Capillarity

Vol. 12, No. 3, p. 72-79, 2024

Current minireview

Numerical simulation of multiphase multi-physics flow in underground reservoirs: Frontiers and challenges

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Keywords:
Numerical simulation
multiphase flow
spontaneous imbibition
pore scale
darcy scale

Cited as:
Liu, P., Zhao, J., Li, Z., Wang, H. Numerical simulation of multiphase multi-physics flow in underground reservoirs: Frontiers and challenges. Capillarity, 2024, 12(3): 72-79.
https://doi.org/10.46690/capi.2024.09.02

Abstract:
This paper explores significant advancements in the numerical simulation of multiphase, multi-physics flows within underground reservoirs, driven by the necessity to understand and manage complex geological and engineered systems. It delves into the latest research in numerical simulation techniques at both the pore and Darcy scales, emphasizing the integration of traditional methods with emerging machine learning technologies. Key simulation methods reviewed at the pore scale include the lattice Boltzmann method, level set method, phase field method, and volume of fluid method, each offering unique advantages and facing limitations related to computational efficiency and stability. Special attention is given to spontaneous imbibition, where capillary action facilitates the movement of wetting fluids into porous media. Discussions at the Darcy scale focus on macroscopic simulation methods that simplify microscale interactions but face challenges in accurately modeling the multiscale and heterogeneous nature of fractured media. Furthermore, an overview of the basic principles, limitations, and potential of integrating machine learning algorithms with traditional numerical methods emphasizes their role in enhancing simulation efficiency and stability. Future research will aim to address existing challenges and maximize the use of advanced computational technologies to refine the accuracy, efficiency, and practical applicability of multiphase and multifield flow simulations in underground reservoirs.

1. Introduction

Underground reservoirs are complex systems where mechanical, thermal, chemical, and hydraulic processes interact in a coupled manner. Key challenges in various geo-energy development and geological sequestration projects—including shale gas and coalbed methane extraction, oil reservoir exploitation, geothermal energy development, carbon dioxide sequestration, underground gas storage, and the geological disposal of high-level radioactive waste—stem from the necessity to simulate multi-scale, multi-phase, and multi-field coupling phenomena within these reservoirs. In addition, spontaneous imbibition, the process in which a wetting fluid displaces a non-wetting fluid within porous media due to capillary forces, plays a critical role in enhancing recovery mechanisms (Hatiboglu and Babadagli, 2008; Zahasky et al., 2019; Cai et al., 2021). This phenomenon significantly influences oil extraction, environmental remediation, and other applications where fluid transport in porous media is essential. Effective simulation of spontaneous imbibition is vital for optimizing these processes and improving recovery efficiency (Cai et al., 2014). Over the past decades, significant advancements in numerical methods tailored to these challenges have emerged, grounded in diverse mechanical and thermal principles (Taron

Yandy Scientific Press

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Received May 12, 2024; revised June 4, 2024; accepted June 23, 2024; available online June 26, 2024.

et al., 2009; Izadi and Elsworth, 2015; McDermott et al., 2015; Viswanathan et al., 2022). Among these, methods based on continuum mechanics, such as the finite volume method, finite element method (FEM), extended finite element method, boundary element method, and phase field method have gained widespread application (McDermott et al., 2015; Guo et al., 2024). Simultaneously, approaches based on discontinuum mechanics, such as the discrete element method (DEM), displacement discontinuity method, and numerical manifold method, have been developed to address the challenges posed by the inherently discontinuous nature of geological porous media (Fleissner et al., 2007; Zheng et al., 2015; Chukwudozie et al., 2019).

Despite these advancements, current numerical methods largely remain restricted to handling simpler couplings of thermal, hydraulic, mechanical, and chemical processes (THMC). The exploration into more complex conditions and the intricate couplings present in real-world scenarios is still in its infancy. Furthermore, the significant computational cost of these simulations mean that most are still confined to theoretical research, with limited application at an engineering scale. This has led to a pressing need for the development of more efficient algorithms that can leverage parallel computing and other strategies to enhance computational performance and manage the vast complexities of practical engineering problems. This paper aims to review the commonly used numerical simulation methods at both the pore scale and the Darcy scale, elucidating their applicability, strengths, and limitations. Particularly, it highlights how machine learning algorithms have begun to influence numerical simulation, providing significant breakthroughs in efficiency and stability. The paper also identifies critical challenges and outlines future directions for research in the field, setting the stage for a deeper integration of advanced computational techniques in geological engineering.

