



中國地質大學

# 新增博士生导师遴选申请

## 附件材料

申 报 人	王宇航
二 级 单 位	环境学院
职 称	特任教授

2023年11月

## 1. 学历学位证书



# The University of Tulsa

Upon recommendation of the Faculty of the Graduate School and the McDougall  
School of Petroleum Engineering hereby confers upon

**Junfang Wang**

the degree of

**Master of Science in Engineering**

with all its honors, rights, and privileges.

Given under the Seal of the University at Tulsa, Oklahoma, on this  
thirty-first day of July, two thousand and fifteen.

*J. Duane Gibson*

Chairman of the Board of Trustees

*Kevin C Bice*

Secretary of the University



A stylized, handwritten signature in dark ink.

President of the University

*David A. Hagquist*

Dean of the College



# University of Wyoming

The Trustees of the University by virtue of the authority vested in them and on the recommendation of the faculty of the

College of Engineering and Applied Science

Have conferred the degree of

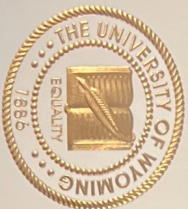
Doctor of Philosophy

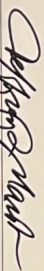
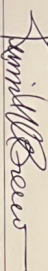
Petroleum Engineering

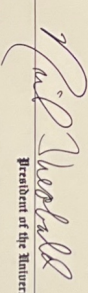
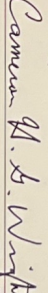
on

**Buhang Wang**

with all the Rights, Privileges, and Honors pertaining thereto,  
given at Laramie, Wyoming, on the 14th day of August, in the year  
Two thousand twenty



  
President of the Trustees  
  
Secretary of the Trustees

  
President of the University  
  
College Dean



## 2. 博士后工作证明

Date August 11, 2020  
Our reference 67540/EWI/CS  
Telephone +31(0)15-2789000  
E-mail HRServices@tudelft.nl  
Subject Employment contract  
ID 918788/0

This is an employment contract between:

Y. Wang;

and

Delft University of Technology (hereinafter TU Delft),

- Y. Wang was born on May 16, 1990 and lives at the following address: 309-S 10TH ST APT 26, LARAMIE WY 82070, USA.
- Delft University of Technology is located at Stevinweg 1, 2628 CN in DELFT and is registered with the Chamber of Commerce, entry number 27364265. The university is represented in this contract by Prof.dr. J.E.J. Schmitz, Dean of the faculty Electrical Engineering, Mathematics and Computer Science. This is in accordance with Article 20 of the TU Delft Mandate Regulations (2007)

TU Delft and Y. Wang are entering into this employment contract under the following conditions:

**Duration of the temporary employment contract**

Your appointment at TU Delft commences on September 1, 2020 and is a temporary employment contract lasting until September 1, 2022. This employment contract ends by operation of law on this date. Your appointment is subject to Article 2.3 para.1 of the Collective Labour Agreement for Dutch Universities (hereinafter CAO NU). This employment contract may be dissolved before the end of the term. Premature termination is subject to the notice periods in the CAO NU.

Employment is on the strict condition that you are eligible for a residence permit which allows you to work at the TU Delft.

**Position**

You are appointed to the position of Researcher to the faculty Electrical Engineering, Mathematics and Computer Science, department of Delft Institute of Applied Mathematics, in the research group of Numerical Analysis. The following job profile and level from the University Job Classification System (UFO) apply: "Onderzoeker 4" (010840).

**Probationary period**

A probationary period of two months applies. During the probationary period the employment contract may be dissolved by TU Delft or yourself with immediate effect. During this period the provisions concerning termination of the contract do not need to be observed.

**Working hours and holiday hours**

At TU Delft full-time work means 38 hours a week. In accordance with this contract you work 1.0 FTE, that is 38 hours a week. As part of the flexible working hours scheme, you have chosen to work 40 working hours per week. This means you are entitled to 328 holiday hours per calendar year. In the calendar year 2020 you are entitled to 109 holiday hours.

**Salary / holiday allowance and year-end bonus**

Your salary is € 3,491.00 gross per month, in accordance with salary scale 10, step 5. This is based on the UFO job profile and level of your position. The incremental date is September 1.

In addition to this, in the month of May you receive a holiday allowance of 8% of your salary and in December a year-end bonus of 8.3% of the salary.

You receive your salary specification in digital form every month. You state your agreement to receiving a digital salary specification.

Initialled TU Delft:



Initialled Y. Wang:



### **30% rule**

We will assess with you whether you meet the qualifying conditions for a tax free allowance on extraterritorial expenses, as described in the "Uitvoeringsbesluit loonbelasting 1965" (the 30% rule).

### **General work-related expenses**

You receive monthly compensation for work-related expenses. This compensation is a maximum of € 27.00 net per month calculated in proportion to the agreed working hours and is paid together with the salary. This compensation is part of the Work-Related Expenses Scheme. TU Delft reserves the right to change or discontinue this compensation.

### **Commuting allowance**

You receive a monthly commuting allowance. This is a maximum of € 20.00 net per month calculated in proportion to the agreed working hours and is paid together with the salary.

