

EXAMPLE PROBLEMS

The module UNSATCHEM is developed from the variably saturated solute transport model HYDRUS-1D [Šimůnek *et al.*, 1997], and thus the water flow and solute transport parts of the model have been tested earlier. Therefore both example problems solved in this section concentrate on the demonstration of the chemical features of the model.

Two example problems are presented in this section. The first example simulates an infiltration process into a relatively dry soil column. This example shows predicted differences between the equilibrium and kinetic precipitation-dissolution model. The second example simulates a furrow irrigation problem

1. Example 1 - Column Infiltration

This example is based on the one used in the documentation of the code SWMS_2D [Šimůnek *et al.*, 1992] to compare results obtained with the SWMS_2D and UNSAT2 [Davis and Neuman, 1983] codes. It originally simulated a one-dimensional laboratory infiltration experiment discussed by Skaggs *et al.* [1970]. This example was altered for the purposes of this report to include multicomponent chemical transport.

The soil water retention and relative hydraulic conductivity functions of the sandy soil are $\theta_r=0.02$, $\theta_a=0.02$, $\theta_s=\theta_m=0.35$, $\theta_k=0.2875$, $\alpha=0.0410 \text{ cm}^{-1}$, $n=1.964$, $K_s=0.000722 \text{ cm s}^{-1}$, $K_k=0.000695 \text{ cm s}^{-1}$. The sand was assumed to be at an initial pressure head of -150 cm. The soil hydraulic properties were assumed to be homogenous and isotropic. The column was subjected to ponded infiltration (a Dirichlet boundary condition) at the soil surface, resulting in one-dimensional vertical water flow. The open bottom boundary of the soil column was simulated by implementing a no-flow boundary condition during unsaturated flow ($h<0$), and a seepage face with $h=0$ when the bottom boundary becomes saturated (this last condition was not reached during the simulation). The solution composition of the water initially present in the soil profile is that of a calcite supersaturated well water from the Wellton-Mohawk Irrigation District (well # 15 [Suarez, 1977]: $\text{Ca}_T=12.2$, $\text{Mg}_T=9.7$, $\text{Na}_T=37.5$, $\text{K}_T=0.3$, $\text{Cl}_T=31.1$, $\text{SO}_{4T}=22.1$, alkalinity=6.5 $\text{mmol}_c\text{L}^{-1}$). Calcite undersaturated Colorado river water from the Grand Valley ([Rhoades and Suarez, 1977]: $\text{Ca}_T=2.63$, $\text{Mg}_T=1.05$, $\text{Na}_T=2.55$, $\text{K}_T=0.06$, $\text{Cl}_T=1.94$, $\text{SO}_{4T}=2.03$, alkalinity=2.33 $\text{mmol}_c\text{L}^{-1}$) was used as the solution composition of the infiltrating water. The simulation was run at a temperature of 25 °C and the soil CO_2 concentration was assumed to be equal to the atmospheric CO_2 (0.000333). The precipitation-dissolution of calcite was considered either as an equilibrium or kinetic process with a calcite surface area of $0.02 \text{ m}^2\text{l}^{-1}$ of soil. The bulk density of the soil was taken as 1.3 g cm^{-3} and molecular diffusion as $0.02 \text{ cm}^2\text{s}^{-1}$. Longitudinal dispersivity was equal to zero. Activity coefficients were calculated with the Debye-Hückel equation. Cation exchange was not considered in this example.

Figures 1 and 2 show the water content and tracer concentration profiles, respectively, at various times. Calcium concentration and alkalinity profiles at various times for both equilibrium and kinetic calcite precipitation-dissolution are shown in Figures 3 and 4, respectively. Calcite profiles at various times for both equilibrium and kinetic calcite precipitation-dissolution are shown in Figure 5.

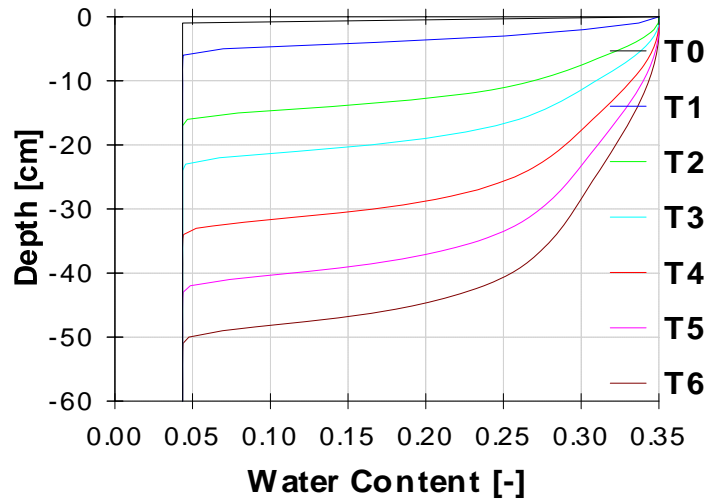


Figure 1. Water content profiles at various times for example 1.

