Migration and Retention of a Heavy NAPL Vapor in the Unsaturated Zone

International Research Training Group **nupus**

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VEGAS Versuchseinrichtung zur Grundwasser- und Altlastensanierung

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Nupus Conference Freudenstadt, 16 - 19 March 2014

Motivation

Spreading and migration of contaminants in the unsaturated zone may occur as liquid or gas. Vapor (gas) plumes may accumulate in subsurface parts of buildings or sink towards the groundwater table.

- Does migration of vapors from a liquid spill in the unsaturated zone pose a potential threat to underlying aquifers?
- How does a contaminant vapor plume migrate in the unsaturated zone and how is it influenced by the component's properties?
- Do physical processes (e.g. adsorption) retard migration in porous media and how does water saturation affect the behavior?

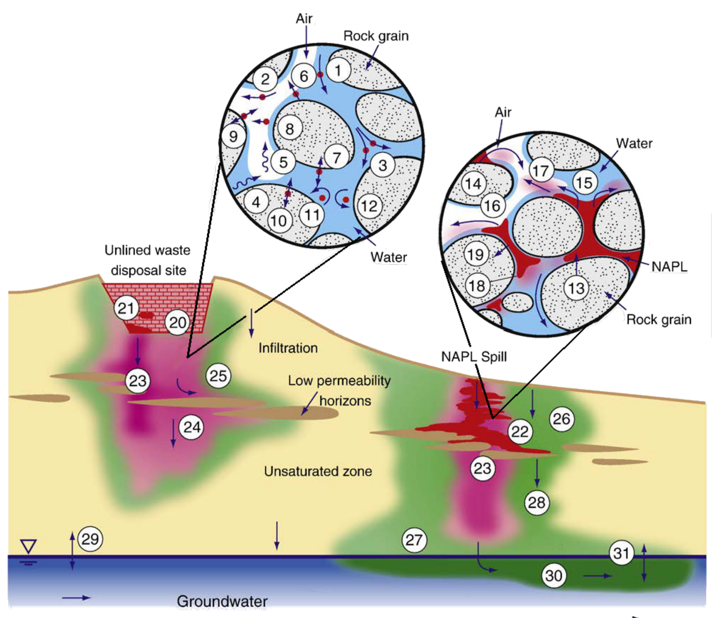

Figure 1: Contamination in the unsaturated zone [3].

Vapor Migration

Column experiments to quantify density-driven vapor migration of carbon disulfide (CS_2) in dry porous media.

Darcy's law and Rayleigh number for vapor transport [4]:

$$q = -\frac{k}{\mu}\nabla(P + \rho g z)\,;\, Ra_m = \frac{gkL(\rho_S - \rho_\infty)}{\mu D_{eff}}$$

Migration is dependent on molecular mass and vapor pressure of contaminant.

Vapor migration experiment:

- 1-D column experiments (L = 4 m)
- Boundary conditions
  - Glass beads:
    - $k_{coarse} = 1.5 \times 10^{-9}\,m^2$
    - $k_{medium} = 2.6 \times 10^{-10}\,m^2$
  - Injection of heavy NAPL vapor (CS_2) in middle of column
  - Top/bottom: constant pressure (p_{atm})
- Concentration measurement over time

