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The Relevance of Fluid and Porous Media Properties for DNAPL Migration and Entrapment: A Numerical Evaluation of Laboratory Experiments

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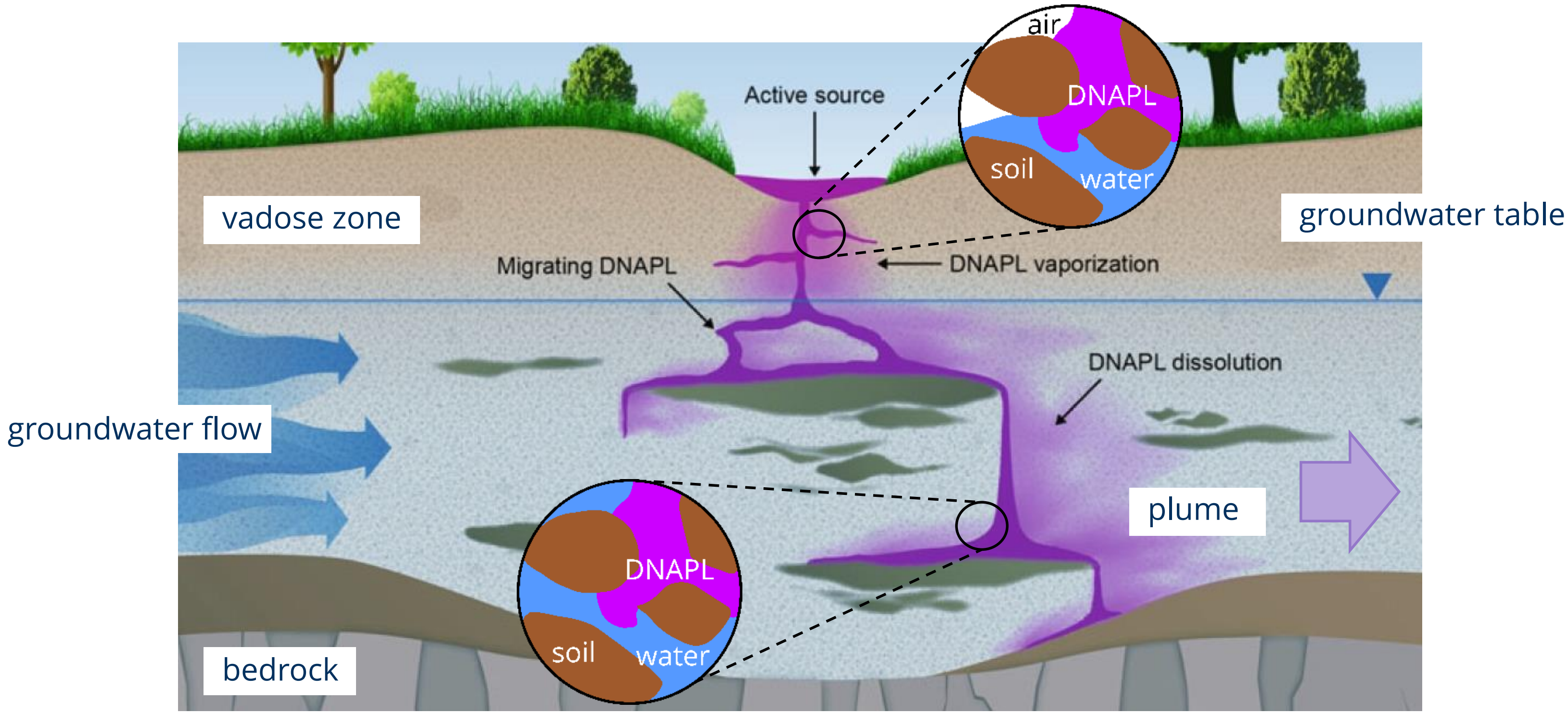
Background

- Ongoing worldwide contamination of groundwater bodies by compounds belonging to the chemical group of Dense Non-Aqueous Phase Liquids (DNAPLs) ▶ next slide

