Application of MRST to the Simulation of LNAPL Transport in Groundwater

Ehsan Ranaee[1], Giovanni Porta[2], Monica Riva[2], Fabio Inzoli[1], Alberto Guadagnini[2]

[1] Dipartimento di Energia, Politecnico di Milano

[2] Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano

Scopes : Computational tools specifically developed for petroleum engineering applications are potentially transferrable to simulating contamination processes taking place in soil-water systems. Since operational conditions (e.g., confinement, consolidation, solid surface properties, and operating pressures) can be different from those encountered in a deep reservoir, feasibility studies should aim at assessing the feasibility of such applications.

Aims : We assess the ability of the MRST toolkit (Lie, 2019) to simulate soil contamination by light non-aqueous phase contaminants (LNAPL). We did so upon relying on a compositional formulation of the governing equations employed for reservoir simulations.

Key objectives : (*i*) compare the MRST solution against that provided by other specialized software packages and (*ii*) discuss uncertainties arising from the parameterization of the system.

Assumptions : (compositional model): (*i*) the components form at most three phases of vapor hydrocarbon (gas), liquid hydrocarbon (oil) and water; and (*ii*) there is no mass exchange between the water phase and the hydrocarbon (gas-oil) phases.

Mathematical model :

We rely on an Equation-of-State (EOS) based compositional formulation (Moyner and Tchelepi, 2017 for details) of the system of equations and assume hydrocarbon migration in isothermal conditions.

$$\frac{\partial(\phi\rho_w S_w)}{\partial t} + \nabla\cdot(\rho_w \mathbf{u}_w) = q_w$$

$$\frac{\partial\left(\phi\left[X_i\rho_o S_o + Y_i\rho_g S_g\right]\right)}{\partial t} + \nabla\cdot\left(X_i\rho_o\mathbf{u}_o + Y_i\rho_g\mathbf{u}_g\right) = X_i\rho_o q_o + Y_i\rho_g q_g$$

$$X_i = \frac{x_i W_i}{\sum_{j=1}^{N_c} x_j W_j};\ Y_i = \frac{y_i W_i}{\sum_{j=1}^{N_c} y_j W_j}$$

$$\boldsymbol{u}_\alpha = -\frac{k_{r\alpha}}{\phi\mu_\alpha}K(\nabla p_\alpha - \rho_\alpha g\nabla z), \qquad \alpha = w, o, g$$

$$f_{io}(p, T, x_1, \ldots, x_{N_c}) - f_{ig}(p, T, y_1, \ldots, y_{N_c}) = 0$$

$$S_w + S_o + S_g = 1 \qquad \sum_{i=1}^{N_c} x_i = 1 \qquad \sum_{i=1}^{N_c} y_i = 1$$

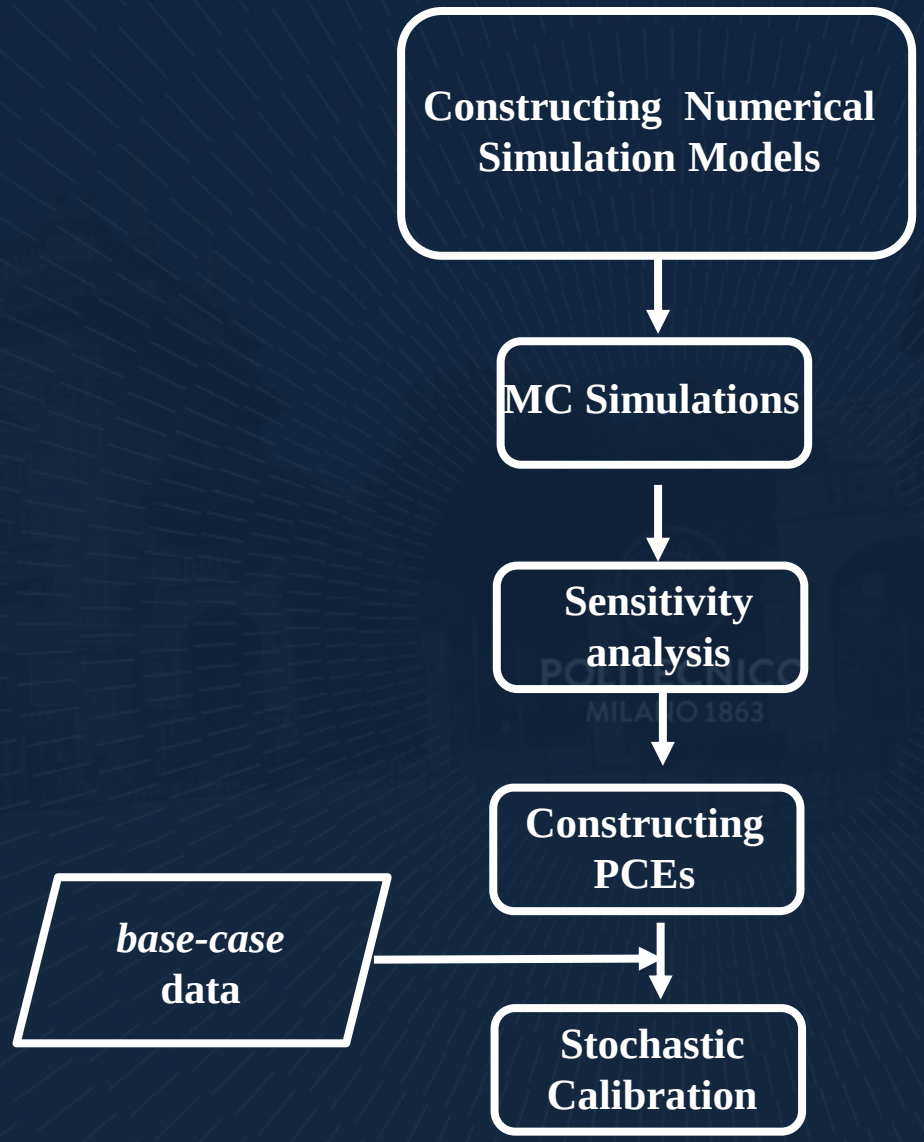
Workflow

- Our study is keyed to the assessment of uncertainties associated with simulation of multiphase-multicomponent flow migration in contaminated sites.

- We do so by constructing and calibrating a numerical simulation models and evaluating their capabilities (in a sensitivity-based calibration framework) to reproduce some predefined “base-case” responses.

