Supplement of

Geophysically based analysis of breakthrough curves and ion exchange processes in soil

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S1   Experimental setup

S1.1   Soil composition

The soil used in this work was a calcareous loamy sand. For the heterogeneous experiment, washed sea sand was also used. Soil texture was evaluated by a hydrometer experiment (based on Stokes' law). The percentages of sand, silt and clay in each of the soils are presented in Table S1.

Table S1. Texture of the porous media

Soil	Sand (%)	Silt (%)	Clay (%)
Loam	93.2	4.1	2.7
Sea sand	99.8	0.2	0

S1.2   Column packing

The air-dried soils were passed through a $< 250 \mu m$ sieve. For the homogeneous experiments, $310g \pm 2g$ of soil was packed in the column with an average packed bulk density of $1.37 g/cm^3$. For the heterogeneous profile, a $3cm$ layer of sand was packed between the two middle electrodes. The total weight of soil compacted was $312g$ and the packed bulk density was $1.379 g/cm^3$. After the packing, columns were saturated from the bottom with the background $NaCl$ solution until the EC of the outflow solution was equal to that of the inflow.

S2 Modeling adsorbed reactive species using σ'' data

The imaginary conductivity data of the $Na^+ - Ca^{2+}$ exchange experiment in loamy soil was normalizes and used as a proxy to the adsorbed Ca^{2+} concentration. The data set was flipped around the horizontal axis ans then normalized such that the first σ'' value (before any Ca^{2+} adsorption) is 0 and the final σ'' value (the end of the experiment) is 1. The geometric and transport model parameters of the simulations presented in the main text were used to calculate dissolved species concentrations. Then, the adsorbed concentration was calculated and compared to SIP data (see Fig. S1). Alternatively, the normalized imaginary conductivity can be used to calibrate the transport model (i.e. to obtain the dispersivity and adsorption coefficient). The obtained values are within 6% of the values obtained by the σ'-based calibration.

As can be seen in Fig.S3, the initial increase in σ'' is not captured by the model. An accurate depiction of this initial stage of the exchange process requires a more complex model that includes non-equilibrium processes.
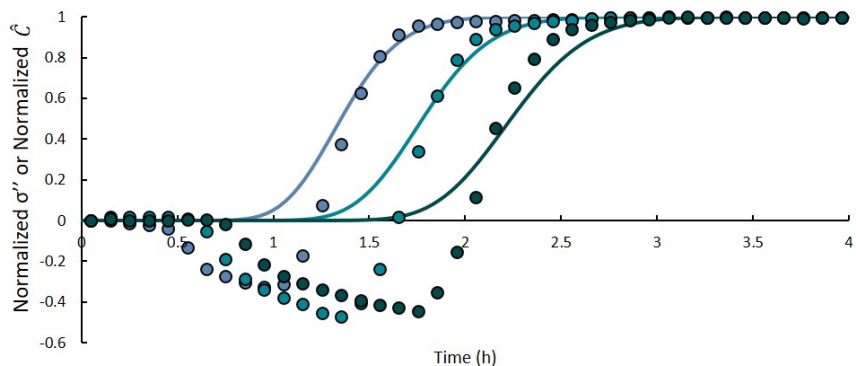

Figure S1. Normalized imaginary conductivity at $1Hz$ versus time at the three channels (serving as a proxy for adsorbed concentration) and its HYDRUS-based model fit