In addition to the monthly commuting allowance, you may choose a mobility allowance through the Individual Terms and Conditions of Employment Options Scheme (IKA).

### **Individual Terms and Conditions of Employment Options Scheme (IKA)**

You are entitled to put together a part of your terms and conditions of employment package yourself as part of the IKA scheme.

### **Location**

Your work location is Delft. TU Delft reserves the right to change your work location if it feels that this is necessary for the proper performance of your job.

### **Pension Scheme**

You participate in the pension scheme of the General Pension Fund for Public Employees (*Algemeen Burgerlijk Pensioenfonds*, ABP). TU Delft registers you with the General Pension Fund for Public Employees (ABP), that administers the pension scheme. An employee's pension contribution is withheld from your salary each month. You can find the details of the ABP pension fund at [www.abp.nl/english/](http://www.abp.nl/english/).

### **Confidentiality**

You are obliged to keep all information derived from your position confidential. This concerns information about your own work, but also information about TU Delft and the people who work there. This obligation of confidentiality remains in force after the termination of the employment contract. The obligation of confidentiality does not apply to information that is available through public sources.

### **Ancillary activities**

Work performed for third parties, whether paid or unpaid, is subject to certain rules and obligations. For example, you are obliged to report such ancillary activities. Moreover, you may not carry out ancillary activities until you have received written approval from TU Delft. This approval may be subject to certain conditions. For example a publication obligation in the case of an academic position.

These rules and obligations are in line with the Sectoral Scheme Covering Ancillary Activities (that forms part of the CAO NU) and the TU Delft Implementing Regulation which is based on this.

### **Intellectual Property Rights**

All intellectual property rights ensuing from your work during your appointment at TU Delft accrue fully to TU Delft. This is prescribed by law and applies worldwide.

You can find more information on intellectual property rights in Section 3 of the CAO NU.

Initialled TU Delft:



Initialled Y. Wang:





**Collective Labour Agreement and schemes and regulations on terms and conditions of employment**

The CAO NU, and any future versions thereof, applies to this employment contract and forms an integral part of it. You can read the text of the CAO NU at [www.vsnv.nl/en\\_GB/cao-universiteiten.html](http://www.vsnv.nl/en_GB/cao-universiteiten.html).

The TU Delft schemes and regulations on terms and conditions of employment, codes of conduct and academic integrity, and any future versions thereof, apply to this employment contract and form an integral part of it. An overview of these schemes and regulations on terms and conditions of employment, codes of conduct and academic integrity can be found at the end of this contract. The schemes and regulations themselves can be found on the website <https://www.tudelft.nl/en/employment-conditions/>, where they are available for you to read. By signing this employment contract you declare that you are familiar with the contents of these schemes and regulations.

**Unilateral changes clause**

TU Delft has the right to change the content of this employment contract unilaterally if the importance to TU Delft of doing so is so great as to outweigh, by the standards of reasonableness and fairness, your interests.

**Applicable law**

This employment contract is subject to Dutch law. Any disputes relating to this employment contract shall be settled in the Dutch courts.

The agreements and conditions above are agreed by TU Delft and you and are drawn up in duplicate and signed in Delft on August 11, 2020.

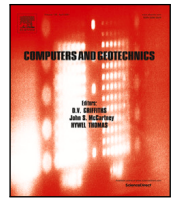


.....  
Prof.dr. J.E.J. Schmitz



.....  
Y. Wang

### 3. 近 5 年代表性学术成果



## Research Paper

# Accurate modeling and simulation of seepage in 3D heterogeneous fractured porous media with complex structures

Luyu Wang<sup>a,b,c,\*</sup>, Yuhang Wang<sup>a,b</sup>, Cornelis Vuik<sup>a</sup>, Hadi Hajibeygi<sup>b</sup>

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## ARTICLE INFO

## Keywords:

Fractured porous media  
Three-dimensional modeling  
Seepage  
Discrete fractures  
Inclusions  
Heterogeneity

## ABSTRACT

The past decades have witnessed an increasing interest in numerical simulation for flow in fractured porous media. To date, most studies have focused on 2D or pseudo-3D computational models, where the impact of 3D complex structures on seepage has not been fully addressed. This work presents a method for modeling seepage in 3D heterogeneous porous media. The complex structures, typically the stochastic discrete fractures and inclusions, are able to be simulated. A mesh strategy is proposed to discretize the complex domain. In particular, a treatment on the intersected elements is developed to ensure a conforming mesh. Then, numerical discretization is provided, in which the flux interactions of fractures, inclusions and surrounding rock matrix are included. Numerical tests are performed to analyze the hydraulic characteristics of 3D fractured media. First, the developed framework is validated by comparing numerical solutions with the results of embedded discrete fracture model. Next, the effects of orientation, aperture and radius of fractures on fluid flow and equivalent permeability tensor are analyzed. The variations of pressure distribution are studied in heterogeneous and homogeneous media. Finally, the hydraulic properties of a medium with complex structures are investigated to show the difference of hydraulic feature between fractures and inclusions.