- We rely on stochastic approaches and advantage from acceptance-rejection sampling (ARS) algorithm to perform calibration of the simulation model with an objective to reproduce base-case values.

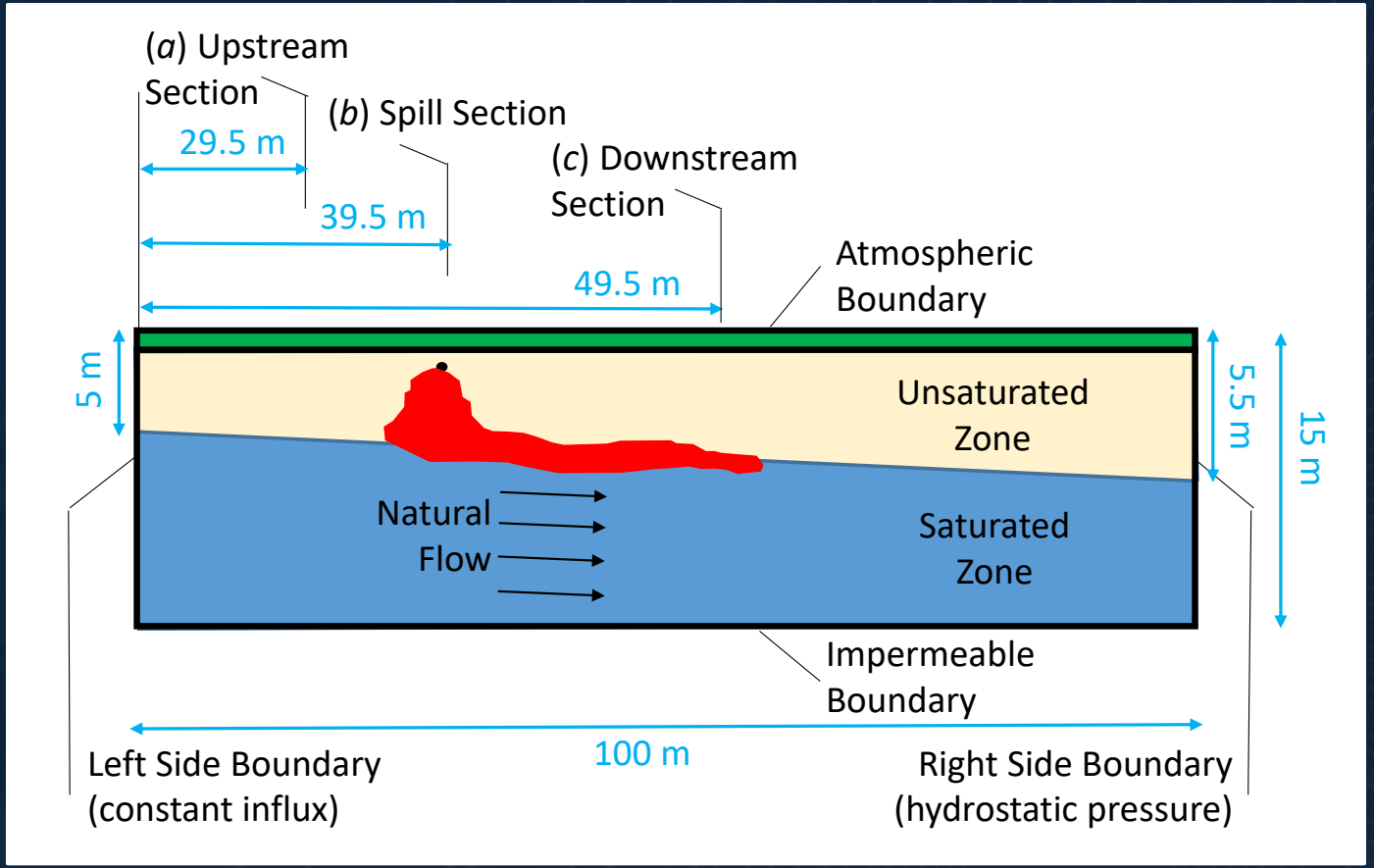
- We take advantage of Polynomial Chaos Expansions (PCE) as surrogate models to perform ARS calibrations in reduced computational costs.



We rest on problem n. 7 of the TMVOC user guide (Pruess and Battistelli 2002) to assess the capability of MRST to characterize LNAPL transport in the subsurface.

- porosity is set to 30 %
- horizontal and vertical permeability are set to 4 darcy and 1 darcy, respectively.
- Tortuosity is set to zero.

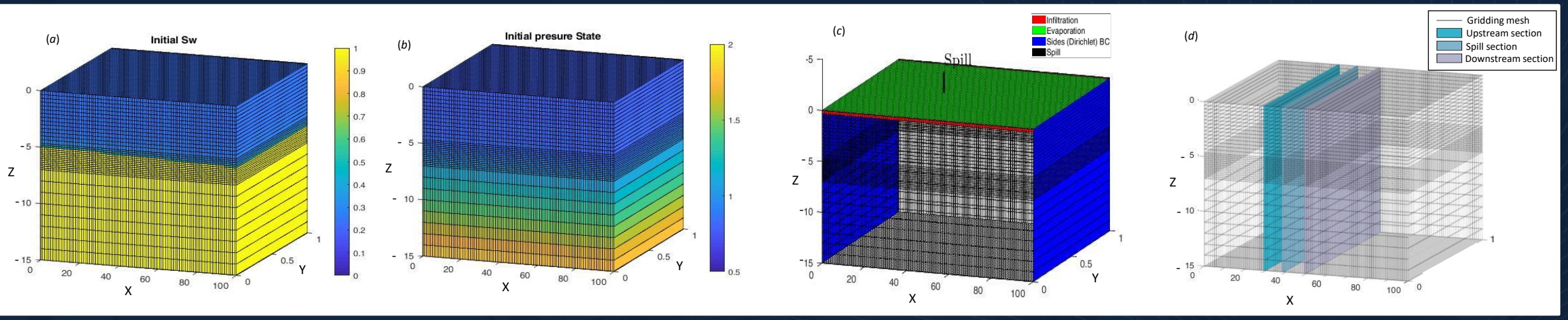
The analyzing problem is a sequence of three stages :
(1) generation of steady flow prior to NAPL spill,
(2) NAPL spill in the unsaturated zone,
(3) redistribution of NAPL.



