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

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Background

What are Kinetic interface sensitive tracers (KIS tracers)? Why is it important?

Objectives

To get a better understanding of KIS tracers developement.

Lab Experiment

Column Experiment.

Numerical Modeling

Discretisation effect, boundary effect, sensitivity analysis.

Results

Breakthough behavior of non-wetting phase and KIS tracer products.

Conclusions

Background

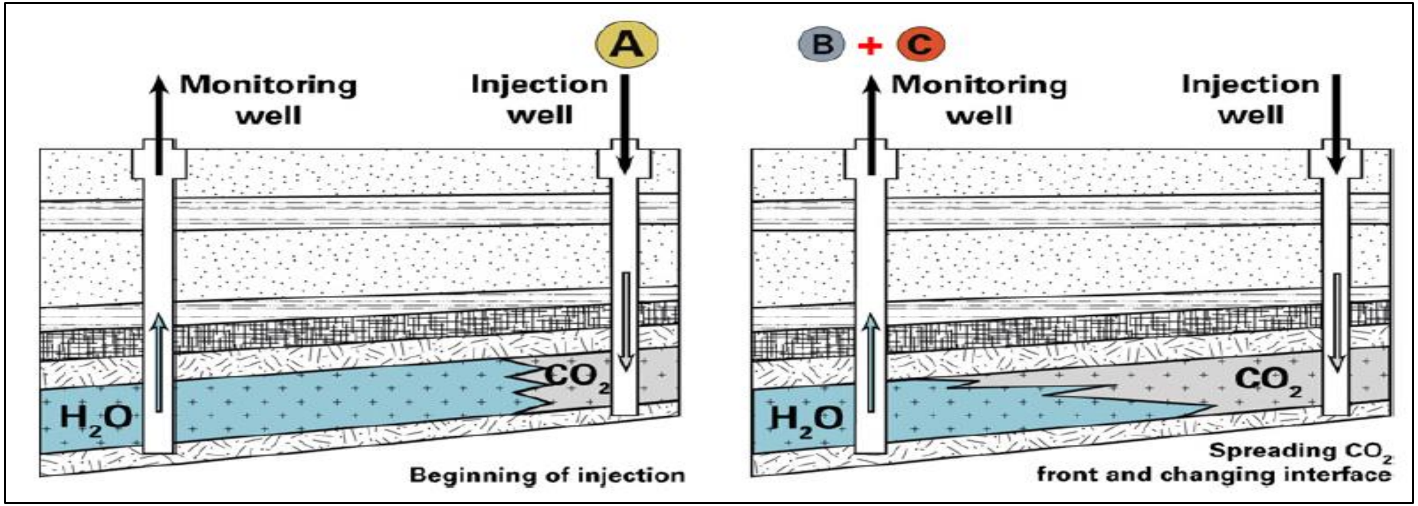


Fig. 1 Injection well: Injection and spreading of scCO2 together with dissolved KIS tracer. Monitoring well: Measurement of KIS tracer reaction products in the brine, Schaffer et al. 2013

Background

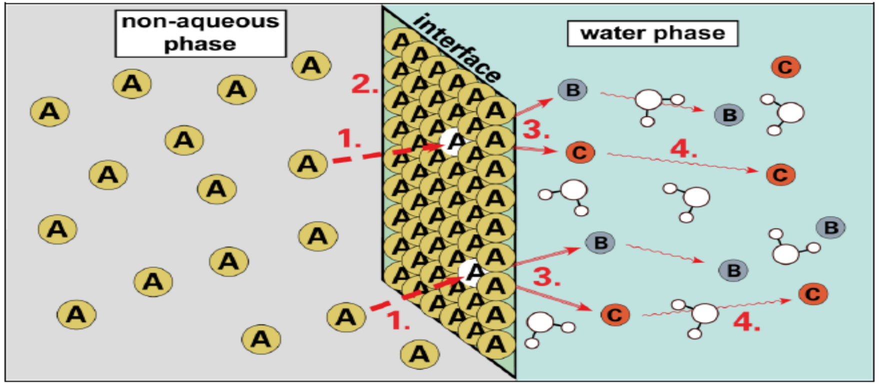
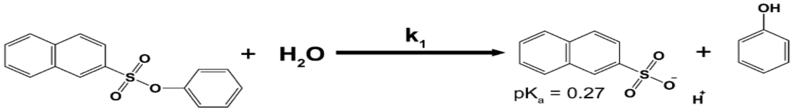


