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Quantifying the impact of viscosity variations induced by a chemical reaction on mixing efficiency in porous media

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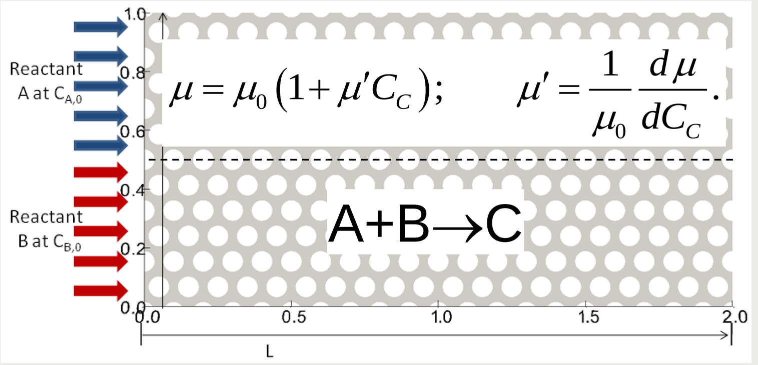
Overview

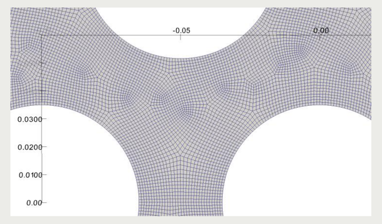
- Mixing-induced reacting flows in porous media can be used to develop subsurface flow for enhanced subsurface natural resource recovery and carbon sequestration
- In this work, we examine the case of reaction products that change the viscosity of the fluid to evaluate :
  - the impact of viscosity variations on mixing efficiency in porous media
- Computationally powerful & highly parallelized pore-scale model implemented in the SIERRA/ARIA finite element CFD code is used to examine:
  - flow in porous media with chemical reaction dependent viscosity

Pore Scale Modeling

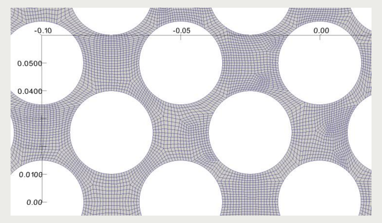
- Mixing-induced chemical reactions can alter fluid properties (viscosity and density), mixing efficiency, and shear rate for engineered solutions



$$\mu = \mu_0 (1 + \mu' C_C); \qquad \mu' = \frac{1}{\mu_0}\frac{d\mu}{dC_C}.$$



Loosely packed array
Porosity = 0.556
Grain diameter = 0.07 cm



Closely packed array
Porosity = 0.434
Grain diameter = 0.03 cm

μ is the viscosity of the solvent. Thickening (μ' >0) and thinning (μ' <0) viscosity with product concentration (C_c) by bimolecular reaction

Incompressible Navier-Stokes equation: Velocity (*u*) at pore scale

Multicomponent Reactive Transport at pore scale

Δt

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right) C_A = D_A \nabla^2 C_A - kC_A C_B$$
$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right) C_B = D_B \nabla^2 C_B - kC_A C_B$$
$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right) C_C = D_C \nabla^2 C_C + kC_A C_B$$

⇒

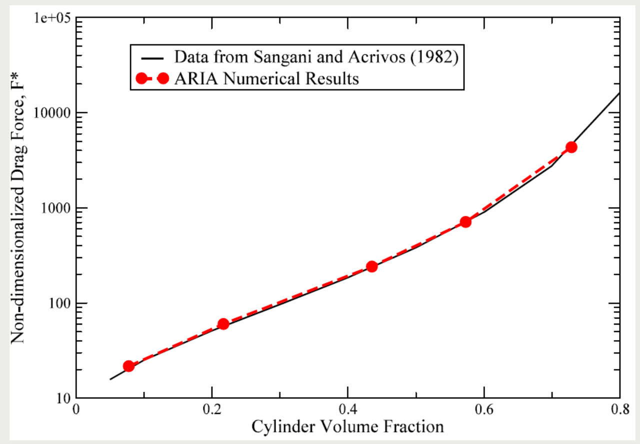
$$\left(\frac{\partial}{\partial t} + Pe\,\mathbf{u}\cdot\nabla\right) c_A = \delta_A \nabla^2 c_A - Da\ c_A c_B$$
$$\left(\frac{\partial}{\partial t} + Pe\,\mathbf{u}\cdot\nabla\right) c_B = \delta_B \nabla^2 c_B - Da\ c_A c_B$$
$$\left(\frac{\partial}{\partial t} + Pe\,\mathbf{u}\cdot\nabla\right) c_C = \nabla^2 c_C + Da\ c_A c_B$$

