

## Pore Scale Modelling of Carbon Capture and Sequestration.

Payton, R.L.<sup>1</sup>, Yizhuo, S.<sup>1</sup>, Kingdon, A.<sup>2</sup>, Hier-Majumder, S.<sup>1</sup> 2019. Kingdon, A. 2019.

1. Royal Holloway University of London, Department of Earth Sciences, Egham Hill, Egham, TW20 0EX, UK
2. British Geological Survey, Keyworth, Nottingham, NG12 5GG, UK

Poster H33N-2193 : presented at 2019 AGU Fall Meeting, San Francisco, CA, USA, 9-13 Dec. <https://agu.confex.com/agu/fm19/meetingapp.cgi/Paper/516278>

### Abstract

Carbon capture and storage (CCS) has been identified as an area of research interest due to its potential for reducing the global greenhouse effect. CCS typically involves injection of supercritical CO<sub>2</sub> into abandoned oil and gas reservoirs or saline aquifers with sufficient porosity and permeability. CO<sub>2</sub> is trapped by a number of mechanisms which differ in security with storage in carbonate minerals (geological carbon storage) being the most secure long term mechanism. Consequently, it is important to understand the behaviour of reactive flows and what influences the mineralisation process to occur so that the CCS process can be optimised as a tool for reducing the greenhouse effect.

In this work, we present a novel methodology based on 3D models of connected pore structures extracted from micro computed tomography (microCT). The pore geometry is used to build a representative volume in which fluid flow and mineral precipitation takes place. We numerically solve the governing equations of coupled advection-diffusion-reaction using Finite Element Discretisation. The performed simulations describe advection and diffusion of an injected CO<sub>2</sub> brine as well as reaction of this fluid phase with the pore walls to form carbonate minerals. A series of different Damköhler (Da) and Péclet (Pe) numbers are employed to investigate the effect on mineralisation and brine migration of differing advective, diffusive and reactive strengths in the system. We complement our microscale model of porous flow with a regional scale model taking into account geological structures relevant to the subsurface of the UK Geoenergy Observatories Cheshire Energy Research Facility Site, UK.

# H33N-2193: Pore Scale Modelling of Carbon Capture and Sequestration

Ryan L Payton<sup>1</sup>, Yizhuo Sun<sup>1</sup>, Andrew Kingdon<sup>2</sup> and Saswata Hier-Majumder<sup>1</sup>

Dept. Earth Sciences, Royal Holloway University of London<sup>1</sup>, British Geological Survey<sup>2</sup>  
ryan.payton.2015@live.rhul.ac.uk



- We present a reactive flow model describing mode of H<sub>2</sub>CO<sub>3</sub> transport at both regional (2D) and micro (3D) scales.
  - Increasing porosity results in a shift from a channelised migration front to a tabular front.
  - Greater porosity and higher anorthite fraction both lead to higher CaCO<sub>3</sub> precipitation.
  - At the micro scale, throat radii <25μm control reduction in effective porosity by precipitation.

## 1. Introduction

Carbon capture and sequestration (CCS) is considered by many to be a major component in the solution for tackling anthropogenic climate change. The mode of transport of the reactive H<sub>2</sub>CO<sub>3</sub> phase is of importance to understand how it affects mineralisation. We examine the impact of porosity and anorthite fraction on regional transport and anorthite fraction and connected porosity on micro scale transport.

## 2. Regional Scale CCS

$$\begin{aligned}
 (1) \quad & \nabla \cdot \mathbf{u} = 0 & (2) \quad & \phi \mathbf{u} = -\frac{k}{\mu} (\nabla p + \rho g \hat{\mathbf{z}}) \\
 (3) \quad & (1 - \phi) \frac{\partial c_1}{\partial t} = -\Gamma_1 & (4) \quad & (1 - \phi) \frac{\partial c_2}{\partial t} = \Gamma_2 \\
 (5) \quad & \phi \frac{\partial c_0}{\partial t} + \phi \mathbf{u} \cdot \nabla c_0 = \phi D \nabla^2 c_0 - \Gamma_0 + f_c \\
 (6) \quad & \text{CaAl}_2\text{Si}_2\text{O}_8(s) + \text{H}_2\text{CO}_3(aq) \rightleftharpoons \text{CaCO}_3(s) + \text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4(s)
 \end{aligned}$$

Equations 1-6: Regional scale numerical model governing equations.

$$\begin{aligned}
 (7) \quad & \mathcal{D}a = \frac{L \Gamma_0}{\mathbf{u}_0} & (8) \quad & \mathcal{P}e = \frac{L \mathbf{u}_0}{D}
 \end{aligned}$$

Equations 7&8: Definition of non-dimensional terms.

Fig. 1a

- Low porosity promotes formation of distinct channels.
- Greater porosity results in a planar migration front and a reduction in migration extent.

Fig. 1b

- Greater An fraction causes more reaction and consequently a reduced migration front.

