Numerical simulation of kinetic interface sensitive tracers in laboratory column experiments with COMSOL Multiphysics

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Introduction: The kinetic interface-sensitive tracers (KIS tracers) are used to give a partial picture of the spreading, mixing and plume migration of supercritical carbon dioxide ($scCO_2$) in the deep saline aquifer by estimating the interfacial areas between $scCO_2$ and brine during the injection of $scCO_2$. To get a better understanding of the KIS tracer reaction and transport processes in the two-phase flow system, a novel modeling approach with respect to specific interfacial area was developed in COMSOL Multiphysics®.

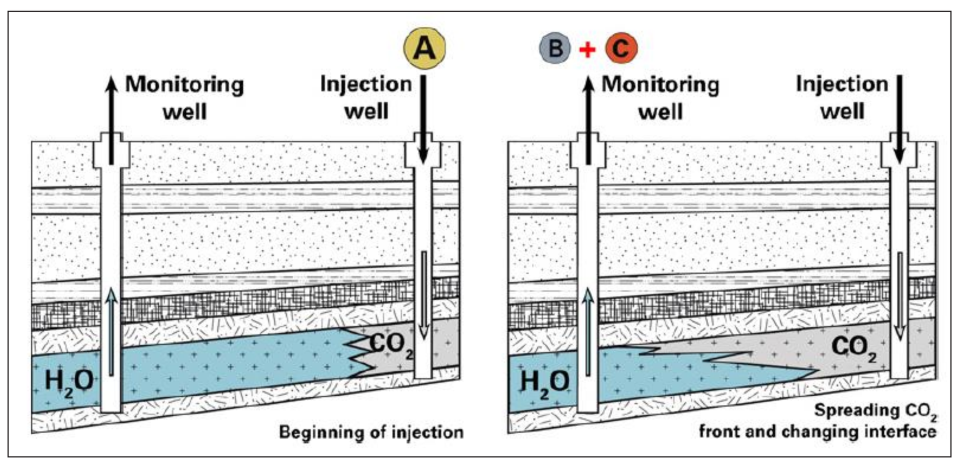

Figure 1. KIS tracer application in the field, Schaffer et al. 2013

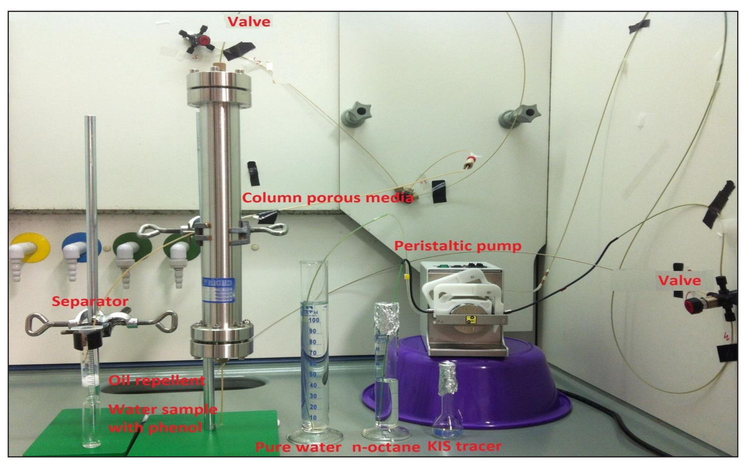

Figure 2. Experiment set-up

Computational Methods: The two-phase flow system was built up by applying the pressure-saturation equations using the Coefficient Form PDE interface. And the Solute transport process was simulated in the Solute Transport interface, based on the mass balance equation of each component in each phase. By introducing the interface mass transfer rate $r^{\kappa}_{n\to w}$, which linearly depends on the kinetic reaction rate $Rc^{\kappa}_{n\to w}$, specific interfacial area a_{wn} and fractional occupancy of the adsorption sites θ_{κ}, the specific mass flux of the reaction products into the water phase can be expressed.

Two-phase flow system: pressure saturation formulation

$$\begin{bmatrix} 0 & -\phi\cdot\varrho_w \\ 0 & \phi\cdot\varrho_n \end{bmatrix}\cdot\begin{bmatrix} \frac{\partial p_w}{\partial t} \\ \frac{\partial S_n}{\partial t} \end{bmatrix} = \nabla\cdot\begin{bmatrix} k\cdot\varrho\cdot k_{rw}/\mu_w & 0 \\ k\varrho k_{rn}/\mu_n & k\varrho k_{rn}/\mu_n\cdot\frac{dp_c}{dS_n} \end{bmatrix}\cdot\nabla\cdot\begin{bmatrix} p_w \\ S_n \end{bmatrix}$$