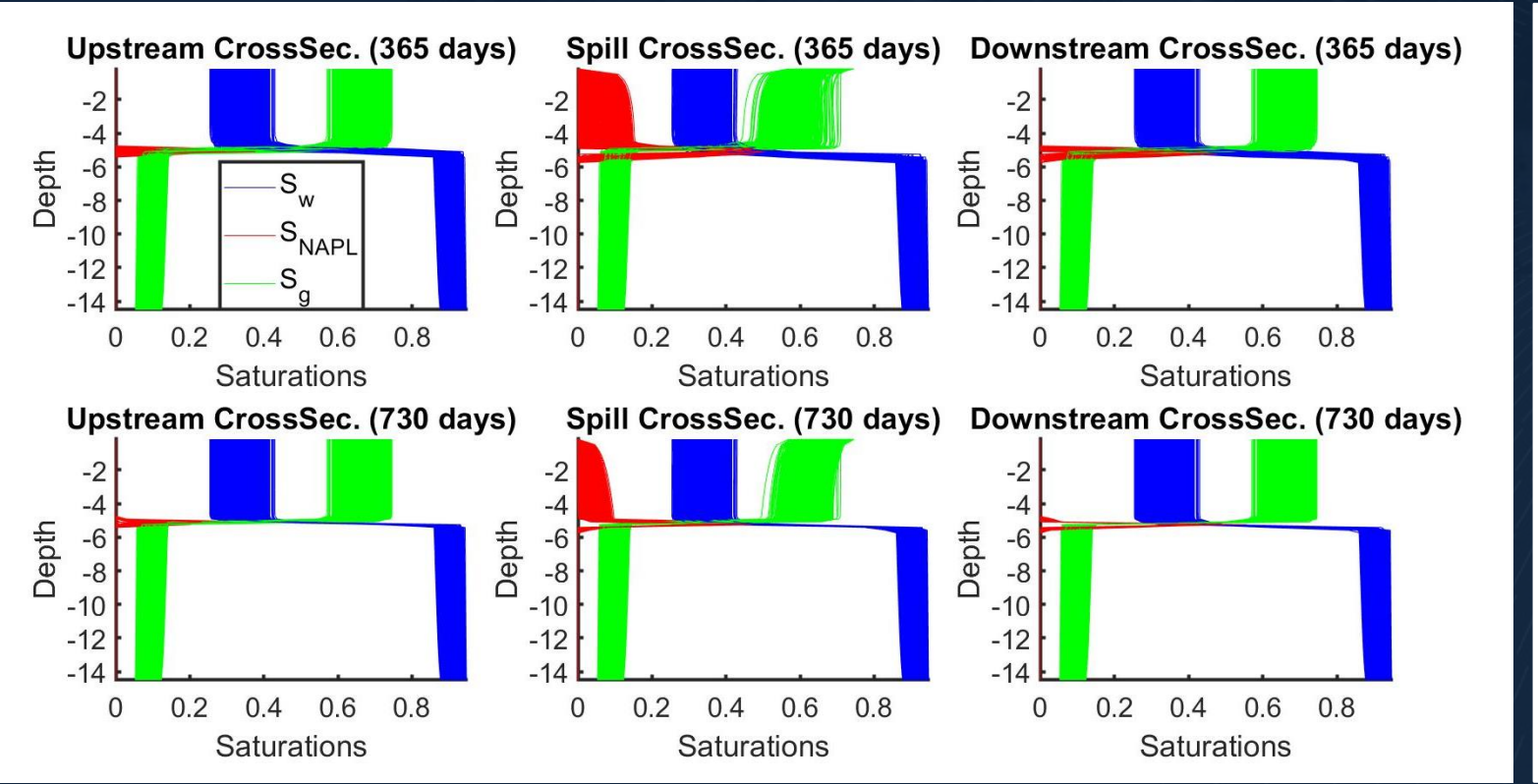
Compound	Mass flux [kg/s]
n-pentane	7.5×10^{-6}
benzene	3×10^{-7}
toluene	1.8×10^{-6}
p-xylene	3×10^{-6}
n-propylbenzene	3×10^{-6}
n-decane	1.44×10^{-5}

Base case

Compound	Molecular formula	Molecular weight [g/mol]	Solubility [mg/l]	Boiling point [°C]	Vapor pressure [atm]	C_{oc} [ml/g]	log C_{ow} [-]	H [-]
	Alkyl benzenes							
benzene	C_6H_6	78	1780	80	0.13	8.1×10^1	2.13	0.22
toluene	C_7H_8	92	515	111	0.038	2.3×10^2	2.69	0.27
p-xylene	C_8H_{10}	106	215	138	0.012	5.9×10^2	3.18	0.23
-propylbenzene	C_9H_{12}	120	52	159	0.0044	1.5×10^3	3.69	0.42
	Straight chain alkanes							
n-pentane	C_5H_{12}	72	38.5	36	0.68	9.8×10^2	3.45	52
n-decane	$C_{10}H_{22}$	142	0.052	174.	0.0017	1.9×10^5	6.25	190