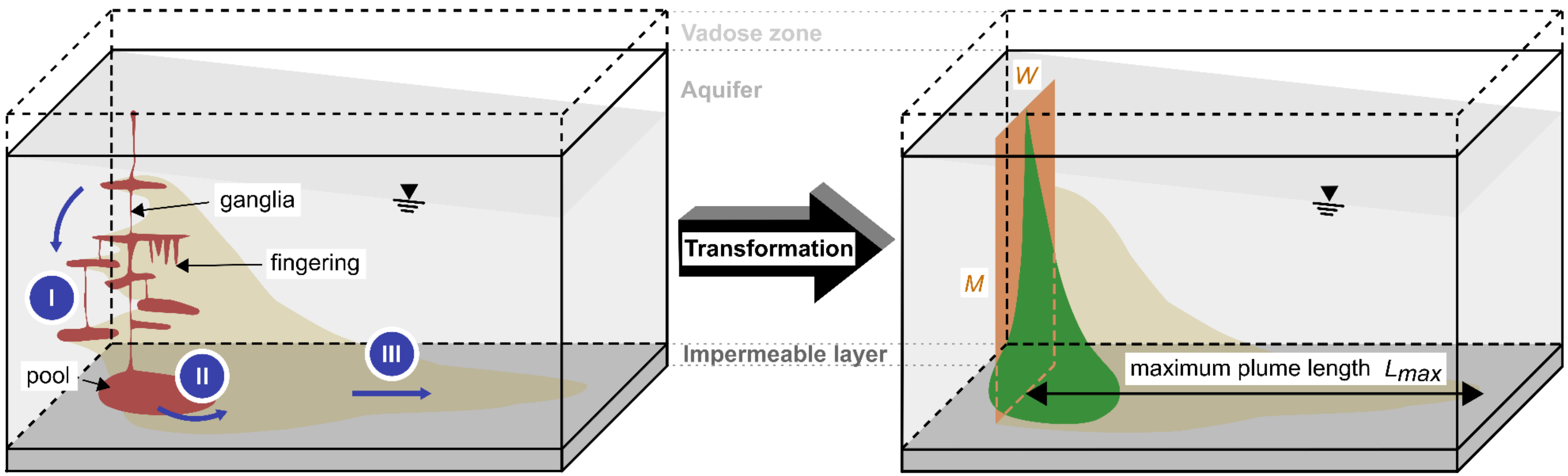
Background (modified after [1])



Background

- Ongoing worldwide contamination of groundwater bodies by compounds belonging to the chemical group of Dense Non-Aqueous Phase Liquids (DNAPLs)
- DNAPLs are toxic, mutagenic, highly persistent, and soluble in water (may reach wells used for water abstraction), so that assessment and remediation are essential
- Source zone geometry (SZG) has major influence on dissolved contaminant plumes, but often considered as over-simplified SZG
- Exploration of SZGs limited by technical/economical constraints
- Complex processes vs. poor knowledge on SZGs [2] next slide

Concept of DNAPL contamination [2]



- DNAPL source zone
- DNAPL plume
- Over-simplified implementation of source zone geometry (*W*... width, *M*... thickness)
- Effective source zone geometry
- I Phase migration
- II Mass transfer from organic to aqueous phase
- III Advective-dispersive transport incl. sorption and reactions

Goals

- Enhance understanding of DNAPL source zone formation
- Identification of factors relevant for phase migration

