BUNDESGESELLSCHAFT
FÜR ENDLAGERUNG

COMPARING UNCERTAINTY QUANTIFICATION METHODS FOR MODELLING RADIONUCLIDE TRANSPORT IN NUCLEAR WASTE DISPOSAL SYSTEMS

1st URS PhD Workshop

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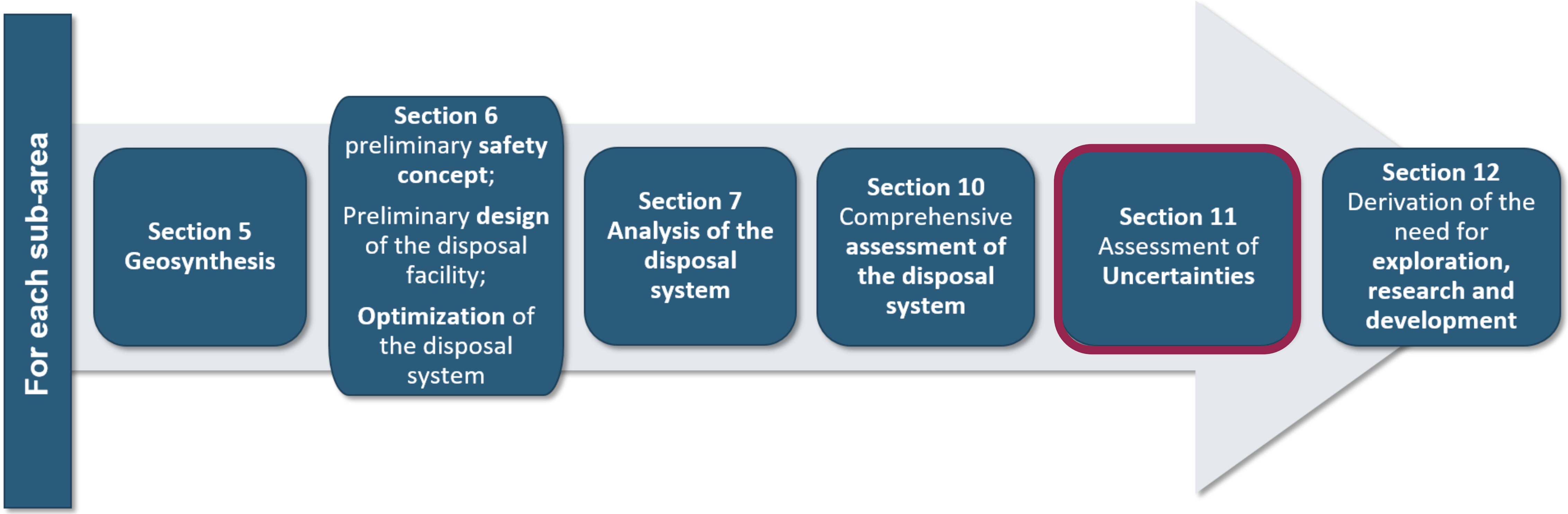
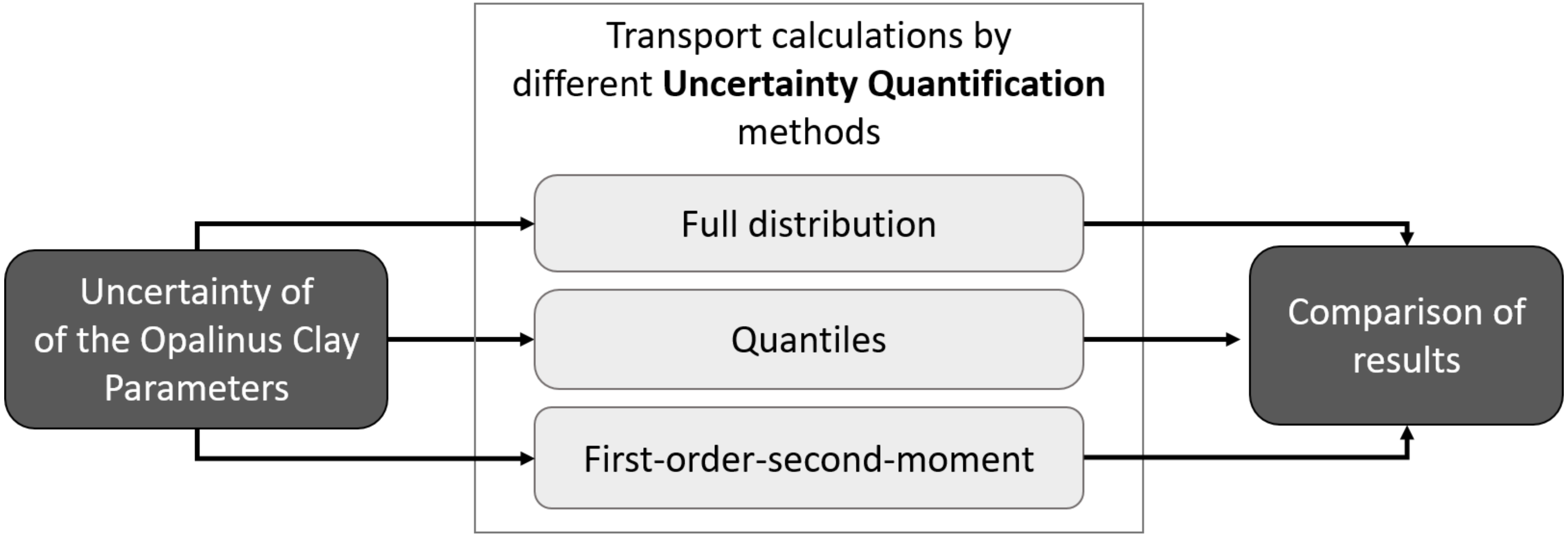
INTRODUCTION AND MOTIVATION