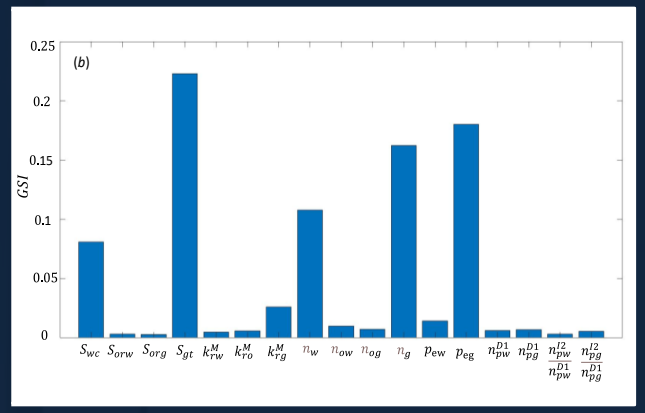


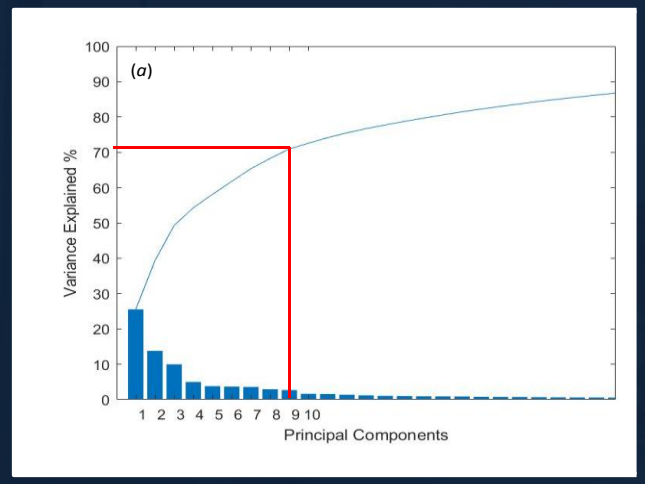
MC simulations

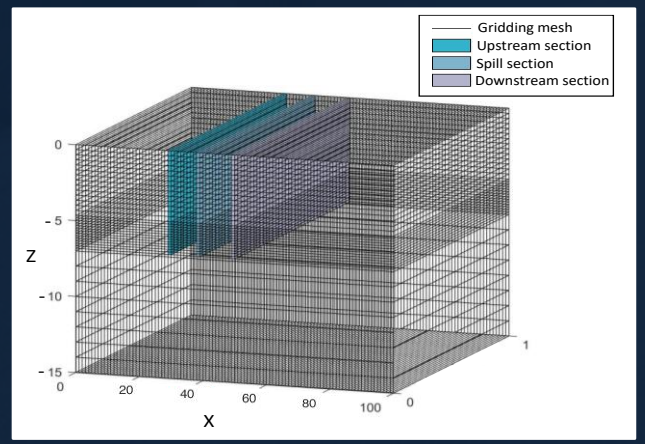


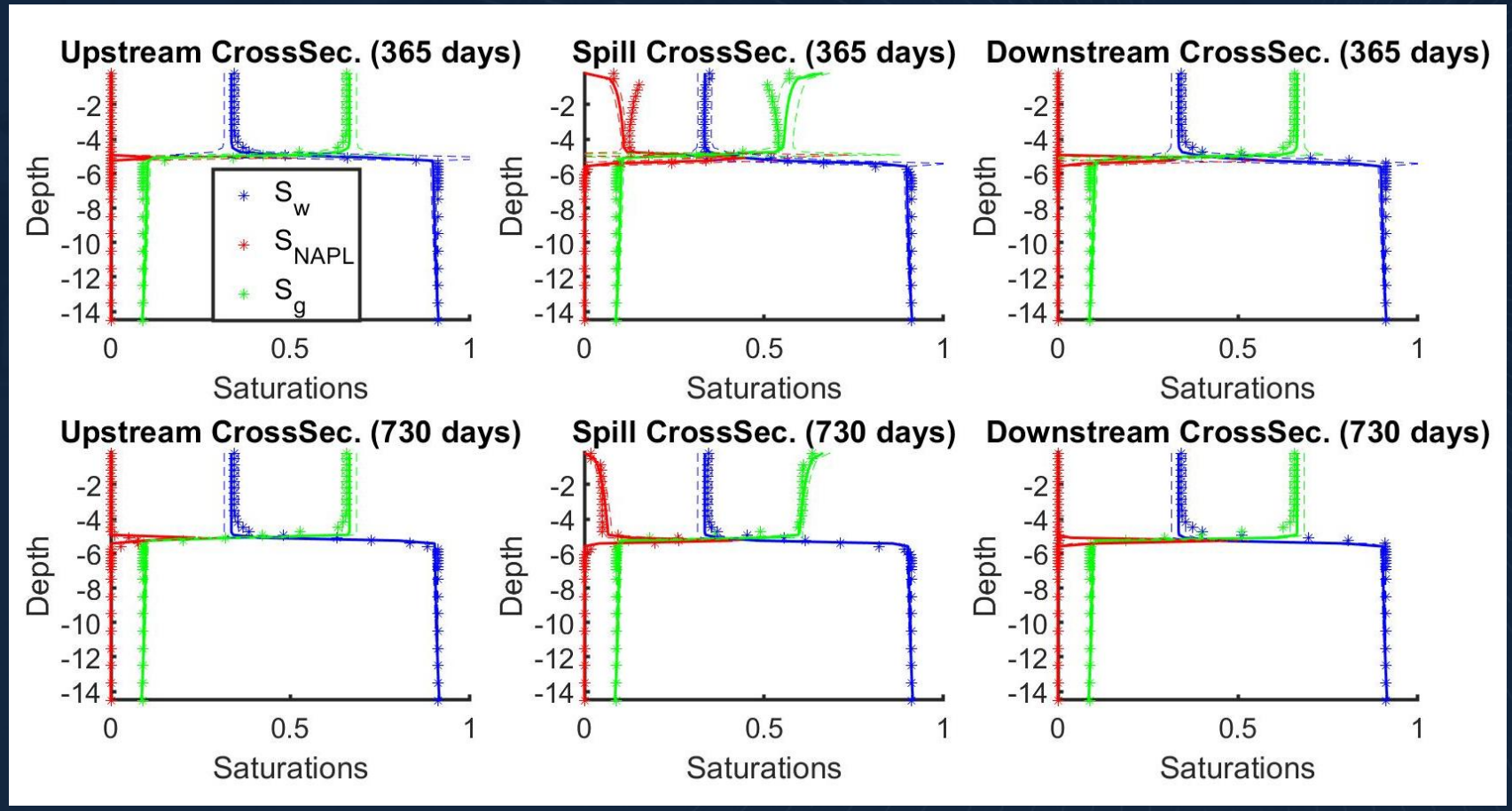
	Properties	Confidence interval $[U_{\theta f}^{-}, U_{\theta f}^{+}]$
Saturations ending points	$\theta_1 = S_{wc}$	[0.2, 0.3]
	$\theta_2 = S_{row}$	[0, 0.1]
	$\theta_3 = S_{rog}$	[0, 0.1]
	$\theta_4 = S_{gt}$	[0, 0.1]
Relative permeability ending points	$\theta_5 = k_{rw}^{M}$	[0.8, 1]
	$\theta_6 = k_{ro}^{M}$	[0.6, 0.8]
	$\theta_7 = k_{rg}^{M}$	[0.4, 0.6]
Relative permeability model parameters	$\theta_8 = n_w$	[3, 5]
	$\theta_9 = n_{ow}$	[3, 5]
	$\theta_{10} = n_{og}$	[3, 5]
	$\theta_{11} = n_g$	[3, 5]
Capillary pressure model parameters	$\theta_{12} = p_{\mathrm{ew}}$ [kPa]	[0, 2]
	$\theta_{13} = p_{\mathrm{eg}}$ [kPa]	[0, 2]
	$\theta_{14} = n_{pw}^{D1}$	[2, 3]
	$\theta_{15} = n_{pw}^{I2} / n_{pw}^{D1}$	[2, 3]
	$\theta_{16} = n_{pg}^{D1}$	[2, 3]
	$\theta_{17} = n_{pg}^{I2} / n_{pg}^{D1}$	[2, 3]

