Introduction to special section on Modeling of Pore-Scale Processes

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1. Introduction

[1] In recent years pore-scale modeling of flow through porous media has gained much popularity. This can be attributed to advances in visualization of the actual pore space (and fluid distributions), to very high image resolution, and to the steady increase in computing power. The latter allows the incorporation of processes on the scale of individual pores in models that are close to the continuum scale. At the same time, research into physical and chemical processes in the fluids occupying individual pores, and interactions with the solid phase, have continued. The visualisation capability has greatly contributed to the accurate modeling of the pore space.

[2] The popularity of pore-scale modeling was reflected in a sizable special session at the XVIth Conference on Computational Methods in Water Resources (CMWR), which was held in Copenhagen in June 2006. Expanded papers from this conference have been submitted for inclusion in this special section on Modeling of Pore-Scale Processes. The selection of papers represents an excellent cross section of the current research in this area, as outlined below. Contributors to the section tend to work mainly in the areas of hydrocarbon recovery, water resources or both, although the applications of the presented research are significantly wider.

[3] Pore-scale modeling began with the representation of a porous medium as an interconnected network of cylindrical tubes complemented with simple rules for flow through the tubes, to calculate macroscale flow and transport characteristics such as relative permeability and dispersion coefficients. These macroscopic properties were in turn taken as input in macroscopic or continuum-scale models for flow and transport. With respect to this basic goal, little has changed in the almost 60 year history of pore-scale modeling. *Blunt* [2001] and *Blunt et al.* [2002] have provided some excellent reviews of the corresponding literature.

[4] However, what has changed in recent years is the level of detail at which various processes and also the pore space itself are modeled. Especially in the area of (multiphase) flow there has been a drive to predict flow characteristics starting from pore space information of high-resolution thin section and X-ray computed microtomography images. This stands in contrast to the more traditional methods, in which (idealized) geometrical and topological network characteristics are matched to relatively simple macroscale data, to predict more complicated properties. However, in practice the distinction between the two approaches is not as large as it appears. For example the detailed pore space is often mapped onto an idealized network and some information (such as wettability) is currently only available from macroscopic data. Both approaches are represented in this special section and prove to be equally useful. The above discussion of ''detailed'' versus ''idealized'' approaches reveals what is probably the most important question in pore-scale modeling: What are the really important characteristics and pore-scale processes that are both necessary and sufficient to predict certain macroscale properties? For a long time, in the absence of large computing power, the idealized approach has worked with a minimum number of necessary parameters, which are often not sufficient. However, the increase in computing power has allowed the incorporation of many features and additional parameters, some of which are probably not necessary for a given process. It may be clear that the requirements of, in particular, the detail in which the pore space is modeled, depends on the process in question. Moreover, investing computational resources in unnecessary details reduces the opportunity to scale up to a reasonable macroscopic scale. To answer the above problems, the often employed heuristic attitude to network modeling needs to be complemented by more rigorous mathematics, such as the upscaling methods described in some of the papers in this special section.

[5] Apart from the papers that aim to work through the full prediction trajectory from pore space to macroscopic process, a number of other papers have taken a deliberately simplified approach to work out the unresolved details of a given process in, for example, a single pore, with the aim of incorporating these in a network model. In the overview of the papers in the special section, presented below, a broad distinction is made between the papers that deal with multiphase flow and those that deal with dispersion and reaction.

[6] Finally, special mention needs to be made of the development and application of the lattice Boltzmann (LB) method in pore-scale modeling, which features more or less prominently in many of the papers. This method is used almost routinely to calculate single-phase flow patterns, hence absolute permeabilities, in irregular (pore) geometries. More sophisticated versions of the LB method are applied and developed for two-phase flow, as well as for

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multicomponent reactive transport. These versions can provide very accurate flow and transport calculations, but the computational cost is high, hence the scale, or in fact the dimension (two dimensions), of the considered porous media has to be small.