MODEL BENCHMARK AND APPROACH

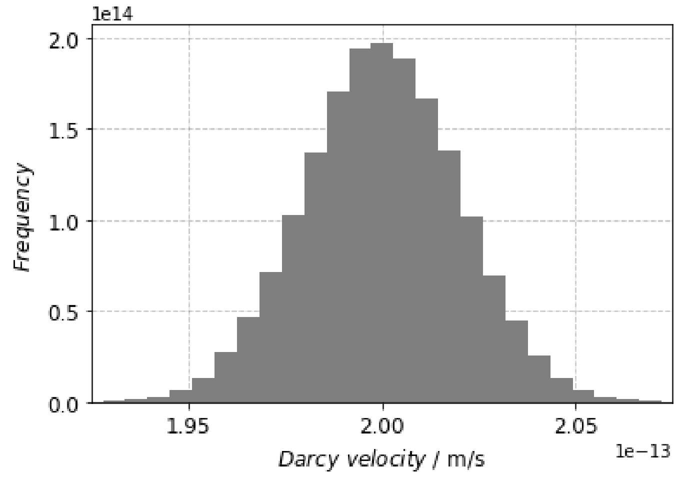
- 1D model of the Opalinus Clay
- Analytical solution by Van Genuchten (1981) for advection, sorption and decay [1]
- Migration of iodine 129