KIS transport: mass transport equation

$$\phi S_n\frac{\partial c_i}{\partial t} + \phi c_i\frac{\partial S_n}{\partial t} + \nabla\cdot(\mathrm{c_i}\mathbf{v_i}) - \nabla\cdot\left[(\mathrm{D_{dis,i}} + \mathrm{D_{dif,i}})\nabla \mathrm{c_i}\right] = -\mathrm{r_i}$$

$$\phi S_w\frac{\partial c_j}{\partial t} + \phi c_j\frac{\partial S_w}{\partial t} + \nabla\cdot(\mathrm{c_j}\mathbf{v_j}) - \nabla\cdot\left[(\mathrm{D_{dis,j}} + \mathrm{D_{dif,j}})\nabla \mathrm{c_j}\right] = \mathrm{r_j}$$

Effective mass transfer rate

$$-\frac{d(c)}{dt} = r^{\kappa}_{n\to w} = \theta_{\kappa}\cdot Rc^{\kappa}_{n\to w}\cdot a_{wn}$$

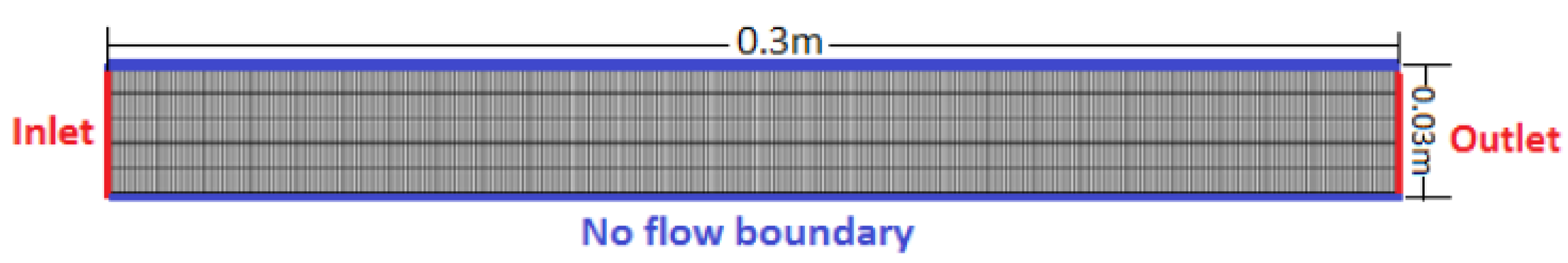

Figure 3. Boundary conditions, inlet boundary follows Neumann boundary condition; outlet boundary (Dirichlet Boundary condition or Neumann boundary condition); no flow boundaries follow Neumann boundary condition.

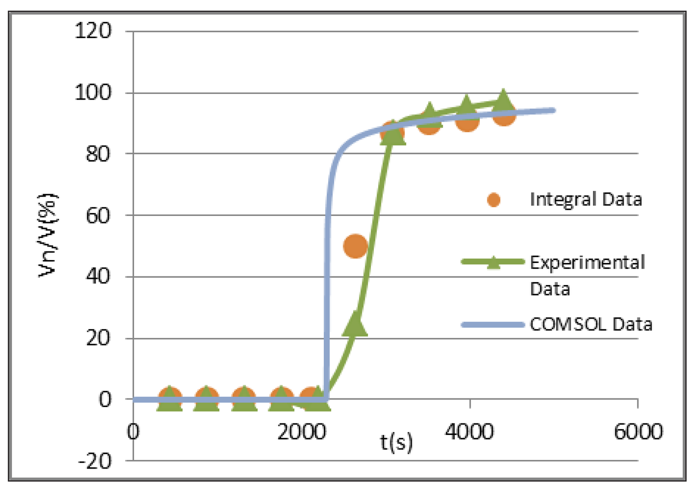

Figure 4. BTC of Sn

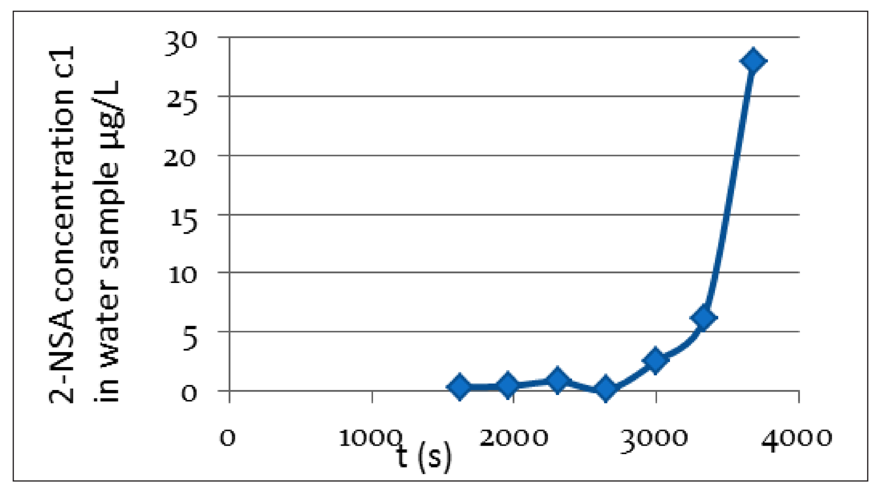

Figure 5. BTC of 2-NSA

Results: The breakthrough curves (BTC) of non-wetting phase saturation and the concentration of KIS tracer reaction product are shown in Figure 4 and Figure 5. The development of non-wetting phase saturation *Sn*, specific interfacial area *awn*, KIS tracer concentration *c* and KIS tracer product concentration *c2* along the column were analysed (Figure 6).