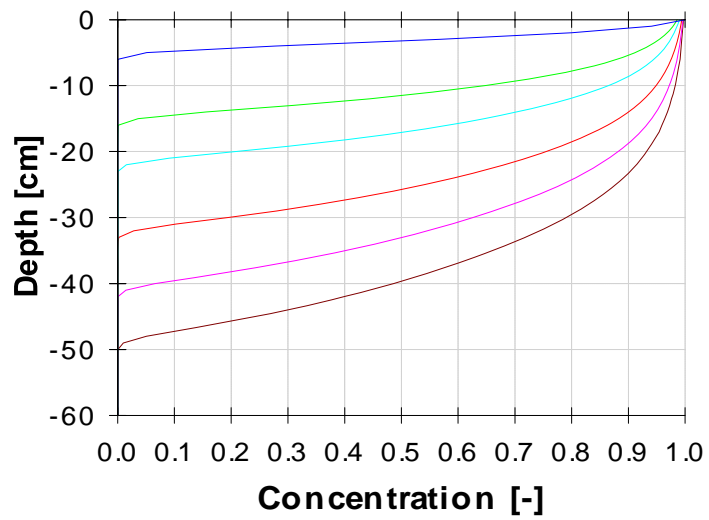


Figure 2. Tracer concentration profiles at various times for example 1.

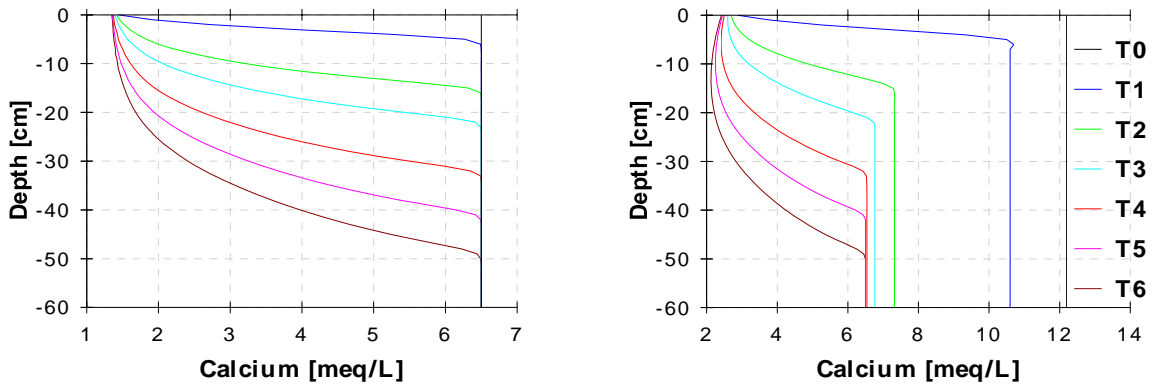


Figure 3. Calcium concentration profiles at various times for a) equilibrium and b) kinetic calcite precipitation-dissolution for example 1.

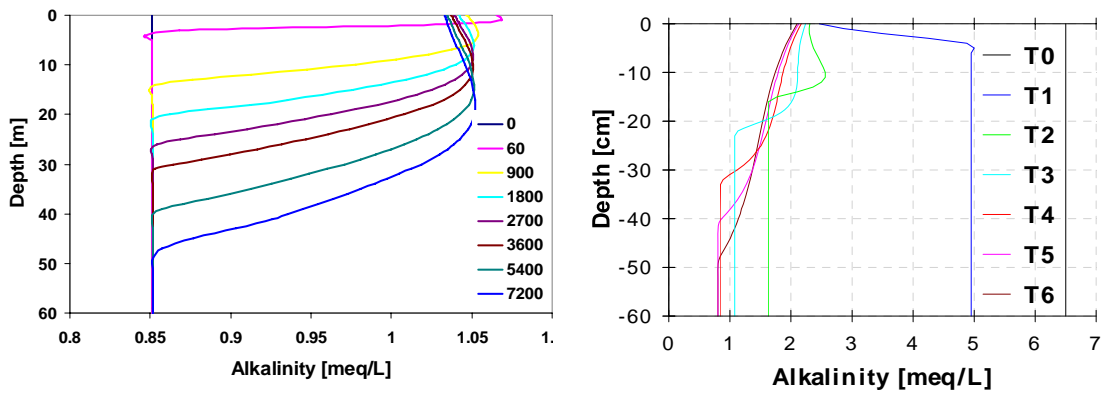


Figure 4. Alkalinity profiles at various times for a) equilibrium and b) kinetic calcite precipitation-dissolution for example 1.