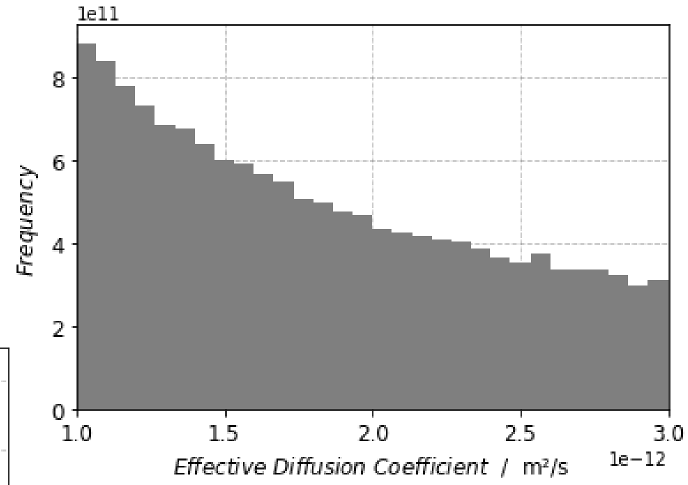
- Modelling domain: 160 m
- Node spacing: 0.4 m
- Simulation time: one million years

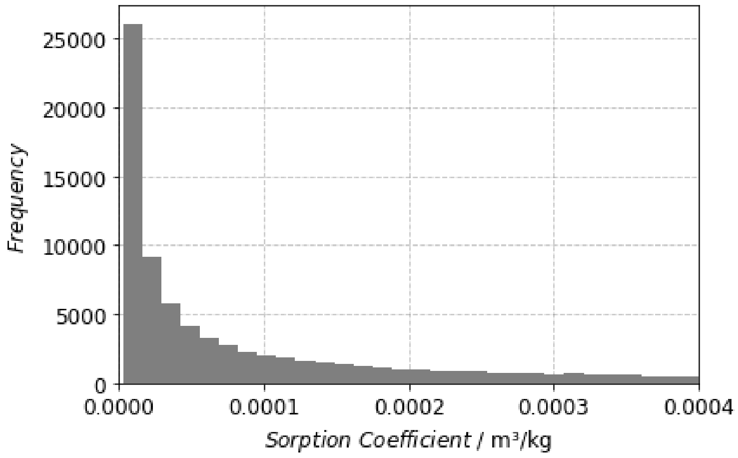


PARAMETERIZATION

Parameter	Value	Reference
Porosity of OPA [-]	0.12	[2]
Bulk Density of OPA [kg/m^3]	2 394	[2]
Darcy velocity in OPA [m/s]	$2 \cdot 10^{-13}$	[3]
Effective diffusion coefficient for ^{129}I in OPA [m^2/s]	$1 \cdot 10^{-12}$	[2]
Kd-value for 129I in OPA [m^3/kg]	$3 \cdot 10^{-5}$	[2]
Half-life of 129I [year]	$1.6 \cdot 10^7$	[2]