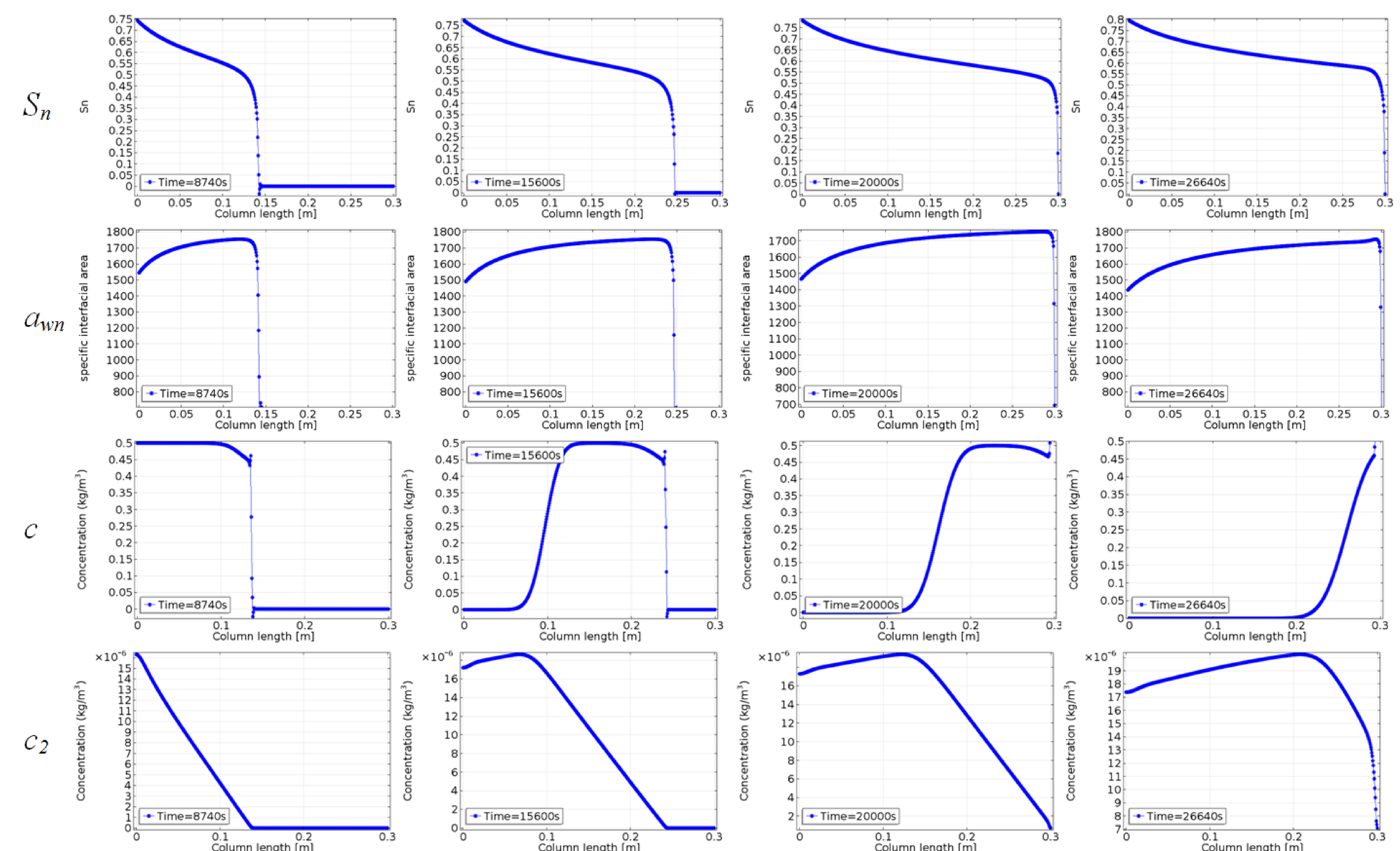

Figure 6. Breakthrough process of *Sn*, *awn* , *c* and *c2*

Conclusions:

1) The tracer reaction and transport processes in two-phase flow system can be well simulated with consideration of the kinetic of mass transfer over interface;
2) An average specific interfacial area between the two phases in the column can be estimated;
3) A practical range of kinetic reaction rate for a more suitable KIS tracer was determined.

References:

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