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

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- We present a reactive flow model describing mode of H_2CO_3 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 $CaCO_3$ precipitation.
- At the micro scale, throat radii $<25\,\mu m$ 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_2CO_3 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

$$(1)\quad \nabla \cdot \boldsymbol{u} = 0 \qquad\qquad (2)\quad \phi \boldsymbol{u} = -\frac{k}{\mu}(\nabla p + \rho g \hat{\boldsymbol{z}})$$

$$(3)\quad (1-\phi)\frac{\partial c_1}{\partial t} = -\Gamma_1 \qquad (4)\quad (1-\phi)\frac{\partial c_2}{\partial t} = \Gamma_2$$

$$(5)\quad \phi\frac{\partial c_0}{\partial t} + \phi\boldsymbol{u}\cdot\nabla c_0 = \phi D \nabla^2 c_0 - \Gamma_0 + f_c$$

$$(6)\quad CaAl_2Si_2O_{8(s)} + H_2CO_{3(aq)} \rightleftharpoons CaCO_{3(s)} + Al_2Si_2O_5(OH)_{4(s)}$$

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

$$(7)\quad \mathcal{D}a = \frac{L\Gamma_0}{\boldsymbol{u_0}} \qquad\qquad (8)\quad \mathcal{P}e = \frac{L\boldsymbol{u_0}}{D}$$

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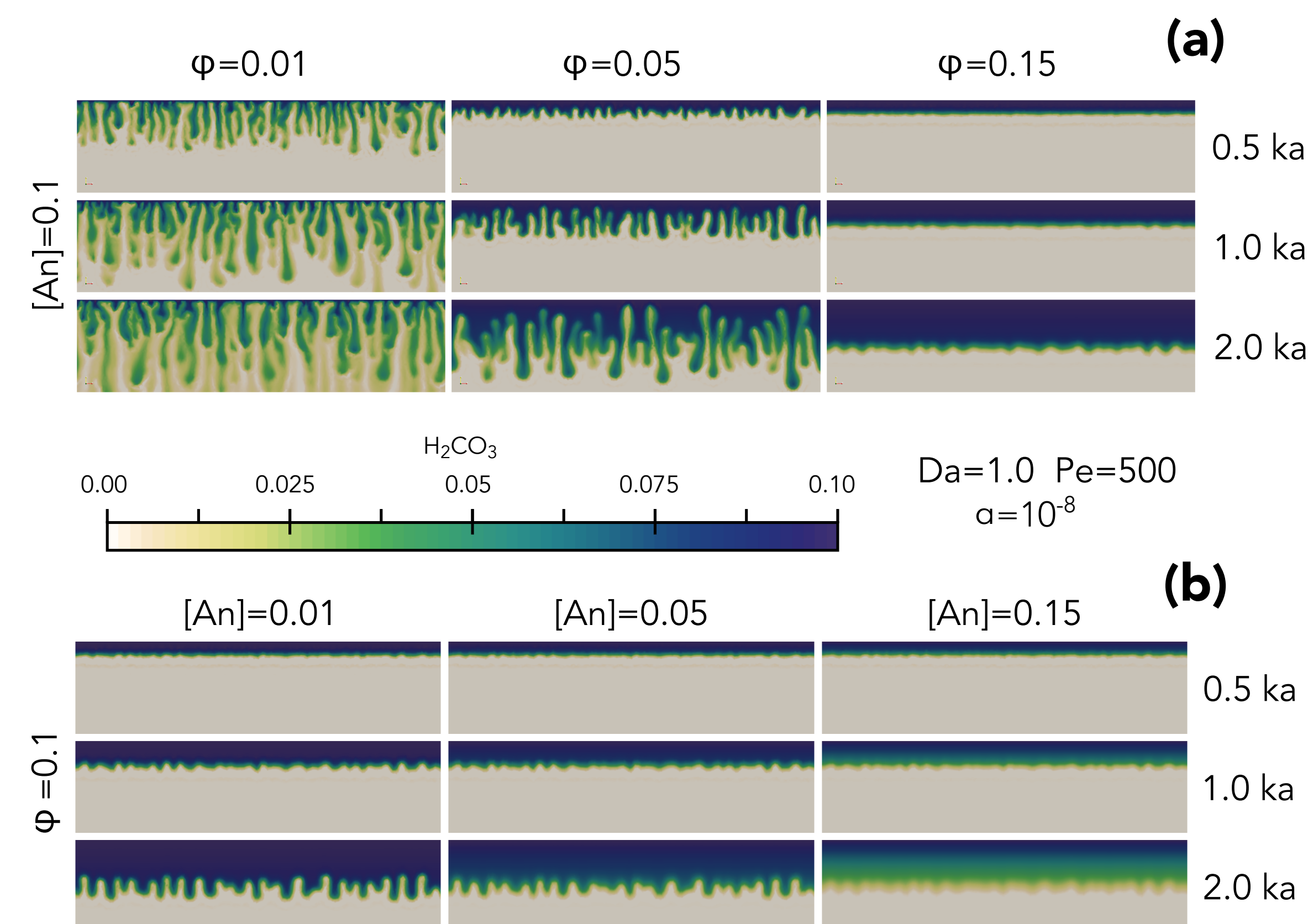- Greater An fraction causes more reaction and consequently a reduced migration front.

