trong mẫu vật liệu có cấu trúc rỗng tại bước thời gian t (được ký hiệu là dz/dt) được diễn tả như là mao dẫn độc lập bởi phương trình Poiseuille. Khi đó, phương pháp Newton được áp dụng để liên hệ giữa bước thời gian số và thời gian thực của các mô phỏng with bước thời gian số bạn đầu đã được cho sẵn. Thuật toán SGP (từ nghiên cứu trước đây của nhóm nghiên cứu của chúng tôi), để đánh giá sự chính xác của thuật toán SGP, chúng tôi áp dụng mô hình SGP cho hai trường hợp nghiên cứu (có cùng mẫu vật liệu có cấu trúc rỗng, nhưng với hai loại chất lỏng khác nhau). Kết quả số từ mô hình SGP suy ra thời gian thực từ các bước thời gian số cụ thể. Khi đó, những dự đoán số sử dụng phương pháp SGP tại những thời gian thực này được so sánh với kết quả số được tính từ các phương pháp số khác, trong đó phương trình cân bằng khối lượng được giải với việc sử dụng mô hình van Genuchten và mô hình Brooks-Corey để diễn tả đường cong mao dẫn. Chúng tôi chính bày sự phát triển của phương pháp gradient percolation tự tổ chức, được xét trong trường hợp khuyeesch tán chất lỏng ở trạng thái chưa có phản ứng hóa học cho phép cung cấp các mô phỏng số theo thời gian thực với sự giảm thời gian mô phỏng theo tỷ lệ 1/100 (đúng như kỳ vọng từ nghiên cứu trước đó của nhóm nghiên cứu của chúng tôi).

Từ khoá: Percolation, tự tổ chức, mao dẫn, vật liệu có cấu trúc rỗng, mô phỏng số

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