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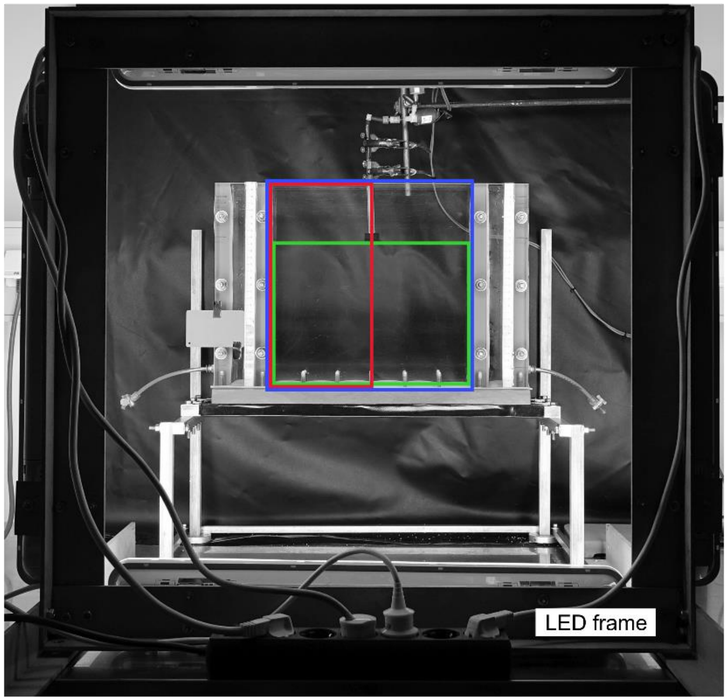
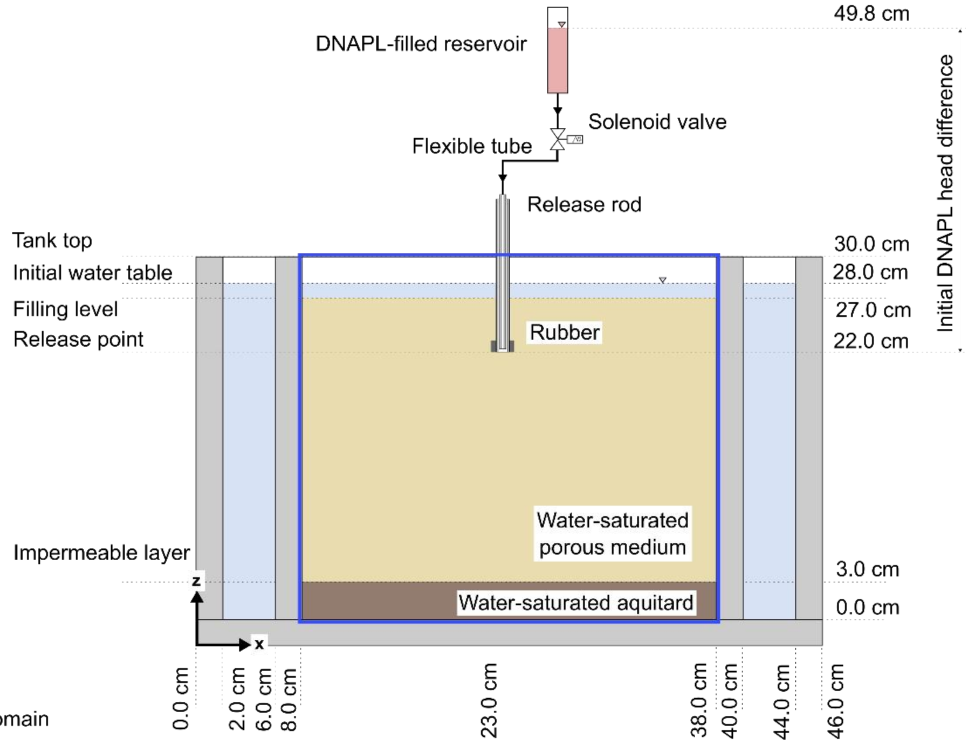
Approach

- Perform experimental trials to generate observation data
- Develop and apply image processing and analysis (IPA) framework
- Definition of reference model base-case scenarios
- Calibration of numerical multiphase flow model against IPA data
- Estimation of uncertainties and parameter relevance