UNCERTAINTY QUANTIFICATION METHODS AND RESULTS 1/2

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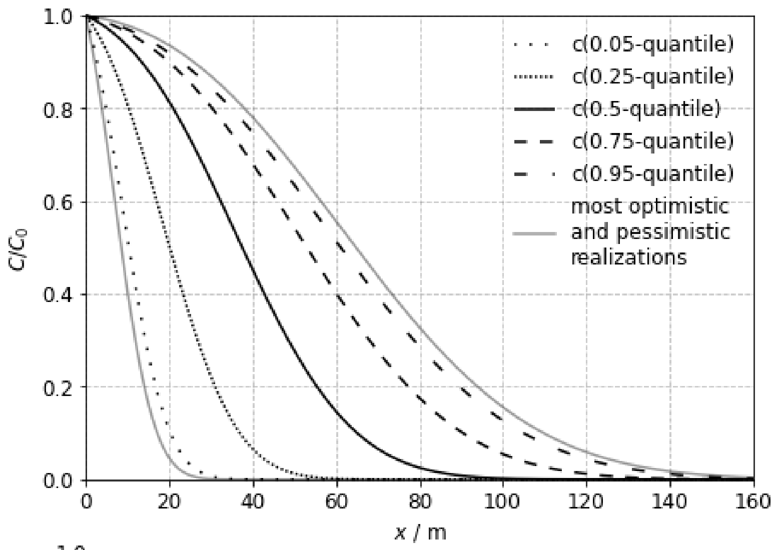
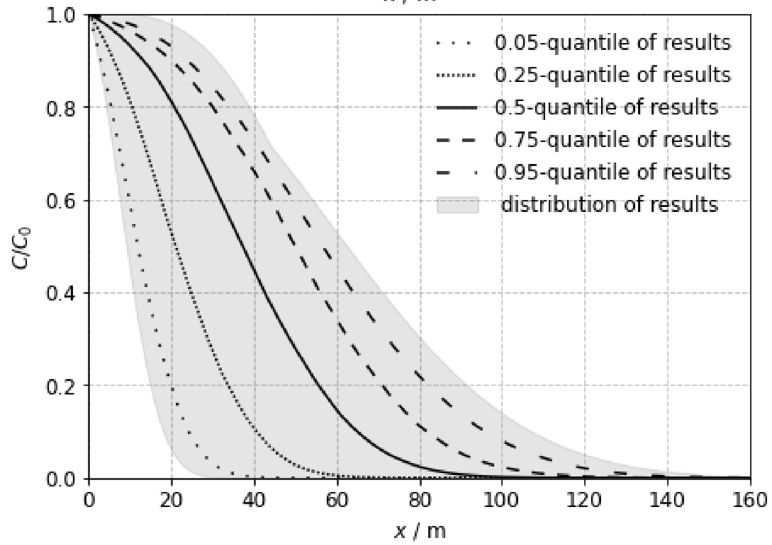
1. Calculations based on quantiles and intervals of distributions
   - sample of 100,000 elements from each parameter distribution
   - 0.05-, 0.25-, 0.5-, 0.75- and 0.95-quantile, the minimum and maximum values as input for transport calculations (7 calculations)
      - ➢ results: set of discrete values
2. Uncertainty Quantification based on full distributions
   - 100,000 calculations
   - Monte-Carlo-Sampling of uncertain parameters
      - ➢ results: 100,000 results, from which statistical properties can be calculated





