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Abstract

Hydrogeochemical modelling of soil salinisation, alkalinisation and sodification: Presentation and calibration of the PASTIS model. Irrigation allowed improving agriculture productivity in arid regions. However, in some places, irrigation was at the origin of gradual changes in soil physicochemical properties. These changes led after several years of cropping to losses in fertility. Such salinisation processes have been noticed in irrigated areas of the Sahelian African sub-region as in Mali, Senegal and Niger. Avoiding salinisation requires properly understanding and quantifying the relationships between water regime and the chemical processes occurring within a soil profile. In this respect, models incorporating the various physical and chemical mechanisms could be useful tools in evaluating and designing irrigation strategy. We present the model PASTIS coupling water flow, solute transport and chemical processes. Ion exchange and mineral precipitation/dissolution are modelled using first-order kinetics. A transport experiment was carried out on an undisturbed soil column equipped for soil solution sampling at various depths. Ion exchange isotherms of the soil were calibrated from batch experiments. Hydrodynamic dispersion of the column was calibrated from a Chloride breakthrough curve and model inversion. Measured breakthrough curves for K, Ca, Na, Mg reveal the existence of non-equilibrium and a kinetic coefficient has been calibrated for cation exchange. The model represents correctly the chemical breakthrough curves.

Résumé

Modélisation hydrogéochimique des processus de salinisation, alcalinisation et sodisation des sols : présentation et calage du modèle PASTIS. L'irrigation est indispensable à l'amélioration de la productivité agricole des terres dans les régions arides. Cependant, elle peut conduire localement à une dégradation progressive des propriétés physico-chimiques des sols et une baisse de la fertilité. Ces processus de salinisation des sols ont été mis en évidence dans différents périmètres irrigués dans les pays sahéliens comme le Mali, le Sénégal ou le Niger. La prévision et la prévention de ces risques requièrent une meilleure compréhension et quantification des relations entre le régime hydrique sous l'influence de l'irrigation et l'évolution des propriétés des sols. Dans ce but, le développement d'un modèle intégrant les différents déterminants physiques et chimiques de ces évolutions représente un outil pour l'évaluation et la conception de stratégies d'irrigation. Le modèle PASTIS couplant les flux hydriques, le transport des solutés et les réactions géochimiques est présenté. Les échanges ioniques et la précipitation ou dissolution des minéraux sont modélisés sous la forme d'une cinétique d'ordre 1. Une expérimentation a été mise en œuvre sur un monolithe de sol équipé pour le prélèvement de la solution à différentes profondeurs. Les isothermes d'échange ont été calées à partir d'expérimentation en réacteur fermé. La dispersion hydrodynamique a été calée par une méthode inverse à partir de l'élution des chlorures. Les courbes

d'élution des cations K, Ca, Na et Mg mettent en évidence l'existence d'un non-équilibre et un coefficient cinétique pour les échanges de cations a été utilisé pour le calage du modèle. Le modèle reproduit correctement l'élution des différents solutés.

Introduction

Development of irrigation allowed improving agriculture productivity in arid regions. However, in many places a decrease in soil fertility was observed after several years of cropping. Salinisation, sodification and allalinisation that may conduct to degradation of soil structure inducing soil crusting and reduction of permeability are one of the major causes of this loss of soil fertility (Ghassemi, Jakeman *et al*. 1995; Tyagi 1996). Such salinisation processes occur in arid region where high evaporation leads to concentration processes of soil water. This is the case in irrigated areas in the Sahelian African sub-region as in Mali (Bertrand, 1985; Bertrand and N'Diaye, 1994; Barral and Dicko, 1996), in Senegal (Boivin *et al*., 1998) and in Niger (Marlet, 1996). Geo-chemical processes of salinisation are fairly well known and studied. However, the time it takes to reach a certain level of soil sodicity depends not only on chemical processes but also on the different phenomena controlling water flow and water balance in the profile. So, developing strategies to avoid salinisation or to try to recover good soil physical properties requires not only to understand and quantify chemical mechanisms but also to take into account transport phenomena and their impact on chemistry.