2. Multiphase Flow and Pore Space Reconstruction

[7] *Okabe and Blunt* [2007] present a pore space reconstruction method for a complex type of porous medium, such as carbonate reservoirs. A multiple-point statistics approach is used to generate a three-dimensional (3-D) model from 2-D high-resolution thin section images showing micropores, which are combined with a lower resolution microtomography image that include larger pores and vugs. Absolute permeabilities computed using the lattice Boltzmann method are in agreement with measured values.

[8] *Jiang et al.* [2007] introduce an improved method for extraction of the geometrical and topological network that represents the pore structure of a porous medium, centered around an efficient thinning algorithm to determine the medial axis of the pore space. Additionally, they describe partitioning of the pore space in ''nodes and bonds'' and the determination of geometrical features, such as radii and shape factors. The functionality of the method is demonstrated through network extraction from microtomography images of three sandstones.

[9] *Øren et al.* [2007] use a previously developed, geologically based reconstruction technique to rebuild virtual rocks for two heterogeneous sandstones from the North Sea. The method is based on explicit simulation of the geologic process by which the sandstones are formed. The authors also obtain 3-D X-ray microtomography images of the actual rock samples. They compute effective material and transport properties for the X-ray images and compare these to the same properties for the virtual rocks and to available experimental data. For both sandstones the authors compare two-point correlation functions, local porosity distribution, NMR response, elastic, conductive and flow properties of the X-ray images and the virtual rocks. The study indicates that the process-based technique can be successfully used to reconstruct virtual rocks that capture the properties of the pore space in heterogeneous sandstones necessary to predict effective material and transport properties (using direct pore-scale simulations).

[10] *van Dijke et al.* [2007] consider a particular three-phase flow property of a single pore, i.e., the precise criteria for the existence of thick conducting fluid layers, such as oil layers residing between gas in the oil-wet centre and water in the water-wet corners of the pore. These thermodynamic criteria for formation and removal of layers are consistent with the capillary entry conditions for the accompanying three-phase bulk displacements. This is essential for accurate pore-scale modeling of three-phase flow, in particular for drainage of the layer phases at low saturations.

[11] A. Al-Kharusi and M. J. Blunt (Multiphase flow predictions from carbonate pore space images using extracted network models, submitted to *Water Resources Research*, 2006) follow through the entire prediction trajectory starting from 2-D thin section images, creating an equivalent network model and finally predicting two-phase flow properties for a carbonate rock sample. Good agreement between experimental data and network simulations is obtained for absolute permeability, as well as for the mercury intrusion and primary drainage capillary pressure curves. Subsequently, waterflood and secondary drainage capillary pressure curves are matched by varying the contact angle distribution. Using this wettability information, good predictions are obtained for the relative permeabilities during the various two-phase flow processes.

[12] *Schaap et al.* [2007] apply a two-phase LB simulator to model capillary pressure curves for drainage and imbibition in a section of a glass bead porous medium. Good agreement with experimental observations is achieved for air-water experiments, with less favourable agreement for water-Soltrol experiments, possibly due to a nonzero contact angle.

[13] *Gladkikh et al.* [2007] use previously developed network modeling techniques for petrophysical interpretation of logging data. A numerically created random dense packing of equal sized spheres is used as a model porous system. Details of geologic processes are added by modeling cementation of the grains. Porosity and mean value of grain size are extracted from NMR logging data. A network is then generated using Delaunay tessellation of sphere centers, which is utilized to simulate single-phase flow. The authors apply the approach to two Berea sandstone cores and compare the predicted absolute permeabilities against measured values. They also apply the method to a water well for which logging and core analysis data were available.

[14] Similar to the above study *Motealleh and Bryant* [2007] use a network that was built on the basis of a dense random packing of spheres, to investigate the effects of irreducible water saturation on the permeability of the nonwetting phase. Porosity of the system was altered by varying the amount of cementation. The authors study the geometry of the wetting phase bridges left between the gain gaps to understand the effects of reduction in the area open to the flow of the nonwetting phase on its effective permeability. A qualitative comparison of the results to the experimental data is presented. They also perform a simple bead pack experiment to study the precipitation of salt due to evaporation of water from brine left in the system after drainage by air. The model is used to explain salt precipitation mechanisms and consequent reduction in the effective permeability of the nonwetting phase.