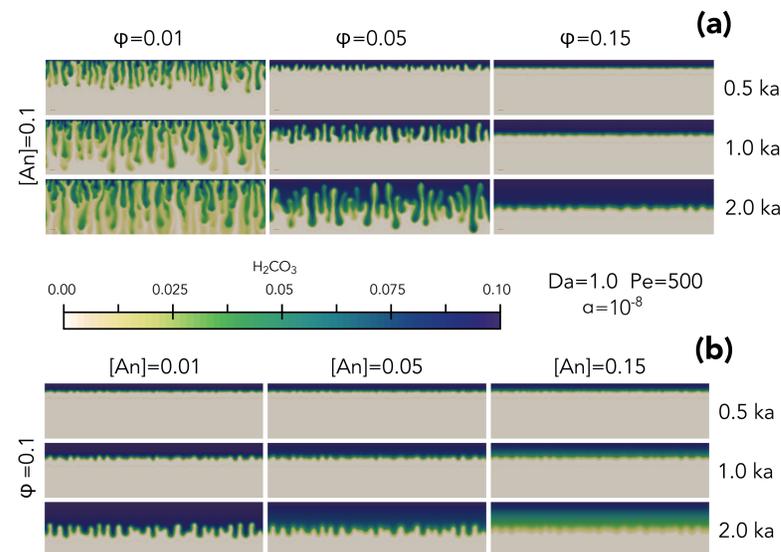


Figure 1: Top down migration front of H<sub>2</sub>CO<sub>3</sub> under variable porosity (a) and An fraction (b) up to 2,000 years simulated time.

$$\begin{aligned}
 (9) \quad & \nabla \cdot \mathbf{u} = 0 & (10) \quad & \mu \nabla^2 \mathbf{u} - \nabla p = 0 \\
 (11) \quad & \frac{\partial c_1}{\partial t} = -\Gamma_1 & (12) \quad & \frac{\partial c_2}{\partial t} = \Gamma_2 \\
 (13) \quad & \frac{\partial c_0}{\partial t} + \mathbf{u} \cdot \nabla c_0 = D \nabla^2 c_0 - \Gamma_0
 \end{aligned}$$

Equations 9-13: Micro scale numerical model governing equations.

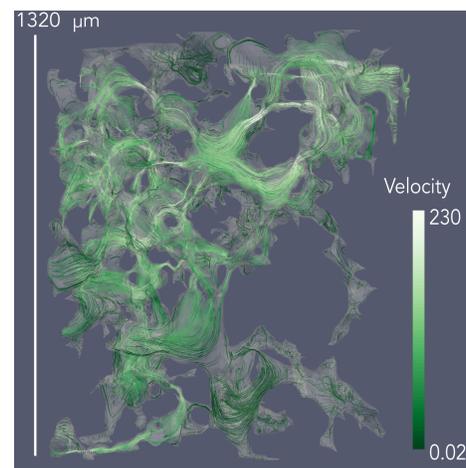


Figure 3: Nondimensional velocity streamlines through connected pore space. Colourmap is in logarithmic scale.

Fig. 2a

- Increasing An fraction results in a larger mass of CaCO<sub>3</sub> stored, increasing by ~300 MT from 5-25% An.
- Increasing reactivity (Da) results in a greater mass stored.

Fig. 2b

- Increasing porosity causes a greater mass of CaCO<sub>3</sub> to be stored.
- A shallower curve here suggests porosity is not as influential as An fraction on mass stored.

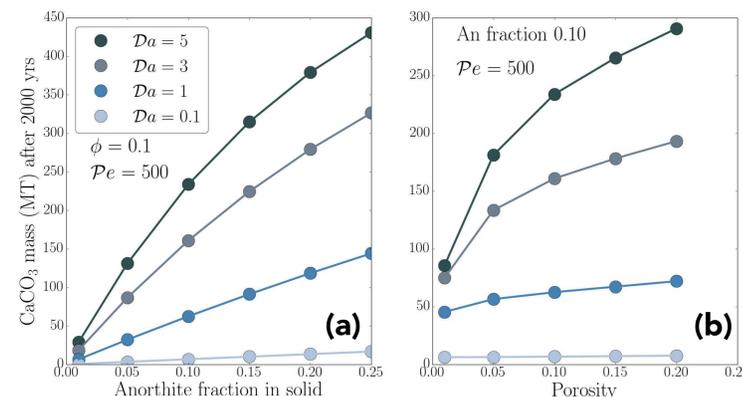


Figure 2: The relationship between An frac (a) and porosity (b) with mass of CaCO<sub>3</sub> precipitated from the H<sub>2</sub>CO<sub>3</sub> and Ca reaction. Greater Da increases the strength of this reaction.

## 3. Micro Scale CCS

We imaged a sample of Brae sandstone from the North Sea using μCT. We investigate the mode of transport of H<sub>2</sub>CO<sub>3</sub> under groundwater flow conditions through connected porosity.

Fig. 3

- Main flow channels are highlighted in brighter colours.
- Deprived areas are shown by darker colours.
- A clear central highway is seen despite complete connectivity.