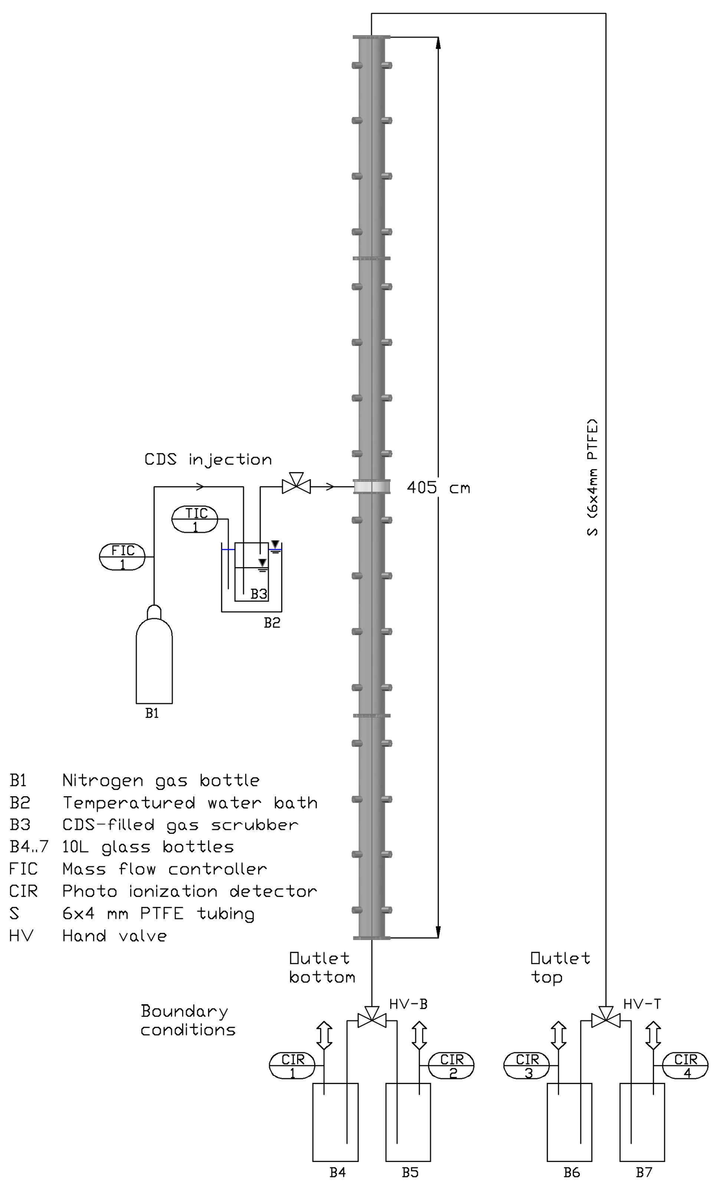

Figure 2: Flow chart of vapor migration experiment set-up.

Numerical simulation to understand physical principles for migration:

- 1-D 2p2cni model
- Initial hydrostatic pressure distribution
- Model including boundary set-up (tubing)

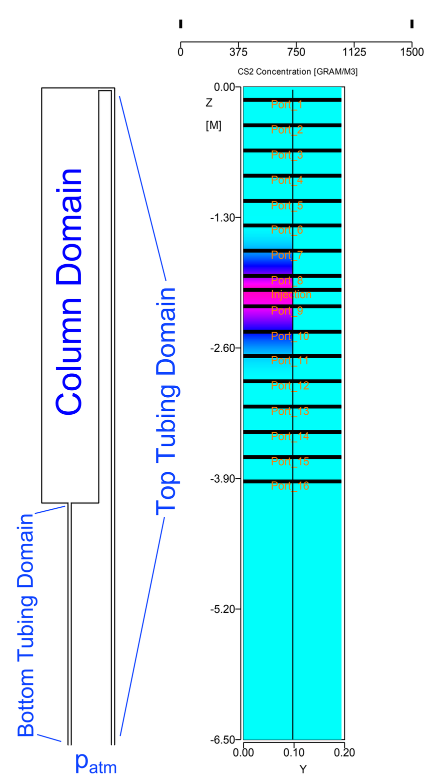

Figure 3: Numerical model set-up.

Preliminary results of investigation:

- Description of density-driven vapor migration
- Observed acceleration as an effect of boundary conditions.
- Physical principles of migration process are understood
- Transport dependent on permeability and total mass of contaminant
- Migration behavior reproduced in 1-D numerical simulations