2. Pore-scale numerical simulation methods

At the pore scale, a variety of numerical simulation methods are utilized to investigate multiphase flow phenomena within porous media. These methods include lattice Boltzmann method (LBM), level set method, phase field method, and volume of fluid method (VOF) (Meakin and Tartakovsky, 2009). Each technique offers distinct advantages and is subject to specific limitations. The LBM is a mesoscopic approach that models fluid flow by tracking particle distributions across a lattice grid. It is particularly valued for its computational efficiency and ability to handle complex geometries. However, the LBM can encounter numerical stability challenges, especially at low Reynolds numbers or high Damkohler number, limiting its applicability in certain scenarios (Eshghinejadfard et al., 2016). The level set method serves as an interface tracking tool to model and delineate fluid interfaces. This involves setting initial interfaces and boundary conditions, then solving the Navier-Stokes equations alongside the mass conservation equation to simulate multiphase flows (Herreros et al., 2006). While powerful, the level set method demands substantial computational resources, particularly for complex geometries or large-scale simulations. The phase field method calculates the evolution of phase field functions with appropriate boundary conditions to model various multiphase flow behaviors in porous media (Ahammad et al., 2017). Its strength lies in handling complex interface topologies, but it requires significant computational investment similar to the level set method. The VOF method uses an Eulerian framework to simulate multiphase flows by explicitly tracking fluid interfaces on a fixed grid. However, it faces significant challenges in accurately capturing thin interfaces and resolving sharp gradients, which can affect the fidelity of the simulation, particularly in spontaneous imbibition processes (Carciofi et al., 2011). Celebrated for its versatility and accuracy in capturing fluid interfaces and phase distributions, the VOF method faces challenges in resolving thin interfaces and accurately capturing sharp gradients, which can affect simulation fidelity.

In the context of simulating spontaneous imbibition, these methods are evaluated for their effectiveness in modeling the capillary-driven displacement processes (Wang et al., 2023a; Mahmood et al., 2024). The LBM, with its ability to handle complex pore geometries and interface dynamics, is highly suitable for simulating spontaneous imbibition, though it may require stability enhancements for high capillary numbers. The level set and phase field methods, while computationally intensive, provide interface tracking capabilities essential for accurate imbibition modeling. The VOF method, though versatile, may face challenges in accurately capturing the thin fluid interfaces characteristic of spontaneous imbibition processes (Liu et al., 2022; Zhou et al., 2024).

In multi-field simulations at the pore scale, coupling different physical or chemical fields-such as fluid flow, heat conduction, stress changes, and chemical reactions-is crucial. This coupling is typically achieved through the simultaneous resolution of governing equations for each field, integrating coupling terms and establishing appropriate boundary conditions to reflect their interdependencies. The LBM has made significant progress in handling multi-field coupling processes, such as coupling fluid flow with heat transfer or chemical reactions, due to its flexibility in managing various transport phenomena. For instance, LBM has been successfully applied to simulate the simultaneous transport of heat and mass in porous media, as well as reactive transport processes involved in geologic carbon sequestration (Chen et al., 2022). To simulate multiphase flow in porous media, fluid-fluid and fluid-solid interactions must be incorporated. There are various approaches to introducing interaction forces, resulting in different multiphase LB models: the color-gradient model, pseudopotential model, and free energy model, among others (Liu et al., 2016). For solute transport problems, an additional distribution function is required to capture the mass transport process. When dealing with mass transport between different constituents, suitable interfacial conjugate conditions must be developed to manage concentration and flux jumps at interfaces. In some scenarios, solid surfaces may react with chemical solutions, necessitating reaction boundary conditions. Recently, various single- or multi-phase reactive transport models have been developed to describe physicochemical processes during geological carbon sequestration (Wang et al., 2023b). The LBM is also widely used to simulate heat transfer processes across

different constituents in porous media. Under unsteady-state conditions, special attention is required for conjugate heat transfer between different constituents. These physical and chemical processes can be efficiently resolved within the LBM framework, which is particularly advantageous for handling complex boundaries, making it an ideal tool for analyzing multi-field coupling multiphase flow problems in porous media (Qin et al., 2019).

