International Journal of Rock Mechanics and Mining Sciences 106 (2018) 269–277

Contents lists available at ScienceDirect

International Journal of Rock Mechanics and Mining Sciences

journal homepage: www.elsevier.com/locate/ijrmms

Prediction of permeability and formation factor of sandstone with hybrid lattice Boltzmann/finite element simulation on microtomographic images

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ARTICLE INFO

Keywords:
Digital rock physics
Computed tomography
Hydraulic permeability
Formation factor

ABSTRACT

In Fontainebleau sandstone, the evolution of transport properties with porosity is related to changes in both the size and connectivity of the pore space. Microcomputed tomography can be used to characterize the relevant geometric attributes, with the resolution that is sufficiently refined for realistic simulation of transport properties based on the 3D image. In this study, we adopted a hybrid computation scheme that is based on a hierarchical multi-scale approach. The specimen was partitioned into cubic sub-volumes for pore-scale simulation of hydraulic permeability and formation factor using the lattice Boltzmann method. The pore-scale results were then linked with finite element simulation in a homogenized scheme to compute and upscale the transport properties to specimen scale. The simulated permeability and formation factor have magnitude and anisotropy that are in good agreement with experimental rock physics data. Together with simulated and measured values of connected porosity and specific surface area, they provide useful insights into how pore geometry controls the evolution of the transport properties.

1. Introduction

The upper crust of the Earth is composed of rocks with a pore space made up of geometric features with very different morphology and scale, including relatively equant pores on the submicron scale and elongated fractures that may extend over hundreds of km. In most instances, these features are interconnected, thus constituting a percolative structure for hydraulic and electrical transport. A fundamental understanding of the transport properties of rock is of importance in many natural resources and environmental applications. Hydraulic permeability controls the migration, trapping, and extraction of conventional and unconventional hydrocarbon resources.[1] It influences contaminant transport, potential leakage of radionuclides in a waste repository, as well as the transient development and maintenance of excess pore pressure in hydrogeological settings.[2] Permeability may impact not only transport of pore fluid but also mechanical and failure behaviors in relation to the stability of a seismogenic system and induced seismicity.[3,4] Another transport property of importance is the electrical conductivity, which together with related AC properties such as induced polarization and streaming potential, provide useful geophysical tools for exploration in the oil and gas, as well as mining industries.

Both transport properties have been characterized in the rock physics laboratory under confining and pore pressures comparable to crustal settings. The electrical transport (characterized by the conductivity σ) is made up of two components: bulk conductivity σ_{bulk} through the pore fluid, and conductivity σ_s along the surface of the grains.[5] If the surface conduction component can be isolated from the overall conductivity σ, then the bulk conduction component can be identified. To decouple the effect of pore geometry from that of the electrolyte conductivity on the bulk conductivity of a rock saturated by a fluid of conductivity σ_w, one typically considers the formation factor: $F=\sigma_{\mathrm{w}}/\sigma_{\mathrm{bulk}}$, which has been observed to be related to the porosity (by Archie's law, an empirical power law). In contrast, the permeability k (which spans over 14 orders of magnitude in geomaterials) cannot be as simply related to the porosity, with the implication that other geometric attributes (such as pore size and connectivity) also exert important control over hydraulic transport.[5]

A fundamental understanding of transport properties would, therefore, hinge on a deeper understanding of the geometric complexity of the pore space. Traditionally, pore space in rock is imaged using optical and scanning electron microscopes. Supplementary information on the geometry of the pores and throats may also be gained from mercury porosimetry[6] and nuclear magnetic resonance (NMR) imaging.[7] Furthermore, recent advances in 3D imaging techniques such as laser scanning confocal microscopy (LSCM)[8] and X-ray computed

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https://doi.org/10.1016/j.ijrmms.2018.04.020
Received 29 June 2017; Received in revised form 23 January 2018; Accepted 8 April 2018

tomography (CT)[9] have provided enhanced perspectives on pore geometry complexity. Attributes such as pore dimension statistics, connectivity, and specific surface area can readily be characterized quantitatively.

In recent years, CT imaging has proved to be an effective tool in digital rock physics for probing both the mechanical and transport behaviors. In particular, for a clastic rock such as sandstone the void space is dominated by relatively equant pores connected by throats that are sufficiently large for direct imaging using X-ray microCT, and such data have elucidated the 3D geometric complexity[9] and its control over poromechanical properties[10–16] as well as mechanical failure and strain localization.[14,17–20] The first such attempts in digital rock physics were by Spanne et al.[21] and Auzerais et al.[22] who acquired CT images with a synchrotron X-ray source and analyzed the geometric attributes and transport properties of Fontainebleau sandstone samples with nominal porosities of 19.7% and 15.2%, respectively.

Fontainebleau sandstone is monomineralic and does not show significant variability in quartz grain size or sorting. However, it has a wide variability in porosity (2–30%) attributed to different degrees of silicification during its diagenetic evolution.[23] A systematic study of its acoustic and transport properties and their dependence on porosity was conducted by Jacquin[24] and Bourbie and Zinszner,[25] who observed that the relation between hydraulic permeability and porosity undergoes a transition from high to low porosities. Above a crossover porosity of ~9%, the permeability and porosity are related by a power law with a constant exponent of ~3.05. Below this crossover, permeability decreases drastically with decreasing porosity, manifested by an exponent value up to 7.3. This significant reduction of permeability in the low-porosity regime is attributed to the corresponding decrease in pore connectivity that ultimately leads to the percolation threshold at a porosity of ~4%.[26,27] Since then, Fontainebleau sandstone has been the focus of extensive research in both experimental and digital rock physics for several decades. Nevertheless, there remain a number of outstanding questions, such as the discrepancies between calculated and measured effective permeabilities, relationships between formation factor and permeability under different porosities, and effects of microstructural attributes, such as pore size distribution, pore connectivity and effective hydraulic radius, on the porosity-permeability relationship.[13,28–31] The objective of the present study is to revisit some key issues related to hydraulic and electrical transport.