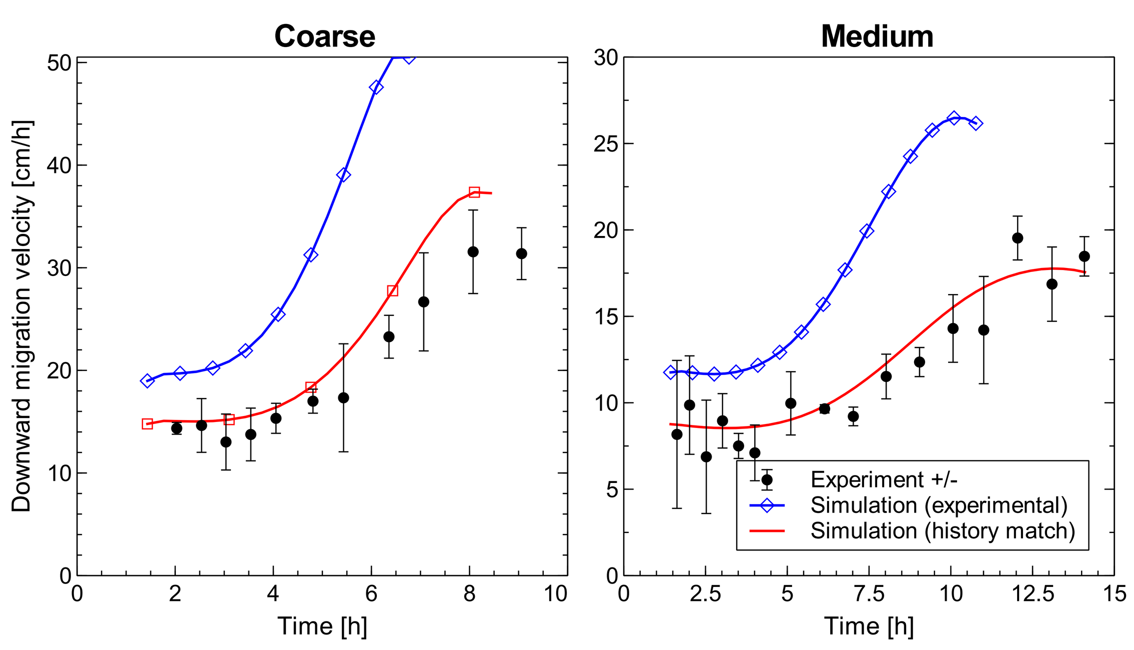

Figure 4: Downward velocity of vapor migration experiments and simulations.

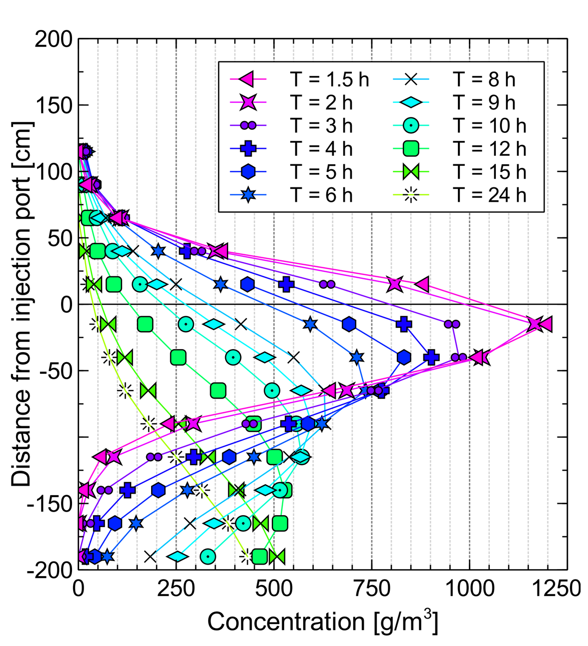

Figure 5: Concentration profiles in column experiment.

Vapor Retardation

Column experiments to quantify retardation of CS_2 vapor in unsaturated zone and its dependency on porous media and water saturation.