## 1. Introduction

Modeling of seepage in fractured porous media is of great interest in geotechnical engineering and geoscience applications (Hajibeygi et al., 2020; Mejia et al., 2021; Wang et al., 2022a). In practice, fractures are randomly distributed in the geological fields, and they have contrasting hydraulic properties compared to that of the rock matrix (Berkowitz, 2002; Kolditz et al., 2012; Adler et al., 2013). As a result, fractures play a critical role in determining the dynamics of flow and transport in such fractured systems.

There are different approaches for numerical investigation of fractured porous media. They can be mainly divided into two categories. The first category is related to the geological modeling techniques and the geostatistics (Yin and Chen, 2020; Jacquemyn et al., 2021; Cañamón et al., 2022), which also studies the distribution law of natural fractures from the perspective of the statistical methods. In this category, field investigation provides the massive data of geological information of fractures. The researchers do not focus on numerical simulations, such as the seepage and deformation simulations, but study the statistical characteristics of fracture networks. However, the second category

focuses on the numerical methods related to hydraulic and mechanical processes of the deformable fractured media, in which the finite element method and the finite volume method are the commonly used numerical approaches (Karimi-Fard and Durlofsky, 2012; Wang et al., 2020, 2022b; Hajibeygi et al., 2020; Sui et al., 2022). In the presented study, we mainly focus on the second category.

Three representative numerical models have been widely used to simulate seepage in fractured porous media, namely, (a) the equivalent continuum model (ECM) (Ghahfarokhi, 2017; Chung et al., 2018; Wang et al., 2022a), (b) the discrete fracture network (DFN) (de Dreuzy et al., 2013; Hyman et al., 2015), and (c) the discrete fracture model (DFM) (Karimi-Fard et al., 2004; Zidane and Firoozabadi, 2018; Wang et al., 2022c). The ECM, which is proposed based on the upscaling technique, is an efficient computational model but it cannot reflect the interaction between the fractures and the rock matrix. Especially, for a fractured medium with a few fractures with large size, the equivalent permeability tensor may not exit. In this case, the ECM does not work. The DFN is a simplified model which neglects flow in the rock matrix. It provides an acceptable solution if the permeability of fractures is

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# CO<sub>2</sub> Storage in deep saline aquifers: impacts of fractures on hydrodynamic trapping

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## ARTICLE INFO

### Keywords:

Geologic carbon storage  
Multiphase flow in porous media  
Embedded discrete fracture model  
Compositional simulation

## ABSTRACT

Natural or induced fractures are typically present in subsurface geological formations. Therefore, they need to be carefully studied for reliable estimation of the long-term carbon dioxide storage. Instinctively, flow-conductive fractures may undermine storage security as they increase the risk of CO<sub>2</sub> leakage if they intersect the CO<sub>2</sub> plume. In addition, fractures may act as flow barriers, causing significant pressure gradients over relatively small regions near fractures. Nevertheless, despite their high sensitivities, the impact of fractures on the full-cycle storage process has not been fully quantified and understood. In this study, a numerical model is developed and applied to analyze the role of discrete fractures on the flow and transport mechanism of CO<sub>2</sub> plumes in simple and complex fracture geometries. A unified framework is developed to model the essential hydrogeological trapping mechanisms. Importantly, the projection-based embedded discrete fracture model is incorporated into the framework to describe fractures with varying conductivities. Impacts of fracture location, inclination angle, and fracture-matrix permeability ratio are systemically studied for a single fracture system. Moreover, the interplay between viscous and gravity forces in such fractured systems is analyzed. Results indicate that the fracture exhibits differing effects regarding different trapping mechanisms. Generally speaking, highly-conductive fractures facilitate dissolution trapping while weakening residual trapping, and flow barriers can assist dissolution trapping for systems with a relatively low gravity number. The findings from the test cases for single fracture geometries are found applicable to a larger-scale domain with complex fracture networks. This indicates the scalability of the study for field-relevant applications.

## 1. Introduction

Carbon dioxide capture and storage is essential to mitigate climate change and global warming. Subsurface geological media provide many opportunities for a long-term secure storage (Eiken et al., 2011). Candidate formations include depleted hydrocarbon fields, saline aquifers and unmineable coal seams. Among them, saline aquifers provide the biggest volumetric storage capacities (Bachu, 2002). Injected CO<sub>2</sub> can be trapped in saline aquifers through different trapping mechanisms, including structural or stratigraphic trapping, residual trapping, dissolution trapping, and mineral trapping (Benson and Cole, 2008). These trapping mechanisms operate at varying time scales of dominance. Structural (also referred to as “stratigraphic”) trapping occurs as soon as the injected CO<sub>2</sub> migrates towards the top of the aquifer

due to the buoyancy forces, and residual trapping takes place at the trailing edge of CO<sub>2</sub> plume mainly after injection ceases (Ide et al., 2007; Juanes et al., 2006). Both of them take effect in relatively early stages of the operation time. In contrast, the dissolution and mineral trapping mechanisms span much longer time periods. Dissolution trapping occurs as early as (usually super-critical) CO<sub>2</sub> contacts the residing undersaturated reservoir brine. The brine charged with dissolved CO<sub>2</sub> molecules becomes denser. This triggers the density-driven convection in post-injection period (Emami-Meybodi et al., 2015; Neufeld et al., 2010; Soltanian et al., 2016). In the meantime, dissolved CO<sub>2</sub> combined with H<sub>2</sub>O forms carbonic acid, which induces the dissolution/precipitation of minerals in the rock (Dai et al., 2020). Since saline aquifers often reside in sandstone formations, in which the principle mineral is quartz, geochemical reactions contributed to mineral trapping are insignificant