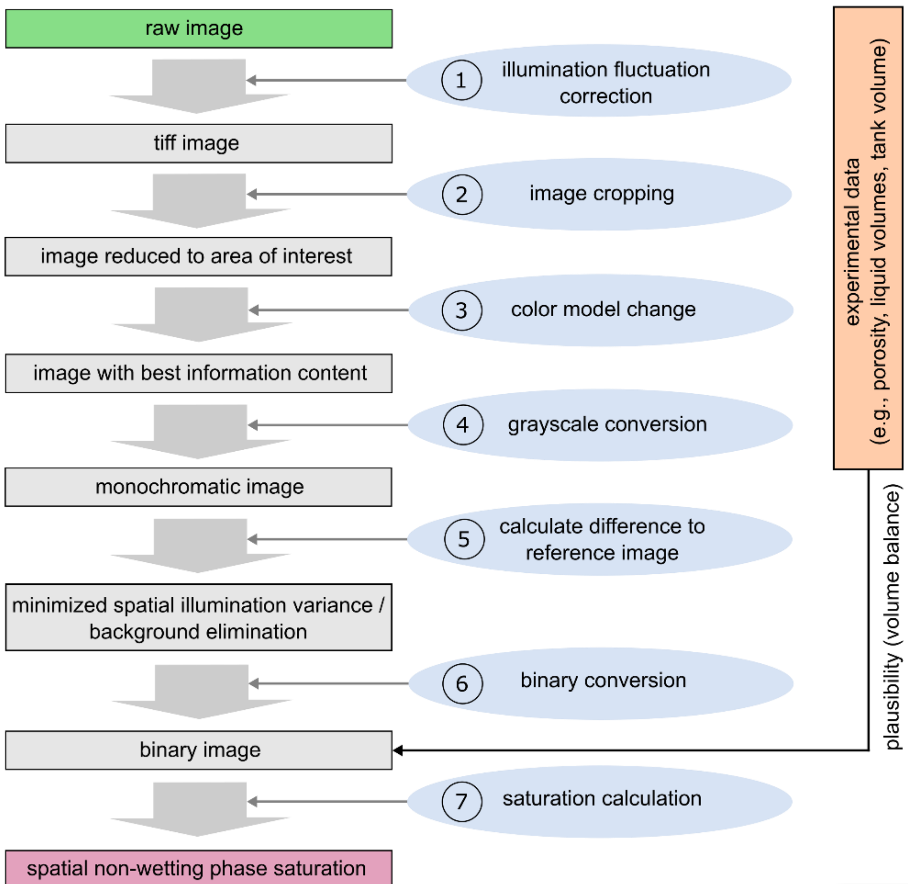
Experimental setup for DNAPL release [3,4,5,6]

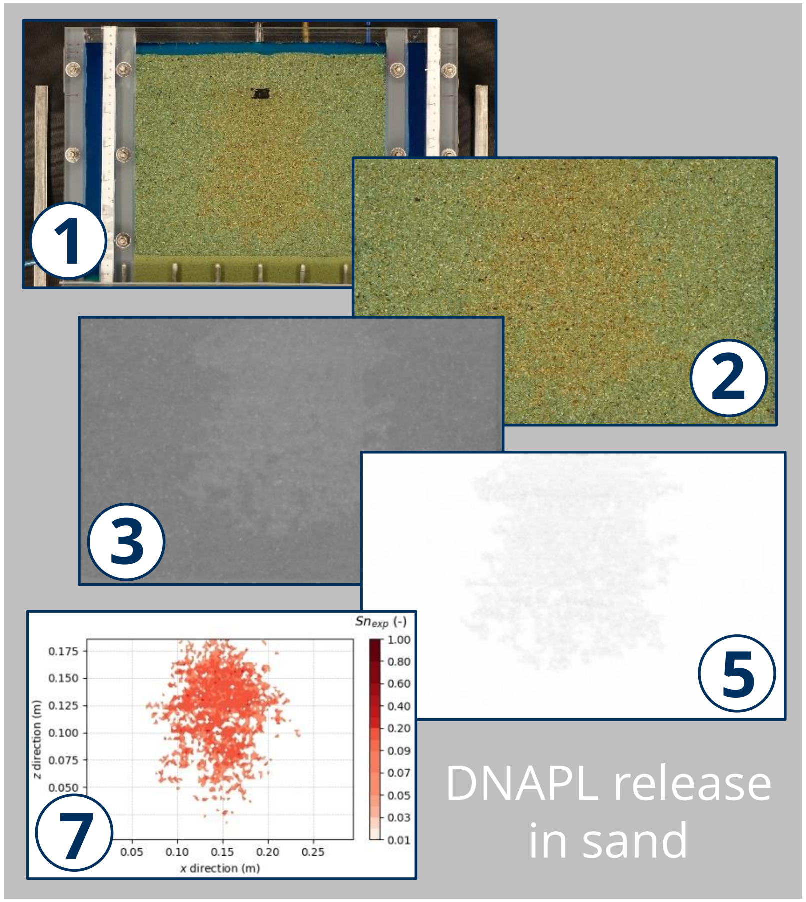




Experiment domain IPA domain TMVOC model domain

IPA framework [3,4,5,6]