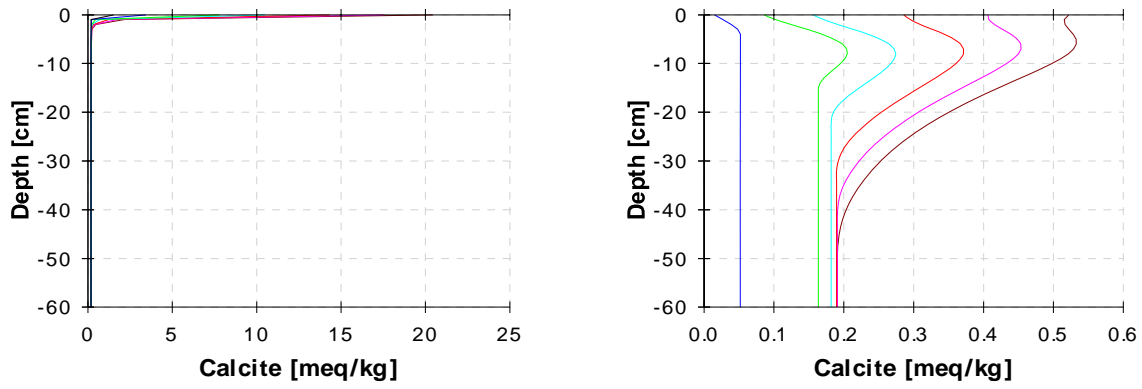


Figure 5. Calcite profiles at various times for a) equilibrium and b) kinetic calcite precipitation-dissolution for example 1.

2. Example 2 - Two-Dimensional Furrow Irrigation Problem

A furrow irrigation problem was used to simulate two-dimensional infiltration of gypsum saturated water into a sodic soil. The simulation of sodic soil reclamation demonstrates the cation exchange feature of UNSATCHEM. The schematic representation of the flow domain for the considered furrow irrigation together with the finite element mesh is presented in Figure 6. It is assumed that every other furrow is flooded with water and that the water level in the irrigated furrow is kept constant at a level of 6 cm. Due to symmetry, it is necessary to carry out the simulation only for the domain between the axis of two neighboring furrows. Free drainage is used as the bottom boundary condition and zero flux is considered on the rest of the boundary. The initial pressure head condition is -200 cm and the soil hydraulic properties are the same as those used in the second example.

The calculation was run at a constant temperature of 25 °C and a CO₂ concentration of 0.01 cm³cm⁻³. Root water uptake and evaporation were neglected. The bulk density of the soil was taken as 1.4 g cm⁻³ and molecular diffusion as 2 cm²day⁻¹. Longitudinal and transverse dispersivities were equal to 2 and 0.2 cm, respectively.

The solution composition of the water initially present in the soil profile is that of the following highly sodic water: Ca_T=0.2, Mg_T=0.0, Na_T=4.8, K_T=0.0, Cl_T=4.6, SO_{4T}=0.0, Alk=0.4 mmol_cL⁻¹. The cation exchange capacity is equal to 100 mmol_ckg⁻¹ and is divided between exchangeable calcium and sodium (a=5.0, a=95.0 mmol_ckg⁻¹). The Gapon selectivity coefficients from *Wagenet and Hutson* [1987] were used ($K_{13}=0.896$, $K_{14}=1.158$, $K_{15}=0.111$). The solution composition of the irrigation water was almost gypsum saturated: Ca_T=32.6, Mg_T=0.0, Na_T=4.8, K_T=0.0, Cl_T=5.0, SO_{4T}=32.0, Alk=0.4 mmol_cL⁻¹. As a consequence of the reactions of the irrigation water with the exchanger composition, cation exchange was the dominant chemical processes in the soil profile. Cation exchange is treated as an instantaneous process in the model.

Figure 7 shows the pressure head profiles for four different times. Steady state water flow was reached approximately after 1.5 days. The distribution of the hypothetical tracer is shown on Figure 8. Figures 9 and 10 present the exchangeable concentrations of calcium and sodium, respectively. The exchange phase concentrations reflect the changes in aqueous Na and Ca concentration. Note the significant lagging of the exchanger front to both the water and tracer front. Also due to the high nonlinearity of Na-Ca exchange, the concentration and exchange fronts are very sharp, in contrast to the more diffuse tracer fronts. After 5 days less than 25% of the profile has been reclaimed to exchangeable sodium percentage less than 15 (which has been the criteria defining the designation sodic soil). The selected cation exchange capacity of 100 mmol_ckg⁻¹ is relatively low. Selection of a higher exchange capacity and associated hydraulic properties of a finer textured soil would enhance both the time required for infiltration, as well as quantity of water required for reclamation.