For multiphase flow in deformable porous media, or fluid-solid coupling processes, different models are needed to describe multiphase flow and solid deformation. One approach uses LBM to simulate multiphase flow and the discrete element method (DEM) to describe solid deformation. Compared to single-phase fluid-solid coupling problems, the challenges lie in managing multiphase-fluid-solid interaction forces in both LBM and DEM, as well as the refilling process when a solid node becomes a pore node due to solid deformation. Fei et al. (2023) developed a coupling algorithm between multiphase LBM and DEM to analyze the droplet impact process on deformable sands, as shown in Fig. 1(c). Another approach is the Darcy-Brinkman-Biot coupling method, which uses a Navier-Stokes-like equation to simulate flow in fractures, the Darcy equation for flow in the matrix, and mass and momentum conservation equations for rock deformation. Liu et al. (2024) applied this method to analyze fracture propagation in deep shale induced by CO_2 injection at the pore level.

3. Darcy-scale numerical simulation methods

In engineering applications, accurately simulating fluid dynamics at the pore scale is often computationally infeasible due to the immense number of pores, particularly across larger domains. As a result, macroscopic simulation methods are predominantly employed, which utilize phenomenological approaches based on statistical parameters such as porosity and permeability to effectively model microscale processes. Based on Darcy's Law, these macroscopic methods assume the porous media to be continuous, simplifying the analysis of fluid flow within porous media and providing an efficient means to address large-scale seepage problems. Therefore, this macroscopic scale is also referred to as the Darcy scale.

Darcy-scale THMC coupling theory encompasses a diverse range of disciplines, including seepage mechanics, rock mechanics, heat transfer, chemistry, and computational mathematics. Within this framework, fluid flow, heat transfer, and chemical reactions are treated as fluid mechanics problems, while the deformation of the rock matrix is addressed as a solid mechanics problem (Liu et al., 2023). Due to the distinct nature of these phenomena, different numerical methods are employed for fluid and solid systems. The Finite Volume Method is commonly used for fluids, and the Finite Element Method is used for solids. Occasionally, a unified Finite Element Method is applied to both systems.

Fig. 2 illustrates the dissolution patterns obtained from solving a THC coupling model using the Finite Volume Method during carbonate rock acidizing, compared with core acidizing experiments. These comparisons demonstrate the Finite Volume Method's effectiveness in capturing dissolution processes under varying injection rates. However, the Finite Volume Method often faces challenges in mesh compatibility when coupling fluid and solid simulations. In contrast, the unified Finite Element Method can suffer from non-conservation issues, leading to convergence problems and non-physical results. To address these challenges, finite element methods that ensure local conservation in fluid systems are essential.

In addressing the complexities of coupled fluid and solid system interactions, solutions can be categorized into fully coupled and decoupled approaches. Fully coupled solutions employ a fully implicit scheme to discretize all equations simultaneously, employing iterative algorithms, typically the Newton-Raphson method, to solve the assembled nonlinear equations at each timestep. Although these methods are demonstrated to be unconditionally stable for linear systems, their stability in nonlinear scenarios remains to be conclusively proven (Heil, 2004). Additionally, the fully implicit scheme generates large equation sets, significantly increasing the computational load for each solution cycle (Lowrie, 2004). This approach also requires the development of new solver programs, making it difficult to integrate with existing simulators.

In contrast, decoupled solutions are often preferred for their simplicity, typically addressing mechanical subproblems first. Notable methods include the drained and undrained splits (Kim et al., 2011a). The drained method, which freezes the pressure during the mechanical step, is known for its conditional stability. Conversely, the undrained method preserves the fluid mass content during mechanical problem-solving and is recognized for respecting the dissipative structure of the continuum problem, proving more reliable in nonlinear applications. However, other sequential approaches have also been explored in reservoir engineering, where the flow problem is addressed prior to the mechanical problem. This introduces methods such as the fixed-strain split, where the total strain rate is maintained constant during the flow solution. Although conceptually simple, the fixed-strain split is only conditionally stable. Alternatively, the fixed-stress split, which has been shown to exhibit stability characteristics similar to the undrained split, offers different convergence and accuracy outcomes. Specifically, the fixed-stress split remains convergent for incompressible systems, unlike the undrained split. Additionally, the fixed-stress split generally requires only two iterations to achieve convergence in linear problems, regardless of the coupling strength and pressure diffusivity, making it preferable in scenarios where the undrained split's accuracy diminishes due to high pressure diffusivity and strong coupling. The fixed-stress split tends to result in less stiff problems, contrasting with the stiffer challenges posed by the undrained split, which necessitates more robust linear solvers. Hence, the fixed-stress split is often recommended for its efficiency and effectiveness in managing these dynamics (Kim et al., 2011b).

