Modelling seawater intrusion in a resin-filled column to study cationic exchange and gypsum precipitation

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INTRODUCTION

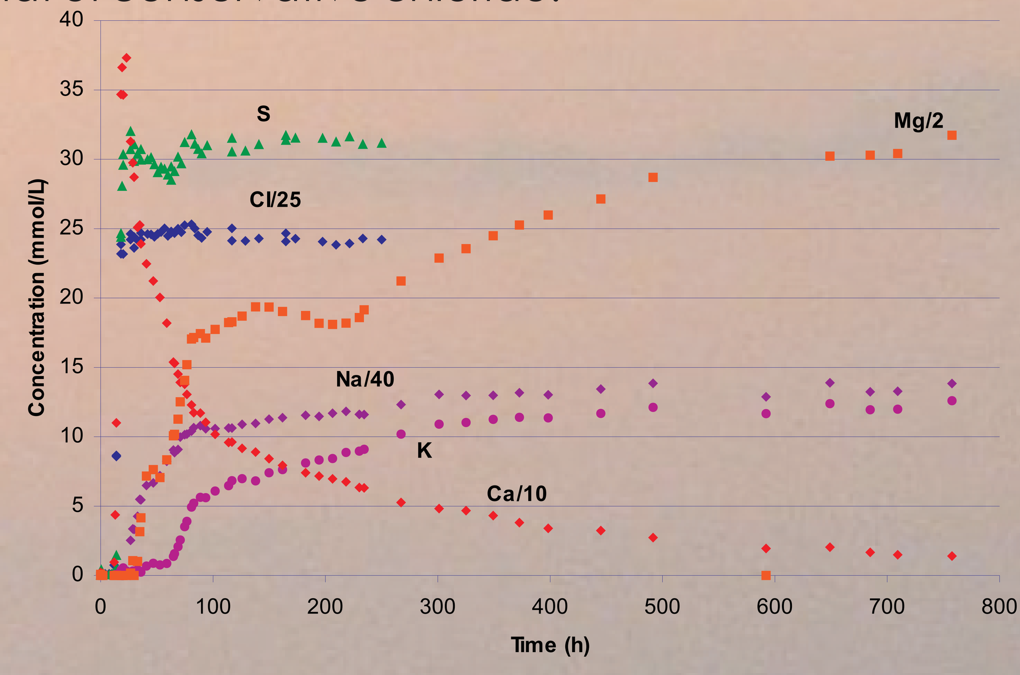
Laboratory column experiments are necessary to the understanding of the reactive transport behavior of inorganic chemical species when dealing with environmental problems such as fresh- or seawater intrusions into aquifers, landfill leaching plumes, or transport of heavy metals in soils and aquifers. In the case of seawater intrusion, cationic exchange is one of the main chemical reactions analyzed [1]. This process occurs when cations from seawater (mainly sodium and magnesium) displace calcium ions on sediment exchange sites.

In previous studies of the reactive transport processes of seawater intrusion [2,3], column experiments were carried out by displacing synthetic freshwater with seawater along a sediment column 100 cm in length. Moreover, application of a multicomponent reactive model [4] to the experimental data showed gypsum precipitation dissolution [5] to be taking place, in addition to cation exchange.

