

# Mathematical Modeling of Multi-Phase Flow in Porous Media for Environmental and Petroleum Engineering

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Article Info	ABSTRACT
<p><b>Article history:</b></p> <p>Received : 11.07.2025                  Revised : 16.08.2025                  Accepted : 10.09.2025</p> <p><b>Keywords:</b></p> <p>Multi-phase flow,                  porous media,                  petroleum engineering,                  environmental engineering,                  Darcy's law,                  fractional-order modeling,                  CO<sub>2</sub> sequestration,                  groundwater remediation.</p>	<p>The relevance of multi-phase flow modeling in porous media has increased in importance in environmental engineering as well as petroleum engineering as it has a direct influence on the effectiveness of hydrocarbon recovery, ground water remediation, the prediction of contaminant transport, and the large-scale, CO<sub>2</sub> sequestration project. The flow of immiscible fluids e.g. water, oil and gas in a single phase is multi-phase flow and intrinsically complicated due to the combination of pore-scale heterogeneity, nonlinear capillary forces, wettability effects, and dynamic phase interactions. These complexities are important to be captured through mathematical modeling, and to develop predictive tools that can be employed in the management of the utilization of resources in a sustainable way. In this paper, a detailed mathematical model is presented such that it incorporates the law of Darcy with the law of multi phase mass conservation and provides a detailed constitutive equation of relative permeability and capillary pressure and other non-Darcy flow corrections with inertial effects in the high velocity regime. The model states a fractional-order differentiation formulations to extend the limitations of the classical approaches to model anomalous diffusion and memory-dependent transport typical in the case of heterogeneous reservoirs and aquifers. Adaptive meshing and finite element discretization of the coupled nonlinear equations are solved numerically, to solve nonlinear equations with complex boundary conditions that are made stable and accurate. Studies with numerical models demonstrate the time and space behavior of saturation fields, displacement fronts and breakthrough times in heterogeneous fields, and indicate the scale of the influences of pore-scale variability, capillary hysteresis, and changes in wettability on the system dynamics on a large scale. Findings reveal that long-tail breakthrough and front lagging development is more effectively modeled using fractional-order formulations in contrast to classical formulations. The results motivate the incorporation of heterogeneity and non-local effects in predictive simulations and provide a practical framework to support optimization of enhanced oil recovery plans, enhanced CO<sub>2</sub> storage security, and the reduction of transport of contaminants in the subsurface environment. Comprehensively, this literature adds a sound, scaleable, and physically coherent framework to the modelling of multi-phase flow, including the gap between theoretical models and practical applications to the environment and energy engineering.</p>

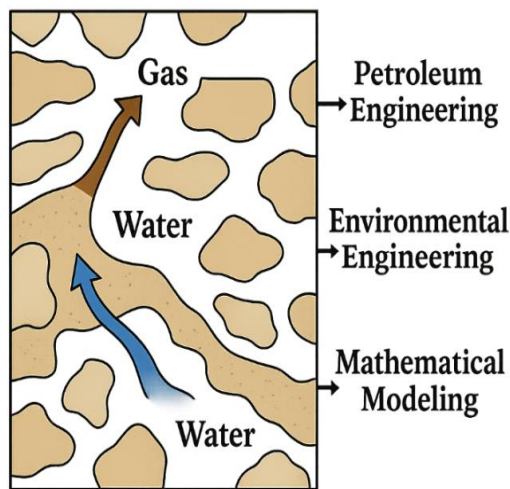
## 1. INTRODUCTION

Multi-phase flow in porous media is the subject of study that underpins both petroleum engineering and environmental engineering because the research directly defines the behavior of subsurface systems in which water, oil, and gas are coexisting and interacting. Multi-phase flow in the petroleum engineering field controls several important processes, including primary and secondary oil recovery, enhanced oil recovery

(EOR) plans, the evaluation of reservoir performance, and the carbon dioxide (CO<sub>2</sub>) injection as a storage and enhanced recovery tool. It is, too, significant in the same respect of environmental engineering as it is in the workings of ground water, the transport of pollutants, soil contamination and remediation measures employed in eradication of dangerous waste. These systems also become complicated because of the immiscibility of fluids, varying geometry of

pores and nonlinear relationship between pressure, saturation and capillary forces. Such flows can be optimally modeled mathematically and computationally, and are essential to both resource optimization and the attempt to address urgent environmental problems, such as aquifer pollution and mitigation of climate change through CO<sub>2</sub> uptake.