Developing and testing models that account for the various physical, biological and chemical mechanisms and their inter-relationships is a key point to be able to design sustainable irrigation strategies. Simunek and Suarez (1994) provided a complete revue of existing models dealing with transport and chemistry. They noted that very few models were available for the unsaturated zone, most efforts having been devoted to the saturated zone. They also pointed out that available models were based on assumptions or simplifications that, in some cases, could be problematic. One limitation that authors discussed was coupling between transport and chemistry that was not really done in an iterative way in the available models. They also show the importance to take into account kinetics for chemistry phenomena considered in models that are not necessarily small as compared to time scales of transport phenomena (convection, dispersion) (Hunter *et al*., 1998). In consequence, accounting for the various sources of non-equilibrium was considered as important and in particular non-equilibrium originating from chemistry (dissolution, precipitation and cation exchange).

In that study, our objectives are to present a model coupling unsaturated water flow, heat flux and solute transport with a chemistry model accounting for kinetically controlled precipitation-dissolution of various minerals and kinetic cation exchange, and to demonstrate its capacity to predict results obtained from a column experiment. The comparison points out the importance of kinetic of the cation exchange process in predicting soil solution composition. The presentation of the model mainly focus on the chemistry and on the coupling between transport and chemistry. The water flow and heat flux modules, more classical, are only briefly described.

Presentation of the PASTIS hydrogeochemical model

The PASTIS model (Predicting Agricultural Solute Transport In Soil), developed by INRA, is presented below (Figure 1). It includes a water flow, a solute transport and a geochemical module.

Water flow

The model is based on a water flow model (Lafolie, 1991) using Richards equation to describe vertical unsaturated water flow in layered soil profiles. This model incorporates a plant growth module not considered in this study. Boundary conditions can handle flux-type

conditions, pressure head conditions and the model can shift from flux-type to pressure-type boundary condition if applied flux exceeds soils intake capacity.

Solute transport

The model is based on the convective dispersive representation of transport. A sink or source term is added to account for production or consumption of the species by chemical processes.

Geochemical reactions

The following major chemical components are considered in the model: S, Cl, K, Na, Ca, Mg, Si and alkalinity. Alkalinity is calculated as the sum of the hydroxyles, carbonate and bicarbonate elements. In the numerical procedure, alkalinity may be modified to maintain charge balance in the solution. The model considers 34 ionic species (Vallès and Bourgeat, 1989). With respect to minerals, the model can take into account up to 26 solid species. However, for the present study, only minerals that may appear in saline and alkaline soils were considered: calcite [$CaCO_3$], sepiolithe [$MgSi_3O_6(OH)_2$] as a Mg-clay mineral, Illite [$Si_{3.5}Al_{2.3}Mg_{0.25}O_{10}(OH)_2K_{0.6}$], gypsum [$CaSO_4.2H_2O$] and halite [$NaCl$] (Marlet *et al*., 1998). The binary cation exchanges, Na-Ca, Na-Mg and Na-K, are defined by selectivity coefficients in the Gaines and Thomas convention (Gaines and Thomas, 1953).

Figure 1. Description of the PASTIS Model and procedures. 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*
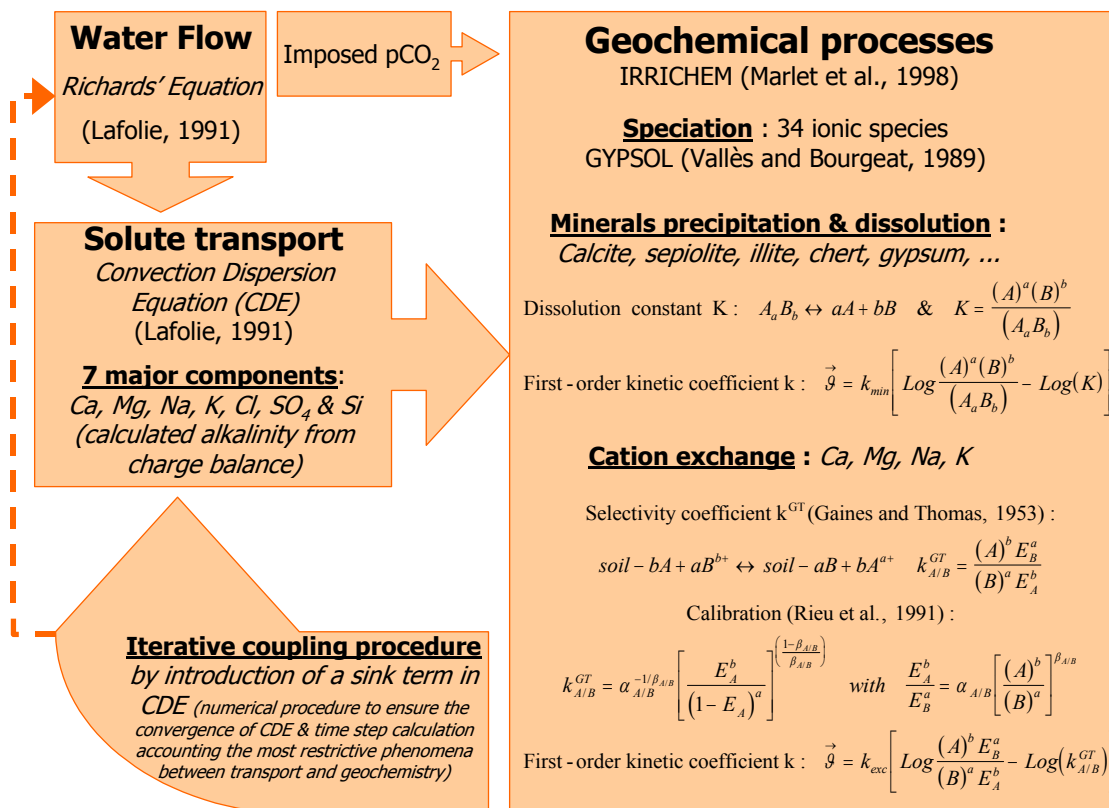
Material and method

