Modeling of Kinetic Interface Sensitive Tracers for Two Phase Immiscible Flow in Porous Media with COMSOL Multiphysics® Alexandru-Bogdan Tatomir^{*1}, Apoorv Jyoti¹, Friedrich Maier¹ and Martin Sauter¹ ¹Dept. of Applied Geology, Geoscience Centre of the University of Göttingen, Göttingen, Germany.

Introduction: Tracer testing are powerful methods for characterization and for understanding the processes occurring in geologic reservoirs. Kinetic Interface Sensitive (KIS) tracer concept has been developed with the intention to estimate the amount of interface between two fluid phases. One direct application is monitoring the spreading of injected supercritical CO2 in geological formations (Schaffer et al. 2013).

The KIS tracer is injected dissolved in the non-wetting phase and undergoes a hydrolysis reaction over the interface resulting in an alcohol and an acid dissolved in the wetting phase. Both alcohol and acid are only present in the wetting phase and there is negligible back partitioning. For the monitoring purposes it is sufficient to track only the acid (tracer) which can indicate the amount of interfacial area between the two fluids.

Results: Two numerical simulations for two different spatial-scales are shown as examples. The model is tested with respect to the sensitivity of different flow and transport parameters (e.g., permeability, porosity, reaction rate, injection rate).





Figure 1. KIS tracer injection with supercritical CO₂

Mathematical Model: The pressure-saturation formulation is chosen among two-phase flow formulations. For closing the system of equations a relationship based on Brooks-Corey

Para	Laboratory	Field Scale
meter	Scale values	values
ϕ	0.2	0.2
k	$1 \cdot e^{-12} [m^2]$	$1 \cdot e^{-10} [m^2]$
	1000 [kg/m ³]	1000 [kg/m ³]
	700 [kg/m ³]	700 [kg/m ³]
λ	2	2
	2000[Pa]	2000[Pa]
	10 ⁵ [Pa]	10 ⁷ [Pa]
	0.0	0.0
Q_{in}	1.0e-4 [kg/m²·s]	1.0e-3 [kg/m².s]
	1.0e-4 [Pa·s]	1.0e-4 [Pa-s]
	1.0e-3 [Pa·s]	1.0e-3 [Pa-s]
$k_{n \to w}^R$	1.0e-6 [kg/m²-s]	1.0e-6

approach among capillary pressure, saturation and interfacial area formulation is used. The strongly coupled, parabolic system of partial differential equations is build using the Coefficient Form PDE interface. The hydrolysis of tracer at follows a pseudo-zero interfaces the fluid-fluid order kinetic reaction and it is implemented with the Solute Transport interface.

Immiscible two-phase flow in porous media

$$-\frac{\partial (S_n \phi \rho_w)}{\partial t} - \nabla \cdot \left(\frac{\rho_w \mathbf{K} k_{rw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g}) \right) - \rho_w q_w = 0$$
$$\frac{\partial (S_n \phi \rho_n)}{\partial t} - \nabla \cdot \left(\frac{\rho_n \mathbf{K} k_{rn}}{\mu_n} (\nabla p_w + \nabla p_c - \rho_n \mathbf{g}) \right) - \rho_n q_n = 0$$

Tracer transport in the wetting phase

$$\phi \frac{\partial C}{\partial t} - \nabla \cdot (C v_w - \phi D \nabla C) - q_{n \to w}^R = 0$$

$$q_{n \to w}^R = k_{n \to w}^R a_{wn}$$

Table 1. Parameters and initial values



-20

-22

-24

0.2

K react=1e-8

K_react=1e-9

0.4 0.6 Time (days)

K react=1e-10

0.8

Figure 5. Lab-scale sensitivity analysis (ϕ , $k_{n \to w}^R$, Q_{in})



$$a_{wn}(S_w, p_c) = a_0 \cdot (S_w)^{a_1} \cdot (1 - S_w)^{a_2} \cdot (p_c^{max} - p_c)^{a_3}$$



Conclusions: The sensitivity studies have investigated the behavior of the tracer concentration, the interfacial area and fluid saturation, with regard to several flow and transport parameters. The simulation results help us gain a better understanding on the behavior of one of KIS tracer's reaction product.

References:

1. Schaffer, M. et al., A new generation of tracers for the characterization of interfacial areas during supercritical carbon dioxide injections into deep saline aquifers: Kinetic interface-sensitive tracers (KIS tracer). International Journal of *Greenhouse Gas Control*, 14, pp.200–208 (2013)

2. Tatomir, A. et al., Modelling of Kinetic Interface Sensitive Tracers for Two-Phase Systems. In M. Z. Hou, H. Xie, & P. Were, eds. Clean Energy Systems in the Subsurface: Production, Storage and Conversion. Springer Series in Geomechanics and Geoengineering, Springer Berlin Heidelberg, pp. 65–74 (2013)

Excerpt from the Proceedings of the 2014 COMSOL Conference in Cambridge