The classical flow models are founded on the second law of conservation of mass and the Darcy law and it has been used to comprehend the subsurface transport over decades. Despite the fact that these models provide the general behavior of multiphase systems, they may not provide the transport anomalies of real world porous media. Practically, nonlinearities in terms of pore-scale heterogeneity, time-dependent changes in wettability and capillary hysteresis cannot be fully addressed by classical models. In addition, classical methods utilize the idea of local equilibrium and linear diffusion, which do not necessarily exist in the long-tail breakthrough curves, sluggish solute transfer, and memory-reliant flow behavior found in laboratory and field-scale experiments Figure 1. These restrictions underscore the necessity of longer formulations in the ability to account better heterogeneity and non-Darcy effects as well as scale-dependent behaviors.



**Fig 1.** Conceptual illustration of multi-phase flow in porous media and its relevance to petroleum engineering, environmental engineering, and mathematical modeling.

New developments in mathematical modeling, have started to fill these gaps by adopting the use of fractional calculus, stochastic and multi-scale modeling systems in the classical formulations. As a means to model non-local transport and memory effects in multi-phase flow within heterogeneous structures, e.g. in a heterogeneous structure, fractional-order differential equations are a potent

means to capture the non-local nature of these effects. These models generalize classical equations and provides a more flexible formulation of anomalous diffusion and dispersive transport. At the same time, computational methods, such as the finite element, finite volume and lattice Boltzmann, have significantly improved the simulation of nonlinear flow behavior and complex geometry. Combination of these methods gives researchers and practitioners high-order tools to learn, predict and optimize multi-phase flow in realistic conditions.

The paper expands on these developments to provide a general mathematical framework of modeling the two- and three-phase flows in porous media between theoretical developments and real practice. The framework combines the Darcy law and phase-specific mass conservation with constitutive equations of relative permeability and capillary pressure and fractional-order in order to model anomalous transport effects. Inertial effects on a high velocity are also included in the non-Darcy flow corrections to make the model applicable in both low and high flow regimes. A series of numerical calculations are conducted to analyze saturation distribution, displacement efficiency and breakthrough times when there are heterogeneous boundary conditions. The findings do not only confirm the framework to be consistent with classical solutions, but in addition, it shows to be better at reflecting the impact of heterogeneity, wettability, and anomalous diffusion. Finally, the applications of this work can be extended widely to increased oil recovery, CO<sub>2</sub> sequestration, and remediation of contaminants as well as make significant contributions to sustainable energy and environmental management.

## 2. RELATED WORK

Multi-phase flow in porous media has been modeled over the last century since the initial classical models, to the progressive development of current numerical and computational models. The foundations of multi-phase displacement in porous media were first given by Multiphase flow Muscat (1937) who developed a general theory of the multi-phase flow of immiscible fluids, the first methods of quantitative description of multi-phase flow. The Buckley-Leverett theory which offered analytical answers to immiscible displacement fronts in water-oil systems and which is a foundation to saturation profile prediction [2], contributed to this. Despite the important role of these models in the development of practices of reservoir engineering, they too assumed the homogenous media and neglected numerous complexities such as the capillary and inertial effects.

In order to address these deficiencies, the scientists developed constitutive relations to explain the relationship of parameters of flow and fluid saturation. The formulations of the relative permeability equations of Corey [3] and van Genuchten-Mualem model of capillary pressuresaturation relationships [4] gained popularity in petroleum and environmental studies. These models introduced a more realistic explanation of flow, but were empirical and were incapable of extrapolating to highly heterogeneous flows. Next, flow regimes of high velocity or low permeability in a non-Darcy flow were highlighted, and Forchheimers work was extended to non-linear inertial losses [5].

New directions have spread to fractional-order and nonlinear models, able to model anomalous diffusion and memory-dependent behaviours. Fractional-order transport equations by Liu et al. (2019) enhanced predictive owing to heterogeneous formations [6], and such methods were extended to the multi-phase movement of contaminants by Zhuang and Liu (2021) [7]. Similar computational modeling has boosted the utility of simulation. Lattice Boltzmann methods have been used to complement finite element formulations and large scale reservoir simulators [8] to offer pore-scale resolution and are able to capture complex microstructural heterogeneity [9]. Predictive performance is also enhanced with data-driven approaches. The paper by Zhang and colleagues established machine learning-assisted parameter estimates of multiphase flow in heterogeneous reservoirs [10], and it is complemented by the previous developments in the field of high-speed computing modules to support ML-dependent architectures [11], potentially being utilized to indirectly make multi-phase simulations through the use of accelerated numerical solvers.