Furthermore, the modeling of underground reservoirs presents unique challenges due to their inherent heterogeneity and multiscale characteristics. These reservoirs feature a diverse range of pore space morphologies and fracture distributions, from nanometer-scale pore throats to kilometer-

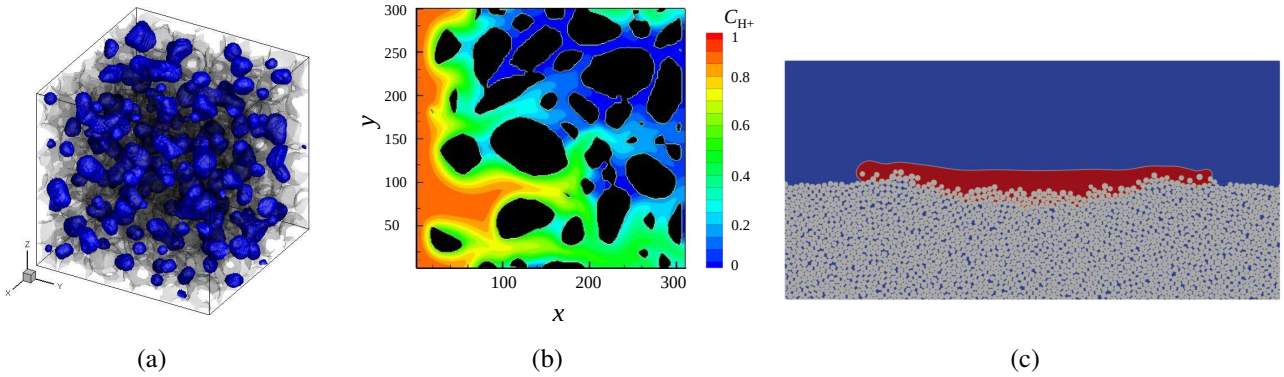

Fig. 1. Typical LBM simulation results of (a) two-phase flow, (b) single-phase reactive transport process and (c) droplet impacting on deformable sands (coupling with DEM).