Retardation of vapor in moist porous media [1, 2]:

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x},$$

$$R = 1 + \frac{\theta_w}{\theta_a K_H} + \frac{\rho_b K_{Dsat}}{\theta_a K_H} + \frac{K_{IA}A_{IA}}{\theta_a}$$

Vapor retardation experiments:

- 1-D column experiments (L = 2 m)
- Upwards flow of CS_2 vapor and conservative tracer (Helium)
- Breakthrough curves at outflow to evaluate retardation

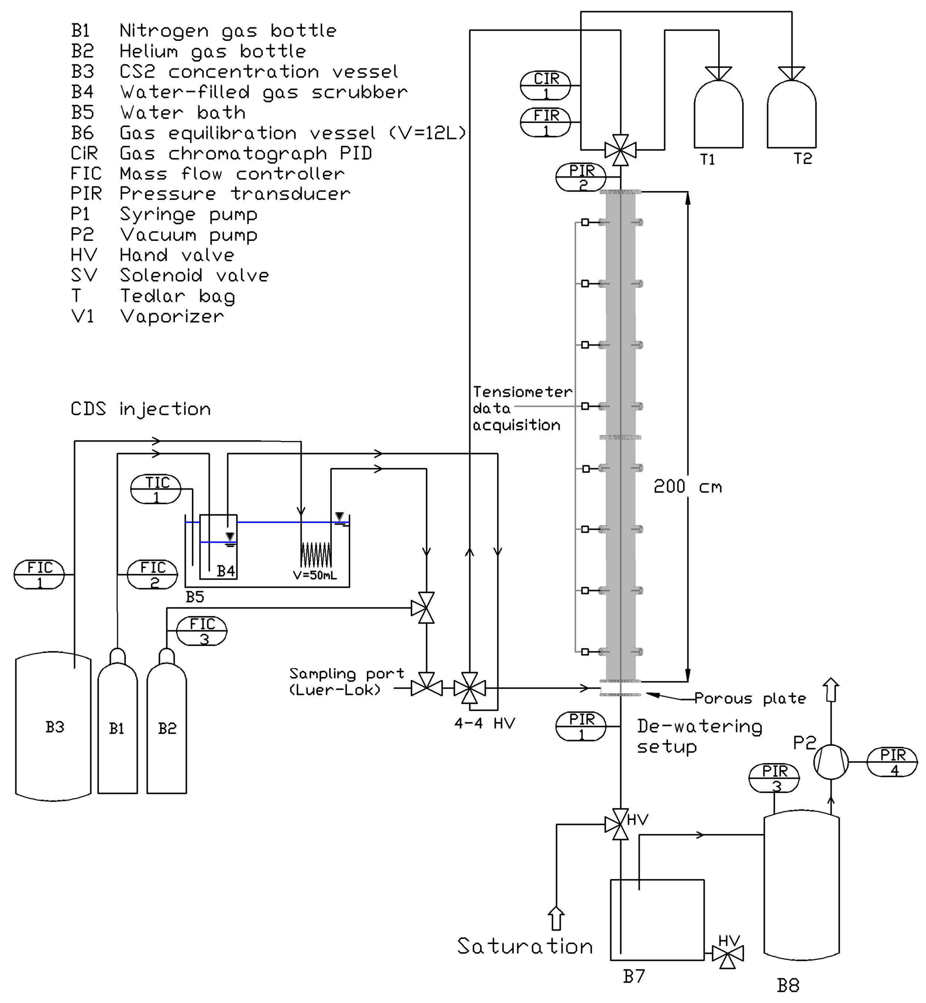

Figure 6: Flow chart of vapor migration experiment set-up.

