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## Editorial

# Multiscale and multiphysics influences on fluids in unconventional reservoirs: Modeling and simulation

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### Abstract:

Unconventional reservoir resources are important to supplement energy consumption and maintain the balance of supply and demand in the oil and gas market. However, due to the complex geological conditions, it is a significant challenge to develop unconventional reservoirs efficiently and economically. At present, unconventional reservoirs are extensively studied, covering a wide range of areas, with special attention to the multiscale characterization of pore structures and fracture networks, description of complex fluid transport mechanisms, mathematical modeling of flow properties, and coupled analysis with multiphysics fields. This work briefly describes the multiscale and multiphysics influences on fluids in unconventional reservoirs, and the modeling and simulation work conducted to analyze them, with the aim to provide some theoretical basis for enhanced recovery from these geo-energy resources. The present article also aims to enhance the community's knowledge of other potential utilizations associated with some unconventional reservoirs, specially related to environmentally-driven projects, including permanent greenhouse gas storage and cyclic underground energy storage.

## 1. Introduction

Unconventional reservoirs are characterized by low porosity, pore throat diameter and permeability. They have special features such as micro- and nano-scale pores, multiscale fracture networks, and varied mineral compositions that make the physics of the fluid transport within them quite complex. These features also impact the fluid-rock petrophysical properties, which thus affect fluid recovery factors, production flow rates and injectivity (Cai and Hu, 2019). Therefore, comprehensive characterization of pore structure, pore-size distributions and in-depth understanding of fluid flow mechanisms are important for efficient development of unconventional reservoirs.

The multiscale and multiphysics nature of fluids in unconventional reservoirs is now widely studied based on labora-

tory experiments, theoretical analyses, and numerical simulations (Yang et al., 2021). This work presents an overview of the research methods and contents commonly used in unconventional reservoirs from different perspectives. With the help of high-precision imaging equipment and fluid injection experiments, three-dimensional (3D) digital cores of unconventional reservoirs can be reconstructed and their pore size distribution and topology can be characterized. Based on that, mathematical models for predicting permeability can be developed by combining various effects. In addition, by combining simulation methods, the flow mechanism and transport properties under multiscale and multiphysics considerations can be examined systematically.

## 2. Multiscale characterization of pore structure

Pore-throat sizes in unconventional reservoirs are in the range of micrometers to nanometers with more than 50% of pore-throat sizes less than  $1\mu\text{m}$  (Zou et al., 2012). The reservoirs key physical properties are obviously different, the pore structure is complex and the heterogeneity/anisotropy is strong and variable on different scales and spatial locations. Thus, geometric descriptions and measurements that can accurately describe pore morphology of unconventional reservoirs at all scales have not yet been found. The development of multiscale natural/artificial fractures and micro-nano matrix pores plays an important role in oil and gas migration and storage. However, this introduces difficulties to the study of microscopic flow laws in unconventional reservoirs. X-Computed Tomography (CT) images and nuclear magnetic resonance test data can usually be regarded as effective approaches to distinguish rock samples into different types. Based on the CT images, gas absorption and high-pressure mercury intrusion experiments, fractal theories are widely used to characterize scale-invariant complexity, heterogeneity, and anisotropy of rock microstructures. It is necessary to ascertain the relationship between the fractal dimension and petrophysical properties, which is closely related to the pore-size distributions and pore-structural characteristics of tight reservoirs (Cai et al., 2020). However, the estimation of fractal dimensions of tight reservoirs is fraught with uncertainties and complexity (Wood, 2021).

Digital core technology refers to the reconstruction of 3D rock structure through a series of algorithms based on scanned images. Such 3D reconstructions facilitate detailed simulation studies. The multiscale digital cores can be constructed through the resolution difference of scanning equipment. Micro-CT provides images of the micro-scale pore structures, while the nano-CT or focused ion beam scanning electron microscope can image pore structures at nano-scale resolutions (Chandra and Vishal, 2021). Multiscale 3D pore-structure models can be constructed by applying image processing technology, leading to the generation of a reliable pore network model (PNM). Such models can be based on pore skeleton lines to obtain the pore size distribution, fractal dimension, surface area and shape factor to achieve multiscale characterization of pores and fractures in unconventional reservoirs.

There are two methods typically used for PNM construction. One is to construct the model based on micro-imaging technology. This method preserves the precise topological structure of the rock formations, as it actually depends on rigorous image processing procedures. The other is to construct a random model that integrates some of the experimental results obtained from real rock formation samples. The models constructed using the second method are representations of real rock samples displayed at the macro scale. Recently, machine learning has been used to reconstruct these complex structures. It is possible for the characteristics of the two-dimensional and 3D structures, obtained from micro-imaging technology or PNM extraction methods to be accurately learned by certain machine learning methods. For example, generative adversarial networks (Goodfellow et al., 2014) can reconstruct

those learned models into homogeneous or heterogeneous 3D structures with similar distribution characteristics to those observed in real rock formations (Mosser et al., 2017; Wang et al., 2021).