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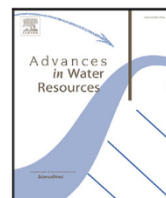
E-mail addresses: [Y.Wang-25@tudelft.nl](mailto:Y.Wang-25@tudelft.nl) (Y. Wang), [c.vuik@tudelft.nl](mailto:c.vuik@tudelft.nl) (C. Vuik), [h.hajibeygi@tudelft.nl](mailto:h.hajibeygi@tudelft.nl) (H. Hajibeygi).

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# Analysis of hydrodynamic trapping interactions during full-cycle injection and migration of CO<sub>2</sub> in deep saline aquifers

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## ARTICLE INFO

### Keywords:

Geologic carbon storage  
Multiphase flow in porous media  
Compositional simulation  
Multiphysics interaction

## ABSTRACT

CO<sub>2</sub> injection into deep saline aquifers has shown to be a feasible option, as for their large storage capacity under safe operational conditions. Previous studies have revealed that CO<sub>2</sub> can be trapped in the subsurface by several mechanisms. Despite the major advances in studying these trapping mechanisms, their dynamic interactions in different periods of a full-cycle process have not been well understood; i.e., they are studied independently at their so-called 'separate time scales of importance'. These mechanisms, however, are dynamically interconnected and influence each other even outside of their main time scale of importance. Besides, previous studies on field-scale simulations often choose grid cells which are too coarse to capture flow dynamics especially in post-injection period. To this end, we develop a comprehensive framework to analyze the flow dynamics and the associated hydrodynamic trapping process, in which the CO<sub>2</sub> injection, migration and post-migration period are all considered in a unified manner. Through illustrative models with sufficient grid resolution, we quantify the impact of different trapping mechanisms and uncertain reservoir properties through a full-cycle process. We demonstrate that the time scale associated with each trapping mechanism indeed varies, yet their dynamic interplay needs to be considered for accurate and reliable predictions. Results reveal that residual trapping is governed by the advective transport in the injection period, and its contribution to the overall trapped amount becomes more significant in systems with lower permeability. Dissolution trapping operates under varying driving forces at different stages. In the injection period, the dissolution process is controlled by advective transport, and later enhanced by the gravity-induced convection in the post-injection period. Such convective transport diminishes the contribution from residual trapping. Our study sheds light on the impact of the coupled reservoir and fluid time-dependent interactions in estimation of the securely trapped CO<sub>2</sub> in saline aquifers.

## 1. Introduction

Carbon dioxide capture and storage (CCS) has been identified as a promising strategy to mitigate climate change due to anthropogenic CO<sub>2</sub> emissions. Given the urgency with respect to limiting global warming, recent decades have witnessed a remarkable increase of research interest around CO<sub>2</sub> storage in subsurface systems (Bui et al., 2018). Of the geological media being considered, hydrocarbon (oil and gas) reservoirs and deep saline aquifers have shown to be successful at pilot and commercial scales (Orr Jr., 2009; Szulczewski et al., 2012; Bachu, 2015). Storing CO<sub>2</sub> in hydrocarbon reservoirs is relatively straightforward, because the geological structures in which buoyant hydrocarbons were retained for quite a long time have proved to be

safe. In addition, the storage capacity could be estimated based on the volume of produced oil/gas assuming hydrocarbons will be completely replaced by CO<sub>2</sub> (Bachu et al., 2007). The storage can become more economically attractive by being combined with enhanced oil recovery (EOR) (Dai et al., 2014; Ampomah et al., 2017) or geothermal energy production (Randolph and Saar, 2011). On the other hand, for CO<sub>2</sub> storage in saline aquifers, the flowing fluids are primarily composed of CO<sub>2</sub> and brine. Due to their distinct mobility contrast and geological heterogeneities, such a displacement process is unstable. Moreover, various trapping mechanisms operating on different time scales add to the complexity in understanding such a dynamic process.

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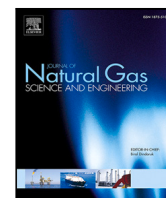
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# Insights into scale translation of methane transport in nanopores