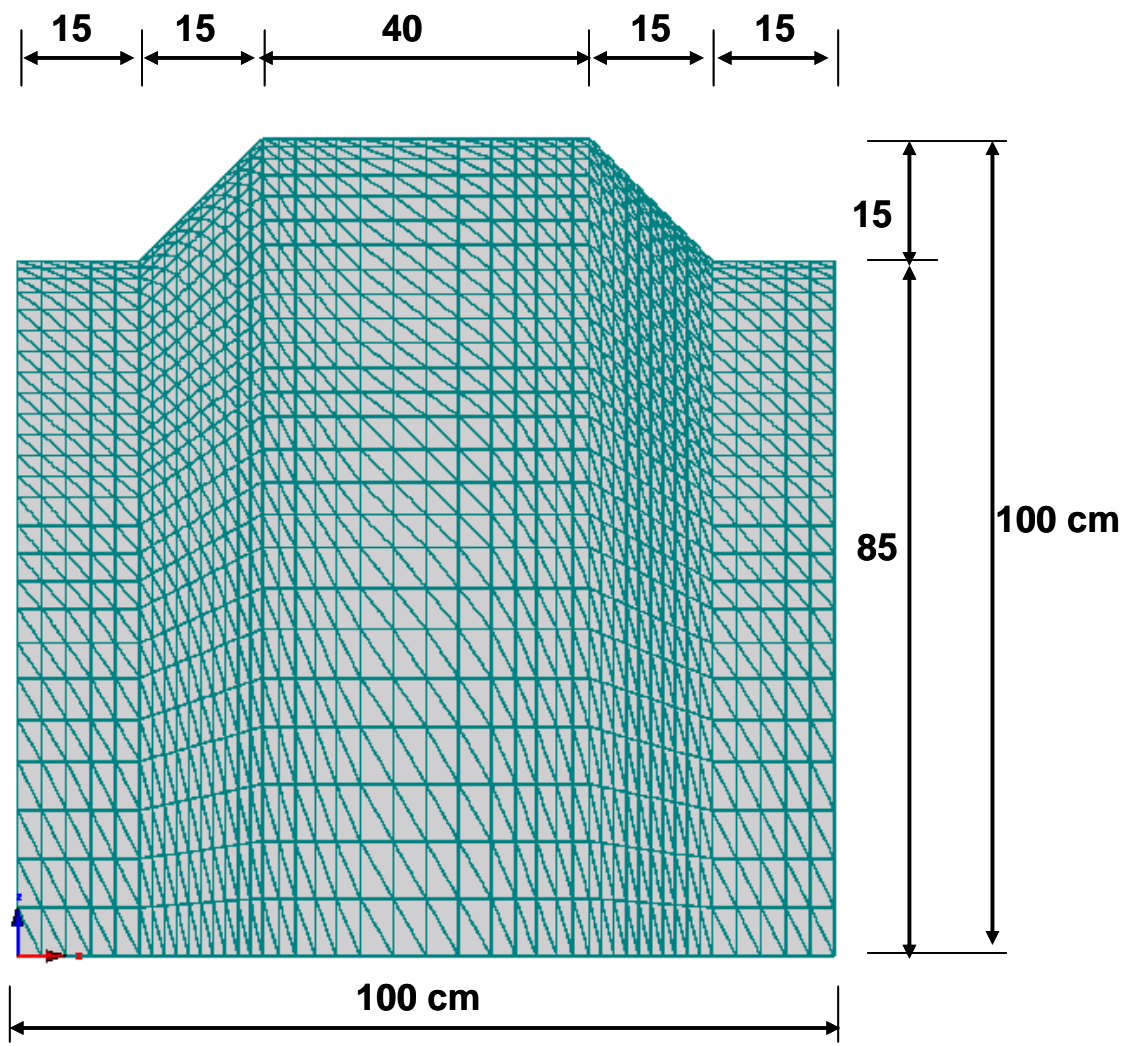


Figure 6. Schematic representation and finite element mesh of the flow domain for the furrow irrigation system for example 2.