Fig. 4

- Highlights the CaCO<sub>3</sub> concentration as a function of time.
- The main channels fill rapidly.
- Low velocity channels are deprived far longer.

Fig. 5

- A narrow throat causes a CaCO<sub>3</sub> build up behind it.
- It takes far longer for peak concentration to be reached beyond the bottleneck.
- This geometry is likely to become isolated and reduce effective porosity.

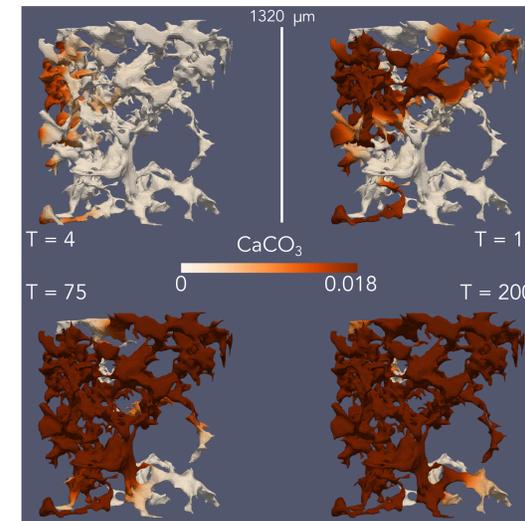


Figure 4: Whole sample CaCO<sub>3</sub> concentration map. Flow is L-R.

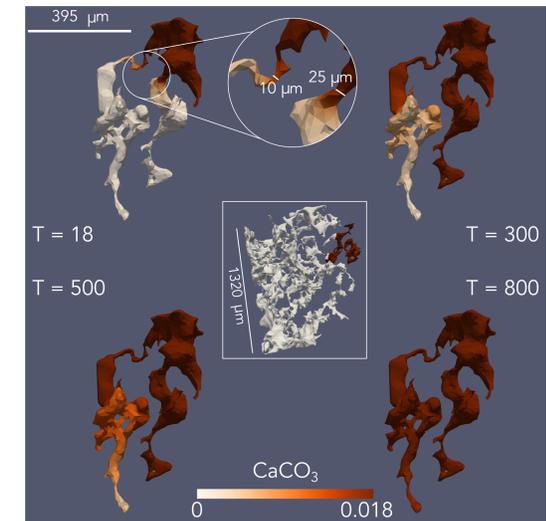


Figure 5: Subsample CaCO<sub>3</sub> concentration map. Flow is from the upper right corner.

Fig. 6

- As the An fraction increases, the peak CaCO<sub>3</sub> concentration does too.
- The large difference in peak CaCO<sub>3</sub> between 5% and 15% shows the importance of lithology in choosing a target formation for CCS.

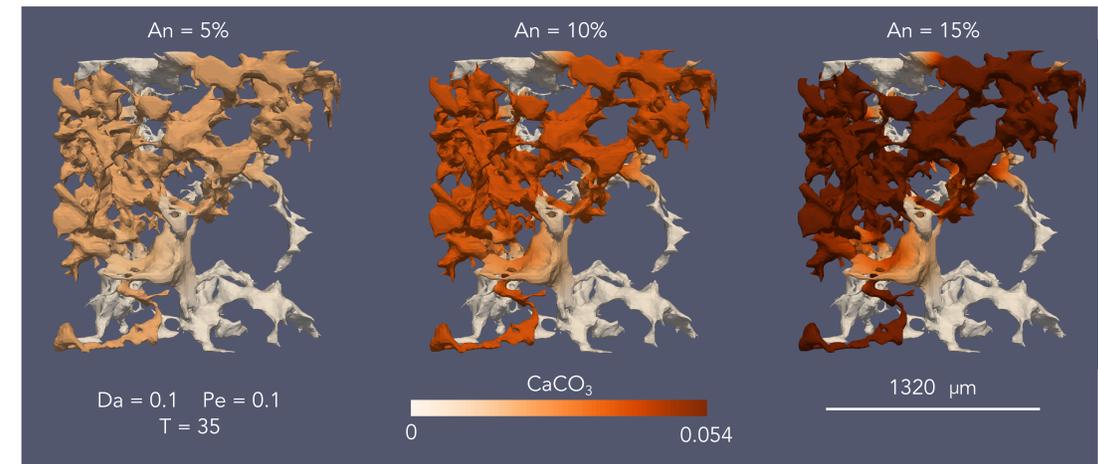


Figure 6: CaCO<sub>3</sub> concentration map for variable An fraction. Flow is from L-R.

## 4. Future Work

1. A method of upscaling of the micro scale model will be developed by simulating CaCO<sub>3</sub> precipitation in μCT images with different porosity.
2. Dimensional analysis of micro scale results to determine mass of CaCO<sub>3</sub> stored in the study volumes.
3. Validation of the micro model through simulation on cemented samples with the cement phase removed to compare precipitation choke points.

## Acknowledgements

This work is financially supported by a NERC studentship with the London NERC DTP. We would also like to thank Oracle for a cloud computing grant. Further thanks to Frank Lehane at RHUL for technical computing support throughout the project.