[15] *Yiotis et al.* [2007] present a pore-scale network model to investigate drying in porous media. The authors study coupling of convective-dispersive mass transfer outside the porous system with the mass transfer processes taking place inside the pore space, e.g., diffusion of liquid vapors. They take into account the effects of wetting layers, left at the pore walls after drying of the bulk fluid, and show that drying rate stays constant while the wetting layers connect the bulk fluid to the external surface. They also report a transition from the abovementioned regime to falling rate regime when the wetting layers become too thin. The results are used to explain experimental observations.

[16] *Helland and Skjæveland* [2007] use a previously developed bundle of capillary tubes model, as a simple representation of pore space, to study two-phase flow. Tubes are equilateral triangle in cross section. The authors incor-

porate wettability alteration scenario to account for contact angle hysteresis. They use thermodynamically consistent threshold capillary pressures for the displacements represented by the changes in the fluid configurations, similar to *van Dijke et al.* [2007]. The model is used to investigate the effects of wettability on the specific oil/water interfacial area for primary drainage, imbibition and secondary drainage in mixed-wet systems. The authors derive analytical expressions for specific interfacial area as a function of saturation and capillary pressure for primary drainage and report curve-fitted functions for imbibition and secondary drainage. They use the model to investigate validity of the conjecture of *Hassanizadeh and Gray* [1993] for water-wet and mixed-wet systems when contact angle hysteresis is taken into account. They probe the question of whether or not hysteresis is present in the relationship between capillary pressure, saturation and interfacial area.

[17] J. M. Nordbotten et al. (On the definition of macroscale pressure for multiphase flow in porous media, submitted to *Water Resources Research*, 2006) propose a new definition for the macroscopic pressure in immiscible two-phase flow, when upscaling the pore-scale microscopic pressure. The definition is based on comparison between (the two-phase extension of) Darcy's law and the volume averaged Stokes equations for fluid flow on the pore scale. The macroscopic pressure is not equal to the intrinsic phase average pressure, unless subscale heterogeneities in material properties or fluid distributions are absent. It is demonstrated how the new definition affects, for example, the calculation of relative permeabilities from network models.

3. Dispersion and Reaction

[18] *Bijeljic and Blunt* [2007] present an idealised 2-D pore-scale network model with the pore size distribution of a Berea sandstone for calculation of the transverse dispersion coefficient. In the pores of square cross section, particles move by advection and diffusion (random walk). Comparison to a number of experiments indicates that the model can predict the trends for the asymptotic macroscopic dispersion coefficient over a broad range of Péclet numbers.

[19] R. S. Maier et al. (Sensitivity of pore-scale dispersion to the construction of random bead packs, submitted to *Water Resources Research*, 2006) investigate the effects of sphere packing variations on the hydrodynamic dispersion coefficient using a previously developed pore-level model. Three-dimensional viscous flow in the pore space between the hard spheres is modeled using lattice Boltzmann method. Motion of tracer particles is handled using the Langevin equation. The authors study the effect of porosity, in uniform and polydisperse bead packs, on the dispersion coefficient. They also investigate the dispersion coefficient in packed beds formed with different compression rate parameters and distributions of distances between neighbors, showing that the more slowly compressed packs have lower dispersion. They also discuss the sensitivity of dispersion coefficient to modifications of the packing algorithm, and study the effects of packing defects and confining walls on the dispersion coefficient.

