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Editorial

Revisiting upscaling in porous media research

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Abstract:
Spatial and temporal upscaling is an important topic for porous media research, due to the large variations in the characteristic scales of pore structures and of physical processes such as multiphase flow. Classical upscaling approach can effectively integrate fine-scale information into large-scale descriptions, but rely on assumptions about homogeneity and boundary conditions. Combining numerical modeling across scales provides an alternative that enables considerations of heterogeneity and more faithful representation of fine-scale physics at the fluid-fluid and fluid-solid interfaces, but the computational cost can be prohibitive. Still, upscaling is faced with challenges of intimate coupling of multiphysics, presence of features such as fracture networks, and limited understandings of physics at different scales. Thus, continued efforts are needed to take advantage of developments in artificial intelligence and multi-scale characterization techniques, to facilitate theoretical, modeling and observational advances in upscaling of processes such as multiphase flow in porous media.

1. Why upscaling

Upscaling integrates some form of representations of fine-scale properties and processes into the coarse-scale analyses. It is an important topic in porous media studies, partly because of the multiscale nature of pore structures (Blunt et al., 2013). The pore size can vary for several orders of magnitude, from nm to mm, whereas observations and scales of practical importance in subsurface energy systems typically range between centimeters (core-scale) and kilometers (field-scale). In the presence of fractures, the variations in structural length scales are even larger, from sub-microns for the apertures of micro-cracks to kilometers in fracture networks (Deng and Spycher, 2019).

Aside from pore structures, the controlling factors of a physical process and its manifestations may also vary across scales. For example, in multiphase flow, molecular interactions at the fluid-solid and fluid-fluid interfaces dictate interfacial tensions and contact angles, which affects the two-phase dynamics at the pore-scale (Cai et al., 2024). In engineering practices, the pore-scale dynamics will influence parameters such as the local displacement efficiency that can be quantified using averaged relative permeability and capillary pressure functions. For mineral precipitation or element deposition, nucleation at the fluid-solid interface is the key process at the nano/micro-scale, which controls the subsequent evolution

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of the pore structures and thus macro-scale properties such as porosity and permeability (Deng and Poonoosamy, 2026). The second example is further complicated by the fact that it is also coupled with fluid flow, as fluid availability at the fluid-solid interface may involve a water film that has a thickness on the order of 10s-100s nm, and properties at the interface (e.g., contact angle) can be altered by mineral coating. At the pore-scale, precipitation in the pore-body versus pore-throat can have drastically different impacts on flow, which manifests at the large scale as different relationships between porosity and permeability.

In addition, upscaling is also needed in the temporal dimension. In general, the time scale of a physical process increases along with its spatial scale, but the scaling varies under different conditions. Take the ripening of bubbles in porous media as an example: in absence of gravity, it is a typical diffusive process and time scales with the square of its length; however, when the diffusive process is driven by gravitational potential, the time scale becomes proportional to the length scale (Feng et al., 2022). Temporal upscaling is the key to identify whether a microscopic or lab-scale observation is practically significant at larger length scales.

2. How to upscale

Different upscaling strategies have been proposed. One approach relies on the use of dimensionless numbers and phase diagrams to guide the upscaling process. For instance, macro-scale equations such as Darcy's law can be derived from pore-scale Stokes flow, when the Reynolds number $\ll 1$ and the viscous force is dominant. When the Peclet number $\ll 1$, and diffusion dominates over advection at the pore scale, a more homogeneous local concentration is expected, which is necessary for the assumption of complete-mixing as used in many large-scale descriptions. The use of dimensionless numbers helps identify important physical processes and regimes under which upscaling methods such as volume averaging and homogenization are applicable. This approach can be simple and elegant but has its limitations. First, the definition of dimensionless numbers may be scale dependent, and thus their applicability across scales is challenged: for instance, mixing at the pore level is not the same as complete mixing over a macroscopic region encompassing many thousands to millions of pores. Second, in evolving porous media, dimensionless numbers that are typically defined based on the initial conditions may become irrelevant following the memory loss of the initial states. Third, the use of dimensionless numbers and upscaling methods including volume averaging and homogenization depend on underlying assumptions of a homogeneous domain or certain boundary conditions (Geers et al., 2017; Keller, 1964).