PCA-based Sensitivity Analysis/ ARS-based Calibration

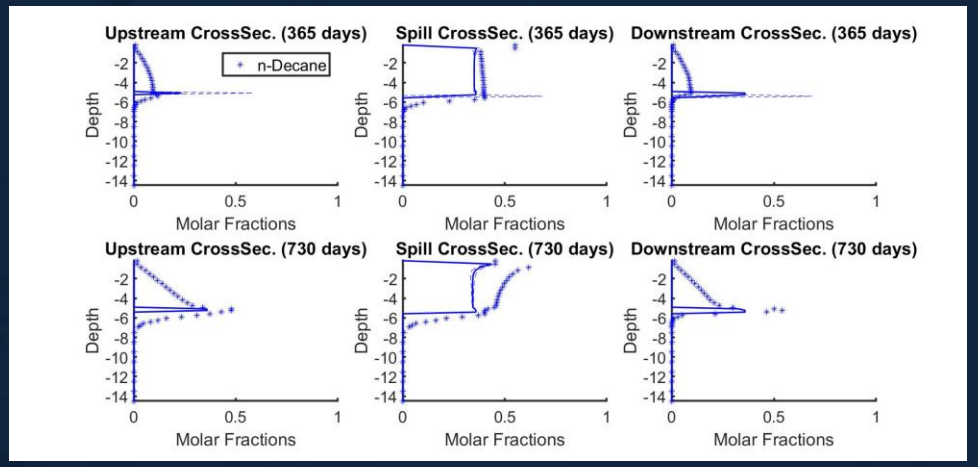


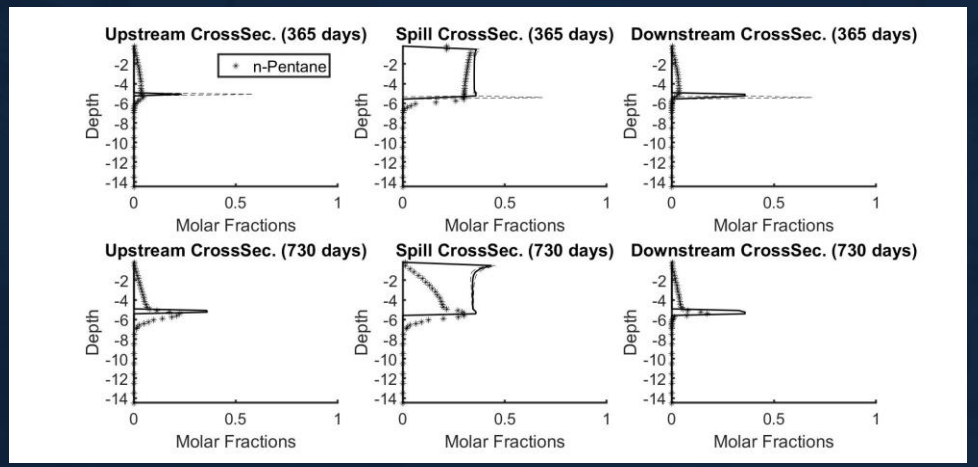


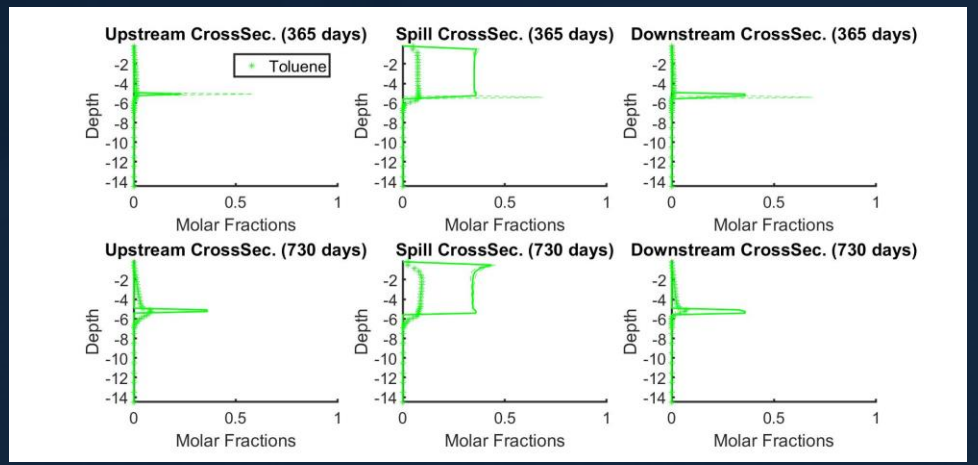


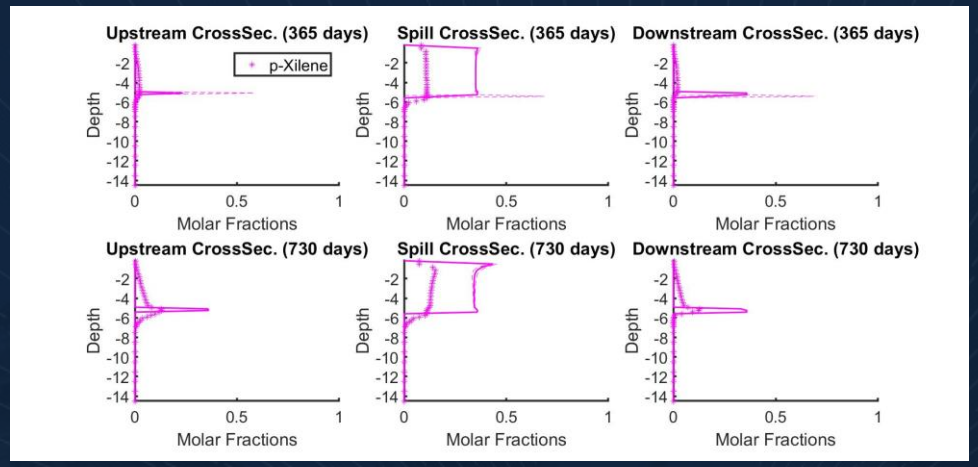


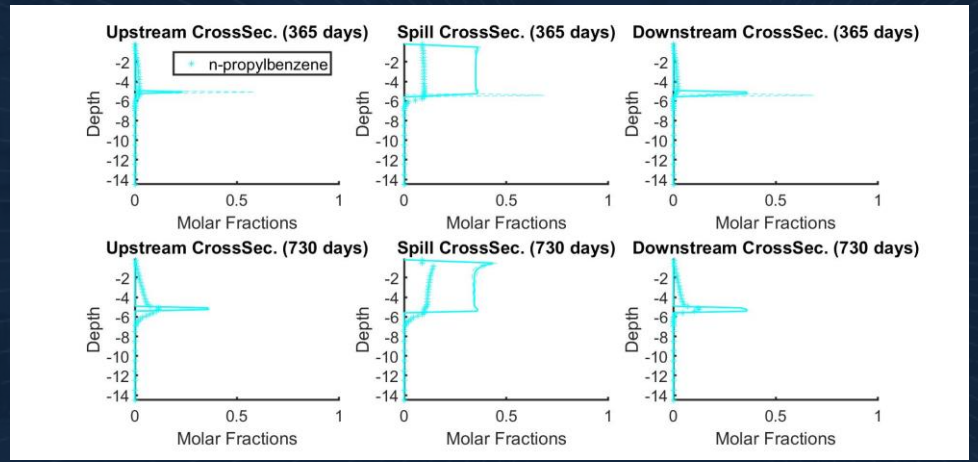
Results

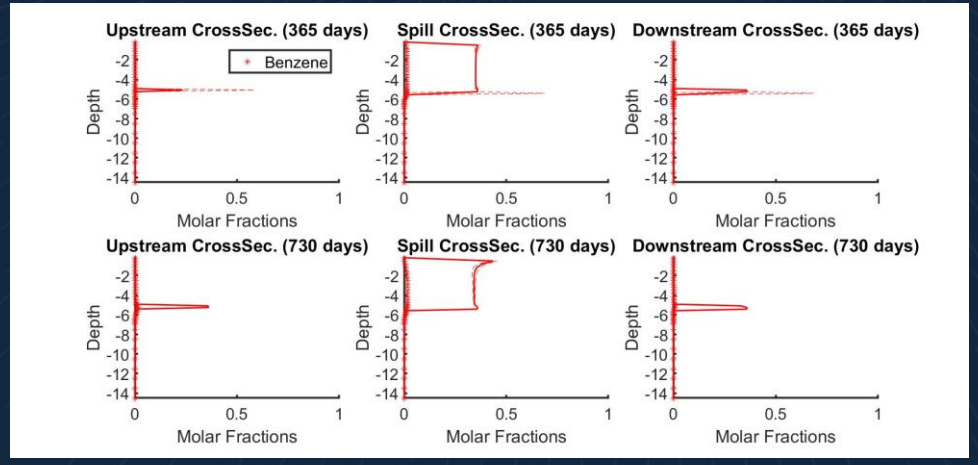

Upstream CrossSec. (365 days)
Spill CrossSec. (365 days)