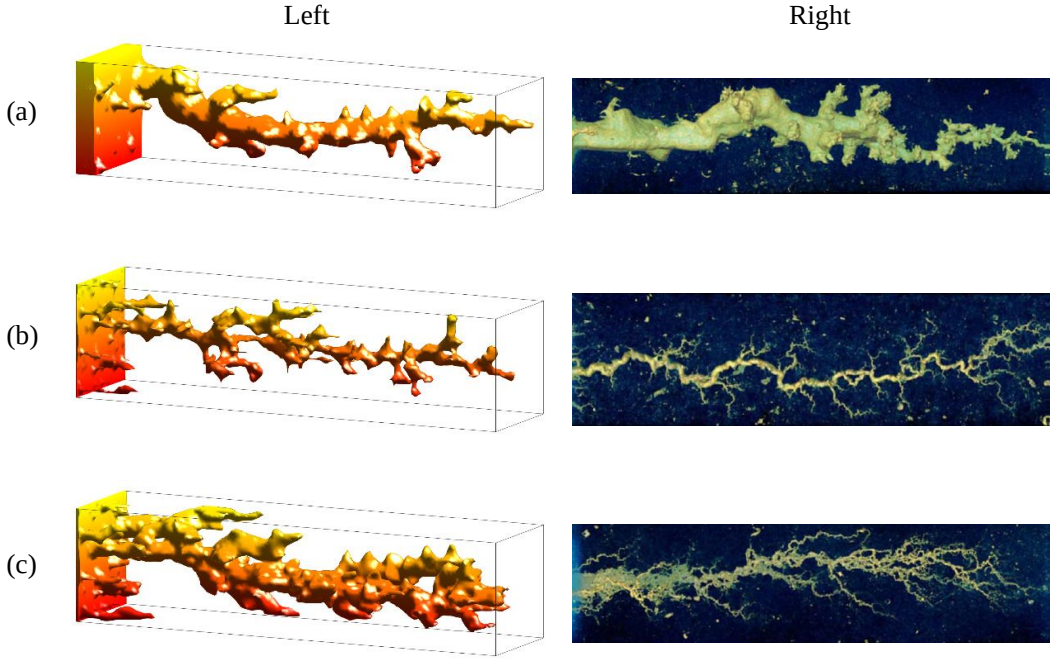

Fig. 2. The simulated dissolution patterns (left) and the experimental observations (right) for (a) low injection rate, (b) medium injection rate, and (c) high injection rate. (Liu et al., 2019).

scale fault zones, encompassing both natural and artificially induced fractures (e.g., from hydraulic fracking). This complexity necessitates advanced modeling techniques capable of capturing various flow mechanisms that range from film flow in small pores to turbulent flow in larger fractures and vugs (Yan et al., 2016; Zhang et al., 2016; Yao et al., 2018). Various models have been proposed to describe these complex systems, including equivalent continuous medium models, dual-porosity models, stochastic continuum models, discrete fracture network models, and hybrid models. Currently, two major challenges exist in studying fluid flow within fractured and vuggy reservoirs: firstly, the mathematical description of two-phase or multiphase flow involving coupled seepage and free flow is complex; secondly, the rules governing fluid exchange between seepage and free flow regions remain unclear. Accurately characterizing the distributions of fractures and vugs, including parameters such as fracture density, spatial location, permeability within fractures, fracture length and orientation, and the sizes and shapes of vugs, remains a formidable challenge. Despite significant advancements in describing the heterogeneity of fractured reservoirs, many issues continue to hinder their practical engineering applications, underscoring the ongoing need for research and development in simulation methodologies.

4. The role of machine learning in numerical simulation

Machine learning algorithms are increasingly utilized in numerical simulations for multiphase, multifield coupled flow problems, offering promising alternatives and enhancements

to traditional methods. These applications can be broadly classified into three categories based on their approach and integration with physical processes.

The first category involves the use of pretrained artificial neural networks to replace computationally intensive parts of numerical algorithms. These neural networks are typically trained using labeled data; hence this approach is referred to as a data-driven method. For instance, Chan and Elsheikh (2018) employed pretrained neural networks to update multiscale basis functions following changes in relative permeability, thereby improving the efficiency of solving multiphase flow problems using multiscale finite element methods. Additionally, Li et al. (2019) demonstrated that phase equilibrium calculations in multi-component numerical simulations accounted for over 50% of total computational time. They proposed a method using deep neural networks to replace these phase equilibrium calculations, enhancing simulation efficiency and overall stability. This stability ensures consistent outputs with given inputs, preventing iterative collapses often caused by poor initial value selection in traditional methods.

The second category integrates physical meaning into neural networks, employing them directly to solve partial differential equations without labeled data. This approach includes the development of Physics-Informed Neural Networks (PINNs) (Li et al., 2021), typically subdivided into two types: Neural-FEM (Finite Element Method) and Neural Operators (Wen et al., 2023). These methods embed physical laws directly into the network, guiding neural networks in solving the residual loss of discretized physical differential equations. Despite their advantage of incorporating physical information, these methods face significant challenges. They exhibit poor extrapolation capabilities; changes in initial and boundary conditions for the same type of partial differential equations often necessitate network retraining, hampering their generalization capability. Additionally, the training process can be challenging due to the sensitivity of physical loss residuals and the abundance of hyperparameters, frequently leading to non-convergence and oscillations during model fine-tuning and training.

Neural Operator networks aim to learn a class of equations to enable rapid solution adjustments in initial and boundary conditions without retraining. Fig. 3 illustrates the typical Fourier neural operator structure for solving two-phase flow problems. While this model type expands the generalization capabilities of PINNs, it still requires labeled data for training due to the function-to-function mapping it performs. This requirement complicates the training process, as purely physical unlabeled equations may not provide sufficient guidance alone. Additionally, some models within this paradigm, like the Fourier Neural Operator, encounter difficulties in gradient computation since they transform data using Fourier transforms, which are not inherently compatible with the automatic differentiation used in many deep learning frameworks.