Figure 1: Top down migration front of H_2CO_3 under variable porosity **(a)** and An fraction **(b)** up to 2,000 years simulated time.

$$(9)\quad \nabla \cdot \boldsymbol{u} = 0 \qquad (10)\quad \mu\nabla^2\boldsymbol{u} - \nabla p = 0$$

$$(11)\quad \frac{\partial c_1}{\partial t} = -\Gamma_1 \qquad (12)\quad \frac{\partial c_2}{\partial t} = \Gamma_2$$

$$(13)\quad \frac{\partial c_0}{\partial t} + \boldsymbol{u}\cdot\nabla c_0 = D\nabla^2 c_0 - \Gamma_0$$

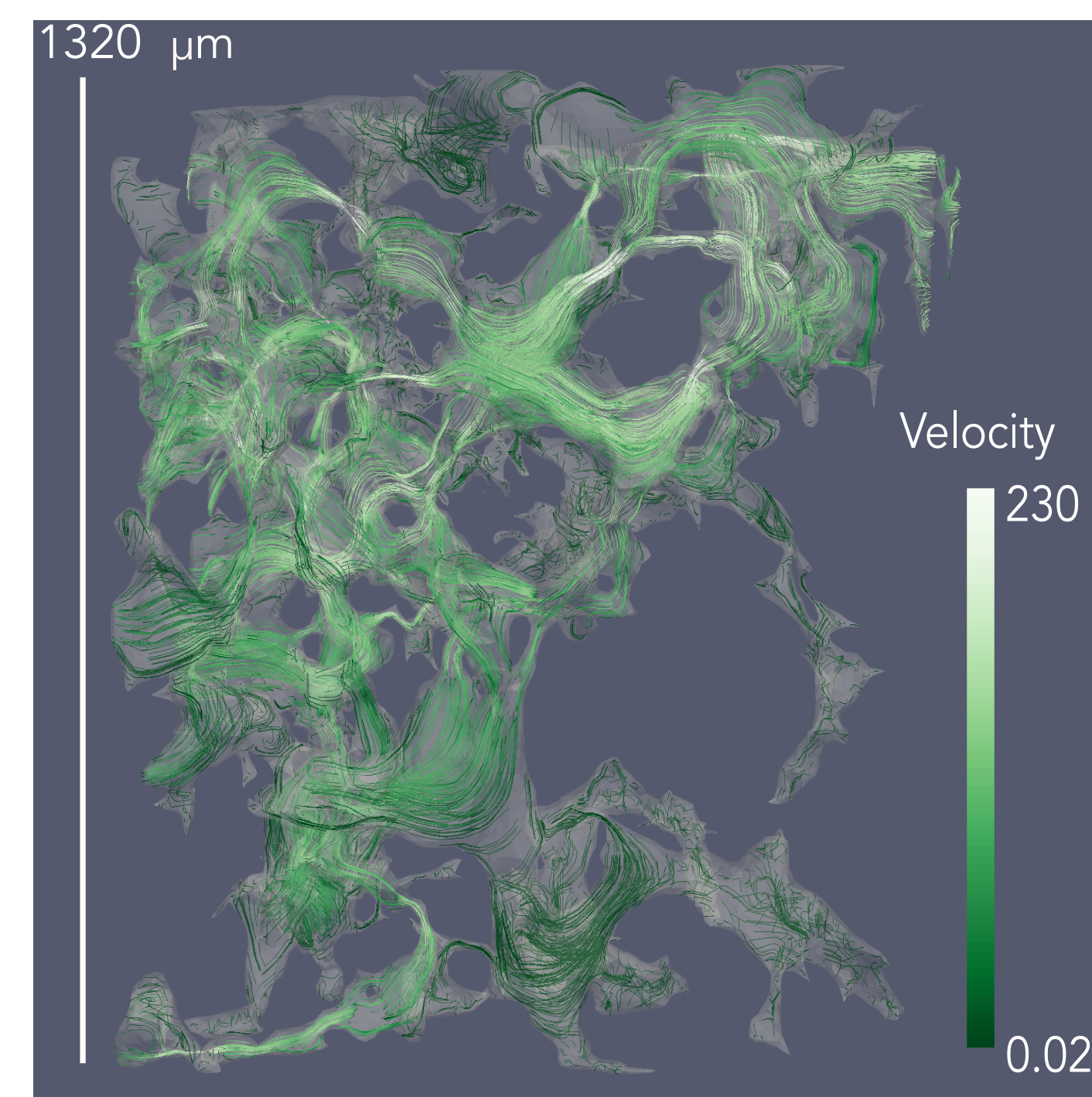**Equations 9-13:** Micro scale numerical model governing equations.