Fig. 2 Schematic representation of all involved processes at the scCO2/water interface during KIS tracer application, Schaffer et al. 2013.

$$\text{Ester } (A_{scCO2}) + H_2O \xrightarrow{k_1} \text{acid } (B_{H2O}) + \text{alcohol/phenol } (C_{H2O})$$



Phenyl naphthalene-2-sulfonate (2-NSAPh)

Naphthalene - 2-sulfonic acid (2NSA)

Phenol

Objectives

1) to develop a novel numerical model to simulate the KIS tracer reaction & transport process in the two-phase flow system based on the lab experiment;
2) to evaluate the development of the specific interfacial area between the two phases during the injection of non-wetting phase.

Experiment

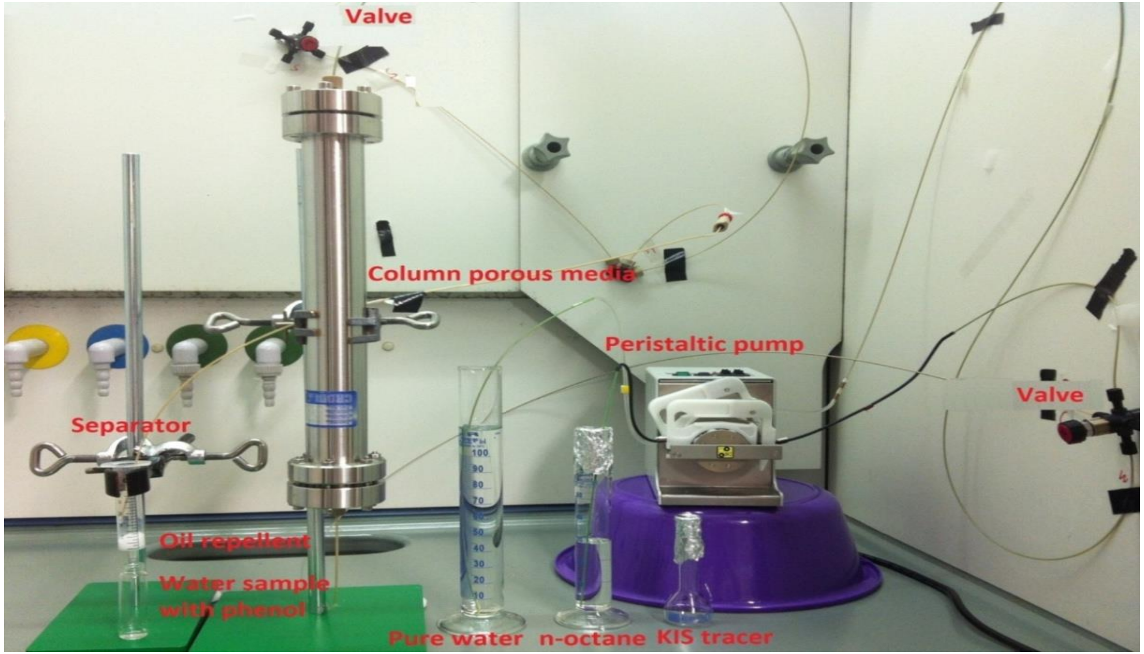


Fig. 3 Experiment set-up

Non-wetting phase: n-octane
Wettingen phase: water

Numerical modeling

1) Two-phase flow - pressure-saturation formulation (Helmig, 1997).