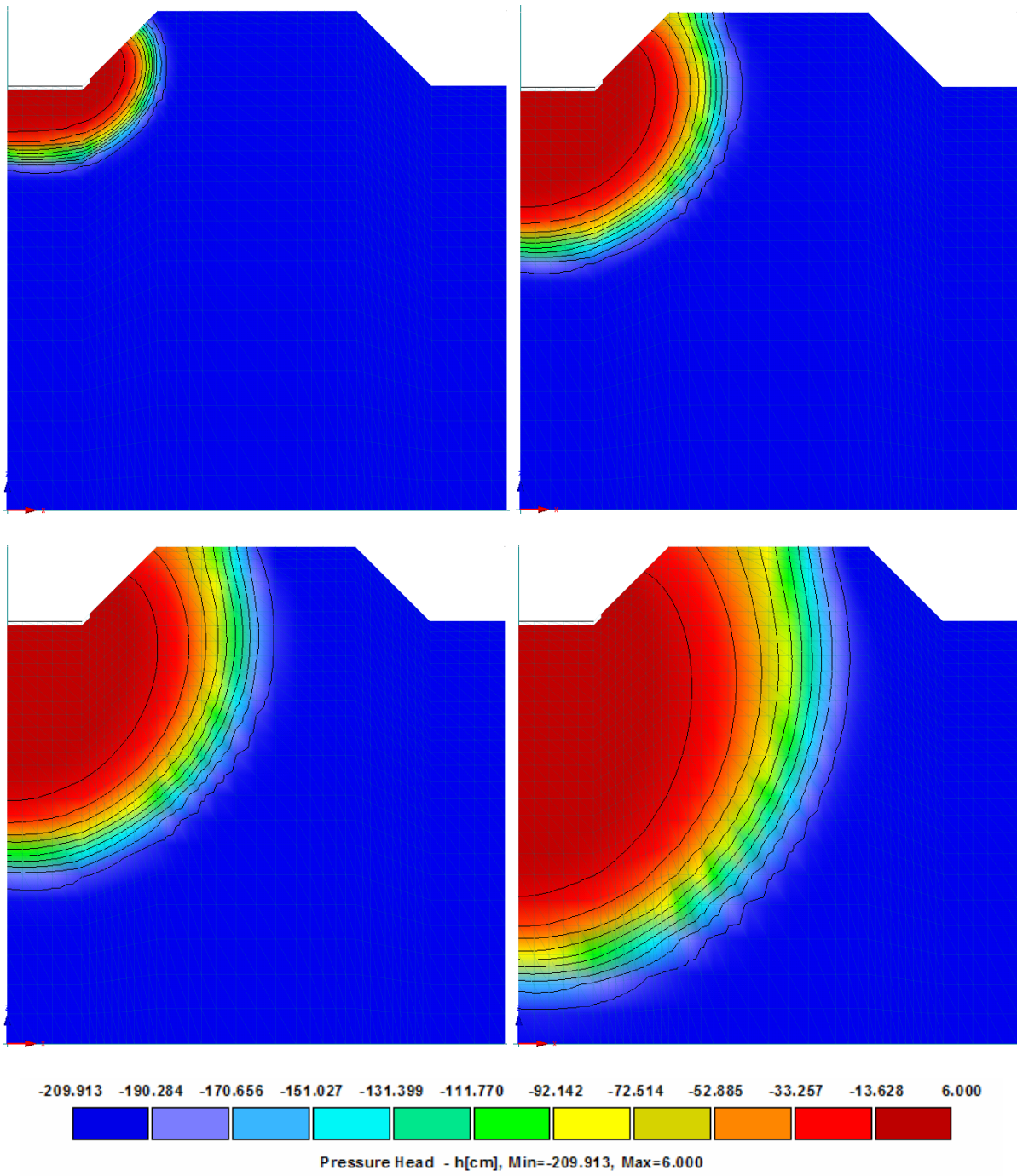


Figure 7. Pressure head (cm) profiles at times: a) 0.1, b) 0.5, c) 1, and d) 2 days for example 2.

