Hydrogeochemical modeling of soil salinisation, alkalinisation and sodification. Presentation and calibration of the PASTIS model

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Though the geochemical processes of alkalinisation, salinisation or sodification are well known, the time changes and distribution of alkalinity, salinity, sodicity and various alterations cannot be predicted precisely within the profile if transport phenomena are not considered. On the other hand, if solute transport models allow one to predict displacement of solutes within the profile, the geochemical mechanisms of alkalinisation play an important role whereas the components of the soil solution are adsorbed on the exchange complex or precipitated. Therefore, it appeared necessary to couple transport and geochemistry to take into account of the hydrological causes of concentration and to predict the chemical consequences and the mineralogical modifications induced by these processes. The PASTIS model (Predicting Agricultural Solute Transport In Soil), developed by INRA, is presented and calibrated.
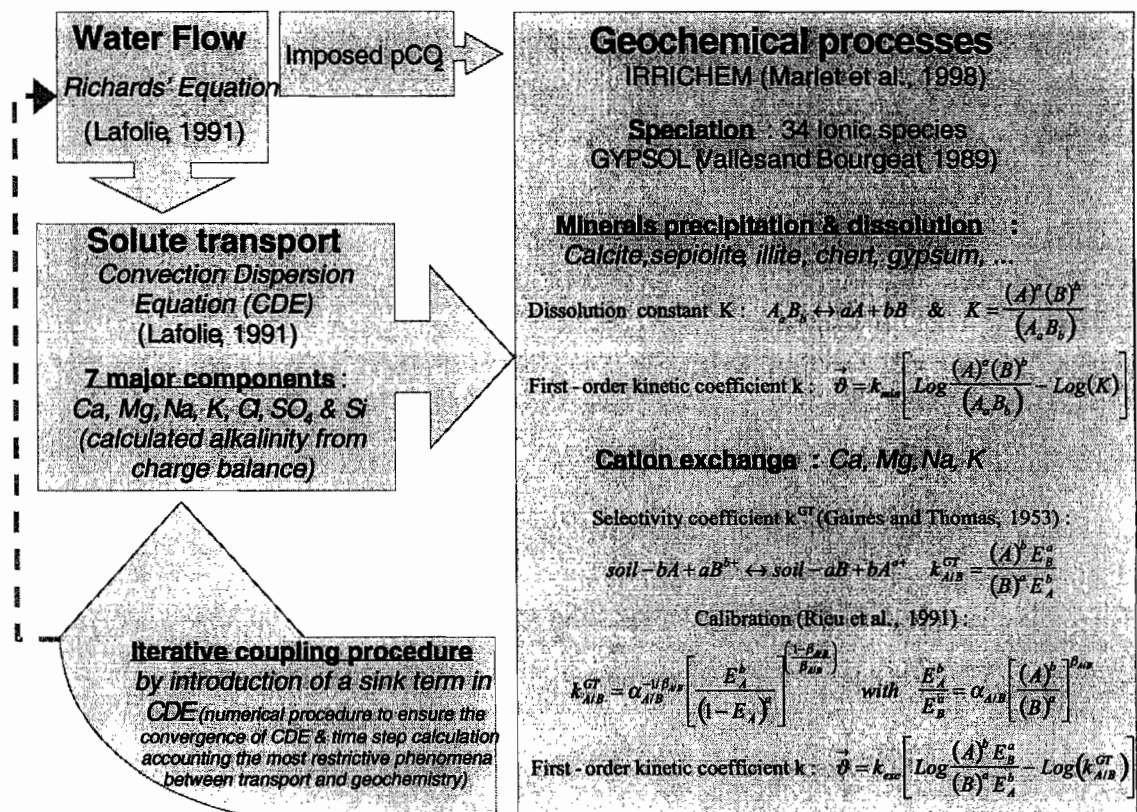
PASTIS presentation

ϑ is the rate of the reaction [mol.l^{-1} s^{-1}], k$_{min}$ [mol.l^{-1}.s^{-1}] and k$_{exc}$ [mol$_c$.l^{-1}.s^{-1}] are kinetic constant for mineral precipitation/dissolution and cation exchange, respectively, R [8.314.10^{-3} kJ. K^{-1}.mol^{-1}] is the gas constant, T is temperature [°K], K is the dissolution constant [-], k^{GT} is the selectivity coefficient in the Gaines and Thomas convention [mol.l$^{(a/b)}$], (A) is the activity of the specie A, E$_A$= X$_A$/(X$_A$+X$_B$) [-] is the charge (or equivalent) fraction of adsorbed component A in the binary exchange A/B and X$_A$ [mol$_c$.l^{-1}] is the charge amount of adsorbed cation A.

