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Pore-Scale Modeling of Multiphase Flow and Transport: Achievements and Perspectives

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When *Irvin Fatt* wrote his classical paper on pore-network modeling (Fatt 1956), he would probably not have thought that this field would become one of the largest fields of research in the porous media discipline. Pore-scale modeling has found its way as an expanding field of research for understanding the physics of flow and transport in porous media. In addition, it is becoming a valuable tool for prediction of petrophysical properties as part of the so-called Digital Rock Physics approaches, thus supplementing and replacing expensive and time consuming laboratory experiments. The recent popularity of pore-level modeling can also be attributed to advances in visualization of the pore space, to very high image resolution, and to the steady increase in computing power. This has made it possible to deal with a multitude of processes in the pore space and interactions with the solid phase (van Dijke and Piri 2007). The focus of this special issue of *Transport in Porous Media* is to provide an overview of some recent developments of various techniques for pore-scale modeling of multiphase flow and reactive transport.

1 Classification of Pore-Scale Methods

The biggest challenge in pore-scale modeling of multiphase flow under transient conditions is the tracking of the fluid–fluid interfaces and contact lines. Determination of the positions and shapes of interfaces in time and space will provide almost all the required information, such as

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saturation, capillary pressure, interfacial areas, and flow patterns. Based on the approach for tracking the interfaces, the models can be classified into sharp and diffuse interface methods.

Traditionally, approaches based on pore-network models (PNM) have been the most common pore-scale modeling methods. Pore-network models require extensive preprocessing (network extraction) to discretize the imaged irregular pore space into simple geometrical objects (nodes and bonds). Then, simplified versions of the relevant conservation laws are solved within this discretized representation using effective parameters for each pore object.

More recently, a variety of approaches have been developed that involve, more or less, direct application of computational fluid dynamics (CFD) to the imaged pore space. But they require complicated discretization within the irregular pore geometry, as well as mesh refinement around, for instance, fluid–fluid interfaces. CFD models can be classified as either continuum or particle based. Examples of continuum-based methods are the Level Set (LS) method (cf. Prodanović and Bryant 2006), the volume of fluid (VoF) method (Hirt and Nichols 1981), and the density functional method (DFM) (cf. Dinariev 2003). Main particle-based methods are the lattice–Boltzmann (LB) method (cf. Gunstensen and Rothman 1993; Pan et al. 2004) and the smoothed particle hydrodynamics (SPH) method (cf. Tartakovsky and Meakin 2005). Particle-based models require extensive post-processing to determine fluid–fluid interfaces and to calculate saturations. Detailed reviews of different pore-scale modeling techniques have been provided by Blunt (2001), Meakin and Tartakovsky (2009), and Joekar-Niasar and Hassanizadeh (2012a).

Suitability of different pore-scale modeling techniques for a given application depends on many aspects, such as the governing equations, assumptions underlying the pore-scale flow and transport equations, as well as the length-scales of the (computational) domain. While the lower scale limit of a pore-scale technique is determined by the scale of the governing equations, the upper scale limit is set by the computational power. For instance, a typical pore-network model considers each pore unit as a computational node, while LB or SPH models may typically consider hundreds of computational points within a single pore unit. Consequently, the simulation scale for the latter models will be much smaller for a given hardware configuration.

2 Content of This Issue

This issue gives an overview of some recent pore-scale modeling works, such as pore-network modeling and LB as upscaling tools for different applications in porous media. Several fundamental concepts are covered in this issue: fundamental understanding of dynamics of two-phase flow using dynamic pore-network models (Joekar-Niasar and Hassanizadeh (2012b)) or LB simulation (Ramstad et al. (2012)), evaluation of petrophysical properties of dual porous media (Bauer et al. (2012)), upscalling of two-phase flow (Tsakiroglou (2012)), diagenetic effects of cementation and compaction on porous media flow (Mousavi and Bryant (2012)), and upscaling of reactive transport (Kim and Lindquist (2012)). Moreover, generation of pore networks based on the statistical properties or direct generation of the network are other main lines of research as discussed in Jiang et al. (2012) and Chareyre et al. (2012).