UNCERTAINTY QUANTIFICATION METHODS AND RESULTS 2/2

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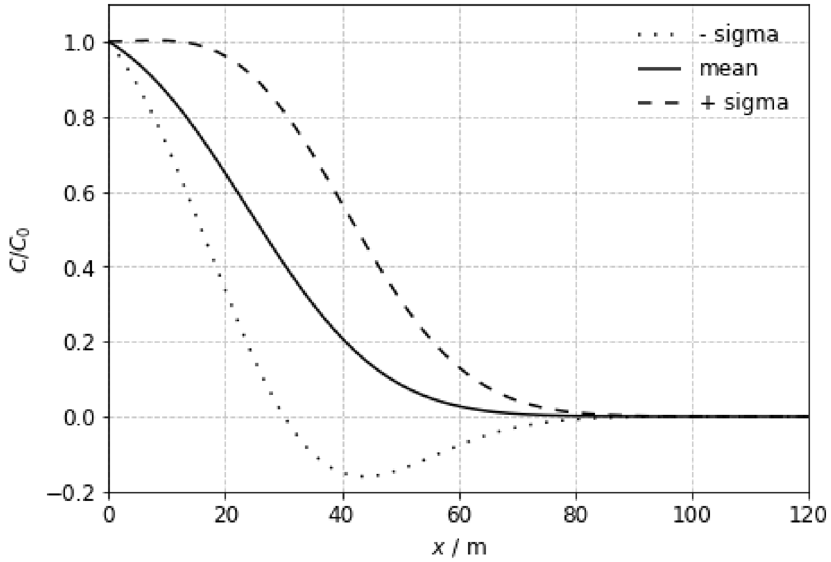
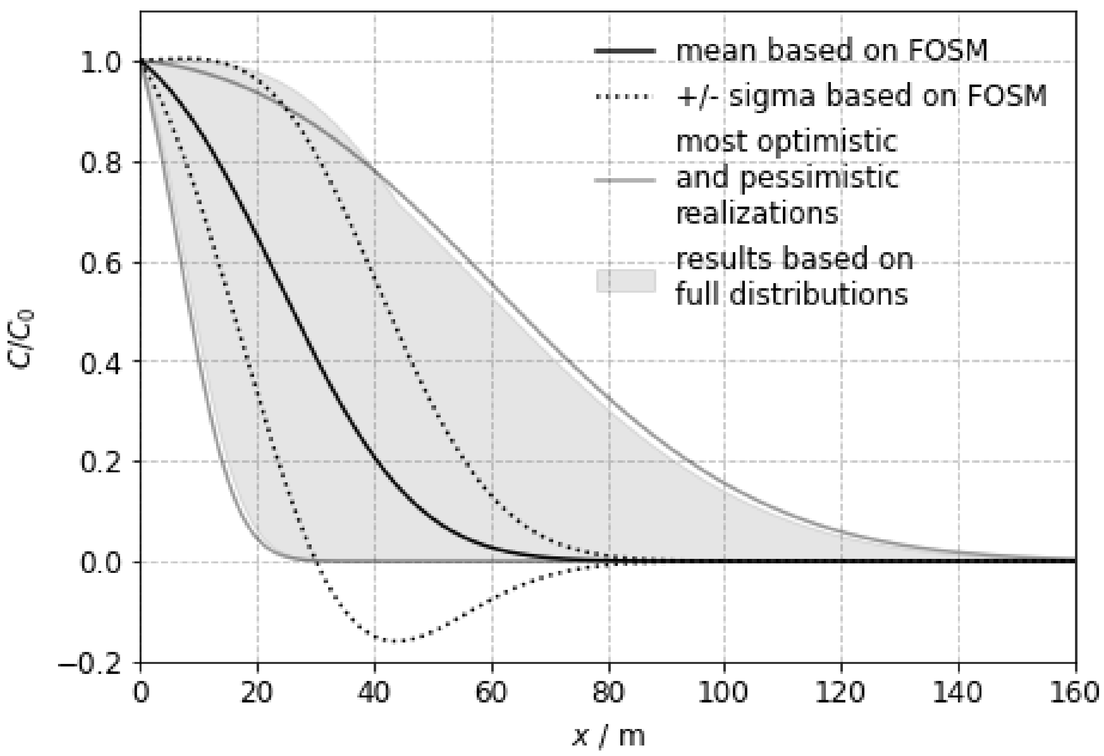
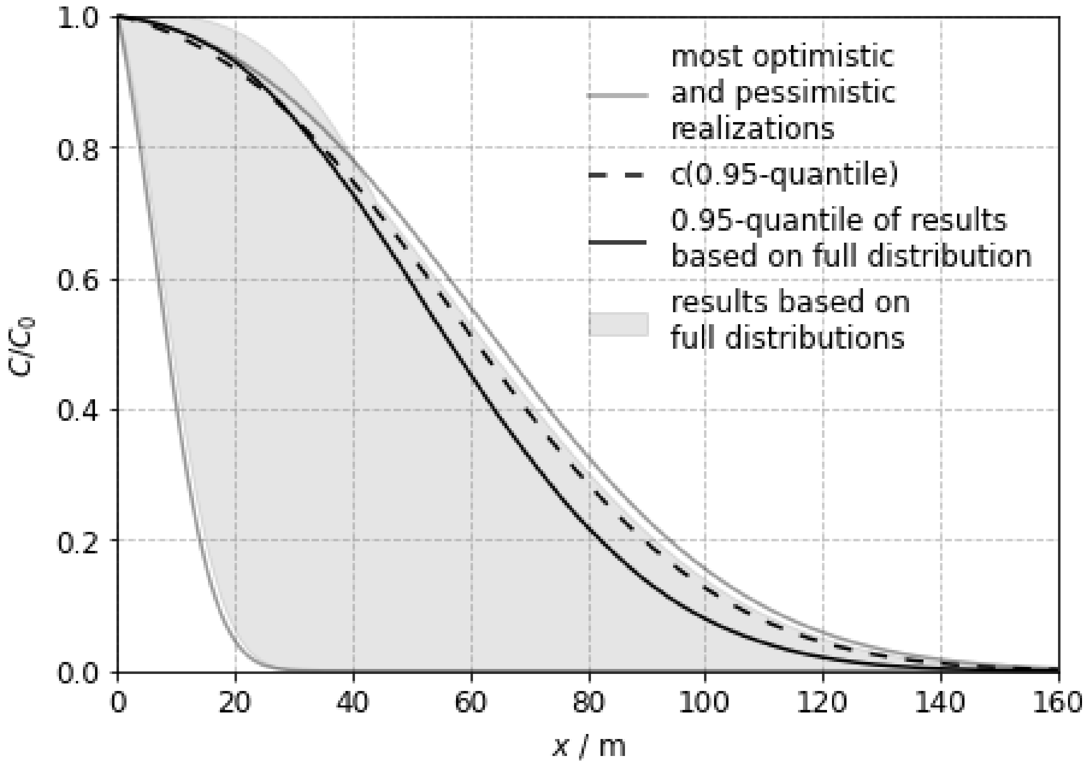
3. First-order second-moment (FOSM) method
   - Based on Taylor-Series Expansion
   - Expansion around the mean of uncertain parameter
   - Requires knowledge of distribution type (normal, log-uniform)
     - ➢ results: mean and variance