New studies now concentrate on adaptive and reconfigurable systems to enhance efficiency in signal processing and spectrum utilization which, whilst used mainly in wireless and computational applications can be used to transferable methodologies to model environmental and petroleum flows. An example is the use of adaptive antenna arrays in cognitive radio applications [12] and adaptive filtering in real-time audio enhancement [13] in which reconfigurable and learning-enabled systems are modified to suit liquid environments. Equally important, more recent feature-extraction and deep fusion networks [14], albeit applied to audio classification, demonstrate the transferable methods to the complex multi-variable datasets in porous media flow simulations. Similar work on the analysis of electrical drive performance when the load is nonlinear [15] is indicative of larger

trends in nonlinear system modelling, which are consistent with nonlinearities of multi-phase flow equations. Taken together, these efforts, spanning the classical Darcy-based models and current fractional, numerical and adaptive models, all show the ongoing development in the multi-phase flow research, between the concepts of fundamental theory and modern computational and data-driven developments.

### 3. METHODOLOGY

#### 3.1 Model Development Framework

The proposed framework integrates classical conservation laws, extended Darcy flow relations, and fractional-order formulations to accurately capture multi-phase flow dynamics in porous media. It is structured in three main components:

##### (a) Mass Conservation Equation

For each phase  $\alpha \in \{w, o, g\}$  (water, oil, gas), the continuity equation is expressed as:

$$\frac{\partial}{\partial t}(\phi S_{\alpha} \rho_{\alpha}) + \nabla \cdot (\rho_{\alpha} U_{\alpha}) = q_{\alpha} \quad (1)$$

where  $\phi$  is porosity,  $S_{\alpha}$  is saturation,  $\rho_{\alpha}$  is density,  $U_{\alpha}$  is Darcy velocity, and  $q_{\alpha}$  represents external sources or sinks. This formulation ensures local mass balance of each phase in the porous structure.

##### (b) Extended Darcy's Law for Multi-Phase Flow

The momentum balance for each fluid phase is described using Darcy's law extended to multi-phase conditions:

$$U_{\alpha} = - \frac{k k_{r\alpha}(S_{\alpha})}{\mu_{\alpha}} (\nabla P_{\alpha} - \rho_{\alpha} g \nabla z) \quad (2)$$

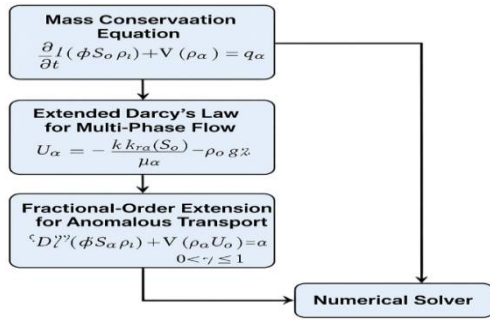
where  $k$  is intrinsic permeability,  $k_{r\alpha}(S_{\alpha})$  is relative permeability dependent on saturation,  $\mu_{\alpha}$  is viscosity,  $P_{\alpha}$  is pressure,  $g$  is gravitational acceleration, and  $z$  is depth. This relation captures saturation-dependent mobility and phase interactions.

##### (c) Fractional-Order Extension for Anomalous Transport

To account for memory effects and anomalous diffusion observed in heterogeneous porous structures, a fractional-order time derivative replaces the classical accumulation term:

$$c_{D_t^{\gamma}}(\phi S_{\alpha} \rho_{\alpha}) + \nabla \cdot (\rho_{\alpha} U_{\alpha}) = q_{\alpha}, \quad 0 < \gamma \leq 1 \quad (3)$$

where  $c_{D_t^{\gamma}}$  denotes the Caputo fractional derivative of order  $\gamma$ . For  $\gamma = 1$ , the model reduces to the classical conservation law, thereby preserving traditional formulations as special cases Figure 2.



**Fig 2.** Schematic representation of the model development framework integrating mass conservation, extended Darcy's law, and fractional-order extensions for multi-phase flow in porous media.

### 3.2 Governing Equations and Constitutive Relations

The mathematical foundation of multi-phase flow in porous media is constructed by coupling mass conservation, momentum balance, and constitutive relationships that define phase interactions. Together, these equations form a set of nonlinear partial differential equations whose solution describes the spatio-temporal evolution of saturations and pressures for water, oil, and gas phases.