Another upscaling strategy involves more explicit representation of the fine-scale behavior. For instance, Density Functional Theory (DFT) calculations and Molecular Dynamics (MD) simulations can provide important interfacial properties. They are particularly useful for tight reservoirs such as shale gas and shale oil formations, where hydrocarbon storage and transport predominantly occur within nanoscale pores of kerogen and clay minerals that are difficult to characterize through conventional laboratory experiments. At these nanoconfined environments, rock-fluid interfacial interactions govern adsorption, wettability and fluid mobility, yet direct experimental observation remains technically challenging and costly. DFT offers quantum-mechanical insights into static interfacial properties, precisely calculating adsorption energies, binding configurations, charge redistribution and interaction forces between hydrocarbon molecules, brine components and shale solid surfaces, which identify favorable adsorption sites and clarify the fundamental driving forces for hydrocarbon retention within nanopores. In contrast, MD simulations capture dynamic molecular behaviors under realistic reservoir temperature and pressure, reproducing confined diffusion, fluid flow, phase change and salinity-dependent wettability evolution inside nanosized pores. By combining quantum-scale static information from DFT with time-resolved dynamic transport descriptions from MD, researchers can systematically unravel adsorption-desorption mechanisms, assess in-situ hydrocarbon storage capacity, analyze how pore geometry and surface chemistry affect fluid deliverability, and provide theoretical guidance for developing efficient enhanced recovery techniques for unconventional tight oil and gas resources. For another example, pore scale models that resolve velocity and concentration fields can be used to derive average / effective properties for large scale modeling. Modeling at the intermediate scales may also be needed (Masoudi et al., 2024). In the case of (multiphase) flow in porous media, pore-network models are often used to connect pore-scale and large-scale modeling (Cui et al., 2022). This is also referred to as recursive upscaling or hierarchical upscaling. The advantage of integrating fine-scale modeling is being able to accommodate spatial heterogeneities, but it can be computationally expensive. Alternatively, surrogate models may be developed for fine scale processes to ensure computational feasibility.

3. Challenges and prospects of upscaling

One challenge for some of the upscaling methods (e.g., volume averaging and homogenization) is the requirement of strong scale separation, while for other upscaling methods (e.g., numerical upscaling) identifying scale specific physics, state variables, parameters and phenomena is still helpful. This can be particularly challenging when in presence of multiple physical and chemical processes, as each one has its own characteristic time and length scale.

The multiphysics nature of many porous media upscaling problems is partially accounted for by constitutive relationships that connect parameters that are associated with different state variables, and is also manifested in the observations that parameters associated with one state variable may be dependent on other physical processes. For example, reactive surface area at the pore-scale typically corresponds to the geometric surface area, whereas at large scale it is used to account for the accessibility of flow and transport. In other words, tracking the physical meanings of the 'same' parameters across scales may be difficult.

In the presence of multiscale fractures, the foundational

assumption of the classical paradigm of porous media upscaling - the existence of a Representative Elementary Volume (REV), a scale at which local averaged properties such as porosity and permeability become statistically stationary and independent of sample size - is challenged. Unlike a granular matrix where heterogeneities are relatively distributed, fractures introduce discrete, high-conductivity pathways that violate the assumption of a continuous and homogeneous medium. Because fractures often exhibit spatial correlation, clustering, and lengths that can span multiple scales, the separation of scales necessary for classical REV-based homogenization becomes obscure (Long et al., 1982). Consequently, the very existence of a scale-invariant REV becomes debatable; measurements can fluctuate dramatically depending on the sampling window, yielding properties that are a function of the sample's intersection with the fracture network rather than a true intrinsic characteristic of the formation. This inherent scale-dependency and non-uniqueness compel the adoption of alternative theoretical frameworks-such as stochastic / fractal continuum models, discrete fracture networks, or dual-porosity theorie-which acknowledge the lack of a well-defined REV. Many seek to characterize flow and transport through statistical distributions of fracture attributes rather than through a single deterministic effective property.

One of the primary goals of upscaling is to filter out redundant fine-scale information, but it may also miss key perturbations that can cause new phenomena (e.g., wormholing) to emerge at the large scale. Hybrid modeling that explicitly integrate models at different scales and only call for fine-scale models when needed is a promising approach for upscaling in porous media, which is capable of capturing such cross-scale phenomena. However, it requires tracking and storage of fine scale fields and transfer of information across scales, and is faced with the same challenge of data scarcity. Detailed fine-scale characterization for a large domain that is needed for powering such hybrid modeling is lacking, and field-scale data that is needed to validate large scale models is scarce along with field data of the key parameters.

The practical need for upscaling is to create reservoir-scale models with coarser grid size, time step, and descriptions of flow physics and chemistry without sacrificing accuracy. In the past, flow-based averaging was promoted to solve such problems, with properties of the coarser grid tuned to match the flow predictions of a finer grid, usually with strongly heterogeneous porosity and permeability fields. Equations solved on the finer and the coarse grid, however, are the same Darcy's law. Today, as the fine-scale flow model is growing more complex with parameters accounting for surface phenomena, deposition chemistry, geomechanics, and fractures ready to emerge, it is highly likely that the targets of coarsening will also need to grow. Not only effective porosity and permeability need to be defined, but also parameters and processes featured in the new fine-scale model.

These needs further highlight one important challenge for upscaling: the lack of fundamental understanding or theories supported by underlying physics at different scales. At the fine scale, mathematical models for mineral nucleation are yet to be developed to account for complex non-classical nucleation pathways, whereas at the large scale, the use of Darcy's law and relative permeability for multiphase flow remains largely empirical.

In summary, upscaling in porous media is a rich research field, which calls for further advances in the fundamental understanding of multiphysical processes, and the development of a practical methodology that better addresses heterogeneity, complex coupling and computational costs. Recent breakthroughs in artificial intelligence, characterization techniques across nano- and field- scale provide new opportunities that are to be explored.

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Conflicts of interest

The authors declare no competing interest.

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