OBJECTIVES

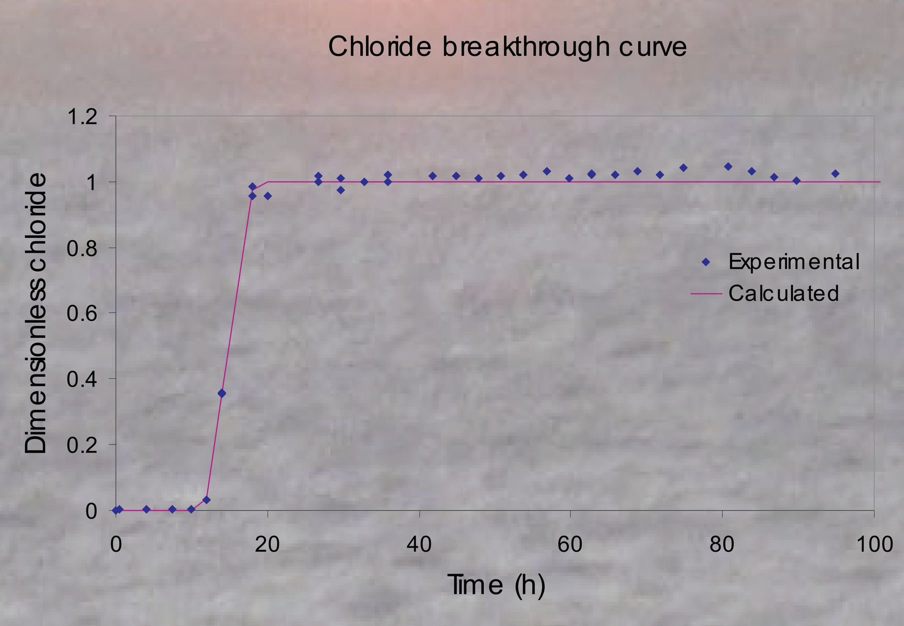
Obtain column transport parameters with ACUAINTRUSION. Modelize with PHREEQC using the calculated transport parameters and exchange coefficients of resin. Different scenarios are considered for precipitation/disolution of gypsum.

An attempt was made to study gypsum precipitation in processes simulating seawater intrusion [6] in a column filled with resin (Duolite C20) of a great cationic exchange capacity (CEC = 15.6 meq/kg). The goal of the 20 time increase in the CEC was to try to obtain a high concentration of calcium, which would produce gypsum precipitation into the column. However, only a very small amount of gypsum precipitated, as can be seen from the elution curve of sulphate (fig. 1), which was nearly synchronous to that of conservative chloride.



Water composition	Freshwater (mmol/L)	Seawater (mmol/L)
Sodium	0	522
Potassium	0	10.3
Calcium	3.13	11.3
Magnesium	0	61.7
Chloride	2.96	606
Sulphate	0	30.2
Bicarbonate	0	2.13

Figure 1. Previous experimental results



Column properties	
Column length	19 cm
Column diameter	2.5 cm
Flow	50 mg/min

Transport parameters	
Peclet number	167.6
Residence time	14.67 h
Darcy's velocity	0.61 cm/h
Porosity	0.47
Interstitial velocity	1.29 cm/h
Dispersion	0.146 cm^2/h
Dispersivity	0.113 cm

Figure 2. Chloride breakthrough curves: experimental (symbol), calculated

COLUMN TRANSPORT PARAMETERS

ACUAINTRUSION [7] a graphical user interface was designed with Microsoft Visual Basic 6.0 to calculate the best fit of the experimental data [chloride concentration (mmol/L) versus experimental time (h)]. This code uses the analytical solution of the convection-dispersion equation (Lapidus and Amundson, 1952) is

$$C(L,t) = C_i + \frac{(C_0 - C_i)}{2}\left[\operatorname{erfc}\left(\frac{L - vt}{\sqrt{4D_L t}}\right) + \exp\left(\frac{vL}{D_L}\right)\operatorname{erfc}\left(\frac{L + vt}{\sqrt{4D_L t}}\right)\right]$$