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 $CaCO_3$ 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 $CaCO_3$ 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 $CaCO_3$ precipitated from the H_2CO_3 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_2CO_3 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 $CaCO_3$ 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 $CaCO_3$ 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.

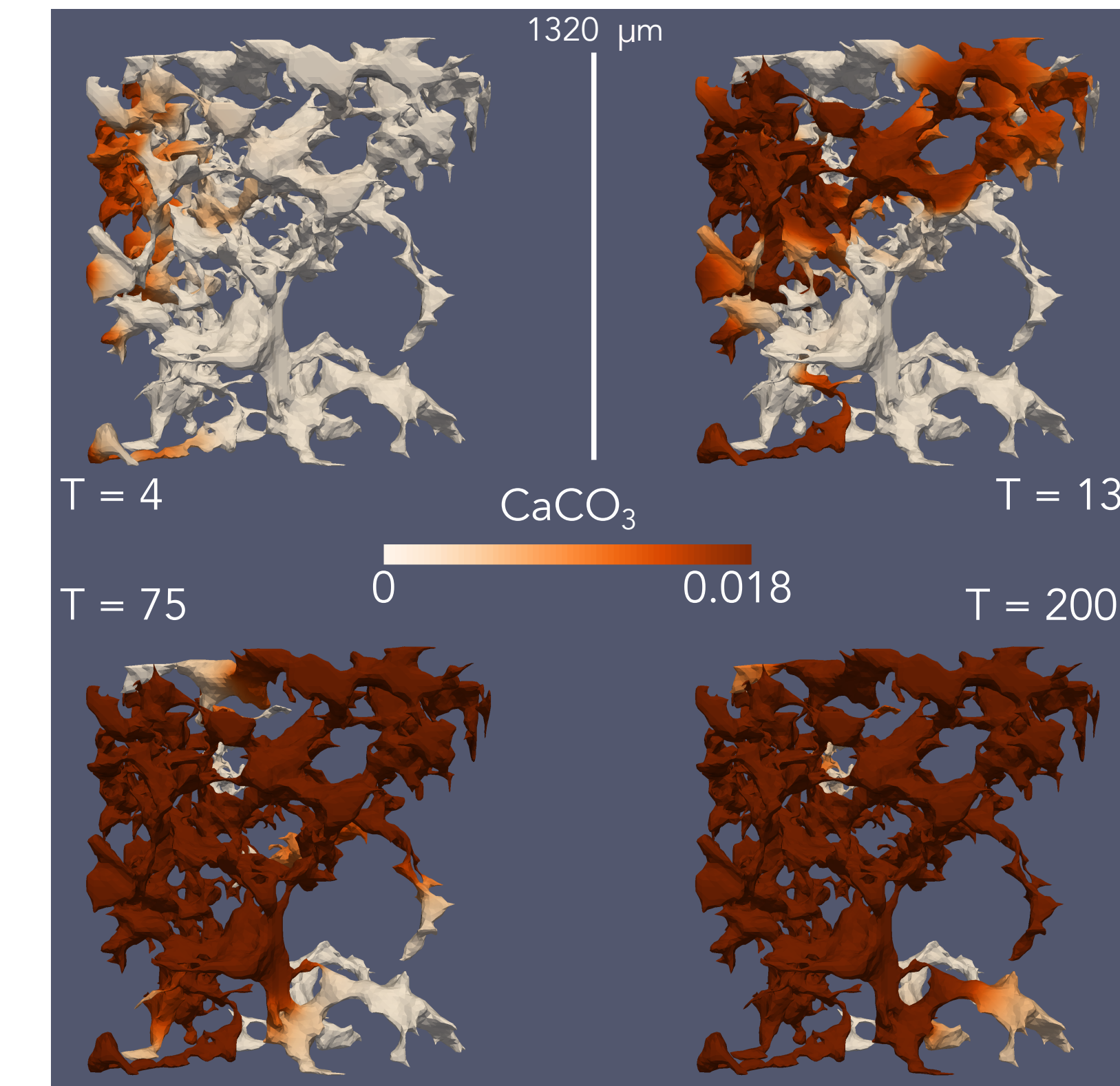**Figure 4:** Whole sample $CaCO_3$ concentration map. Flow is L-R. Da = 0.1, An = 0.05.