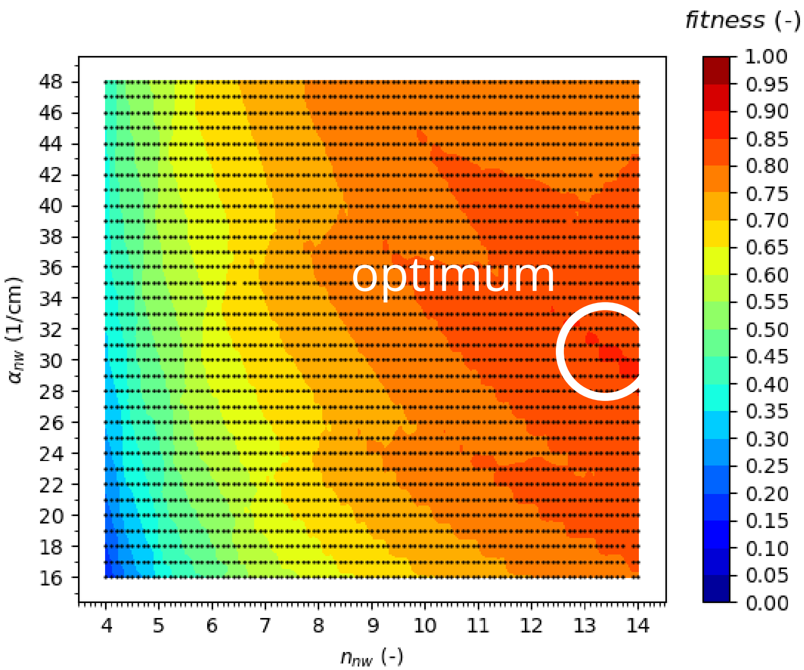




Modeling strategy [4]

- Applied code: parallelized version of TMVOC [7], as implemented in TOUGH3 [8]
- Assumptions: 2-D, two-phase flow, single component, isothermal, homogeneous domain, no diffusion, no degradation, no reactions
- Quantifiable parameters fixed, variation of type curve parameters α_{nw} and n_{nw} [9], manual calibration through Monte Carlo analysis
- Utilization of HPC cluster Taurus (TU Dresden) for simultaneously performing large number of model realizations ($\sum \sim$ 40,000)
- Use of Python 3.x for automatized pre- and post-processing

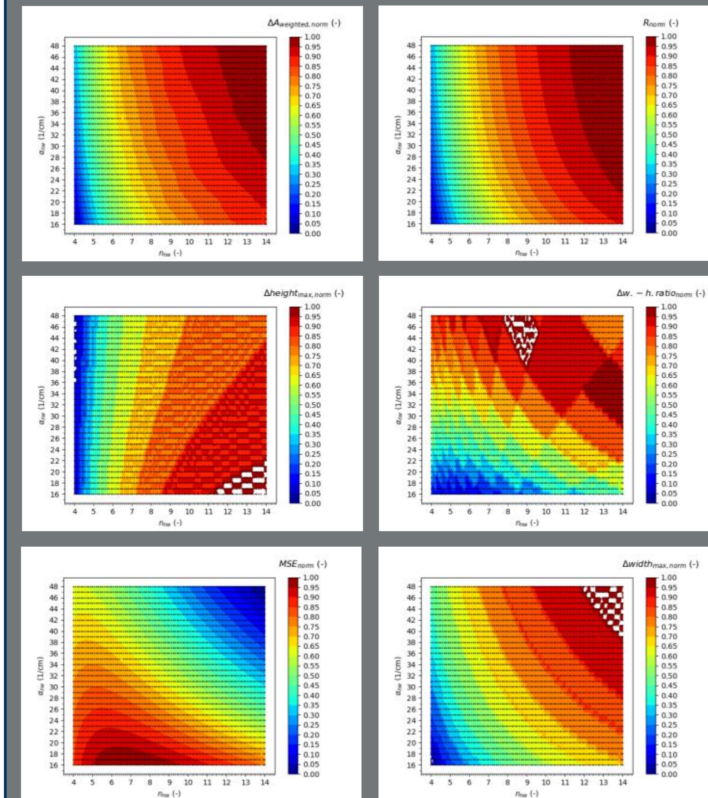
First exemplary results (work in progress) [4]



Model fitness for glass bead scenario at t = 20s (end of release)

