

**Centre for Doctoral Training (CDT):
Geoscience and its Role in the Low Carbon Energy Transition
(2021 start)**

Project Title: Predicting CO ₂ permeation through shale rocks
Host institution: University of Nottingham
Supervisor 1: Sean Rigby
Supervisor 2: Joseph Wood

Project description: This project is aimed at providing key parameters for estimating carbon sequestration. The use of CO₂ to displace methane from unconventional reservoirs, like gas shales, offers the potential for simultaneous improved methane recovery and CO₂ storage. A clear understanding of the mass transport mechanisms is essential for predicting the gas recovery and carbon storage efficiency due to its impact on how far the CO₂ will permeate throughout the reservoir. Unconventional reservoir rocks like shales have complex void spaces, with various surface chemistries and pore types, corresponding to various phases such as organic carbon and inorganic minerals. Due to the high prevalence of microporosity and surface adsorption in shales, the surface diffusion flux constitutes the largest component of the mass transport. Shales also represent a common caprock for aquifers used for carbon storage. This work will aim at predicting the surface diffusion rates, and thence overall mass transport fluxes, from the surface properties of typical reservoir rocks. The parameters thereby obtained are critical inputs for reservoir simulations to predict large-scale gas recovery, storage potential, and seal efficiency.

This work will develop a model for mass transport in heterogeneous rocks using multi-fractal-based models. Many previous studies have shown that the internal surface of shales is fractally rough. The model will use fractal physics to obtain the Arrhenius parameters for small-scale, surface hopping motion using transition state theory, and, also, to predict the larger-scale, anomalous diffusion in heterogeneous fractal void spaces. These parameters will then be incorporated into a model for larger length-scale transport, using percolation theory and critical path analysis to determine the particular rock surface and pore types that control the overall flux within a heterogeneous system. The model will be tested against experimental gas mass transport data for rock core samples.

The impact of the predicted differences in surface diffusion rates in different rock types will be assessed by up-scaling to field scale simulations of the displacement of methane by CO₂ in typical reservoirs. The student will develop expertise in rock core characterisation and permeation/uptake measurements, and reservoir simulation using commercial software.

Stated link to CDT theme: Results will improve design and efficiency of carbon sequestration projects
--

Any Additional Research Costs: None
--

Has access to data been secured? Data will be generated using existing UoN equipment

Career routes: Reservoir simulation; experimental officer (eg in BGS etc)
--