Figure 5: Subsample $CaCO_3$ concentration map. Flow is from the upper right corner. Da = 0.1, An = 0.05.

Fig. 6
- As the An fraction increases, the peak $CaCO_3$ concentration does too.
- The large difference in peak $CaCO_3$ between 5% and 15% shows the importance of lithology in choosing a target formation for CCS.
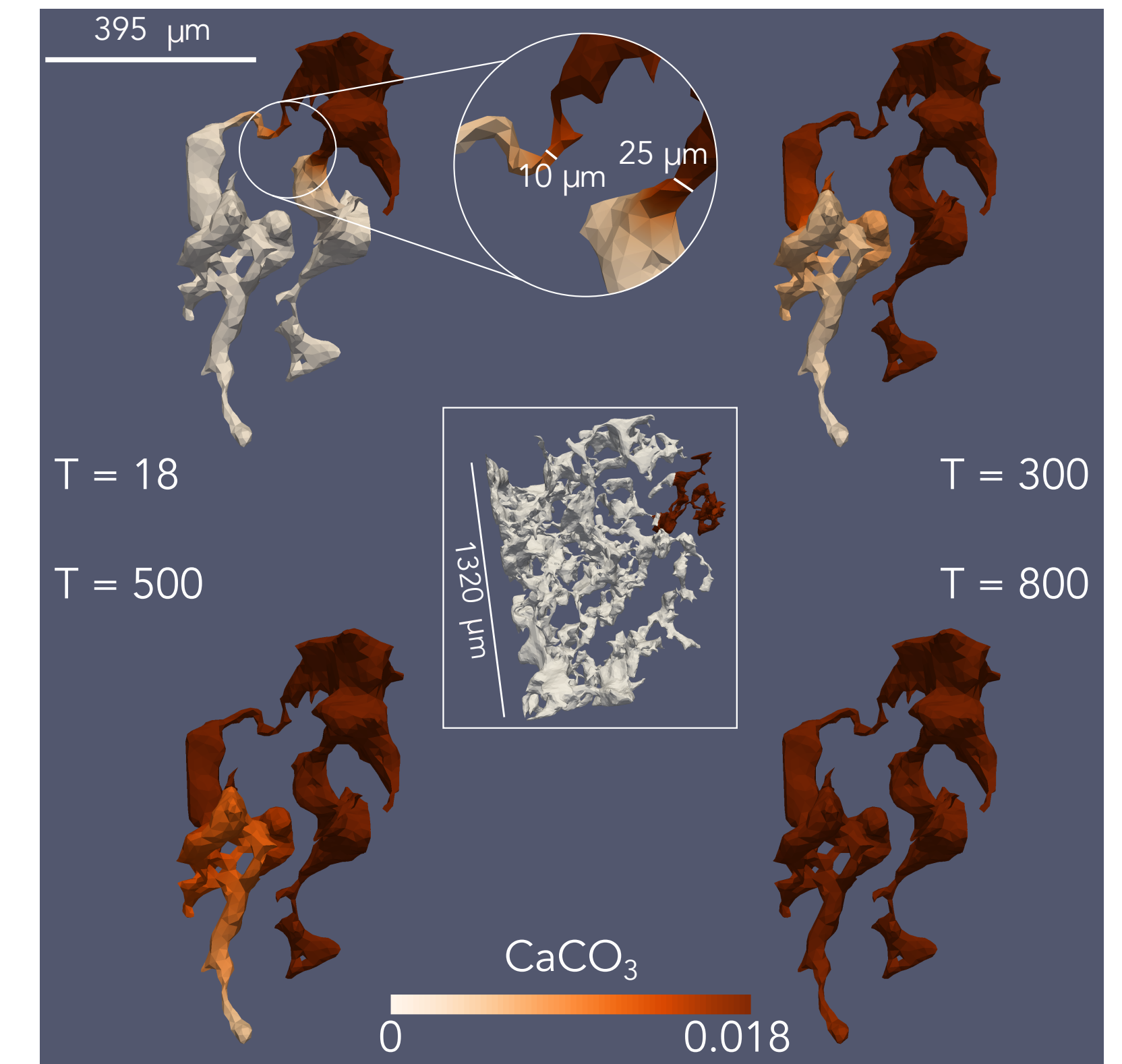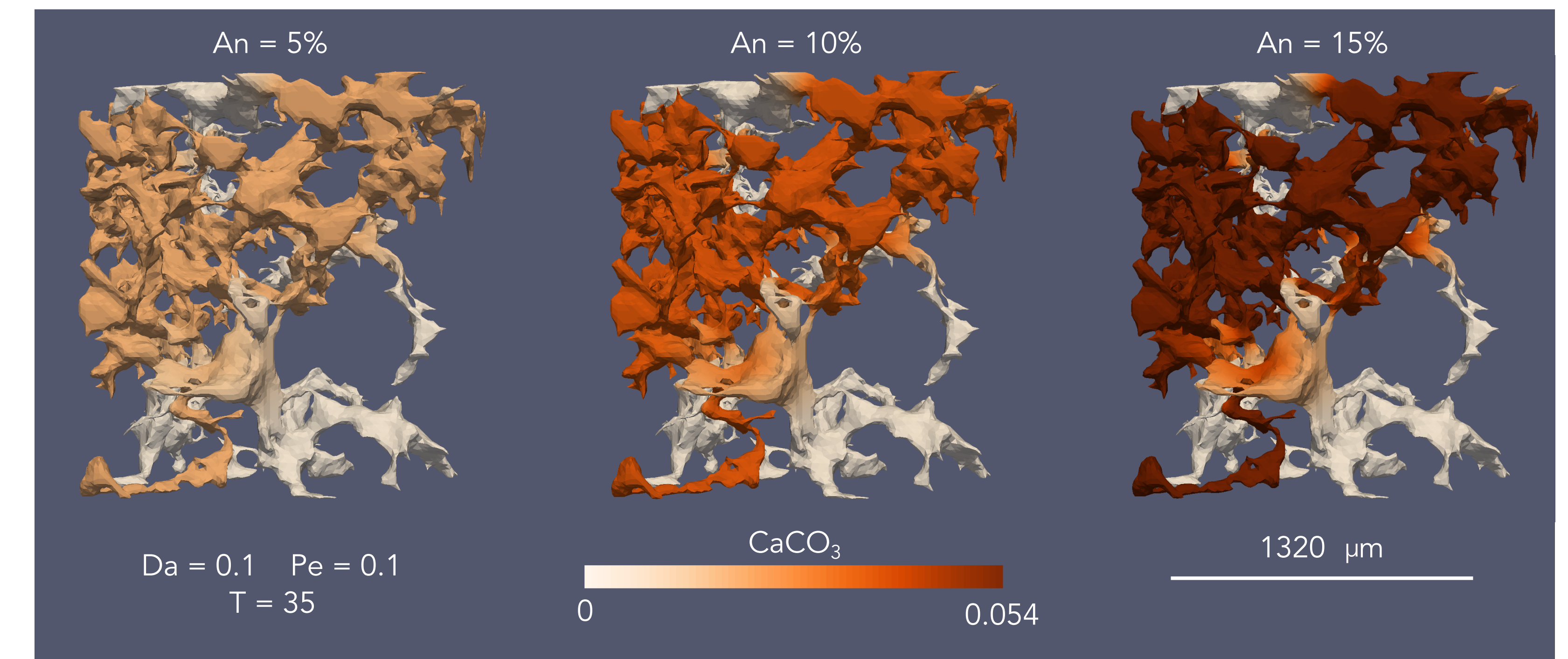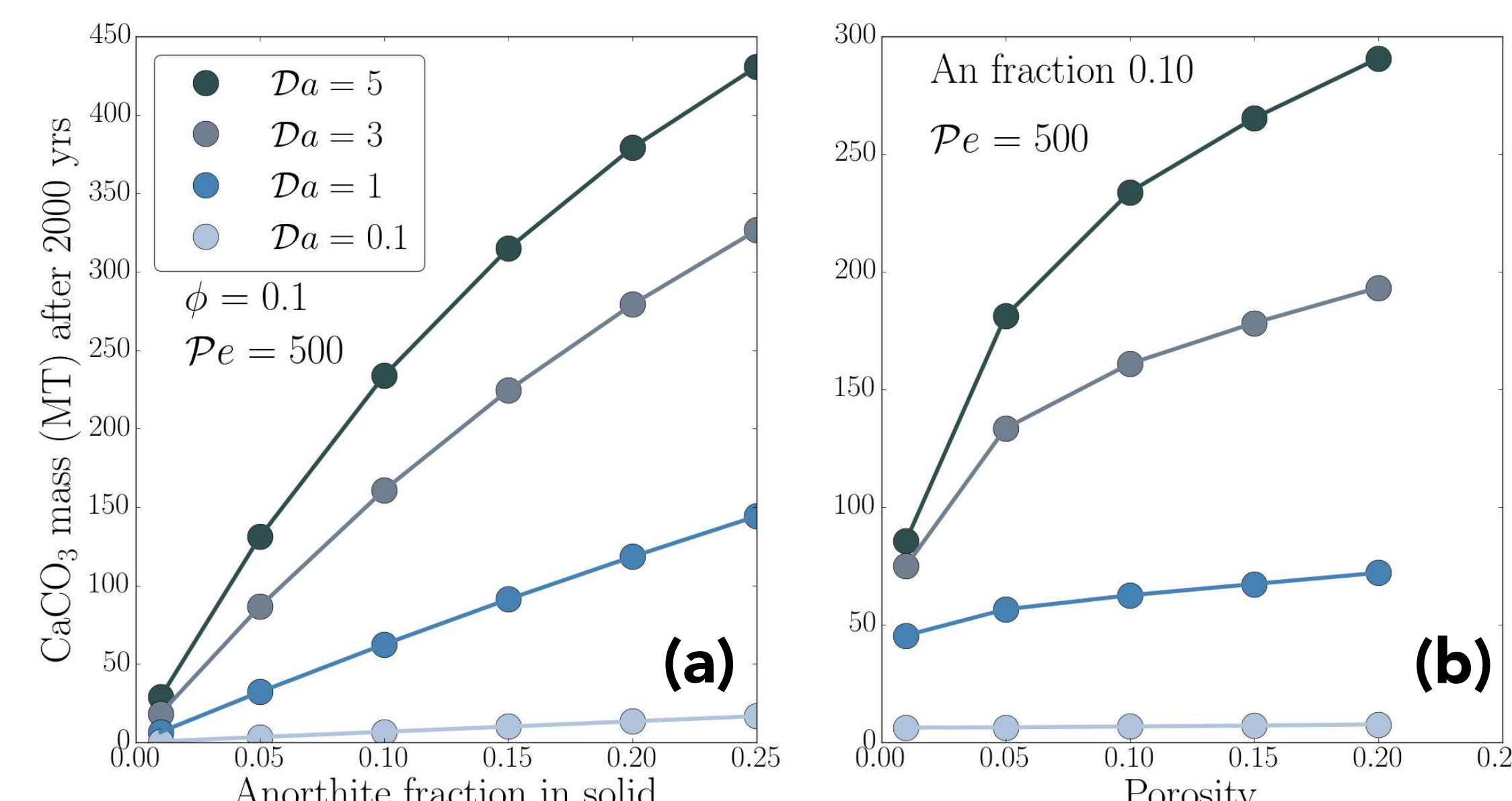

Figure 6: $CaCO_3$ concentration map for variable An fraction. Flow is from L-R. Da = 0.1.

4. Future Work

1. A method of upscaling of the micro scale model will be developed by simulating $CaCO_3$ precipitation in μCT images with different porosity.

2. Dimensional analysis of micro scale results to determine mass of $CaCO_3$ 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