● … model realization
0 … worst fitness
1… best fitness

Partial objective functions



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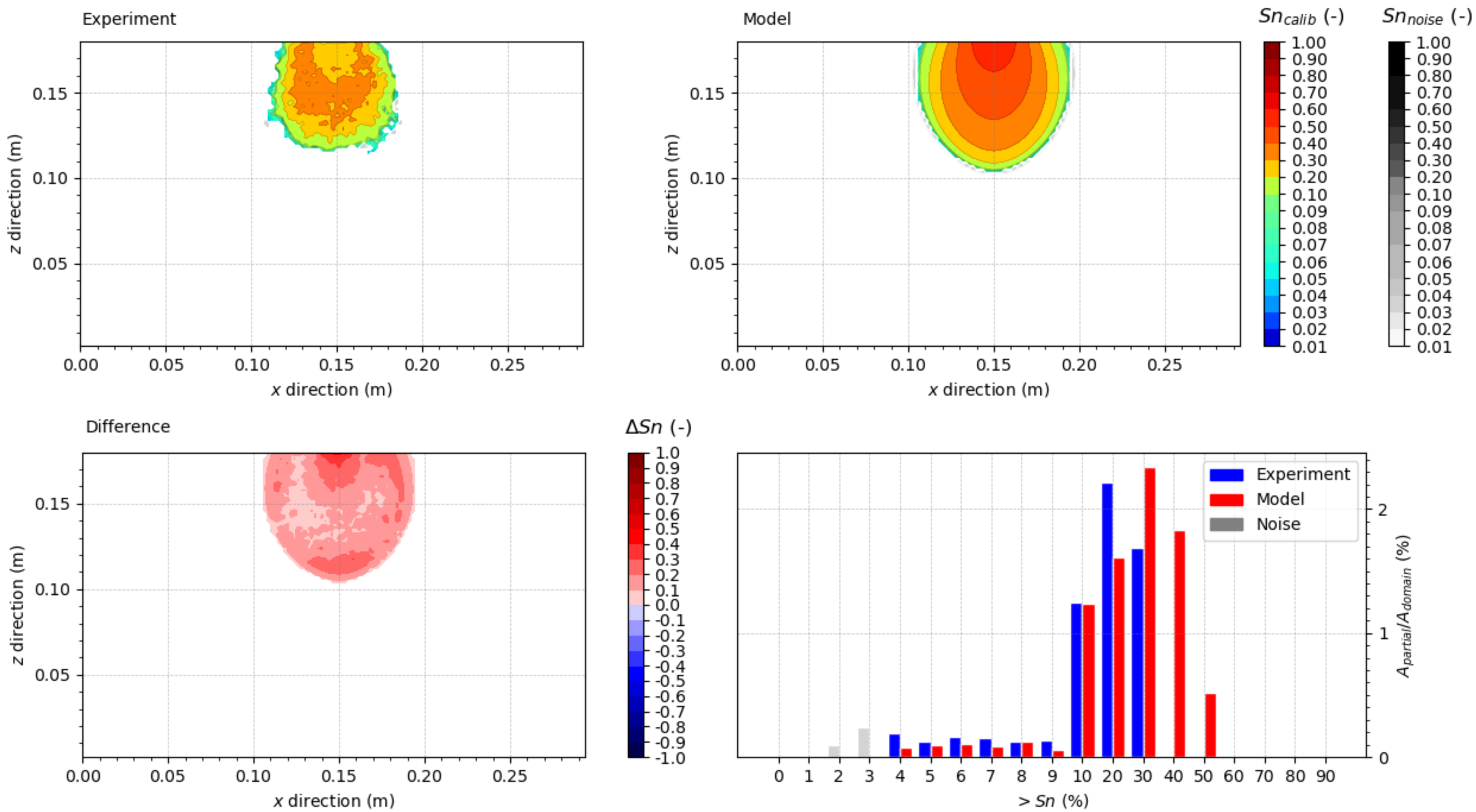

DNAPL saturation distribution for glass bead scenario at t = 20s (end of release)

n_{nw} = 14.0

α_{nw} = 28.0 cm^{-1}

Conclusions

- Model results prove high sensitivity of type curve parameters [4]
- Good agreement between observation and simulation data [4]
- Parts of DNAPL saturation within noise spectrum of IPA data (glass beads: < 4%) [4]

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Outlook

- Finalize calibration for remaining porous media type scenarios [4]
- Quantify and compare uncertainties (experiment, IPA, model) [4]
- Improve relationship between gray-scale intensity and DNAPL saturation to reduce noise spectrum in IPA data
- Add processes to increase system complexity
- Perform SZG predictions

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