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## ARTICLE INFO

### Keywords:

Lattice Boltzmann method

Preconditioning scheme

Rough nanopore

Complex geometry

## ABSTRACT

Accurate prediction of flow behavior in shale matrix is critical for efficient development of shale gas reservoirs. In these systems, the majority of pores are in the nano-size range. As a result, continuum-based approaches may not be appropriate to simulate flow in such systems. Molecular dynamics (MD) simulations are capable of capturing the relevant microscale physics. Their relatively high computational expense, however, restricts MD simulations to rather small systems and domains. This limitation creates a gap between computational need of macroscale systems and capabilities of MD simulations. The lattice Boltzmann method (LBM) is a suitable candidate to bridge this gap. In this work, the multiple-relaxation-time (MRT)-LBM is used to study methane transport in nano-size pores. Adsorption effects near solid boundaries, as well as non-ideal behavior of fluids, are accounted for via incorporating appropriate force terms in LBM. Parameters associated with the force terms in the equation of state are studied in detail, and a workflow is proposed to determine optimal values of these parameters for gas flow in slit pores. Specifically, we establish these parameters such that the range of density values that the model is able to simulate is maximized. We demonstrate this workflow by simulating gas flow where velocity and density profiles from MD simulations are used as reference data. Results from LBM simulations are in good agreement with MD reference data for pores that are 4 nm in width or larger. Moreover, we propose a preconditioning scheme to improve the stability of LBM in dealing with complex geometries. The robustness of this scheme is demonstrated by simulating several roughness geometries. This work motivates the use of LBM in scale translation of the physics of mass transport in more complex permeable media.

## 1. Introduction

Shale gas has become one of the significant hydrocarbon resources owing to advancements in stimulation technologies in recent decades. In shale reservoirs, transport of shale gas is in general a multi-scale process: gas flows through the matrix, which is mainly composed of nano-size pores, followed by a fracture network, and eventually into the wellbore. To study the dynamics of flow and transport in fractured media, many numerical models have been proposed, including dual porosity model (Barenblatt et al., 1960; Blaskovich et al., 1983; Warren and Root, 1963; Wang et al., 2021a), multiple interacting continua model (Pruess, 1985; Wu and Pruess, 1988) and discrete fracture model (Kim and Deo, 2000; Karimi-Fard et al., 2004). These numerical models have advanced our understanding of shale gas flow in fractured media. However, our knowledge of transport in the matrix itself is limited due to the fact that a significant portion of the pores in the matrix are in nano-size range, and that both observing and simulating transport in nanosize pores are challenging tasks.

To study these systems, it is crucial to adopt an approach capable of capturing the physics accurately. Particle-based approaches, e.g., molecular dynamics (MD) simulation and lattice Boltzmann method (LBM), are such potential candidates. MD simulation focuses on interactions at molecular level, therefore, it captures the relevant microscopic physics with high fidelity. This approach has thus received increasing interest recently. Yu et al. (2018) performed MD simulations to investigate transport characteristics of methane in slit nanopores with a fixed width under different pressures. He et al. (2019) used equilibrium and non-equilibrium MD methods to study the key factors that regulate shale gas transport through rough nanopores of shale kerogens whose max pore size is 16 nm. Wang et al. (2021b) studied pressure-driven desorption process of methane in 1–5 nm wide nanoslits using non-equilibrium MD simulations. MD framework is also extended to investigate systems with complex fluids, i.e., multi-phase and multi-component transport in shale nanopores (Yu et al., 2020; Xu

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# Coupled confined phase behavior and transport of methane in slit nanopores

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<sup>c</sup> Department of Mathematics and Statistics, University of Wyoming, Laramie, WY 82071, USA

## HIGHLIGHTS

- A modified extension of PR-EOS for confined phase behavior of methane is proposed.
- The proposed EOS captures shift of critical properties and density phase diagrams.
- The proposed EOS is coupled with lattice Boltzmann method to investigate transport.
- The use of the proposed EOS leads to smaller velocities compared to PR-EOS.
- Transport characteristics of methane in nanopores are pressure-dependent.

## ARTICLE INFO

### Keywords:

Confined phase behavior  
Equation of state  
Rarefied gas flow  
Lattice Boltzmann method

## ABSTRACT

The proximity of the order of magnitude molecular mean free path and pore sizes in nanopores leads to remarkable interactions between molecules and walls. In such systems, the thermodynamic property and the transport behavior of fluids deviate from those at bulk conditions. Molecular dynamics (MD) simulation may be used to investigate the effects of confinement on fluid physics in nano-size pores. However, translating these subscale observations into a larger scale of interest remains a challenging task. In this work, we propose a modified extension of Peng-Robinson equation of state (PR-EOS) motivated and guided by MD simulation results. The shift of critical properties, i.e., pressure and temperature, are evaluated independently. A temperature dependent parameter is introduced to account for the existence of capillary pressure in the two-phase region. This formulation is capable of capturing the shift in critical properties as well as density phase diagrams under various confinement scenarios. We incorporate the proposed EOS in the lattice Boltzmann method (LBM) to study coupled confined phase behavior and transport of methane in nano-size slit pores. Adsorptive strength is determined such that the resulting density ratio matches that from MD simulation. Results indicate that the use of the proposed EOS leads to smaller fluid velocities compared to PR-EOS. This effect is due to stronger interactions between fluid particles under confinement. Also, results show that transport characteristics are impacted by the pressure of the system: in systems with a relatively low pressure, transport seems to be dominated by Knudsen diffusion; however, at a higher pressure, the contribution from viscous flow increases as the pore widens while the influence of Knudsen and surface diffusion diminishes.