Downstream CrossSec. (365 days)
n-Decane
Upstream CrossSec. (730 days)
Spill CrossSec. (730 days)
Downstream CrossSec. (730 days)
Depth
Molar Fractions

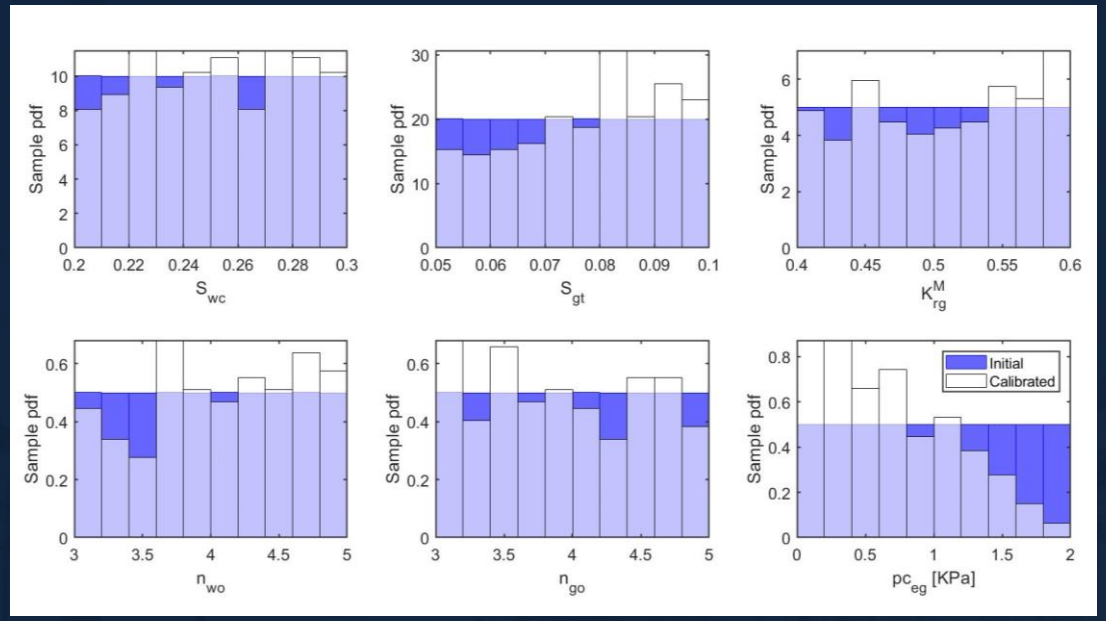

Upstream CrossSec. (365 days)
Spill CrossSec. (365 days)
Downstream CrossSec. (365 days)
n-Pentane
Upstream CrossSec. (730 days)
Spill CrossSec. (730 days)
Downstream CrossSec. (730 days)
Depth
Molar Fractions