$$Pe = \frac{Ul}{D_C} \qquad Da = \frac{kc_{A,0} l^2}{D_C} \qquad \delta_A = D_A/D_C \qquad \delta_B = D_B/D_C$$

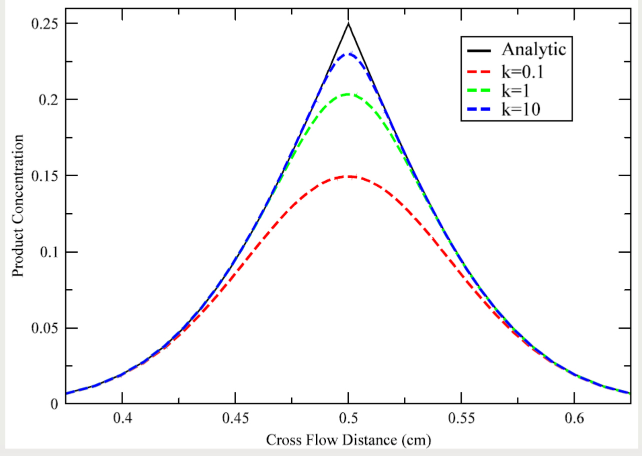
Fluid Viscosity Update

$$\bar{\mu} = \mu/\mu_0 = 1 + \bar{\mu}' c_C \qquad \bar{\mu}' = \frac{C_{A,0}}{\mu_0}\frac{d\mu}{dC_C}$$

