A New Pore Network stochastic generation approach utilising bulk pore characterisation data with application to mudrocks

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With climate change mitigation actions in place, Carbon Capture and Storage (CCS) is by far the most industrially efficient technology to reach net-zero carbon emissions (HM Government, 2018), with current annual capture capacity exceeding 40 million tonnes of CO_2 world-wide (BP, 2020). While supercritical CO_2 is stored in conventional reservoirs or saline aquifers, overlying mudrock formations create a structural trap, preventing CO_2 leakage. Opalinus Clay, generally researched as a repository for radioactive waste, is a perfect candidate for CCS research, with a large dataset of mineralogical and petrophysical properties collected from existing publications (Bossart and Milnes, 2017) and experimental work allowing for good understanding of pore space geometry and underlying flow processes. It is necessary to estimate flow properties, such as permeability and capillary entry pressures, for mudrocks by numerical modelling, as the properties are difficult to obtain from laboratory tests on sample plugs.

Pore Network Modelling (PNM) is a method used for simulating pore-scale physiochemical processes on representative pore networks of sample pore space and estimating the flow properties, and is significantly more computationally efficient than most other methods. Techniques have been developed to extract networks from pore-grain resolved 3D images (Raeini et al., 2017, ThermoFisherScientific, 2020) and to integrate networks for specific sub-volumes of a sample (Ma et al., 2017, Jiang et al., 2013). However, submicron pores in mudrock are abundant and known to form critical flow pathways, but often distributed in a close association with large pores across the whole sample, other than scattered in isolation. This poses practical challenges to apply multiscale tomographic imaging for resolving pores at all scales. Stochastic pore network generation algorithms have been reported (Idowu and Blunt, 2009, Gostick et al., 2009, Jiang et al., 2012), and could be used to create networks where no images are available, but other specific pore characterisation data is present.

This work attempts to create an algorithm, which generates a representative pore network model with pore sizes ranging from sub-nanometre to over a micron, while using direct data input from bulk pore space measurements. An array of nodes was generated randomly based on low pressure adsorption and small angle neutron scattering data, with bonds defined based on nearest neighbours and coordination number. Pore-to-throat aspect ratio and element shape factors were adjusted using mercury intrusion measurements and specific surface area values. Model geometry was calibrated to match total porosity values measured by helium pycnometry. Hydraulic conductivity was modelled following the method used in (Song et al., 2018), which accounts for real gas flow and diffusion effects across a full range of Knudson number. Gas adsorption effects were implemented by changing node and bond effective radii, using methane and carbon dioxide high pressure adsorption isotherms.

The nonlinear system of equations is solved iteratively to achieve effective permeability convergence, using the Pardiso sparse solver interface (Intel, 2021) for improved performance at large model sizes. Calculated results were verified against unsteady state single-phase gas permeability measurements, performed on Opalinus Clay plugs, at a range of confining conditions and absolute pressures.

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