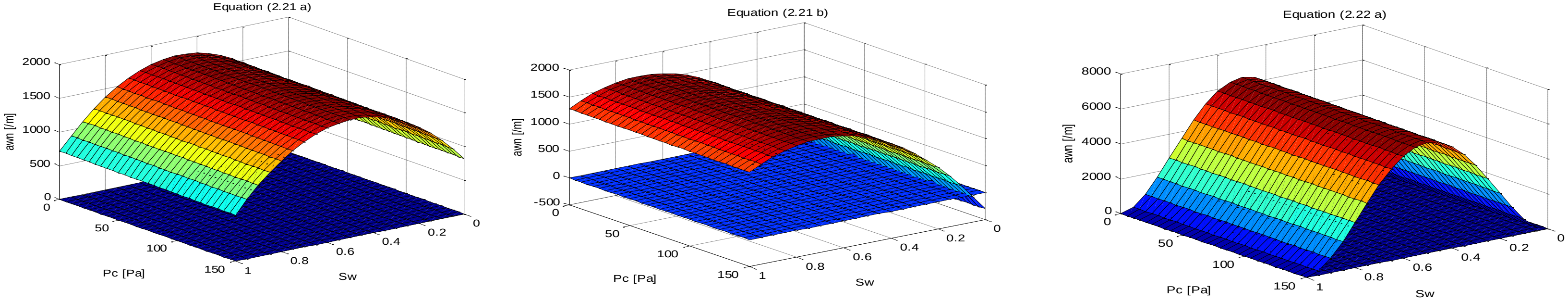
$$L_\alpha(p_\alpha, S_\alpha) := \phi \varrho_\alpha \frac{\partial S_\alpha}{\partial t} + \varrho_\alpha S_\alpha \frac{\partial \phi}{\partial t} + \phi S_\alpha \frac{\partial \varrho}{\partial p}\frac{\partial p}{\partial t} - \nabla \cdot \left\{ \varrho_\alpha \frac{k_{r\alpha}}{\mu_\alpha} \boldsymbol{k} \cdot (\boldsymbol{grad} p_\alpha - \varrho_\alpha \boldsymbol{g}) - \varrho_\alpha q_\alpha \right\} = 0$$

2) Reactive tracer transport- mass transfer (Helmig, 1997)

$$L(\boldsymbol{v}_\alpha, X_\alpha^i) := \int_G \left[\frac{\partial(\phi S_\alpha \varrho_\alpha X_\alpha^i)}{\partial t} + \nabla \cdot \{ \varrho_\alpha \boldsymbol{v}_\alpha X_\alpha^i - \phi S_\alpha \boldsymbol{D}_{pm,\alpha}^i \cdot (\varrho_\alpha \boldsymbol{grad} X_\alpha^i) - r_\alpha^i \} \right] dG = 0$$

3) Specific interfacial area (Hassanizadeh ,1990; Niasar et al, 2010; Niessner ,2008)

$$a_{wn} = \frac{A}{V}$$



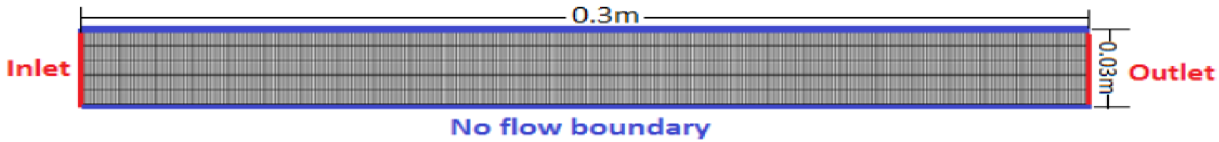
$a_{\alpha\beta}(S_w, p_c) = 849 + 3858 S_w - 0.224 p_c + 0.006 S_w p_c - 3992 S_w^2 - 3992 S_w^2 + 1.283(\mathrm{e}-5) p_c^2$

$a_{\alpha\beta}(S_w, p_c) = -313.6 + 5535 S_w + 0.085 p_c - 0.307 S_w p_c - 3937 S_w^2 - 3937 S_w^2 - 5(\mathrm{e}-6) p_c^2$

$a_{\alpha\beta}(S_w, p_c) = 1 \cdot (S_w)^2 \cdot (1 - S_w)^2 (15000 - p_c)^{1.2}$

Fig. 4 *The pc-Sw-awn relationship*

Numerical modeling



$$r_{n\longrightarrow w}^{\kappa} = \theta_{\kappa} \cdot Rc_{n\longrightarrow w}^{\kappa} \cdot a_{wn}$$

Fig.5 Boundary conditions

Two phase flow model

Pressure-saturation equation

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

$$\frac{dp_c}{dS_n} = \frac{1}{\lambda} \cdot p_d \cdot \left(\frac{1-S_n-S_{wr}}{1-S_{wr}}\right)^{\left(-\frac{1}{\lambda}-1\right)}$$

Inlet -Neumann boundary condition

$$\nabla \cdot \begin{bmatrix} k \cdot \varrho \cdot k_{rw}/\mu & 0 \\ k\varrho k_{rn}/\mu & k\varrho k_{rn}/\mu \cdot p_c{}'(S_n) \end{bmatrix}_{x=0} \cdot \nabla \cdot \begin{bmatrix} p_w \\ S_n \end{bmatrix}_{x=0} = \begin{bmatrix} 0 \\ q \end{bmatrix}$$