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 0.5mmolc.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 CaCl2 solution (EC=2.25 dS.m1 and [Ca2+]=[Cl-]=21 mmolc.l-1) for a 2 months period and a 4-pore volume have been infiltrated.

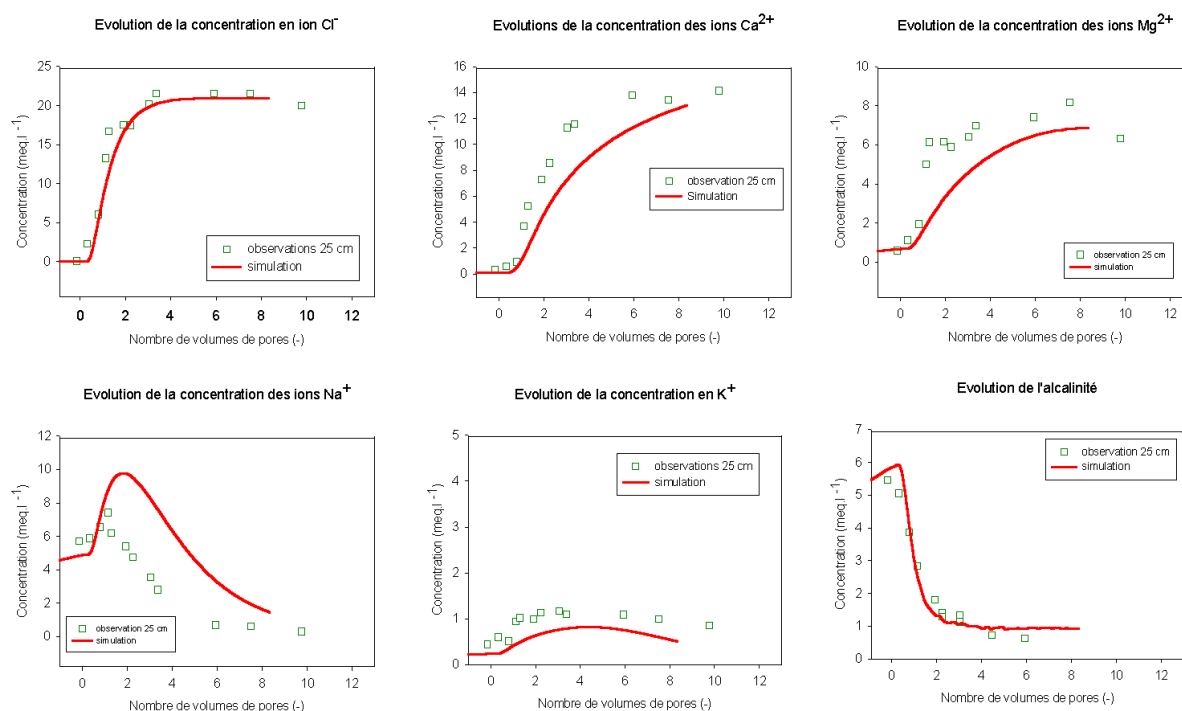**Figure 2. Soil column experiment scheme (Maeght, 1999)**
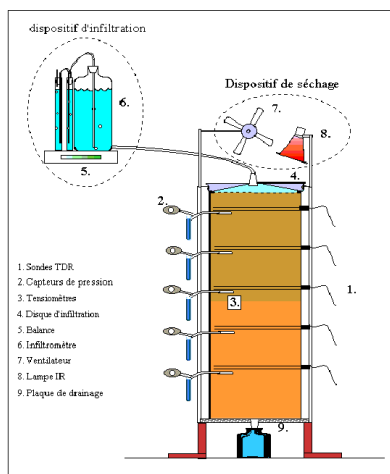
Results