Drag force on an array of cylinders

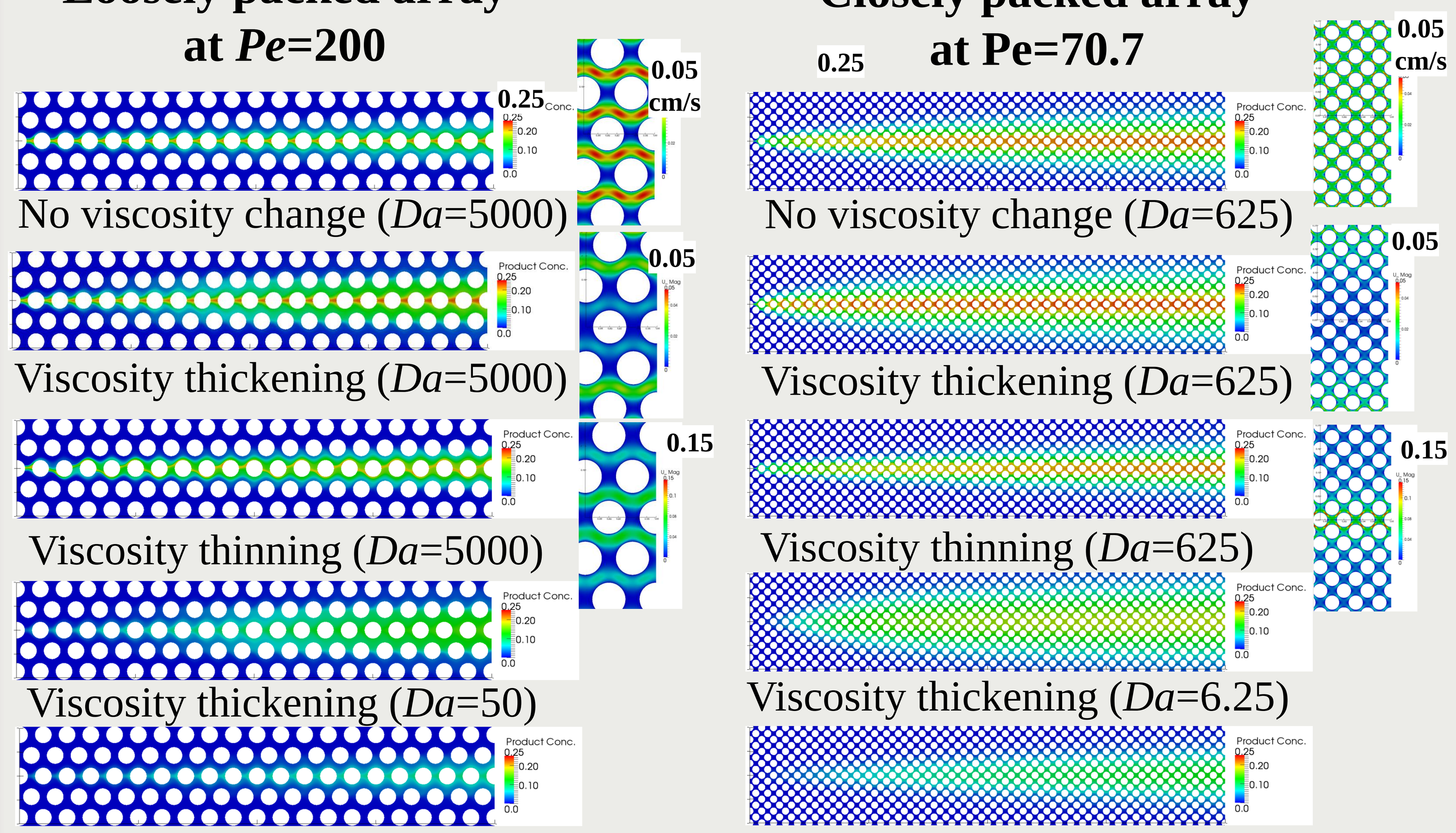