Material and method

The experiment has been achieved in the research center of IRD in Dakar with a soil monolith from Mali of 60 cm high and 23 cm in diameter. Soil texture is loamy sand and CEC equals 0.5mmol$_c$.kg^{-1} In a first step the soil column has been leached with sodic alkaline solution (EC=0.5 dS.m^{-1}) for a 8 months period and a 16-pore volume has been infiltrated until the stability of the composition at the bottom of the column . The saturated hydraulic conductivity has been assessed simultaneously as 11mm.d^{-1}. In a second step the soil column has been leached with a CaCl$_2$ solution (EC=2.25 dS.m^1 and [Ca^{2+}]=[Cl$^-$]=21 mmol$_c$.l^{-1}) for a 2 months period and a 4-pore volume have been infiltrated.
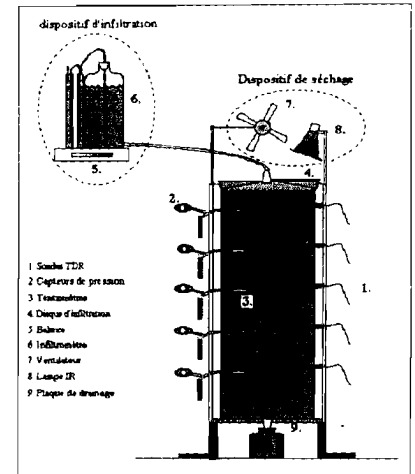
Results
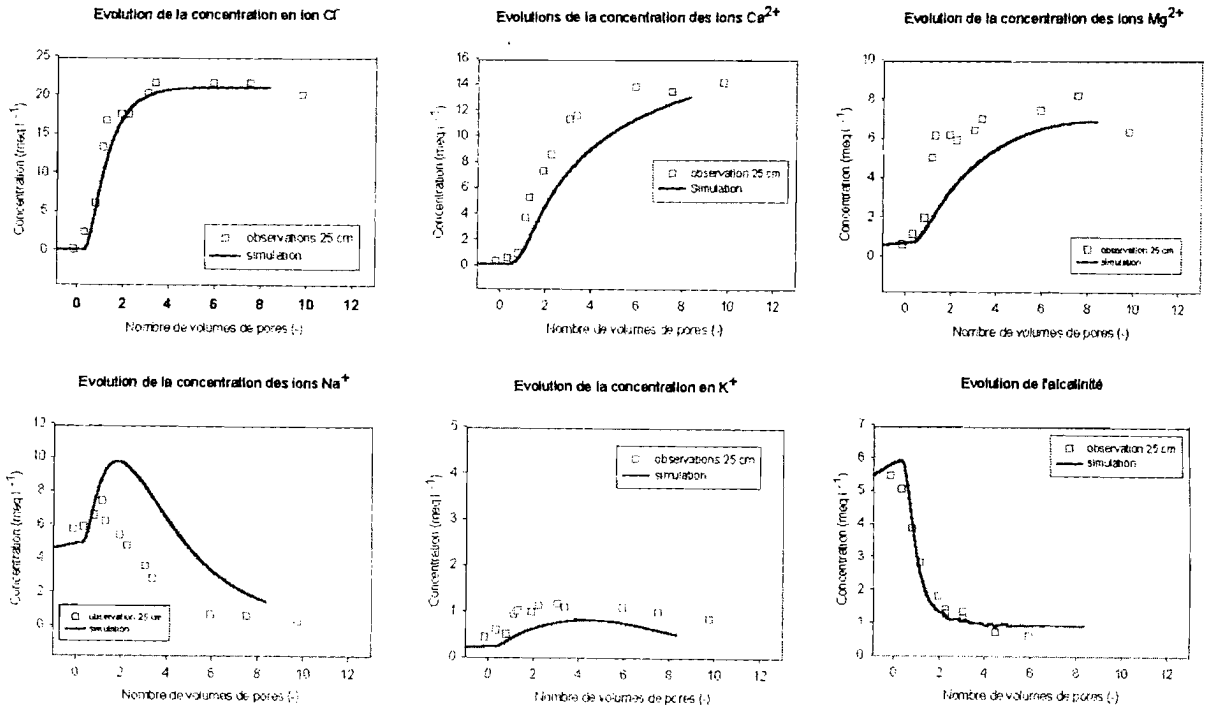
In a first step, the non-reactive solute breakthrough curve has been calibrated according to chloride analysis; dispersivity has been assessed as 1 cm. In a second step the reactive solute breakthrough curves have been calibrated according calcium, magnesium, sodium, potassium and alkalinity, simultaneously. Solute breakthrough curves show a typical situation of non-equilibrium and kinetically control reactions have to be considered. Coefficients of 8.10^{-5} eq.l

$^1.h^{-1}$, $1.2.10^{-5}$ mol.$l^{-1}.h^{-1}$ and $1.2.10^{-6}$ mol.$l^{-1}.h^{-1}$ have been assessed for cation exchange, calcite and silicates (sepiolite and illite) dissolution, respectively.

Conclusion

The results show good agreement between observation and simulation. The model provides an improvement with regard to similar model as LEACHM (Hutson and Wagenet, 1995) or UNSATCHEM (Simunek and Suarez, 1994) due to the use mechanistic geochemical modelling, kinetically control chemical reactions and the introduction of a rigorous iterative procedure for the coupling of geochemical and transport models. The main part of the parameters have been acquired independently and only few parameters for dispersivity and kinetics of chemical reactions have been calibrated.

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