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 (Figure 3). 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.

Figure 3. Comparison between observed and simulated elution curves at 25 cm

Evolution de la concentration en ion Cl⁻ — Evolutions de la concentration des ions Ca²⁺ — Evolution de la concentration des ions Mg²⁺ — Evolution de la concentration des ions Na⁺ — Evolution de la concentration en K⁺ — Evolution de l'alcalinité

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 has been acquired independently and only few parameters for dispersivity and kinetics of chemical reactions have been calibrated.

Bibliography

BERTRAND R. and N'DIAYE M.K., 1994. L'alcalinisation/sodisation, un danger pour les périmètres irrigués sahéliens. Sécheresse, 1994. 5: p. 161-171

BERTRAND R., 1985. Sodisation et alcalinisation des sols de l'Office du Niger (Mali). 1985, CIRAD-IRAT.

BOIVIN P., FAVRE F. and MAEGHT J.L., 1998. Les sols de la moyenne vallée du Sénégal : caractéristiques et évolution sous irrigation. Etude et gestion des sols, 5(4): 235-246.

GAINES G.L., THOMAS H.C., 1953. Adsorption studies on clay minerals. II. A formulation of thermodynamics of exchange adsorption. Journal of Chemical Physic, 21: 714-718

GHASSEMI F., JAKEMAN A.J., NIX H.,1995. Salinisation of land and water resources. Human causes, extent, management and case studies. CAB international, Wallingford Oxon, 526 pp.

HUNTER K.S., WANG Y., VAN CAPPELEN P., 1998. Kinetic modeling of microbially-driven redox chemistry of subsurface environments: coupling transport, microbial metabolism and geochemistry. Journal of Hydology, 109: 53-80.

HUTSON J.L., WAGENET R.J., 1995. An Overview of LEACHM: A process based model of water and solute movement, transformations, plant uptake and chemical reactions in the

unsaturated zone. Chemical Equilibrium and Reaction Models, SSSAJ Special Publication 42: 409-422.

LAFOLIE F., 1991. Modelling water flow, nitrogen transport and root uptake including physical non-equilibrium and optimization of the root water potential." Fertilizer research, 27: 215-231.

MARLET S., 1996. Alcalinisation des sols dans la vallée du fleuve Niger (Niger). Modélisation des processus physico-chimiques et évolution des sols sous irrigation. Montpellier, Ecole Nationale Supérieure Agronomique de Montpellier: 196 p.

MARLET S., VALLES V., LAFOLIE F., CONDOM N., 1998. Hydrogeochemical modelling: a suitable approach to predict the effect of irrigation on soil salinity, sodicity and alkalinity. Communication in: 16th ISSS world congress, August 1998, Montpellier, France.

RIEU M., TOUMA J., GHEYI H.R., 1991. Sodium-calcium exchange on Brazilian soils: modeling the variation of selectivity coefficients, Soil Science Society of America Journal, 55: 1294-1300

SIMUNEK J. SUAREZ D.L., 1994. Two dimensional transport model for variably saturated porous media with major ion chemistry. Water Resources Research 30(4): 1115-1133.

TYAGI N.K.,1996. Salinity management in irrigated agriculture. *In* Sustainability of irrigated agriculture. Pereira L.S. (ed): 345-358.

VALLES V., BOURGEAT F.,1988. Geochemical determination of the gypsum requirement of cultivated sodic soils. I. Development of the thermodynamic model GYPSOL simulating the irrigation water-soil chemical interactions. Arid Soil Research and Rehabilitation, 2:165-177.