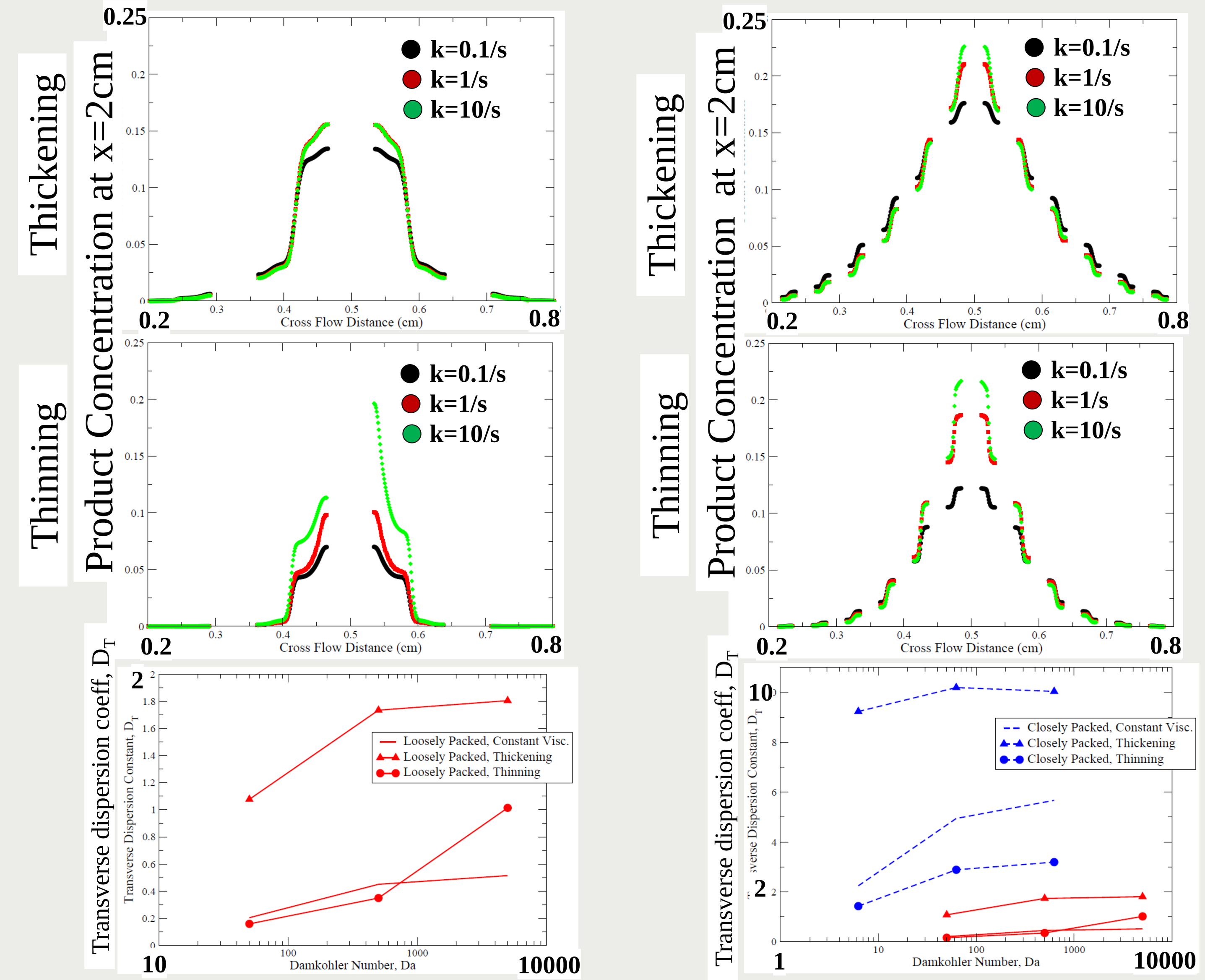
Reaction along a transverse mixing zone with constant viscosity