S3   Model fit and prediction for $ZnCl_2$ transport in treated sand
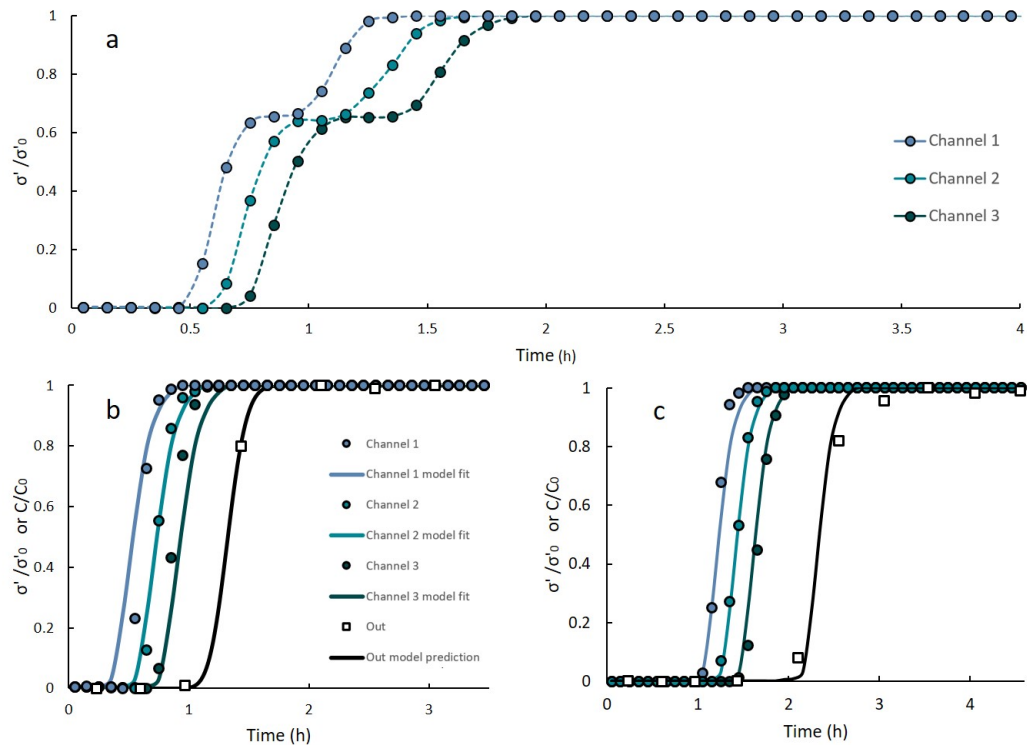
Figure S2. (a) Real conductivity at $1Hz$ versus time at three locations, (b) model fit to the σ'-based initial BT and model prediction for the non-reactive species at the outflow compared to their measured concentration, (c) model fit to the σ'-based secondary BT and model prediction for Zn^{2+} at the outflow compared to its measured concentration.

S4   Chemical measurement comparison between the homogeneous and heterogeneous profiles
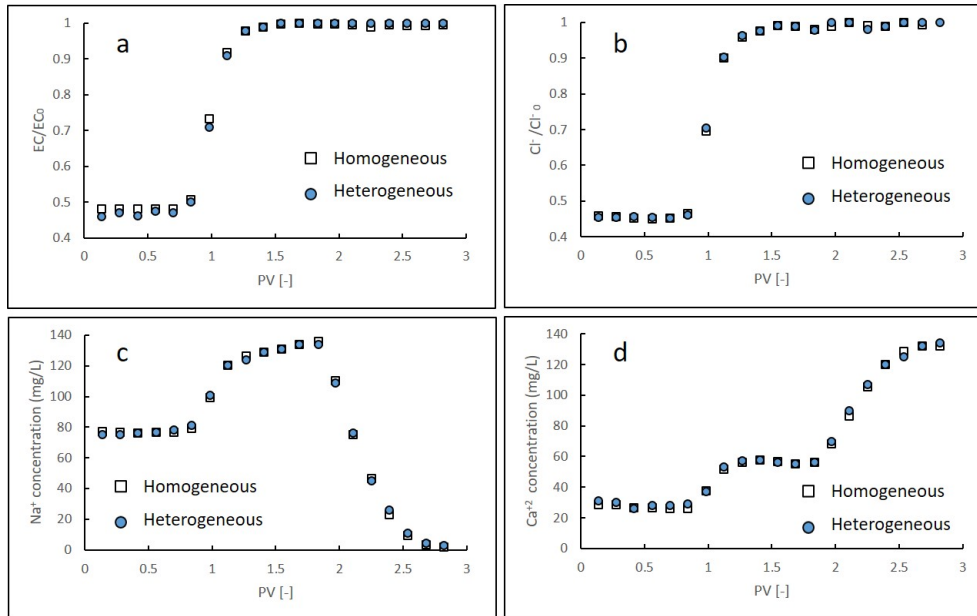
Figure S3. A comparison between the homogeneous and heterogeneous profiles (presented versus PV): (a) $\frac{EC}{EC_0}(-)$, (b) $\frac{Cl^-}{Cl_0^-}(-)$, (c)Na^+ concentrations (mg/L) and (d) Ca^{2+} concentrations (mg/L)