## 1. Introduction

Shale gas, which is composed of methane primarily, is an unconventional resource that has become a significant source of natural gas due to the advancements in stimulation techniques. The transport process of methane is in general a multi-scale process: methane flows through the organic nanopores, followed by the fracture network, and eventually into the wellbore. Despite great advances in discretization schemes for simulating flow in fractured reservoirs [1–6], and

predictions of pore pressure and stress field via coupling of flow and geomechanics using the model proposed by Biot [7–10], the transport mechanism of shale gas in the matrix, where a majority of pores are nano-size [11–14], may not be fully understood. Under such confined conditions, measuring fluid properties or visualizing fluid flow via experimental techniques is a challenging task. On the other hand, numerical simulation becomes an efficient alternative. This work focuses on developing a physics-based description for confined phase behavior of methane, and on coupling the developed formulation with a

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# Water Resources Research

## RESEARCH ARTICLE

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## Scaling Analysis of Two-Phase Flow in Fractal Permeability Fields

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### Key Points:

- A generalized analytical scaling relation is derived for two-phase flow in permeable media subject to self-similar heterogeneity
- Numerical results from a high-resolution simulator agree with predictions of the derived scaling relation
- Nonlinear flows scale with the degree of nonlinearity in the asymptotic regime

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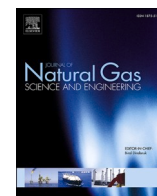
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**Abstract** Fluid mixing in permeable media is essential in many practical applications. The mixing process is a consequence of velocity fluctuations owing to geological heterogeneities and mobility contrast of fluids. Heterogeneities in natural rocks are often spatially correlated, and their properties, such as permeability, may be described using fractal distributions. This work models the fractal characteristics of such permeability fields in which the covariance function is expressed as a power-law function. A generalized scaling relation is derived relating various fractal permeability fields using the magnitude of their fluctuations. This relation reveals the self-similar behavior of two-phase flow in such permeable media. To that end, a recently developed, high-resolution numerical simulator is employed to validate the analytically derived scaling relations. Two flow problems are considered in which flow is governed by (1) a linear and (2) a nonlinear transport equation. Due to the probabilistic representation of the fractal permeability fields, a sensitivity study is conducted for each flow scenario to determine the number of realizations required for statistical convergence. Scaling analysis is performed using ensemble averages of simulated saturation profiles and their mixing lengths. Results support the validity of the developed scaling relation across the range of investigated flow conditions at intermediate times. The dynamics of linear flow in the asymptotic regime is affected by the correlation structure of heterogeneity. In nonlinear flow, scaling behavior appears to be dominated by the degree of nonlinearity.

**Plain Language Summary** Multiphase flow in subsurface permeable media plays a fundamental role in many natural and engineering processes, such as remediation of contaminated aquifers, geological carbon storage, and petroleum reservoir engineering. In all these instances, variability of the media's properties and contrasts of density and viscosity of the flowing phases may lead to significant velocity fluctuation at the pore scale and mixing of the fluids at the macroscale. Optimal design and exploitation of these subsurface resources require accurate and predictive macroscale descriptions of the flow processes. This work investigates the impact of spatial heterogeneity on flow characteristics using a probabilistic description for the permeability field. We demonstrate a relation between flow behaviors in various self-similar fields with a power-law covariance structure. Our findings may help to predict flow behavior in geological formations without the need to conduct full-scale simulations.

## 1. Introduction

Flow and transport in permeable media in the context of the subsurface is receiving a growing interest due to the wide range of applications that rely on an in-depth understanding of such processes. Natural permeable media consist of matrices of grains interspersed with interconnected pores. To capture the dynamics of subsurface flow, mathematical modeling and numerical simulation play essential roles. Given the availability of information regarding the exact geometry, pore-scale modeling and simulation studies provide a detailed understanding of interactions between fluids and solids in permeable media (Bijeljic & Blunt, 2006; Celia et al., 1995; Liu et al., 2014; Mehmani & Tchelepi, 2019; Prodanović & Bryant, 2006). An accurate understanding of physical mechanisms of flow and transport at pore-scale is critical to deriving predictive macroscopic descriptions, which account for disparate length scales and are indispensable in simulating flow in large-scale systems. These mathematical descriptions rely on macroscale variables such as saturation, porosity, and permeability, and they are formulated using conservation laws (LeVeque, 1992). Darcy's



# Pore-scale simulation of gas flow in microscopic permeable media with complex geometries

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## ARTICLE INFO

### Keywords:

Lattice Boltzmann method  
Rarefied gas flow  
Slip model  
Microscopic permeable media

## ABSTRACT

Lattice Boltzmann method (LBM) is an efficient tool to perform direct numerical simulation of gas flow in micro-size pores. Despite great advances in LBM and its use in describing gas flow in micro-size channels in slip and transitional flow regimes, exploring formulations that are able to capture flow behavior in domains with complex boundary geometries remains a challenging task. As a result, the impact of complexities in pore structures on gas flow may not be fully explored using LBM. In this study, we propose to use the combined bounce-back and Maxwellian diffusive reflection scheme to capture the slip velocity with a new set of slip coefficients. Optimal values of slip coefficients are determined using a gradient based method, where the results from the linearized Boltzmann equation is used as the reference solution. The proposed formulation is further validated against predictions from molecular dynamics simulation in the presence of complex geometries by introducing obstacles of different shapes in straight channels. LBM with the proposed boundary treatment is then used to investigate gas flow in a synthetic microscopic permeable medium. Results indicate that gas exhibits different flow configurations as Knudsen number varies, and apparent gas permeability appears to have up to a second-order dependency on the reciprocal mean pressure in slip and transitional flow regimes.