Pore Scale Modeling Results

Product concentration and flow velocity change

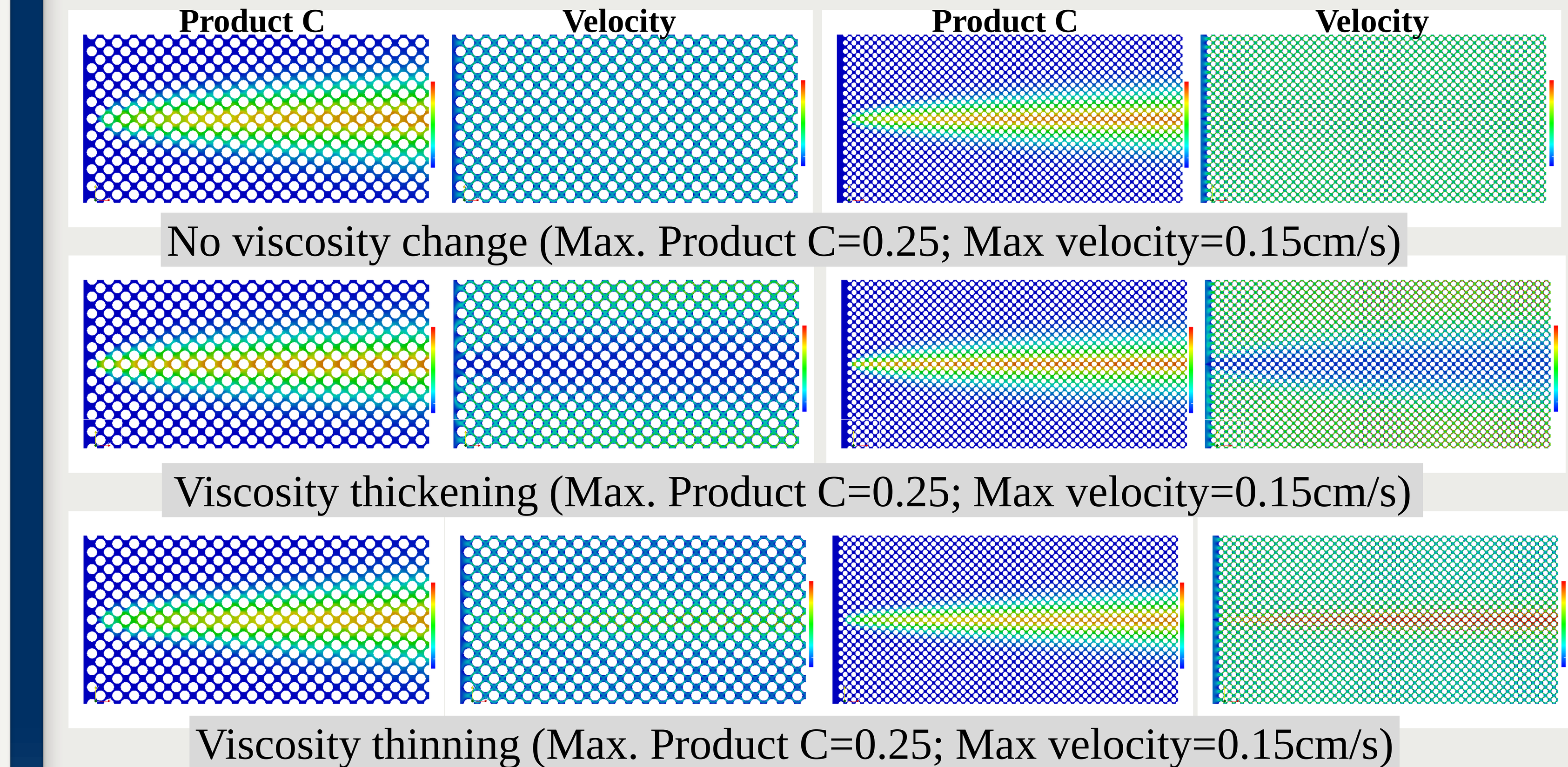


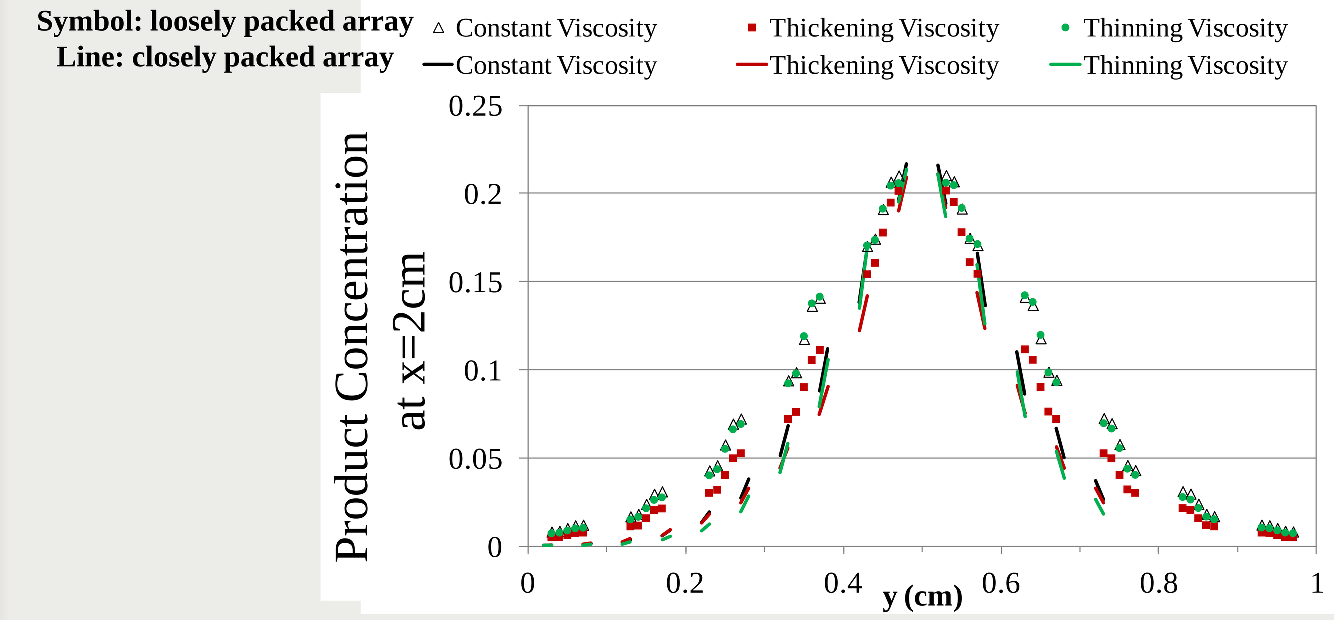


- More reaction product was formed when fluid viscosity increases with increasing product concentration (viscous thickening) than the opposite case (viscous thinning)
- Enhanced mixing at pore scale leads to enhanced reaction rates at high *Da* and lower porosity due to the higher interfacial area and smaller diffusion time scale
- Thinning viscosity creates flow focusing along the mixing line, resulting in streamline compression and lower transverse dispersion
- Flows with viscous thinning reactions can become unstable at high *Da*, leading to enhanced mixing and reaction rates under high *Pe* and higher porosity

Pe=7 & *Da*=62.5

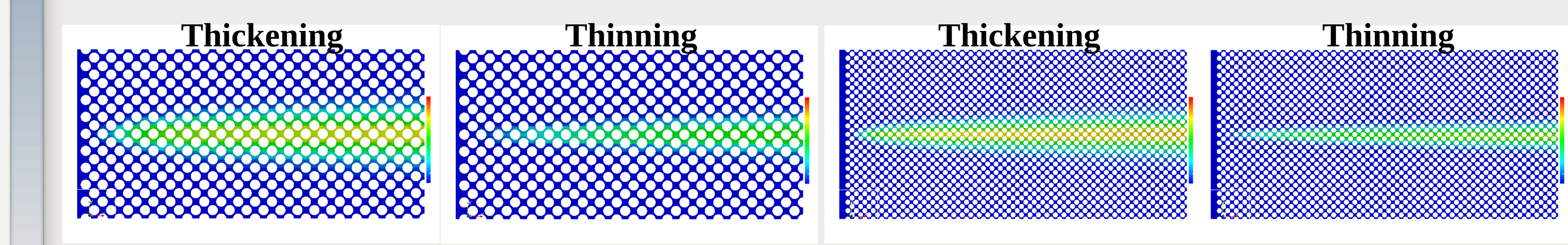
U_{in}=0.01cm/s & *k*=2.5/s | U_{in}=0.02cm/s & *k*=10/s





Pe=70 & *Da*=62.5

U_{in}=0.01cm/s & *k*=0.25/s | U_{in}=0.02cm/s & *k*=1/s



- At *Pe*=7 and *Da*=62.5, the effect of viscosity variations on product concentration at the end of domain was minimal in both packed arrays
- At *Pe*=70 and *Da*=62.5, the effect of viscosity variations on product concentration is significant in both packed arrays
- This comparison shows that at a moderate *Da* (62.5) a case with the lower *Pe* has more significant dependence of the overall reaction rate on Pe. A range of Da and Pe values need to be tested.

- Pore scale model with high performance computing capability will be used to test experimental results with emulsion-stabilizing nanoparticles in order to find optimal delivery of engineered solutions under a variety of pore-geometry conditions

References: • Davison, S. M., H. Yoon, and M. J. Martinez, 2012, Pore scale analysis of the impact of mixing-induced reaction on viscosity variations, Advances in Water Resources, 38, 70-80.

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