[20] *Jacobsen* [2007] uses a reactive transport model within a 2-D pore-scale flow domain, including several active and stagnant pores, to study the distribution of redox and other geochemical processes in intergranular and intragranular microniches in a groundwater system. The model indicates that a separation of redox processes within the pore space is possible, if the stagnant pores are deep and narrow and the rate of organic matter decomposition is fast. However, in most aquifers the organic matter reactivity will be so low that substantial lumps of organic matter are required to produce methanogenic conditions. Otherwise, sulfate reduction will take place in the stagnant pores. The redox processes may lead to localized secondary processes occurring at the grain scale.

[21] *Johnson et al.* [2007] present a review of recent advances that have helped improve our understanding of the retention/release of particles (10 nm to 10 μm) in saturated porous systems, particularly wedging in solid grain contacts. The authors revisit experimental and pore-scale modeling efforts concerned with the transport of biological and nonbiological particles in porous media. They first discuss the similarities between transport of biological and nonbiological particles, and then continue with discussions on classic filtration theory and the processes causing deposition. This is followed by a review of interaction forces between colloids and porous media and the impact of energy barriers on deposition. They also look at the influence of surface heterogeneity on particle attachment in porous media and review new observations that require new models of particle filtration, which include the impact of pore domain geometry, retention in flow stagnation zones, and deposition in grain-to-grain contacts. They argue that recent improvements in our understanding of retention mechanisms may allow the development of correlations that easily predict colloid transport distances in the presence of an energy barrier.

[22] *Kang et al.* [2007] describe improvements of a 2-D LB pore-scale model for multicomponent reactive transport in porous media. In particular, the distribution function boundary condition for the total solute concentration, which is strictly mass conserving, is rigorously derived and implemented in both four-speed and nine-speed lattices. LB simulations of reactive transport in various chemical and geometrical systems are compared with analytic expressions or numerical continuum simulation results. Compared to the nine-speed model, the four-speed model has comparable accuracy and better computational efficiency.

[23] *Lichtner and Kang* [2007] apply the LB model of *Kang et al.* [2007] to solve the reactive transport equations at the pore scale, and volume average the results to fit a multiscale continuum model. Provided that sufficient resolution of the pore-scale geometry can be obtained, the pore-scale model can be used to determine the most appropriate form of continuum formulation (single, dual, or multiple continua) that best fits the upscaled pore-scale simulation and, simultaneously, provide parameters for constitutive relations in the multiscale continuum formulation.

[24] A. M. Tartakovsky et al. (Mixing-induced precipitation: Experimental study and multiscale numerical analysis, submitted to *Water Resources Research*, 2006) use a previously developed particle-based dynamic method (smoothed particle hydrodynamics) to model reactive transport at the pore scale. The authors extend their model to investigate mixing induced supersaturation and precipitation of reaction products in a 2-D porous system. They present a new form of homogeneous and heterogeneous reaction terms in the ad-

vection-dispersion equation that take into account nonuniform concentration distributions and localized reactions. Additionally, the authors take into account the effect of the changing pore geometry, due to precipitation, on the reaction rates in the Darcy scale representation of diffusion equations. Finally, a qualitative comparison is made between simulation results and observations from an experiment, in which two different solutes were injected into a 2-D flow cell showing precipitation of calcium carbonate at the interface.

[25] *Wood* [2007] investigates the longitudinal and transverse dispersion coefficients for inertial flow conditions. A subpore-scale description of mass and momentum balances and the relevant boundary/initial conditions are presented without eliminating the inertial term. An upscaling approach based on volume averaging is presented to mathematically homogenize the microscale mass and momentum balance equations for the Darcy scale systems. To eliminate the microscale deviation term a closure problem is formulated, where the deviation of a dependent variable is determined as a function of its spatial average, which is solved both analytically and numerically. Normalized longitudinal dispersion coefficient versus Peclet number is compared against the experimental data. The author shows that the power law exponents measured for the experimental data are well represented by the theory. It is concluded that the inertial effects to predict longitudinal dispersion are small. The author also compares the predicted normalized transverse dispersion coefficient to the available experimental data and presents a revised version of previously proposed dispersion regimes to reflect the effect of flow field.

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