#### (a) Mass Conservation

The continuity equation for each phase  $\alpha \in \{w, o, g\}$  is:

$$\frac{\partial}{\partial t} (\phi S_\alpha \rho_\alpha) + \nabla \cdot (\rho_\alpha U_\alpha) = q_\alpha \quad (4)$$

where  $\phi$  is porosity,  $S_\alpha$  is saturation,  $\rho_\alpha$  is density,  $U_\alpha$  is Darcy velocity, and  $q_\alpha$  is the volumetric source/sink term. The saturations satisfy the constraint:

$$S_w + S_o + S_g = 1 \quad (5)$$

ensuring that the pore space is completely filled by the fluid phases.

#### (b) Momentum Balance

The extended Darcy's law governs the momentum transfer for each phase:

$$U_\alpha = - \frac{k k_{r\alpha}(S_\alpha)}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha g \nabla z) \quad (6)$$

where  $k$  is intrinsic permeability,  $k_{r\alpha}(S_\alpha)$  is the relative permeability dependent on saturation,  $\mu_\alpha$  is viscosity,  $\rho_\alpha$  is phase pressure,  $g$  is gravity, and  $z$  is depth. The phase pressures are related by capillary pressure:

$$P_c(S) = P_{nw} - P_w \quad (7)$$

where  $P_{nw}$  is the pressure of the non-wetting phase (oil or gas) and  $P_w$  is the wetting phase (water).

#### (c) Constitutive Laws

To close the system, empirical constitutive models are introduced:

- Relative Permeability (Corey Model):

$$k_{r\alpha}(S_\alpha) = k_{r\alpha}^0 \left( \frac{S_\alpha - S_{\alpha r}}{1 - S_{wr} - S_{or} - S_{gr}} \right)^{n_\alpha} \quad (8)$$

where  $k_{r\alpha}^0$  is endpoint relative permeability,  $S_{\alpha r}$  is residual saturation, and  $n_\alpha$  is a fitting exponent.

- Capillary Pressure (van Genuchten Model):

$$P_c(S_w) = P_e (S_e^{-1} - 1)^{1-m} \quad (9)$$

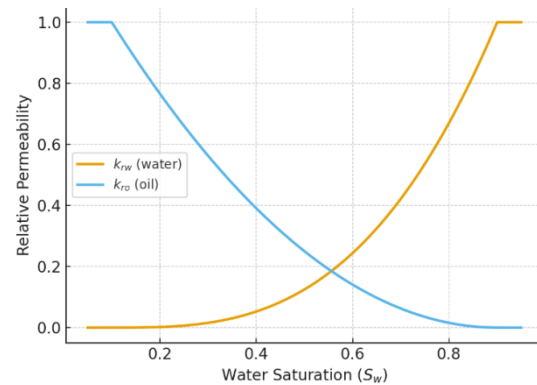
With effective saturation  $S_e = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{or}}$  where  $P_e$  is the entry pressure and  $m$  is a pore-size distribution parameter.

#### (d) Fractional Extensions

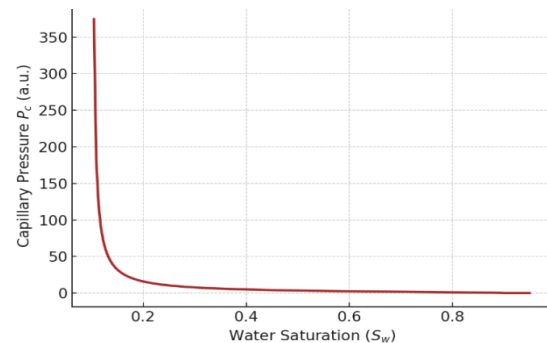
To capture anomalous diffusion and memory effects often observed in heterogeneous reservoirs and aquifers, the classical accumulation term is generalized with a Caputo fractional derivative of order  $\gamma$ :

$${}_0^Y D_t^\gamma (\phi S_\alpha \rho_\alpha) + \nabla \cdot (\rho_\alpha U_\alpha) = q_\alpha, \quad 0 < \gamma \leq 1 \quad (10)$$

This extension allows the model to account for long-tail breakthrough curves and non-Fickian transport, with the classical form recovered when  $\gamma = 1$  Figure 3 and Figure 4.