## 1. Introduction

This work is concerned with rarefied gas flow where the size of the molecular mean free path (MFP), defined as the average distance traveled by gas molecules between each two successive collisions, is significant compared to the characteristic length of the flow field (Muntz, 1989). This type of flow is encountered in a variety of applications such as aerodynamics, heat transfer, micro-electro-mechanical systems (MEMS), and natural gas production from unconventional formations (Ho and Tai, 1998; Barber and Emerson, 2006; Javadpour et al., 2007; Jiang and Younis, 2015; Wang and Shahvali, 2016; Yuan and Rahman, 2016). Unconventional reservoirs, such as shale, are mainly composed of heterogeneous nano-scale pore structures (Loucks et al., 2009; Saraji and Piri, 2015; Zolfaghari et al., 2017). Understanding mass transfer in these permeable media requires careful treatment of their complex geometries at the pore-scale. Such an understanding is paramount to translating dominant physical mechanisms across the wide range of scales present in such systems, and developing appropriate macroscale descriptions (Chen et al., 2015; Ning et al., 2015; Zhao et al., 2016b; Yu

et al., 2017). This work focuses on pore-scale flow simulation (Prodanović and Bryant, 2006; Meakin and Tartakovsky, 2009; Blunt et al., 2013; Mehmani and Tchelepi, 2018) that captures flow dynamics, such as slip velocity in nano-pores with complex geometries, accurately and efficiently.

Selecting an appropriate simulation approach requires close attention to the physical scales and the ensuing flow regimes that are expected to develop in the simulation domain. Knudsen number ( $K_n$ ) is a dimensionless number that serves that purpose well; it is the ratio of MFP to the characteristic length of the flow field (Chambre and Schaaf, 2017). Four flow regimes are delineated using  $Kn$  number: continuum flow ( $K_n < 0.001$ ), slip flow ( $0.001 < K_n < 0.1$ ), transitional flow ( $0.1 < K_n < 10$ ), and free molecular flow ( $K_n > 10$ ). In the continuum flow region, gas flow is described by the continuum fluid mechanics, where the Navier-Stokes (N-S) equation applies with no-slip boundary conditions. As the Knudsen number increases ( $0.001 < K_n < 0.1$ ), velocities near solid walls become nonzero due to more frequent interactions between gas molecules and walls. In such cases, N-S equation with slip boundary conditions may be used. Further increases in  $K_n$

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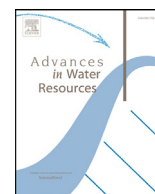
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# An extension of Darcy's law incorporating dynamic length scales

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## ARTICLE INFO

### Keywords:

Multiphase flow  
Nonequilibrium models  
High-resolution methods  
Flow instability

## ABSTRACT

We propose a physics-based, macroscale formulation of multiphase porous-media flows that both honors the validity of Darcy's law in steady or near-steady flows and accommodates the effects of heterogeneities and nonlinearities in unsteady flows. The new formulation recognizes that parameters characterizing the system operate at different length-scales. In particular, the use of Darcy's law, predicated on the assumption of near-steady flows, requires dynamic length scales, owing to the possibility of rapid fluctuations in rock properties and fluid saturations attributable to heterogeneity and nonlinearity. We accommodate these dynamic length-scales through dynamic spatial averaging. The length and position of the averaging window are characterized by the length of the mixing zone and the direction of propagation of information in the transport process. We validate the proposed formulation by comparing highly accurate, two-dimensional numerical solutions against core-scale displacement experiments. The proposed paradigm is consistent with the classical multiphase Darcy formulation, in the sense that the latter also represents the results of an averaging approach.

## 1. Introduction

Accurate mathematical description of multiphase flows in porous media is essential in many practical problems, including groundwater contaminant remediation, geological storage of CO<sub>2</sub>, and petroleum reservoir engineering (House et al., 2006; Juanes, 2008; Qiao et al., 2018). Bench- or field-scale simulation of fluid displacement processes in these applications requires macroscale mathematical formulations, which replace the details of flow in the pores with spatially averaged descriptions (Abriola and Pinder, 1985; Bear, 2013; Jiang and Younis, 2015; Wang and Shahvali, 2016; Chabanon et al., 2017). These formulations involve partial differential equations (PDEs) arising from the conservation of mass, momentum and energy (LeVeque, 1992). This paper presents a new formulation of porous-medium flow, based on length-scale averaging, that accommodates effects associated with spatially heterogeneous media and the nonlinearities inherent in multi-fluid flows.

Darcy's law represents the classic macroscale expression of the conservation of momentum for a single fluid phase flowing in a porous solid. It establishes a linear field equation in which the macroscale (Darcy) velocity is proportional to the gradient of a field potential such as the pressure or hydraulic head (Whitaker, 1986). Strictly speaking, Darcy's law is valid for low Reynolds-number, single-fluid, steady flows in which fluid inertia is negligible (Hubbert, 1956; Whitaker, 1986; Dullien, 2012; Neuman, 1977). In some regimes, such as slow flows in

nearly homogeneous porous media, it is reasonable to treat the flow as nearly steady, since fluid parcels encounter slowly fluctuating rock properties. However, unless the steady-state velocity field is established, in highly heterogeneous media the hypothesis of nearly steady flow may not be valid, especially at displacement fronts.