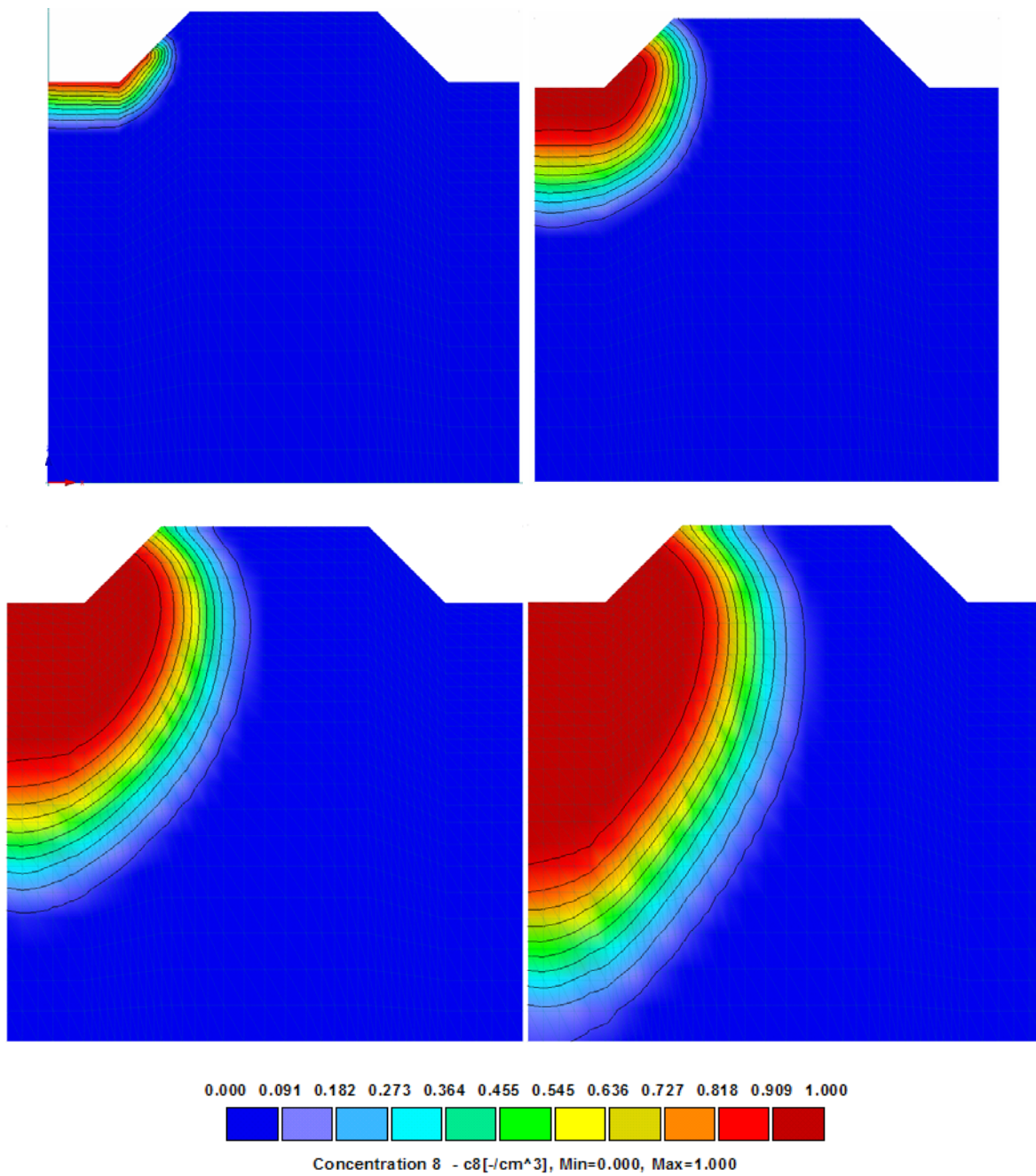


Figure 8. Tracer concentration (-) profiles at times: a) 0.1, b) 1, c) 3, and d) 5 days for example 2.