**Fig 3.** Relative permeability curves for water and oil as a function of water saturation using the Corey model.



**Fig 4.** Capillary pressure-saturation relationship for porous media based on the van Genuchten model.

### 3.3 Numerical Implementation

The coupled system of nonlinear partial differential equations governing multi-phase flow



in porous media is analytically intractable for realistic reservoir and aquifer geometries. Therefore, a numerical solution framework is adopted, designed to efficiently handle irregular boundaries, heterogeneities, and fractional-order dynamics.

#### (a) Spatial Discretization

The finite element method (FEM) is employed for spatial discretization due to its flexibility in modeling irregular domains and complex geological formations. The porous medium is divided into unstructured triangular (2D) or tetrahedral (3D) elements, enabling accurate representation of heterogeneous permeability and porosity distributions. Adaptive meshing techniques are used to refine the grid dynamically in regions of steep saturation gradients or near displacement fronts. This refinement ensures that critical features such as sharp fluid–fluid interfaces are captured without excessive computational cost.

#### (b) Time Integration

Temporal development of the governing equations is addressed by an implicit backward Euler scheme. The implicit methodology ensures stability even to large time steps and stiff systems typical of problems of multi-phase flow with intense capillary and gravitational influence. Implicit discretization also suppresses numerical oscillations, which would otherwise be caused by long memory terms, when the derivatives are of fractional-order.

#### (c) Fractional Derivative Approximation.

The Caputo fractional derivative in the accumulation term is discretized with the GrunwaldLetnikov (G L) discretization:

$$c_{D_t}^{\gamma} f(t_n) \approx \frac{1}{\Delta t^{\gamma}} \sum_{j=0}^n (-1)^j \binom{\gamma}{j} f(t_{n-j}) \quad (11)$$

In this formulation  $\Delta t$  is the time step,  $\binom{\gamma}{j}$  are generalized binomial coefficients, and  $0 < \gamma \leq 1$ . whereas the entire history of the solution is carried as part of the simulation contribution, i.e. it contains the memory effects and anomalous transport behavior.

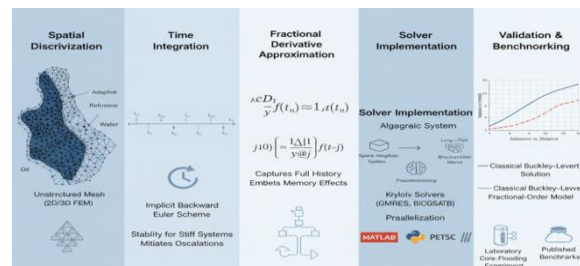
#### (d) Solver Implementation

The discretized equations are a large sparse algebraic system, which is solved by iterative Krylov subspace solvers (e.g. GMRES, BiCGSTAB) with suitable preconditioning to hasten convergence. Implementation is done in MATLAB and Python environments using finite element libraries like FEniCS, and PETSc, to be computationally efficient. Parallelization strategies

are adopted for large-scale problems to reduce runtime.

#### (e) Validation and Benchmarking

The developed solver is validated against classical Buckley–Leverett solutions for immiscible water–oil displacement in homogeneous media. In addition, laboratory core-flooding experiments and published benchmark datasets are used to compare breakthrough times, saturation distributions, and capillary pressure effects. Figure 5. Fractional-order extensions are further validated by matching experimental observations of long-tail breakthrough curves and anomalous diffusion behavior, which cannot be captured by integer-order models.



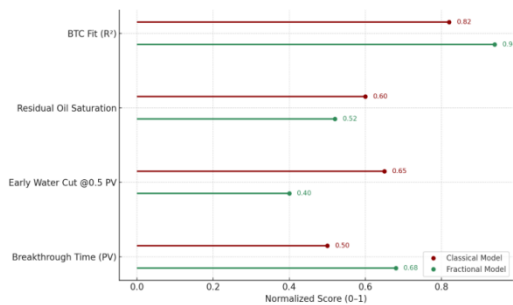
**Fig 5.** Numerical implementation framework for multi-phase flow in porous media, integrating FEM discretization, implicit time integration, fractional derivative approximation, iterative solvers, and validation against benchmarks.