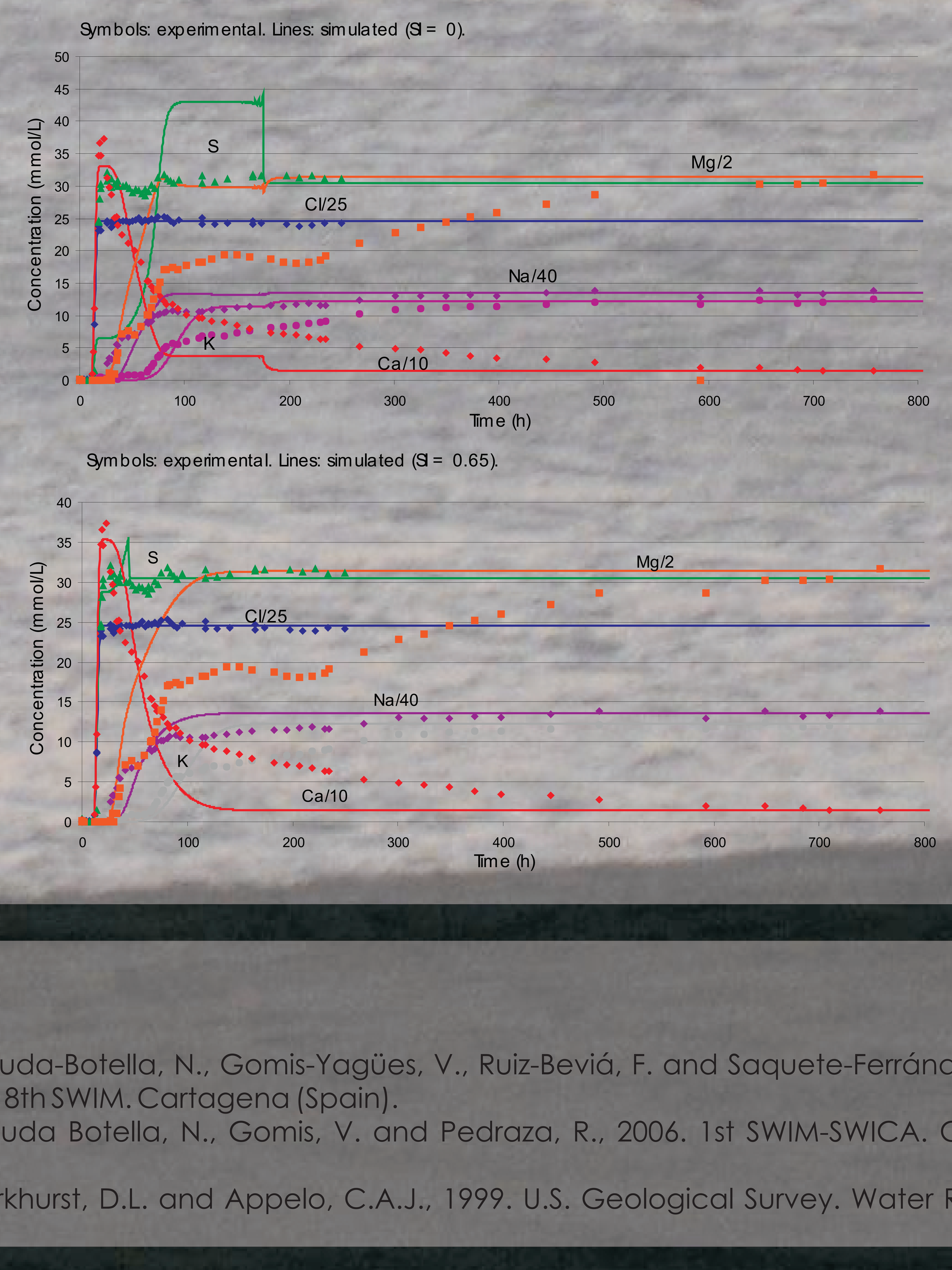
Where
$C(L,t)$ is the chloride concentration at the output stream of the column,
C_i, the initial concentration of the chloride in the freshwater,
C_0, the concentration of chloride in the seawater,
L, column length,
t, time,
v, interstitial water velocity in the direction of propagation (equal to Darcy velocity divided by porosity, or u/ε), and
D_L, longitudinal dispersion coefficient.

REACTIVE TRANSPORT MODEL

PHREEQC (Versión 2) is a computer program for speciation, batch reaction, and one-dimensional transport calculations, distributed free of charge by the U.S. Geological Survey (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/index.html). The windows version of the program has an intuitive, user-friendly interface. Numerous options and capabilities make PHREEQC useful for finding solutions to many practical problems in hydrogeochemistry.

RESULTS

The Saturation Index (SI) of gypsum has been modified in different scenarios. In the case of SI = 0 gypsum precipitation/disolution must have occurred. Differences can be attributed to local equilibrium. Simulation results are improved by taking SI = 0.65. The predicted elution curves in the first stages of advance of the intrusion front are in agreement with experimental results. Differences in the last stages are probably due to the variation in the value of the exchange coefficients with salinity.



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