Bauer et al. (2012) present a dual-pore-network approach (D-PNM) based on μ-CT images at different length scales of bimodal porous media. Their multiscale method supplements a pore network at the coarser scale with pore elements representing the underlying finer scale (microporosity), and is used to calculate petrophysical properties. Tsakiroglou (2012) also presents a multiscale method and shows how his pore-network model can be used as an upscaling tool for two-phase flow properties. Similarly, Kim and Lindquist (2012) use a pore-network model as a tool to upscale reaction rates from the pore to the core scale.

Mousavi and Bryant (2012) present simulations of two-phase flow properties in pore-network models, for which the pore topology and geometry have been modified to represent the diagenetic effects of cementation and compaction.

Jiang et al. (2012) present a workflow for the construction of pore networks that are statistically equivalent to networks extracted directly from 3D-rock images. They discuss whether the extracted pore networks are statistically representative for the generation of pore networks extracted at multiple length scales. Chareyre et al. (2012) present a new method for the direct construction of the pore network for a dense sphere packing and they simulate Stokes flow in the pore space. Their results agree well with high resolution finite-element calculations. The method is proposed as a framework to study the induced forces of the fluid acting on grains in a porous medium.

Joekar-Niasar and Hassanizadeh (2012b) present a full dynamic pore-network model that considers two separate pressure fields for two phases. It simulates the evolution of fluid–fluid interfaces and their appearance and disappearance. They have simulated several drainage and imbibition events (including scanning curves) to investigate the relation between capillary pressure, saturation, and specific interfacial area under non-equilibrium conditions. Finally, Ramstad et al. (2012) present a LB model for two-phase flow for a network based on X-ray microtomography images of Bentheimer and Berea sandstone. The model is able to mimic both unsteady and steady-state experiments for measuring relative permeability.

3 Outlook

The papers in this special issue provide a limited but still diverse overview of applications of pore-scale models that can be used for multi-scale modeling and upscaling (Bauer et al. 2012; Tsakiroglou 2012; Kim and Lindquist 2012); dynamics of multiphase flow in porous media (Joekar-Niasar and Hassanizadeh 2012b; Ramstad et al. 2012) as well as effects of topological changes of porous media on flow properties (Mousavi and Bryant 2012; Jiang et al. 2012; Chareyre et al. 2012).

Although there have been significant achievements in pore-scale modeling, many open questions remain. For example:

- *Consistency across pore-scale models* Different methods of pore-scale modeling are based on different governing equations for the same physical problem. However, the consistency among these models and across different scales is yet to be addressed. In addition, we need to apply our techniques at the appropriate scale. For example, particle-based methods are intrinsically more suited for scales close to the molecular level.
- *Characterization and data management* Imaging techniques provide detailed information about the porous media topology and geometry. With tremendous improvements in image resolution, the available data would be even greater. However, are all these data required to calculate simple petrophysical properties? Moreover, do we need to employ detailed and complicated physically based models to calculate simple and static properties?
- *Multi-physics problems* Many industrial processes involve multiple physical processes, while the pore-scale models often focus on single physical processes. Therefore, we need to determine how multiphysics problems can be included in pore-scale modeling. For example, the structure of, and therefore the flow and transport in porous media, as well as their wetting properties will be altered by geochemical processes in the pore space.

- *Upscaling and coupling across scales* We need to address how information provided by pore-scale models can be used for the improvement of reservoir or large field-scale models? This also raises the question whether current effective parameters, for example relative permeability as function of phase saturation, are still adequate. In addition, upscaling of pore-scale results is necessary to validate against experimental observations at larger scales.

These are examples of fundamental questions that need to be studied for further development and wide range of application of pore-scale models.

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