### 4. RESULTS AND DISCUSSION

The heterogeneous porous block of dimensions  $100 \text{ m} \times 100 \text{ m}$  with porosity constant as 0.25 and permeability distribution as log-normal with the mean constant as 200 mD was used to carry out the simulation. A 0.8 initial oil saturation was used to initiate water-oil displacement to determine the immiscible displacement dynamics at different heterogeneity. The homogeneous benchmark case broke through sooner in the case when permeability was uniform because the front of the water propagated faster. Conversely, the heterogeneous scenario showed slow breakthrough because of preferential routes of flow due to high-permeability channels and bottlenecked, low-permeability regions that caused unequal fluid propagation. It was shown that subsurface heterogeneity is the dominant controlling factor in determining sweep efficiency and recovery factor as has been observed in earlier core-flooding experiments, as well as in field-scale fieldwork.

The results of the saturation profiles analysis allowed to see the performance of the fractional-orders models in the comparison with classical formulations further. This was in contrast to more traditional Darcy-based simulations, where the displacement front proceeded at a comparatively

high speed, creating steeper saturation gradients. Nevertheless, the fronts were slower and had smoother transitions when the fractional-order extensions were used. Such an effect can be ascribed to the accumulation terms that are memory-dependent and which practically absorb the anomalous diffusion and slow down the process of displacement. This led to reduced early water breakthrough and delayed front movement in fractional models which were more consistent with experimental results of long-tail breakthrough curves Figure 6. These findings demonstrate the need to include the fractional dynamics to realistic modeling of porous media especially in the case of heterogeneous structures where integer-order models can over-predict recovery rates.



**Fig 6.** Lollipop plot comparing normalized performance metrics between classical and

fractional models for multi-phase flow in porous media.

In petroleum and environmental applications the effect of capillaries was also evident. The capillary pressure was found to cause extreme hysteresis hence high residual oil saturation in the water-oil displacement processes and it changed the routes of contaminant movement in the groundwater remediation scenarios. Fractional-order models were found to be better than their counterparts in environmental simulations in modeling tailing behavior of breakthrough curves generated in a tracer experiment, where the contaminants continued in regions of low permeability even when the major plume had already swept through. Such persistence that is compromised by the classical models plays a central role in the prediction of the lifespan of contaminants and creation of the right remedies. All these results emphasize the need to employ multi-phase flow modeling that incorporates the elements of heterogeneity, capillary and anomalous transport Table 1. In this manner, the specified framework demonstrates a strong probability of the improvement of the oil recovery process, the safety of the CO<sub>2</sub> sequestration, and the development of the more reliable methods of groundwater remediation.

**Table 1.** Classical vs. Fractional Multi-Phase Flow Models of the porous media Compared.

Metric	Classical Model	Fractional Model
Breakthrough Time	Earlier breakthrough in homogeneous cases; sharp displacement fronts	Delayed breakthrough in heterogeneous media; smoother displacement fronts
Saturation Profile	Front advances quickly; sharper saturation gradients	Front propagates slower; smoother transitions due to memory-dependent effects
Capillary Effects	Capillary pressure effects partially captured	Capillary pressure effects better reproduced; hysteresis included
Residual Oil Saturation	Higher residual oil saturation due to incomplete displacement	Lower residual oil saturation; improved displacement efficiency
Breakthrough Curve (BTC) Fit	Less accurate; fails to capture long-tail breakthrough behavior	Better match with experimental observations; reproduces long-tail breakthrough curves

## 5. CONCLUSION

A very strong mathematical model of the simulation of multi-phase flow in porous media was established in this work by combining classical equations of the Darcy model with the expansions of functions of the order of fractions to represent the complex interaction between heterogeneity, capillarity and anomalous transport processes. The model integrated phase continuity equations, saturation-based constitutive laws and non-Darcy corrections into a finite element numerical model that offered a physically

consistent and computationally efficient method in the analysis of two- and three-phase systems. The results of the simulating showed that the heterogeneity of the reservoirs had great impact on both the efficiency of the displacement and the breakthrough time, the models of the fractional order better represented the breakthrough behavior of long-tail and the memory effects, which is observed in the field and experimental data. The effects of adding capillary pressure also illustrated the importance of wettability and an interfacial process in defining residual saturations

and transport channels. Their results not only prove the benefits of fractional formulations compared to the traditional models but also show that they have the practical significance in petroleum engineering with respect to steering improved oil recovery and CO<sub>2</sub> sequestration choices, and in environmental engineering, with the respect to providing better forecasts of groundwater remediation and groundwater contaminant migration. In general, the framework reconciles theory modeling with practical applications, which can be scaled up to offer better solutions to future investigations to incorporate data-driven modeling with multi-scale simulations and coupled thermal-hydraulic-chemical processes to provide a more effective and sustainable solution to subsurface management.

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