## 3. Multiscale characterization of fluid flow

Simultaneously, mathematical simulation methods have been established to analyze the micro-scale system and obtain its upscaled properties, specially the intrinsic permeability. Moreover, apparent gas permeability models have been developed for unconventional reservoirs incorporating the slippage effect, with high accuracy (Wang et al., 2020). These simulation studies have significantly reduced the need for excessive (and costly) experiments. Besides, considering the effects of wettability, micro-fracture distributions and different pore-throat structures to investigate the evolution of imbibition fronts and recovery provides a theoretical basis for flow characteristics of unconventional reservoirs. Fluid-flow simulations can be performed on multiscale pore-structure models (Scheibe et al., 2015). However, the reconstructed pore structure is complex and numerical calculation requires a large amount of computational resources. This can be mitigated to an extent by focusing on a small-scale region of interest. That local area, delineated in a scanned image, can be used to carry out local small-scale simulations or decompose the full-domain of the pore structure into sub-regions, or “sub-domains”. This makes it possible to adopt and apply models reflecting different scales and features more expediently.

Although the flow characterization can be reliably described at each scale by the corresponding scale method, the information between adjacent scales cannot yet be readily integrated with each other. Currently, only empirical formula can be fitted to the data obtained from adjacent scale models to approximately express their uniaxial coupling. In future, it is anticipated that the complicated relationships and information integration between two adjacent scales could be assisted by machine learning to realize complete coupling (Mehmani et al., 2021).

A comprehensive understanding of immiscible two-phase flow in porous media is vital in various fields. Commonly, immiscible two-phase flow is dominated by capillary, viscous, and gravitational forces, which lead to complicated flow mechanisms at the pore-scale. Pore-scale direct numerical simulation and physics-informed data-driven models are powerful tools for studying two-phase flow in porous media (Zhao et al., 2019). Combining such methods offers the convenience and advantage of conducting parametric analysis and the ability to easily obtain velocity and pressure field distributions relating to the defined pore space.

Interface tracking methods have been widely applied in pore-scale simulation to solve complex changes of pore geometries and topology without using model approximations. There are three main interface tracking methods, namely level-set, phase-field, and volume-of-fluid methods. These have been developed as extensions of computational fluid dynamics to multi-phase flow. Among them, the phase-field method, which is thermodynamically based, strictly guarantees mass

conservation and handles the topological changes of the interfaces exactly. Besides, the phase-field method provides a framework for modeling multi-component flow and transport phenomena by linking flow and thermodynamics at the pore scale. To enhance the accuracy of simulation results, two conditions must be met. Firstly, fluid-fluid interfaces should be sufficiently thin to assure that the theoretical model approaches the sharp-interface limit. Secondly, this thin interface must be adequately divided by a fine mesh, which typically requires about 10 grids. On this basis, the phase-field method can be used to study capillary imbibition, enhanced oil recovery and residual oil mechanisms in two-phase flow.

Pore-scale direct numerical simulation, especially in combination with digital core technology, is commonly used to study oil and water transport within the pore space of reservoir rocks. It is applied to complement core-scale experiments and numerical reservoir simulations (Blunt et al., 2013). Based on this method, the flow physics and interfacial evolution dynamics occurring in the pore space under the influence of multiple factors are studied in detail and the rock physical properties are directly calculated. Overall, the concepts presented are focused on the effects of fluid properties, pore structure, operating conditions, boundary conditions, and wettability on two-phase flow in porous media. The pore filling mechanism and displacement pattern under the influence of these factors are qualitatively analyzed, and the petrophysical properties during multiphase flow in porous media are further calculated (Singh et al., 2019). The results obtained by applying such concepts have enriched our understanding of the microscopic flow mechanisms in porous media, which can help improve oil and gas recovery from low-permeability, tight reservoirs. Moreover, machine learning algorithms are now being developed with the capability of learning from the information calculated by direct numerical simulations of fluid flow through pore-structures and applying that learning to predict the immiscible two-phase flow characteristics (Rabbani et al., 2020).