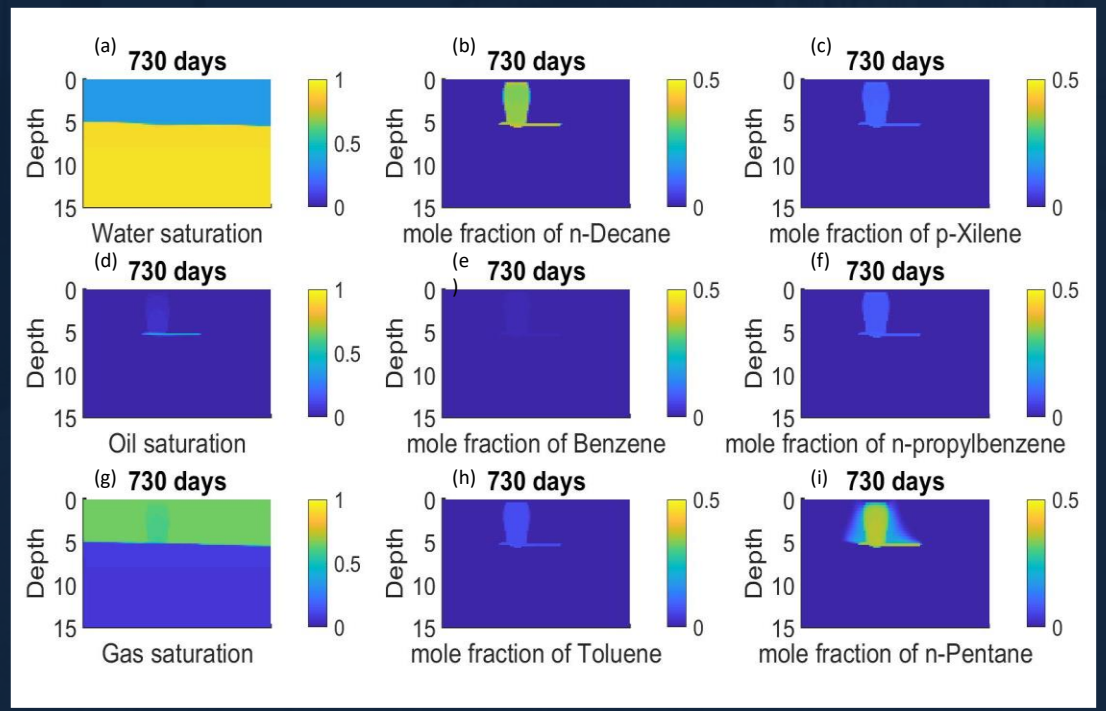

Upstream CrossSec. (365 days)
Spill CrossSec. (365 days)
Downstream CrossSec. (365 days)
Toluene
Upstream CrossSec. (730 days)
Spill CrossSec. (730 days)
Downstream CrossSec. (730 days)
Depth
Molar Fractions


Upstream CrossSec. (365 days)
Spill CrossSec. (365 days)
Downstream CrossSec. (365 days)
p-Xilene
Upstream CrossSec. (730 days)
Spill CrossSec. (730 days)
Downstream CrossSec. (730 days)
Depth
Molar Fractions

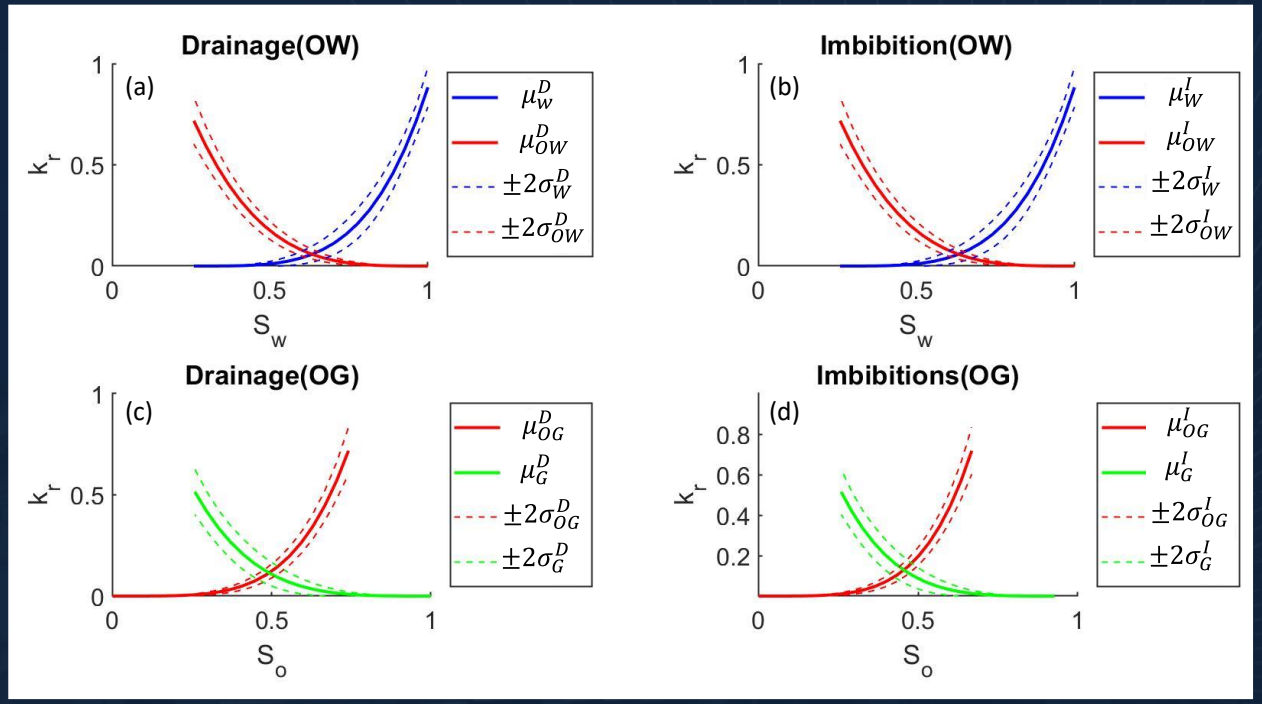

Upstream CrossSec. (365 days)
Spill CrossSec. (365 days)
Downstream CrossSec. (365 days)
n-propylbenzene
Upstream CrossSec. (730 days)
Spill CrossSec. (730 days)
Downstream CrossSec. (730 days)
Depth
Molar Fractions