COMPARISON OF RESULTS





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REFERENCES

1. M. T. VAN GENUCHTEN, “Analytical solutions for chemical transport with simultaneous adsorption, zero-order production and first-order decay,” *Journal of Hydrology,* **49**, 213-233 (1981).
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3. P. BOSSART, F. BERNIER, J. BIRKHOLZER, C. BRUGGEMAN, P. CONNOLLY, S. DEWONCK, M. FUKAYA, M. HERFORT, M. JENSEN, J.-M. MATRAY, J. C. MAYOR, A. MOERI, T. OYAMA, K. SCHUSTER, N. SHIGETA, T. VIETOR, K. WIECZOREK, “Mont Terri rock laboratory, 20 years of research: introduction, site characteristics and overview of experiments”, *Swiss J. Geosci.*, **110**, 3-22 (2017)

BACKUP

Analytical Solution by Van Genuchten (1981)

$$\frac{c}{c_0}(x,t) = H(x,t) + M(x,t)$$

with

$$H(x,t) = \frac{1}{2}\exp\left[\frac{(v-u)x}{2D_p}\right]\operatorname{erf}\left[\frac{Rx-ut}{2(D_pRt)^{1/2}}\right] + \frac{1}{2}\exp\left[\frac{(v+u)x}{2D_p}\right]\operatorname{erf}\left[\frac{Rx+ut}{2(D_pRt)^{1/2}}\right]$$

and

$$M(x,t) = -\frac{c_{\text{ini}}}{c_0}\exp\left(-\frac{\mu t}{R}\right)\left\{\frac{1}{2}\operatorname{erf}\left[\frac{Rx-vt}{2(D_pRt)^{1/2}}\right] + \frac{1}{2}\exp\left(\frac{vx}{D_p}\right)\operatorname{erf}\left[\frac{Rx+vt}{2(D_pRt)^{1/2}}\right]\right\} + \frac{c_{\text{ini}}}{c_0}\exp\left(-\frac{\mu t}{R}\right)$$

where

$$u = v\left(1 + \frac{4\mu D_p}{v^2}\right)^{1/2}$$

and

$$\mu = \frac{\log(2)}{t_{1/2}}\left(1 + \rho\frac{K_d}{\phi}\right)$$

Initial Conditions: $c_{\text{ini}} = 0\ \text{mol/L}$
Boundary Conditions: $c_0 = 1\ \text{mol/L}$