#### 4. Multiscale numerical simulation models

Hydraulic fracturing, an effective method to greatly improve the permeability, has been widely utilized to develop unconventional reservoirs (Barati and Liang, 2014). After hydraulic fracturing, multiscale fractures are generated in the reservoirs. While, the stimulated reservoir volume is usually limited. Acid treatment, which can reduce the rock mechanical strength, is a potential method to enhance the stimulated reservoir volume and improve oil and gas recovery. The multiscale pore structure of unconventional reservoirs is effectively changed by the acid-rock interactions, which involve both physical and chemical processes. The mechanical and petrophysical properties change as well, due to the evolution of the pore structure of the stimulated rock formation. Thus, more connected and widespread fracture networks are formed, leading to more complicated multiscale fluid-flow issues in unconventional reservoirs.

The most widely used models are the continuum media model (CMM) and the discrete fracture network model

(DFNM) (Cacas et al., 1990; Berkowitz, 2002). CMM includes dual-media models, multiple-media models and equivalent continuous-media models. The CMM equates the local influence of fractures to the whole model, focusing on the flow characteristics of the macroscopic region. However, it remains difficult to describe the microscopic flow characteristics of a single fracture in these models. The DFNM uses straight lines or planes, as the characteristic parameters to delineate the fractures and the interconnections of the fractures, in order to represent the distribution of sub-surface fractures in 3D space. The DFNM assumes that fractures are interlacing and that helps to more reliably simulate fluid flow characteristics in fractures. Nevertheless, the DFNM has shortcomings in the mesh divisions it assigns to complex fractures.

In order to overcome the limitations of CMM and DFNM, the embedded discrete fracture network model (EDFNM) has been proposed (Moinfar et al., 2013). In this model, fractures are embedded into the matrix rock meshes, and flow exchange between the matrix and fracture domains is constructed by non-adjacent links. This approach greatly reduces computational cost and is suitable for complex fracture modeling. For the multiscale fracture systems induced by fracture stimulation of tight reservoirs, single CMM, DFNM and EDFNM all have certain limitations. Therefore, CMM is usually used to describe fluid flow in matrix-microfracture systems, and DFNM and EDFNM are applied to simulate fluid flow in large-scale hydraulic fractures. Machine learning algorithms are able to simulate the Navier-Stokes equations (Raissi et al., 2020), enabling them to be used as a bridge to connect these models.

#### 5. Multiphysics and multifield coupling of fluids

Shale formations can generally be considered as a kind of multiscale unconventional reservoir, whose multiscale characteristics are related to the presence of naturally generated organic and inorganic pores, naturally occurring fractures and artificially produced hydraulic fractures. The fluids naturally stored and flowing through shale formations are usually mixtures of gas, oil and formation water. This means that two-phase flow and/or multi-phase flow regimes influence fluid flow in shale reservoirs. Moreover, nanopores in shales are strongly adsorptive, leading to free-state, adsorbed-state, and a small quantity of dissolved-state fluids existing simultaneously in shale formations. The multiple states of fluids make it more difficult to describe their flow through the multiscale pore system, because it tends to involve continuum flow, adsorption-desorption, diffusion and structural distortion. To sum up, fluid flow in shale formation is a complex combination of multiscale, multi-phase, and multiphysics processes, and the relationships between those processes are difficult to describe quantitatively.

The mathematical model is the abstraction, simplification, and approximation of the real fluid flow process, which has been gradually improved in recent years. The pore geometry, pore size distribution, different transport mechanisms, various fluid states, real gas effect, and stress are introduced into mathematical models to describe the flow process in the mul-



tiscale pore system more accurately. The simulation method is another powerful tool to investigate fluid flow in shales and other tight reservoirs. The simulation method can be divided into large-scale and pore-scale simulations according to their computational domain. The former method mainly focuses on field hydraulic fracturing parameter optimization, production prediction, and production mode adjustment. The later method predominantly investigates the flow process visually and is helpful to understand the flow mechanisms through organic and inorganic pore systems. Even though mathematical models and simulation methods are capable of describing fluid flow at specific scales within shales and tight reservoirs, the techniques are far from maturity when applied to the multiscale, multi-phase, and multi-mechanism coupling influencing such formation, in terms of acceptable computational efficiency and accuracy.

Subsurface, unconventional reservoirs are characterized by complex geological conditions such as temperature and pressure, and a gap remains between the conventional simulation results and reality. Nevertheless, pore-structure models and rock-skeleton models can be considered simultaneously in the simulation, and thermal-solid, thermal-fluid, thermal-fluid-solid and thermal-fluid-solid-mechanical structure property coupling models can be constructed to reveal the unconventional rock structure and fluid-flow characteristics under complex conditions. Further work and model development is required to improve the reliability of quantitative models and simulations addressing shales and other tight reservoirs, if these reservoirs are to be used effectively for long-term storage/sequestration of carbon dioxide and short-term storage of hydrogen in the future.

### Conflict of interest

The authors declare no competing interest.

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