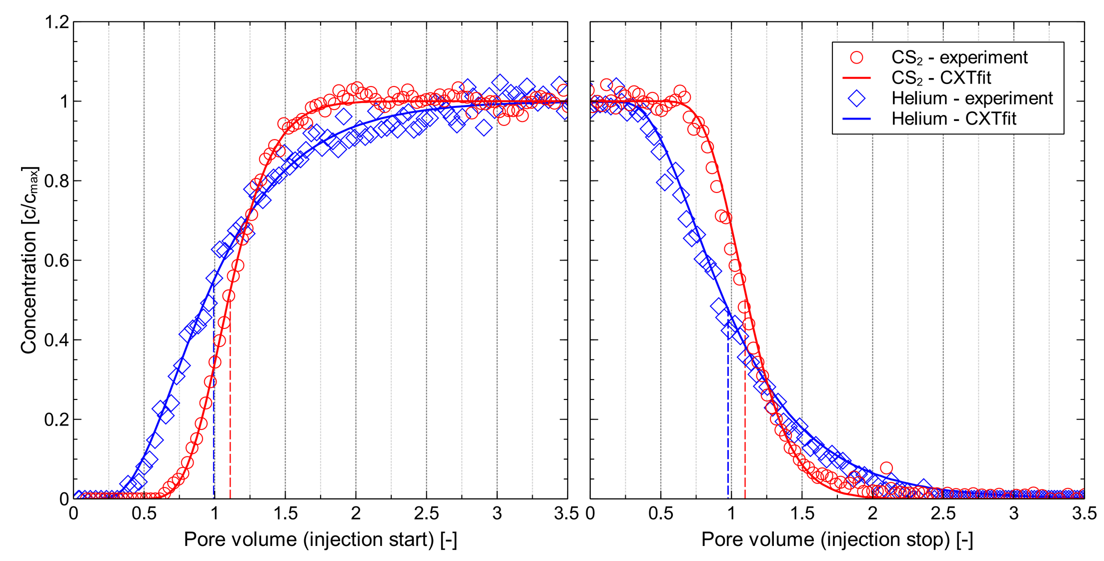

Figure 7: Breakthrough curves (BTC) of CS_2 and conservative tracer Helium in dry porous media.

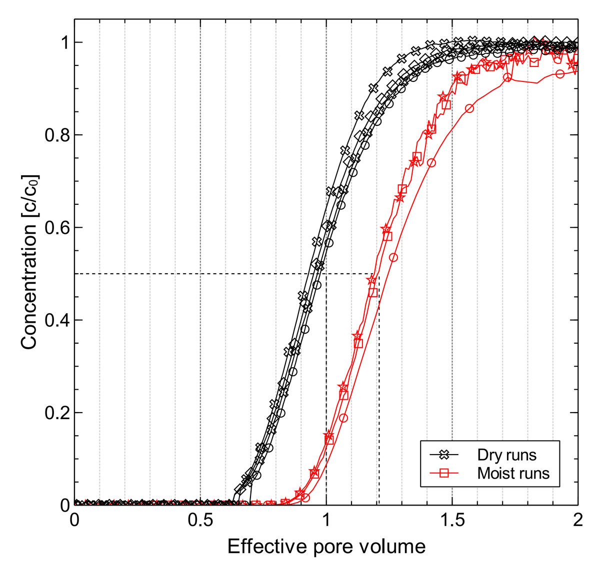

Figure 8: BTC of CS_2 in dry and moist porous media.

Preliminary results:

- Total retardation behavior of CS2 vapor can be quantified based on 1D column experiments
- First experiments indicate that mass transport is reduced by sorption/partitioning processes

Outlook

Vapor migration: additional experiment runs to delineate effect of boundary conditions and validate model.

Vapor retardation: description of retardation as function of porous medium and water saturation variation based on set of column experiments

References

[1] Brusseau, M. L., Popovičová, J., and Silva, J. A. K. (1997). Characterizing gas-water interfacial and bulk-water partitioning for gas-phase transport of organic contaminants in unsaturated porous media. *Environmental Science & Technology*, 31(6):1645–1649.

[2] Popovičová, J. and Brusseau, M. L. (1998). Contaminant mass transfer during gas-phase transport in unsaturated porous media. *Water Resources Research*, 34(1):83–92.

[3] Rivett, M. O., Wealthall, G. P., Dearden, R. A., and McAlary, T. A. (2011). Review of unsaturated-zone transport and attenuation of volatile organic compound (VOC) plumes leached from shallow source zones. *Journal of Contaminant Hydrology*, 123(3-4):130–156.

[4] Seely, G. E., Falta, R. W., and Hunt, J. R. (1994). Buoyant advection of gases in unsaturated soil. *Journal of Environmental Engineering*, 120:1230–1247.

Simulations are performed using the open-source simulator DuMu^x and *Shell*'s Dynamo/MoReS.