Further problems arise in multi-fluid flows. Following Muskat and Meres (1936); Wyckoff and Botset (1936); Leverett (1941), engineers common extend Darcy's law to these flows via the use of nonlinear constitutive relations such as relative permeabilities and capillary pressure. Even though relative permeabilities and capillary pressure are often assumed to be local functions of saturation, they also depend on other nonlinear parameters such as saturation history and composition-dependent rock wettability and fluid viscosities (Avraam and Payatakes, 1995; Tang and Kovscek, 2011; Honarpour, 2018). As with heterogeneities, these nonlinear effects can also call into question the assumption of nearly steady flow, since fluids in the mixing zone at a displacement front may encounter rapidly fluctuating rock properties and fluid saturations. In short, since Darcy's law is predicated on the assumption of steady flows, its straightforward application in highly heterogeneous media and in the presence of nonlinearities neglects the variable length scales over which rock properties and fluid saturations vary.

The new formulation presented in this paper addresses this difficulty, accommodating dynamic length scales through dynamic spatial averaging. The length and position of the averaging window are driven by

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# Analysis of nonequilibrium effects and flow instability in immiscible two-phase flow in porous media

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## ARTICLE INFO

### Keywords:

Multiphase flow  
Nonequilibrium models  
High-resolution methods  
Flow instability

## ABSTRACT

Two-dimensional, high-resolution, numerical solutions for the classical formulation and two widely accepted nonequilibrium models of multiphase flow through porous media are generated and compared with experimental observations from literature. Flow equations for simultaneous flow of two immiscible phases through porous media are written in a vorticity stream-function form. In the resulting system of equations, the vorticity stream-function equation is solved using a spectral method and the transport equation is discretized in space using a central-upwind scheme. The system of equations is solved for a two-dimensional domain using a semi-implicit time-stepper. The solutions reveal behavior that is not apparent in one-dimensional solutions, namely that sharpening of the saturation front caused by the inclusion of a dynamic capillary pressure results in propagation of viscous fingers compared to the classical formulation. The inclusion of nonequilibrium effects in the constitutive relations, in the form of effective saturation, introduces dispersion and smears the otherwise highly resolved viscous fingers in the saturation front. Once developed, the length of the mixing zone in the numerical solutions remains constant with time regardless of the degree of instability. This is contrary to the evolution of the mixing zone observed in unstable flow experiments where, unlike the numerical solutions, the propagation speed of the leading edge of the front appears to increase with time.

## 1. Introduction

An accurate mathematical description of multiphase flow in porous media is essential in many practical applications, such as environmental remediation of the vadose zone and mitigation of green house effects by geological storage of CO<sub>2</sub> in saline aquifers and depleted petroleum reservoirs (Juanes, 2008). Natural porous media consist of matrices of grains interspersed with many irregularly shaped and interconnected void spaces referred to as pores. Attempts to describe, in an exact manner, the geometry of the solid surfaces that bound the flow domain inside a porous medium are futile (Bear, 2013). Given the availability of information regarding the exact geometry of these surfaces (i.e., boundary conditions) in a porous medium, it would be conceivable to treat multiphase flow at the pore level (herein referred to as microscale) using a fluid continuum approach (i.e., the Navier–Stokes equations). Pore morphology aside, a great deal of additional information would be needed to attempt such a theoretical solution to the problem of multiphase flow, e.g., properties and condition of interfaces and mass transfer across them (Bear, 2013). Nevertheless, under the burden of many simplifying assumptions, simplified approaches for pore-level fluid flow

simulation have been developed (Lenormand, 1990; Lenormand et al., 1988; Wilkinson, 1986; Wilkinson and Willemsen, 1983; Witten Jr and Sander, 1981). Field-scale simulation models must, however, deal with immensely disparate length scales from pores to the field (Bear, 2012). To circumvent these difficulties, computationally feasible field-scale models rely on macroscale descriptions of flow through porous media, which use macroscale variables such as saturation, porosity, and permeability.

Mathematical descriptions of flow through porous media are formulated using conservation laws, namely conservations of mass, momentum and energy (LeVeque, 1992). Darcy's law is a macroscale expression of the conservation of momentum for a single phase, and is valid for low Reynolds numbers (very slow flow) (Dullien, 2012; Hubbert, 1956; Whitaker, 1986). In macroscale formulations of multiphase flow through porous media, Darcy's law is extended to multiple phases via the use of constitutive relations, i.e., relative permeability and capillary pressure functions (Leverett, 1941; Muskat and Meres, 1936; Wyckoff and Botset, 1936). Moreover, constitutive relations are known to depend not only on local saturation, but also on a number of other parameters such as saturation history, initial wetting-phase saturation, wettability, interfacial tension, pore geometry and viscosity of fluids

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#### 4. 近 5 年承担主要科研项目

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