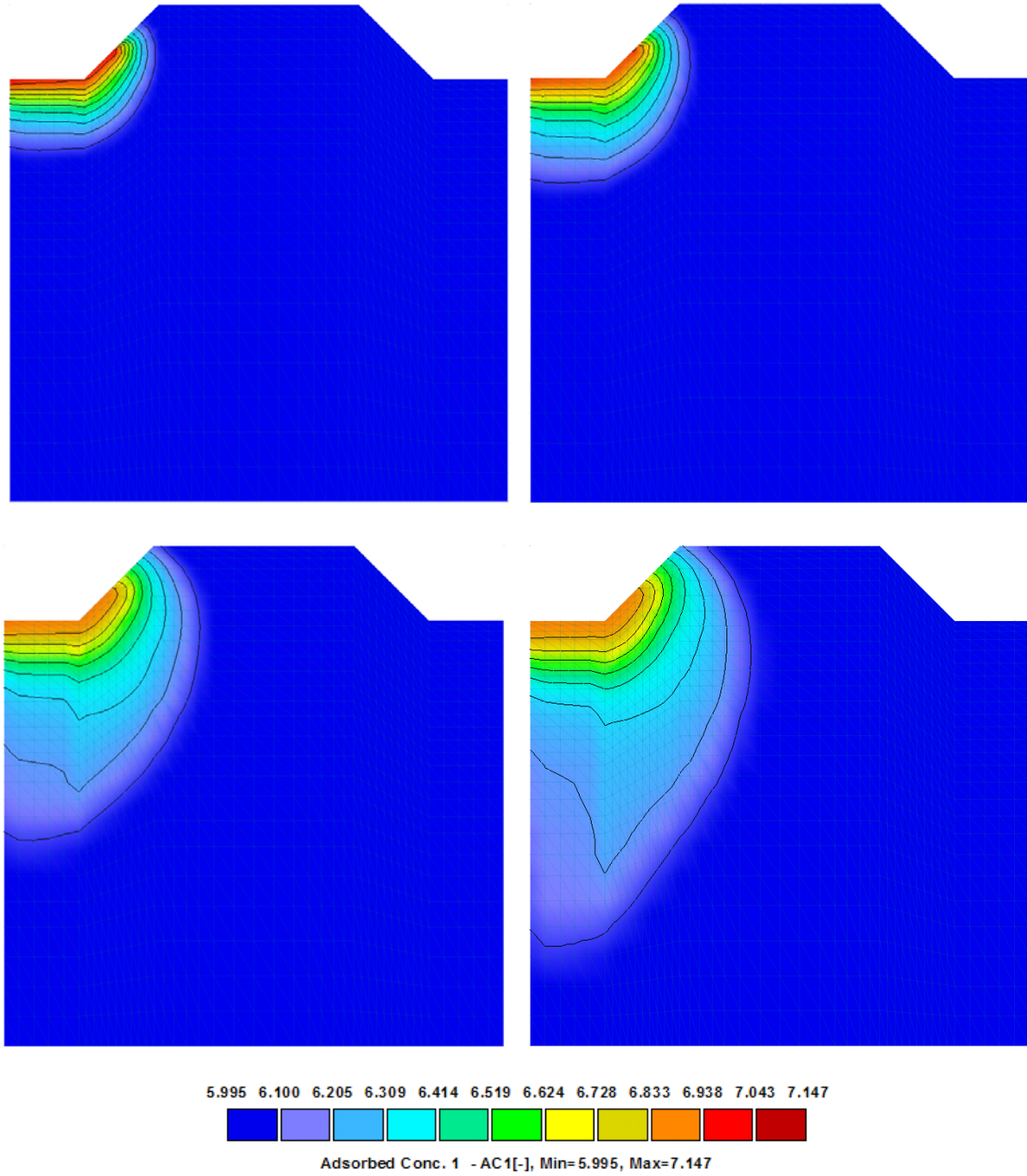


Figure 9. Exchangeable concentrations of calcium (mmol.kg^{-1}) profiles at times: a) 0.5, b) 1, c) 3, and d) 5 days for example 2.

