Advances in Geo-Energy Research

Vol. 21, No. 1, p. 98-100, 2026

Editorial

Artificial intelligence for multiscale subsurface flow in the energy transition

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Keywords:
Artificial intelligence
pore-scale imaging
digital rock physics
multiscale subsurface flow
geological carbon storage
underground hydrogen storage

Cited as:
Zhu, L., Cai, J., Blunt, M. J. Artificial intelligence for multiscale subsurface flow in the energy transition. Advances in Geo-Energy Research, 2026, 21(1): 98-100.
https://doi.org/10.46690/ager.2026.07.10

Abstract:
Artificial intelligence is changing how we observe and predict subsurface flow. Pore-scale research made this shift visible first: segmentation, generative reconstruction, super-resolution and rapid property prediction are making the analysis and physical interpretation of large datasets easier, faster and more accurate. In parallel, rapid predictions for CO_2 storage, underground hydrogen storage and hydrocarbon recovery continue to advance. However, understanding flow in the subsurface is inherently a multiscale process both in space – from micron-sized pores that control displacement processes to carbon dioxide storage sites extending over tens of kilometres – and time – from millisecond displacement to secure storage over millennia. To address this challenge with machine learning tools demands transferability, physical consistency and transparent provenance. In this editorial we explore the current state-of-the-art and provide a personal perspective for the future of artificial intelligence for flow in porous media for the energy transition.

1. Introduction

At the pore scale, interface position, fluid connectivity, trapping, wettability and displacement history shape how fluids move (Blunt, 2017; Wang et al., 2025). Two pore configurations with the same saturation can contain different connected pathways or trapped clusters and can develop differently when flow conditions change. Larger-scale prediction therefore depends on which of these pore-scale distinctions remain important after averaging. Artificial intelligence (AI) can accelerate recognition and prediction. It also brings model credibility to the centre of the science.

2. AI at the pore scale

Pore-scale imaging has provided extensive datasets for training and testing AI models: for instance, X-ray micro-tomography (micro-CT) can routinely generate 10-billion voxel three-dimensional (3D) images in a few seconds to hours, depending on the instrument, at a resolution of typically a few microns. AI has leveraged this information to generate artificial pore structures, including multiphase fluid distributions, to merge datasets at different resolutions to provide super-resolution images with a large field-of-view, and to aid image segmentation and analysis. The first application was the use of generative adversarial neural networks to generate 3D pore structures with representative morphology and permeability statistics (Mosser et al., 2017). For heterogeneous rocks, Cai and colleagues used a 3D generative adversarial network to reconstruct tight sandstone while preserving pore geometry, connectivity and the porosity distribution (Zhao et al., 2021). The result placed heterogeneity, and the topology that carries it, at the centre of evaluation. Pyramid architectures generate larger domains while retaining heterogeneous features across scales (Zhu et al., 2024). Diffusion models

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Yandy Scientific Press

2207-9963 © The Author(s) 2026.
Received June 15, 2026; revised June 29, 2026; accepted July 10, 2026; available online July 12, 2026.

extend the target, producing rock structure and multiphase configurations together (Zhu et al., 2025). Geometry, topology, transport statistics, diversity and usability in flow analysis decide whether these pore-scale models can be used to predict averaged flow properties.

The next application was phase segmentation – taking a raw image of X-ray attenuation and identifying the rock and fluids. Annotation-free supervoxel methods have been shown to preserve saturation, interfacial area, curvature and contact angle while resisting noise (Ye et al., 2025). Cross-scanner domain transfer carries trained models into new conditions (Tang et al., 2025), and super-resolution expands the observable field while recovering multiphase structure (Ma et al., 2025). However, models with high voxel scores may still not give good predictions of connectivity and permeability (Wang et al., 2021). Furthermore, these methods require retraining against benchmark data whenever a new rock or displacement process is considered. To overcome this limitation, in 2026, Blunt's group established SAMamba3D, the first foundational model for zero-shot 3D segmentation of multiphase pore-scale images (Zhang et al., 2026).