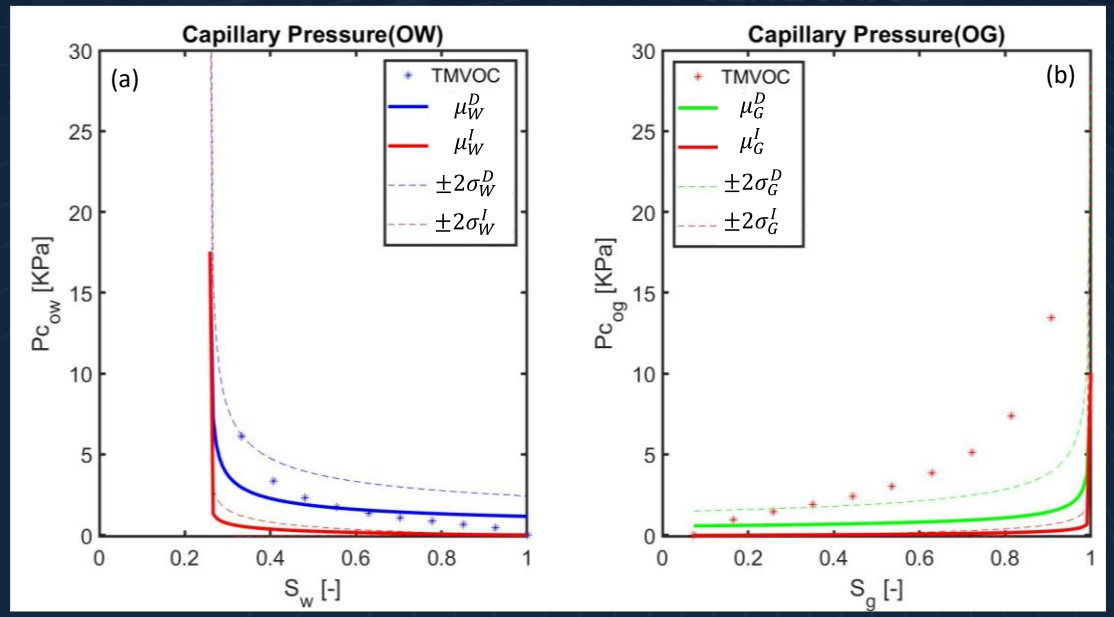

Upstream CrossSec. (365 days)
Spill CrossSec. (365 days)
Downstream CrossSec. (365 days)
Benzene
Upstream CrossSec. (730 days)
Spill CrossSec. (730 days)
Downstream CrossSec. (730 days)
Depth
Molar Fractions


Sample pdf
S_{wc}
S_{gt}
K^M_{rg}
n_{wo}
n_{go}
pc_{eg} [KPa]
Initial
Calibrated


(a) 730 days
Water saturation
(b) 730 days
mole fraction of n-Decane
(c) 730 days
mole fraction of p-Xilene
(d) 730 days
Oil saturation
(e) 730 days
mole fraction of Benzene
(f) 730 days
mole fraction of n-propylbenzene
(g) 730 days
Gas saturation
(h) 730 days
mole fraction of Toluene
(i) 730 days
mole fraction of n-Pentane
Depth

Results


Drainage(OW)
Imbibition(OW)
Drainage(OG)
Imbibitions(OG)
k_r
S_w
S_o
μ_w^D
μ_{OW}^D
$\pm 2\sigma_W^D$
$\pm 2\sigma_{OW}^D$
μ_W^I
μ_{OW}^I
$\pm 2\sigma_W^I$
$\pm 2\sigma_{OW}^I$
μ_{OG}^D
μ_G^D
$\pm 2\sigma_{OG}^D$
$\pm 2\sigma_G^D$
μ_{OG}^I
μ_G^I
$\pm 2\sigma_{OG}^I$
$\pm 2\sigma_G^I$


Capillary Pressure(OW)
Capillary Pressure(OG)
TMVOC
Pc_{ow} [KPa]
Pc_{og} [KPa]
S_w [-]
S_g [-]
μ_W^D
μ_W^I
$\pm 2\sigma_W^D$
$\pm 2\sigma_W^I$
μ_G^D
μ_G^I
$\pm 2\sigma_G^D$
$\pm 2\sigma_G^I$

Concluding Remarks:

- Our study is keyed to the *assessment of uncertainties* associated with simulation of *multiphase-multicomponent flow migration in contaminated sites*.

- We focused on the appraisal of the joint role of relative permeability and *capillary pressure* on responses of a compositional reservoir simulation practices.

- Simulation results show that *LNAPL Spill hardly influence the saturated zone* and LNAPL contaminant phase (as a whole) tend to stay on (or near) the aquifer surface and will not sink to the impermeable bedrock. It will float almost entirely upon the water phase as a film, without significant penetration into the water phase.

- Results show a *symmetrical distribution of LNAPL in the unsaturated zone* (in horizontal direction). In the *saturated zone* the total *VOC mass fraction is shifted along groundwater flow direction*.

- In our test case, *uncertainties are mainly linked to the estimations of relative permeabilities* during both drainage and imbibition conditions; when comparing to the effects of *capillary pressures*.

Concluding Remarks:

- *Molar fraction of each VOC in the NAPL phase is analyzed*. Results show that the amount of each component is primarily related to the mass flux entering in the aquifer, and the variations along the vertical direction are a consequence of the chemical properties of the compounds.

Calibrated model can generally provide reasonable estimation of molar fractions of alkanes (n-pentane and n-decane); hence reference values for molar fractions of alkyl VOCs are overestimated (benzene, toluene, p-xylene, n-propylbenzene).

Key References:

- Pruess, K. Battistelli, A.: TMVOC, a Numerical Simulator for Three-Phase Non-Isothermal Flows of Multicomponent Hydrocarbon Mixtures in Saturated-Unsaturated Heterogeneous Media, Lawrence Berkeley National Laboratory Report LBNL-49375, April 2002.

- Lie, K.A.: An Introduction to Reservoir Simulation Using MATLAB/GNU Octave : User Guide to the MATLAB Reservoir Simulation Toolbox (MRST), Cambridge University Press. (2019). https://doi.org/10.1017/9781108591416

- Møyner, O., Tchelepi, H.: A Multiscale Restriction-Smoothed Basis Method for Compositional Models. SPE Reservoir Simulation Conference, TX. USA 20-22 February 2017. https://doi.org/10.2118/182679-MS