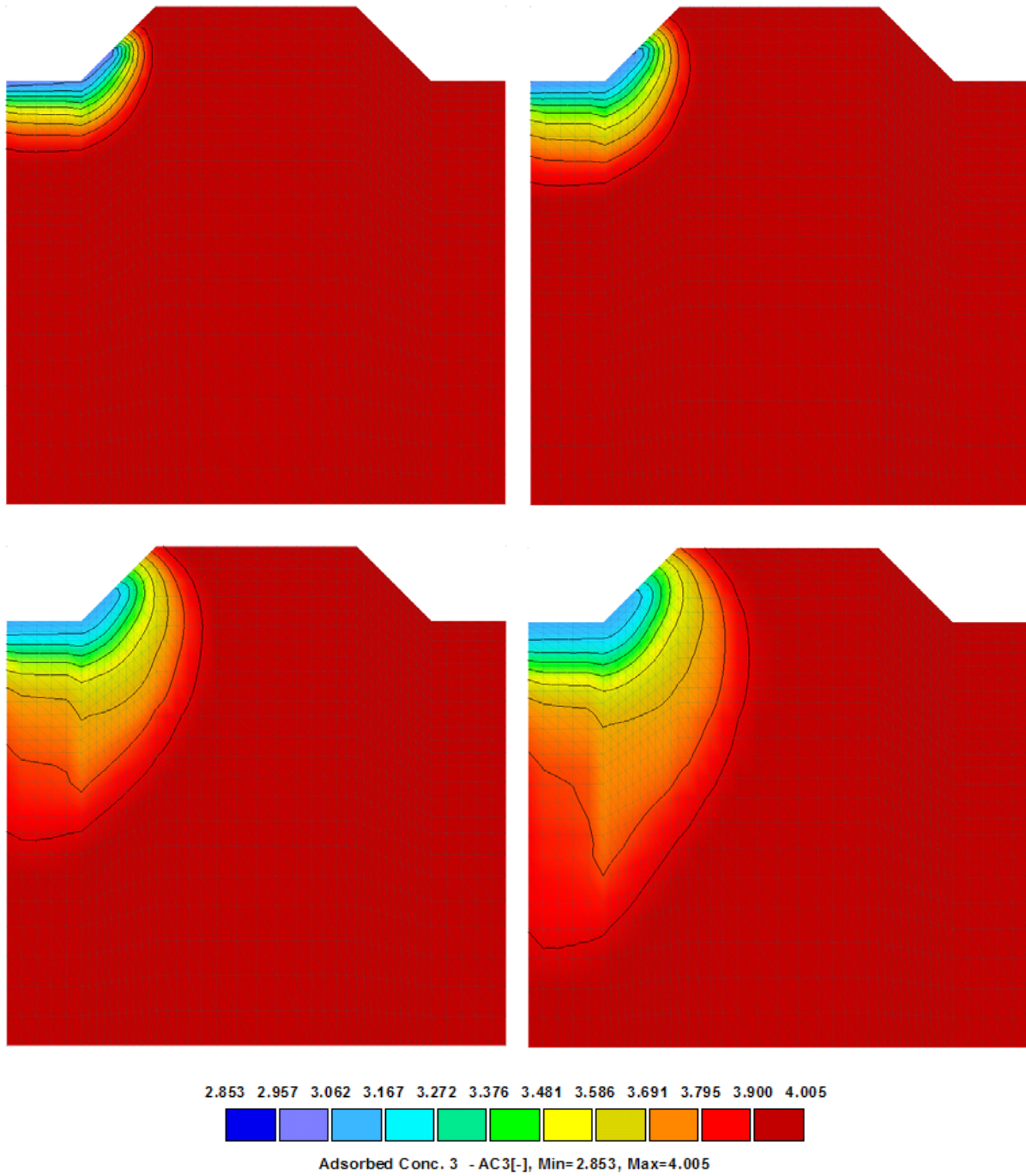


Figure 10. Exchangeable concentrations of sodium (mmol_c.kg⁻¹) profiles at times: a) 0.5, b) 1, c) 3, and d) 5 days for example 2.

References

- Davis, L. A., and S. P. Neuman, Documentation and user's guide: UNSAT2 - Variably saturated flow model, *Final Rep., WWL/TM-1791-1*, Water, Waste & Land, Inc., Ft. Collins, CO, 1983.
- Šimůnek, J., T. Vogel, and M. Th. van Genuchten, The SWMS_2D code for simulating water flow and solute transport in two-dimensional variably saturated media. Version 1.1, *Research Report No. 126*, U.S. Salinity Laboratory, USDA, ARS, Riverside, California, 169 pp., 1992.
- Šimůnek, J., and D. L. Suarez, Two-dimensional transport model for variably saturated porous media with major ion chemistry, *Water Resour. Res.*, *30*(4), 1115-1133, 1994.
- Šimůnek, J., D. L. Suarez, and M. Šejna, The UNSATCHEM software package for simulating one-dimensional variably saturated water flow, heat transport, carbon dioxide production and transport, and multicomponent solute transport with major ion equilibrium and kinetic chemistry, Version 2.0, *Research Report No. 141*, U.S. Salinity Laboratory, USDA, ARS, Riverside, California, 186 pp., 1996.
- Šimůnek, J., M. Th. van Genuchten, and M. Šejna, The HYDRUS Software Package for Simulating Two- and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media, **Technical Manual**, Version 1.0, PC Progress, Prague, Czech Republic, pp. 241, 2006.
- Šimůnek, J., M. Šejna, and M. Th. van Genuchten, The HYDRUS Software Package for Simulating Two- and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media, **User Manual**, Version 1.0, PC Progress, Prague, Czech Republic, pp. 161, 2007.
- Skaggs, R. W., E. J. Monke, and L. F. Huggins, An approximate method for determining the hydraulic conductivity function of an unsaturated soil, *Techn. Rep. No. 11*, Water Resour. Res. Center, Purdue University, Lafayette, IN, 1970.
- Suarez, D. L., Ion activity products of calcium carbonate in waters below the root zone, *Soil Sci. Soc. Am. J.*, *41*, 310-315, 1977.
- Suarez, D. L., and J. Šimůnek, UNSATCHEM: Unsaturated water and solute transport model with equilibrium and kinetic chemistry, *Soil Sci. Soc. Am. J.*, *61*, 1633-1646, 1997.
- Wagenet R. J., and J. L. Hutson, LEACHM: Leaching Estimation And Chemistry Model, A process-based model of water and solute movement, transformations, plant uptake and chemical reactions in the unsaturated zone, *Continuum 2*, Dept. of Agronomy, Cornell University, Ithaca, New York, NY, 1987.