

# Upscaling Heterogeneous Shale Porosity from Nanometer- to Millimetre-Scale in 3-D

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## Abstract

Microstructures and pore systems in shales are key to understanding the role of shale in energy applications, but the characterisation of pores is highly challenging due to their small size and significant heterogeneity at multiple scales. This study proposes a novel multi-stage upscaling procedure to comprehensively investigate the heterogeneous and complex microstructures and pore systems in shales using 3D multi-scale imaging data. Five imaging techniques were used for characterisation from sub-nanoscale to macroscale (core-scale), spanning four orders of magnitude. Image data were collected using conventional X-ray computed tomography (XCT), Micro-CT, nano-CT, Focused Ion Beam Scanning Electron Microscope (FIB-SEM), and Electron Tomography (ET) techniques with voxel sizes of 0.6 nm, 10 nm, 120 nm, 1  $\mu\text{m}$  and 13  $\mu\text{m}$  respectively. Prior to upscaling, a novel two-step analysis was performed to ensure sub-samples were representative. Following this, a three-step procedure, based on homogenising descriptors and computed volume coefficients, was used to upscale the quantified microstructure and pore system. At the highest resolution (nanoscale), four distinct pore types were identified with sizes ranging from 2 nm to 4  $\mu\text{m}$ : intra-organic pores, organic-mineral interface pores, inter-mineral pores and intra-mineral pores. At the sub-micron scale, three pore-associated phases were identified: granular minerals (4-100  $\mu\text{m}$  diameter); phyllosilicate minerals grains (0.2 - 4  $\mu\text{m}$ ); organic matter particles (0.6 - 4  $\mu\text{m}$ ). Equations were derived for the relationship of porous phases and their associated pores at this scale. At the microscale, laminae and fractures were identified and the volume coefficients were recalculated to upscale the pore system to the

macroscale (millimetre). The integrated pore network across three scales principally combines two distinct sub-networks: 1) fractures with thickness of 4 -30  $\mu\text{m}$ , primarily parallel to the bedding, 2) a global, web-like pore network between phyllosilicate minerals with sizes in the range 6-50 nm and coordination numbers 2-5, and 3) a localized, cluster-like connected pore network lying within porous organic matter with sizes in the range 200 - 800 nm with coordination numbers 5 - 9. The accuracy of the upscaling methodology predicting the total porosity within 7.2% discrepancy from helium porosity. The pore geometry and network were further validated by pressure-dependant permeability measurements. The results provide a unique perspective to understanding heterogeneous rock types, The implications of the results for gas and liquid storage space and transport pathways in shales will be significant in many areas, including shale gas, carbon sequestration, nuclear disposal, and hydrogen storage.