Outlet- Dirichlet boundary condition

$$\begin{bmatrix} p_w \\ S_n \end{bmatrix}_{x=0.3m} = \begin{bmatrix} p_{w\_outlet} \\ S_{n\_outlet} \end{bmatrix}$$

No flow- Neumann boundary condition

$$\nabla \cdot \begin{bmatrix} k \cdot \varrho \cdot k_{rw}/\mu & 0 \\ k\varrho k_{rn}/\mu & k\varrho k_{rn}/\mu \cdot p_c{}'(S_n) \end{bmatrix}_{y=0\&0.03m} \cdot \nabla \cdot \begin{bmatrix} p_w \\ S_n \end{bmatrix}_{y=0\&0.03m} = 0$$

Solute transport model

Mass transport equation

$$\begin{cases} \phi S_n \frac{\partial c_i}{\partial t} + \phi c_i \frac{\partial S_n}{\partial t} + \nabla \cdot (\mathrm{c_i} \mathbf{v_i}) - \nabla \cdot [(\mathrm{D_{dis,i}} + \mathrm{D_{dif,i}}) \nabla \mathrm{c_i}] = -\mathrm{r_i} \\ \phi S_w \frac{\partial c_j}{\partial t} + \phi c_j \frac{\partial S_w}{\partial t} + \nabla \cdot (\mathrm{c_j} \mathbf{v_j}) - \nabla \cdot [(\mathrm{D_{dis,j}} + \mathrm{D_{dif,j}}) \nabla \mathrm{c_j}] = \mathrm{r_j} \end{cases}$$

Inlet - Dirichlet boundary condition

$$\begin{bmatrix} c_i \\ c_j \end{bmatrix}_{x=0} = \begin{bmatrix} c_{in} \\ 0 \end{bmatrix}$$

Outlet- Neumann boundary condition

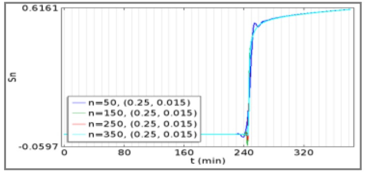
$$-\nabla \cdot \begin{bmatrix} (\mathrm{D_{dis,i}} + \mathrm{D_{dif,i}}) \nabla \mathrm{c_i} \\ (\mathrm{D_{dis,j}} + \mathrm{D_{dif,j}}) \nabla \mathrm{c_j} \end{bmatrix}_{x=0.3m} = 0$$

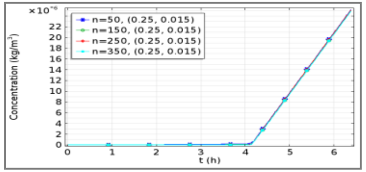
No flow- Neumann boundary condition

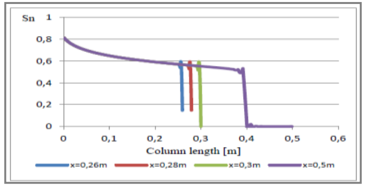
$$-\nabla \cdot \begin{bmatrix} (\mathrm{D_{dis,i}} + \mathrm{D_{dif,i}}) \nabla \mathrm{c_i} \\ (\mathrm{D_{dis,j}} + \mathrm{D_{dif,j}}) \nabla \mathrm{c_j} \end{bmatrix}_{y=0\&0.03m} = 0$$

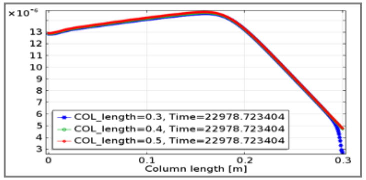
Numerical modeling

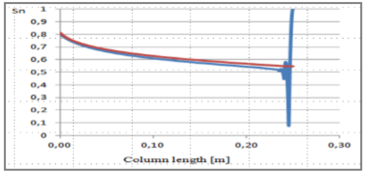
1) Discretization effect
2) Boundary effect
3) Bench marking
4) Sensitivity analysis