Despite the rapid advancement of PINNs in recent years, developing network structures that can operate without labeled data in complex scenarios remains a major research focus. In practical applications, such as numerical simulations of multiphase flows in underground reservoirs, capturing the strong nonlinearities inherent in high-dimensional parameter fields poses significant challenges. Therefore, further efforts and continuous research are essential to extend the application of PINNs in subsurface numerical simulation domains.

The third category, known as physics-constrained deep learning approaches, combines the empirical strengths of data-driven models with the rigor of physics-based models, enhancing both prediction accuracy and generalizability. This approach merges the empirical strength of data-driven models with the rigor of physics-based simulations, ensuring predictions fit the data while complying with fundamental physical principles. By incorporating constraints directly derived from physical equations, such as conservation laws and boundary conditions, into the training process, these models achieve higher fidelity in simulating physical phenomena. This methodology is particularly advantageous in situations where traditional data-driven approaches might falter due to insufficient or noisy data. For example, in simulating fluid dynamics within complex geological formations, physics-constrained models can predict fluid behavior more reliably by adhering to the principles of fluid mechanics enforced through the model architecture and loss functions.

These enhanced models, such as the Theory-guided Convolutional Neural Network (TgCNN), as shown in Fig. 4, go beyond conventional learning paradigms by embedding scientific knowledge into the learning algorithms, allowing them to perform robustly under a wide range of conditions. This is critical for applications like reservoir simulation and climate modeling, where underlying processes are highly complex and multifaceted. The successful application of these advanced models opens new avenues for research and development in numerical simulation, promising significant improvements in how engineers and scientists predict and manage natural and engineered systems.

Overall, integrating machine learning with traditional numerical methods reshapes the landscape of numerical simulation, making it possible to tackle previously intractable problems with improved efficiency, accuracy, and robustness.

5. Challenges and perspectives

Despite significant advancements in simulation technologies for THMC coupled processes in porous media, the understanding of multiphase transport processes within underground reservoirs remains limited.

At the pore scale, challenges in numerical simulation stem from the complex nature of fluid-solid interactions, capillary forces, and chemical reactions. The property variation across different constituents increases the complexity of modeling efforts. In addition, achieving reliable results requires exceedingly fine computational grids, which leads to elevated computational costs, especially for 3D conditions. Current research is focused on advancing simulation techniques such as lattice Boltzmann, volume-of-fluid methods, phase-field methods, which may enhance the handling of interfaces in multiphase flows. The multiphase fluid-solid coupling simulation method requires further study. Furthermore, machine learning is being investigated as a tool to predict behaviors based on data from

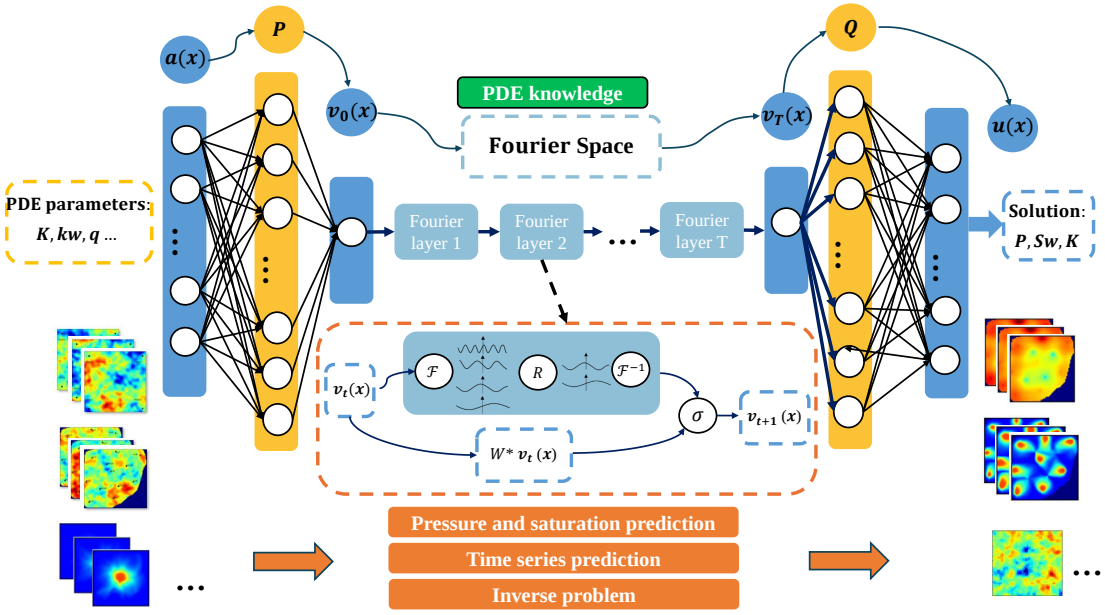

Fig. 3. Fourier neural operator structure for solving two-phase flow problem (Zhang et al., 2022).