The next application for AI is in predicting flow and displacement. PoreFlow-Net maps pore geometry to 3D velocity fields, moving AI from structural description to resolved flow response (Santos et al., 2020). Graph learning moves further into dynamics by predicting multiphase evolution from experimental micro-CT data (Gu et al., 2024). Wang, Zhu and colleagues jointly developed a multimodal graph-network simulator and 3D U-Net framework from 4D microvelocimetry, and showed that a model trained on drainage in a sintered bead pack could partially reproduce particle trajectories and velocity structures (Wang et al., 2026). For a given structure, fluid conditions and history, can a model predict what happens next inside the pore space? Local field errors, conservation, interface motion, trapping, reconnection and rollout stability all enter the test.

Experiments physically ground this prediction problem and provide rich training datasets. For instance, Blunt and collaborators used fast synchrotron tomography to capture dynamic CO_2 invasion at reservoir conditions, and produced complete time-resolved drainage and imbibition datasets in carbonate rock, to reveal intermittent pathway rearrangement during transient and equilibrium multiphase flow (Andrew et al., 2015; Spurin et al., 2020). Four-dimensional velocimetry resolves the velocity perturbations accompanying phase rearrangement (Bultreys et al., 2024). Pore-scale imaging also captures CO_2 trapping at reservoir conditions and hydrogen-brine displacement in sandstone (Andrew et al., 2014; Thaysen et al., 2025). These studies supply observable events, conditions and independent validation targets.

Multiresolution imaging and deep learning have, for instance, enabled permeability prediction for digital porous media at far lower computational cost than direct simulation (Jiang et al., 2023). The field has advanced from isolated properties to complete relations that evolve with state. Xie et al. (2023) combined 3D digital-rock images with wettability and interfacial tension to predict oil-water relative-permeabilities as a function of saturation directly. The relative permeability function records how phase accessibility changes through displacement, so local errors may accumulate into a distorted two-phase response. The whole saturation-dependent function including endpoints, crossover behaviour and sensitivity to fluid-rock conditions must survive testing. Such responses condense complex pore events into quantities whose interpretation still depends on scale, history and uncertainty.

3. AI in subsurface-flow prediction

Beyond the pore-scale tasks, subsurface-flow prediction begins with averaged properties and predicts responses across larger domains that may extend over tens of kilometres in CO_2 storage sites, for instance. A change in scale changes the target and its evidence. Such estimates become valuable when their support scale, boundary conditions and uncertainty remain explicit in interpretation. Process history, anisotropy and unresolved porosity continue to shape effective permeability, capillary pressure, relative permeability and reaction parameters. Laboratory experiments and independent field-scale data, such as pressure measurements, detailed formation evaluation from well logs, seismic images and production history therefore remain decisive tests. Scientific judgement still depends on parameter definitions, domains of validity and honest error reporting.

Beyond property estimation, reservoir-scale research is turning to rapid prediction and the quantification of uncertainty. Deep-learning studies of CO_2 geological storage now point towards physics guidance, interpretability and generative modelling (Wang et al., 2024). Nested Fourier neural operators now deliver real-time, high-resolution CO_2-storage predictions (Wen et al., 2023), while underground hydrogen-storage surrogates are advancing in parallel (Fu et al., 2025). Speed creates room for broader uncertainty analysis, but it also raises the standard for transparent failure reporting. These predictions may still carry the imprint of unresolved structure and local flow processes. Pore-scale understanding may therefore offer physical constraints whose relevance must be judged against geology and observations. Geological uncertainty, observational constraints and operating conditions can all reshape performance, so validation must remain specific to the task.

4. Outlook

Foundational models should be the next direction for the field, with their credibility built on demonstrable transfer across fluids, rocks, wettability conditions and scales. Editorial judgement matters here: the strongest model is the one that sharpens a scientific question and survives the evidence assembled around it. Diverse data, physical evaluation, independent experiments and transparent reporting will determine whether results can accumulate, be compared and be reused. The progress worth pursuing lets speed serve understanding, prediction face testing, and every advance become a reliable starting point for the next discovery.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (No. 42476238).

Conflicts of interest

The authors declare no competing interest.

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