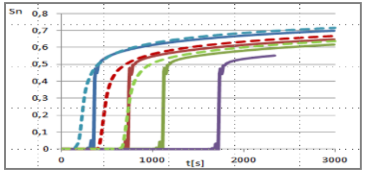


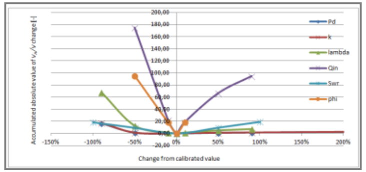


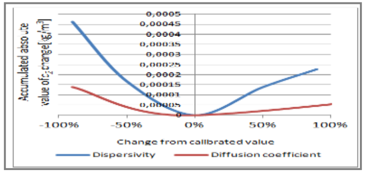






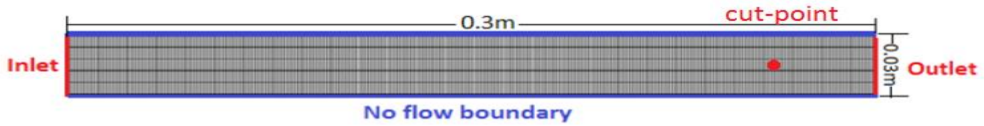






Results

1) Breakthrough curves



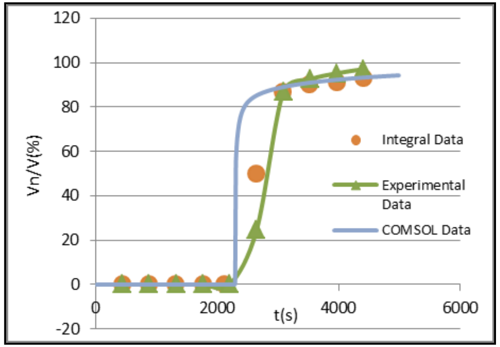


Fig.6 *Experimental and simulated breakthrough curves of n-octane (x=0.25m)*

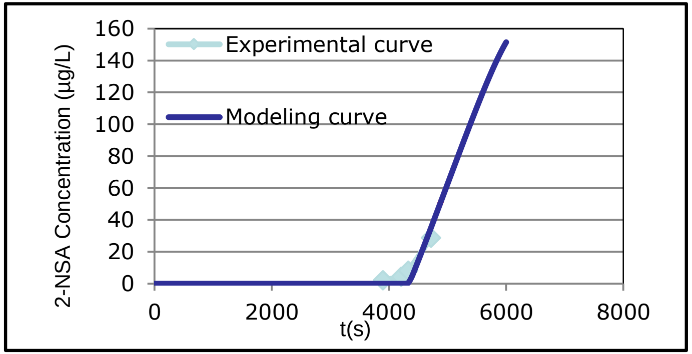


Fig. 7 *Experimental and simulated breakthrough curves of 2-NSA (x=0.25m)*

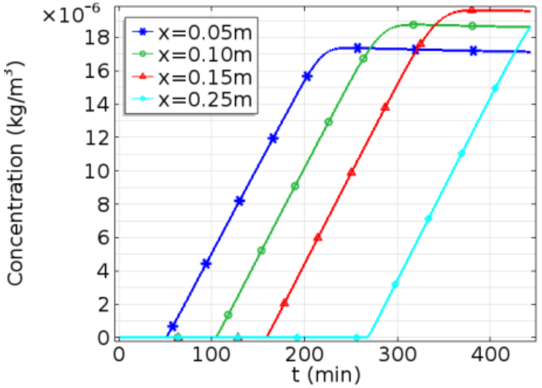


Fig. 8. *Breakthrough curve of c2 at different cut points*

2) Relationship between Sn, awn, C_KIS(c), C_2NSA(C2)