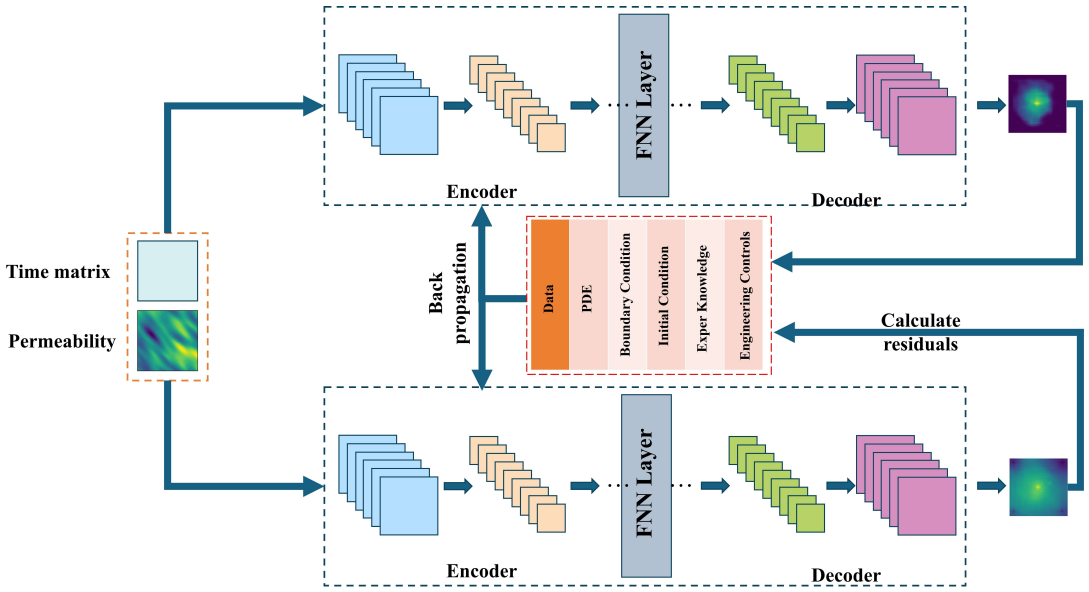

Fig. 4. The network structure of TgCNN (Wang et al., 2022).

numerical simulations and experiments, potentially decreasing computational demands while preserving accuracy.

At the Darcy scale, the primary challenges encompass managing multiscale complexities, intricate boundary conditions, and substantial computational resource requirements. Nonetheless, prospects are encouraging due to advancements in numerical algorithms and the increasing availability of high-performance computing. The integration of machine learning with traditional simulation methods holds promise for substantially improving simulation capabilities. Additionally, innovations such as augmented and virtual reality for visualization could significantly refine the accuracy, efficiency, and applicability of simulations, thereby expanding the frontiers of subsurface flow simulation.

In summary, pore scale and Darcy scale simulations are at a critical point where integrating advanced computational methods, high-performance computing, and machine learning could dramatically improve their accuracy, efficiency, and practical applicability. Continued development in these areas is expected to significantly enhance the capability to understand and manage complex geological processes, with important implications for energy production, environmental protection, and natural resource management.

Acknowledgements

The authors gratefully acknowledge the support from the National Natural Science Foundation of China (Nos.

52374036, 52204032), Natural Science Foundation of Shandong Province (No. ZR2023ME207), Science Foundation of China University of Petroleum, Beijing (No. 2462023QNXZ001), National Key Laboratory of Petroleum Resources and Engineering, China University of Petroleum (Beijing), Science & Technology Department of Sichuan Province (No. 24NSFSC5757).

Conflict of interest

The authors declare no competing interest.

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