To probe the physics behind the contrast in permeability evolutions between the high- and low-porosity regimes in Fontainebleau sandstone, Lindquist et al.[9] used a synchrotron X-ray source to image the pore spaces of four samples with nominal porosities 7.5%, 13%, 15% and 22%, respectively. They quantitatively analyzed the pore geometry, and furnished the segmented data to Arns et al.[34] for computation of the formation factors, which showed good agreement with experimental measurements. Arns et al.[35] followed up with computation of permeability using the lattice Boltzmann (LB) method. Whereas the agreement between the simulated and laboratory data was reasonable in the high-porosity regime, it was not as satisfactory for the sample with 7.5% porosity, with a variability of 2 orders of magnitude in the LB simulated permeability. This discrepancy is suggested to be related to a combination of image resolution and discretization effects in Arns et al..[35] However, in a parallel study, Thovert et al.[36] investigated another Fontainebleau sandstone sample of porosity 6.92%, that had been scanned at a comparable resolution. In contrast, the analysis in Thovert et al.[34] on the geometry, percolation and electrical conductivity seemed to indicate that the image resolution in 35 could be adequate.

A robust simulation in the low-porosity regime of the permeability and connectivity loss is key to understanding how pore geometry, percolation and transport evolve with diagenesis in a sedimentary rock. In recent years, there have been significant advances in both X-ray CT imaging and numerical computation. If indeed image resolution of Lindquist et al.[9] is inadequate for permeability simulation in this regime, one may readily acquire new CT data for the sample at a more refined resolution with current facilities. Meanwhile, leveraging recent advances in computational poromechanics such as 15 and 16 to analyze this rather unique set of digital rock physics data may also bring new insights and clarification. Furthermore, comprehensive experimental studies of Fontainebleau sandstone[29] have recently been undertaken, which may lead to further understanding of the constraints and potential issues on the simulation-based digital rock technology related to geometrical attributes, image resolutions and other numerical issues.

Our computation scheme is based on a hierarchical multi-scale approach.[15,16,37] The specimen was partitioned into small representative elementary volumes (REV) for pore-scale calculation of transport properties. Unlike previous studies that used different numerical techniques (e.g. LB method for permeability and finite difference method for formation factor), we here employed LB simulations for both types of transport, which may provide a more consistent basis for synthesizing permeability, formation factor and geometric attributes. The pore-scale LB results were then linked with finite element (FE) simulation in a homogenized scheme to compute formation factor and permeability tensor at specimen-scale.

2. Numerical analysis

2.1. Fontainebleau sandstone and X-ray CT imaging

The Fontainebleau sandstone data set was presented by Lindquist et al.[9] who characterized cylindrical samples (diameter 4.52 mm) of the same length cored from 4 blocks of measured porosities 7.5%, 13%, 15% and 22%. X-ray CT imaging was performed at the X2-B beam line of the National Synchrotron Light Source at Brookhaven National Laboratory. With a linear voxel size of 5.7 µm in all three directions, the $795 \times 795 \times 512$ reconstructed image sections were padded to a volume of $800 \times 800 \times 512$ voxels.

The images were encoded in 8 bits ($0-255$). Lindquist et al.[9] used an indicator Kriging algorithm to segment the CT data, and this binary data set of Fontainebleau sandstone has been widely used in computational studies.[32–35] Nevertheless, in this study we did not adopt this binary data set, but instead started with the 8-bit data. In parts of the data for the 15% porosity sample, we observed "ring" artifacts, that may have been induced by slight differences in the column-by-column response of the CCD detectors, with resultant small variations in grey level that got propagated through the data sets during the reconstruction and appear in cross-sectional images as rings.[11] Accordingly, we decided not to include this sample in this study, and simply focused on CT data for the three samples FB75, FB13 and FB22 with total porosities of 7.5%, 13%, and 22%, respectively. In this study, segmentation of the data was performed using the default option of the auto-thresholding module of the software ImageJ, which is a variation of the IsoData algorithm for two-phase segmentation proposed by Ridler and Calvard.[38] This modulus is selected after visual inspections of the binary images generated from all 16 algorithms available in ImageJ. Geometrical attributes were then extracted from the segment images; a flood-filled algorithm was adopted to identify the connected porosity, and Crofton formula was used to characterize the surface area. Details of the flood-filled algorithm and the Crofton formula can be found in 39,40.

2.2. Estimation of effective permeability and formation factor via hybrid lattice Boltzmann/finite element simulations

In this work, effective permeability and formation factor were calculated using a hybrid lattice Boltzmann/finite element (LB/FE) scheme as a cost-efficient alternative to direct numerical simulations.[15,16,28,37] In the hybrid scheme, we first use a region growing algorithm to distinguish the isolated pore space from the connected one. Then, the connected pore space of a numerical specimen is divided into cubic unit cells of identical sizes ($190 \times 190 \times 190$ voxels, with volume of $(1.08\,\text{mm})^3$); within each unit cell made up of, a Poisson problem and