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Experimental and Numerical Study of Carbon Dioxide Geological Storage in Coal –**A Comparative Analysis with the application of Positron Emission Tomography Imaging.**

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With the global energy mix predominantly fossil fuel based¹, carbon dioxide (CO₂) capture, utilisation and geological storage (CCUS) is a key tool in reducing anthropogenic CO₂ emissions. One of the main challenges facing CCUS in coal seams is the loss of injectivity due to CO₂ coal swelling²⁻⁷. This work aims to improve the understanding of CO₂ transport mechanisms in coal by applying in-situ Positron Emission Tomography (PET) imaging to obtain direct images of CO₂ flow in coal, allowing for better CO₂ geosequestration techniques.

This work presents a comparative history matching analysis between a one-dimensional Advection Diffusion Equation (ADE) model and experimental data obtained from in-situ PET imaging during core flooding. Traditional core flooding methods usually rely on assumptions that flow within samples is piston like, possibly leading to inaccuracies during modelling<sup>8 \lt /sup>. The use of PET imaging provides an actual representation of gas flow behaviour and serves as a ground truth point of reference during history matching. This comparative analysis focuses on determining how the diffusion coefficient of CO₂ in coal changes vis-à-vis coal properties such as initial adsorbate molecules, coal swelling and their effects on gas (particularly CO₂) diffusion within coal samples.

[¹¹C]CO₂ was utilised as the PET radiotracer during core flooding experiments to directly image carbon dioxide (CO₂) diffusion dynamics and mechanisms within coal samples. A 1-D ADE model in MATLAB was then history matched to experimental data for the purpose of obtaining the diffusion coefficient that best represented what was observed. Additionally, X-Ray μCT imaging technology was utilised to obtain high resolution (30μm) images of the core samples. Machine learning algorithms were then applied to these CT images as a method of digital image segmentation to obtain a good estimate of sample porosity, further improving the accuracy of the 1-D ADE model. In-situ PET scans allow for a dynamic observation of gas flow during the core flooding experiment as well as a source on which gas diffusion effects can be confirmed through the use of history matching with a 1-D ADE model in MATLAB and subsequently back calculating the diffusion coefficient of best fit from the ADE model that accounts for key core flooding parameters such as coal porosity, gas flow rate and type of injected gas.

The results show that stable diffusion coefficients arise when samples are dry and an inert gas (He) is used as the carrier gas. In the cases of competitive adsorption between methane (CH₄) and CO₂ in samples that were CH₄ saturated show a decreasing diffusion coefficient. Diffusion coefficients in CO₂ saturated samples were in the order of 100 times lower than in samples that were not exposed to CO₂ prior to injection. This indicates that coal swelling has a significant impact on the ability of gas to effectively diffuse in the coal matrix. These findings further develop the body of knowledge surrounding CO₂ geosequestration in unmineable coal seams and contributes to the optimisation of CCUS processes during the transition to low-carbon and renewable energy sources.

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