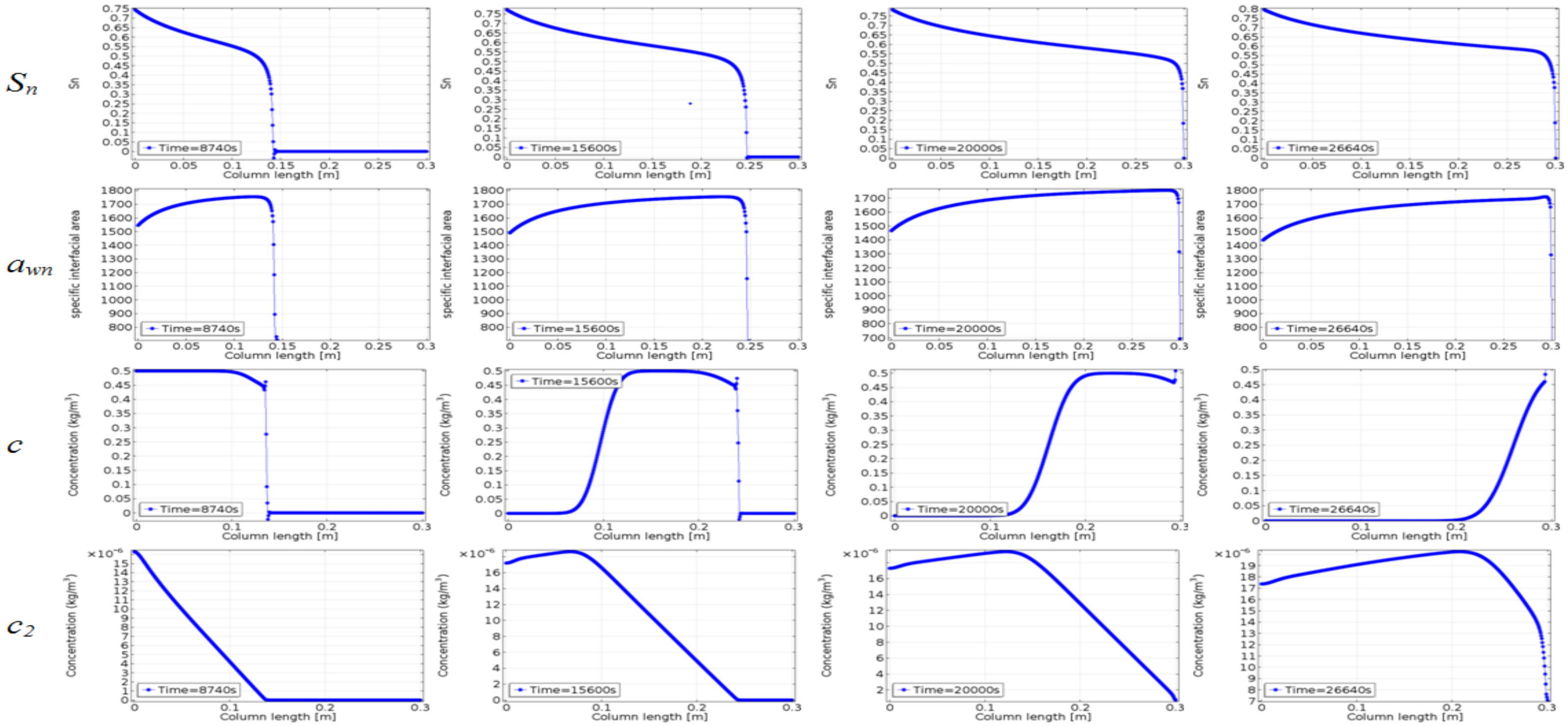


Fig. 8 Breakthrough process of S_n, a_{wn}, c and c_2 along the colum porous media at different time step

Conlusion

1) The numerical model can be used to simulate the two-phase flow system and tracer reaction and transport processes;
2) An average specific interfacial area between the two phases in the column is around 1650/m at the final stage.

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Thank you for your attention!

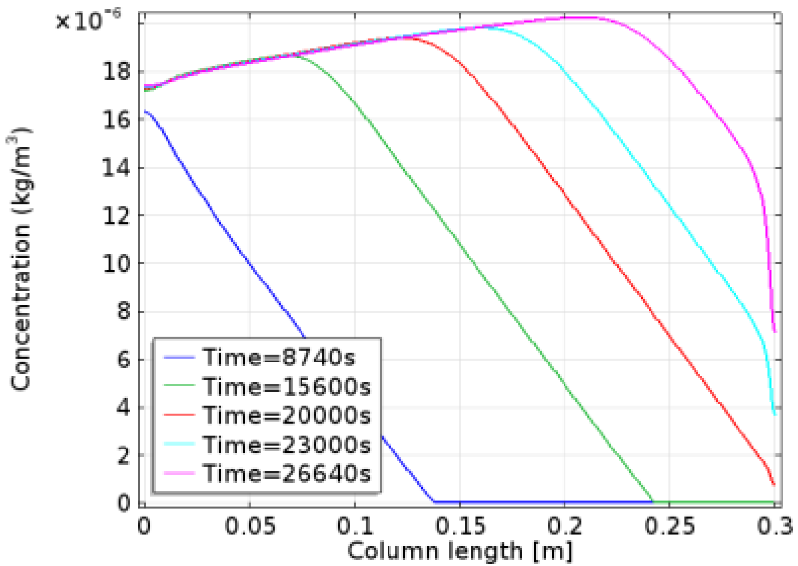

Figure 5. 36 Distribution curves of phenol concentration c_2 at different time point