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Combination of a crop model and a geochemical model as a new approach to evaluate the sustainability of an intensive agriculture system

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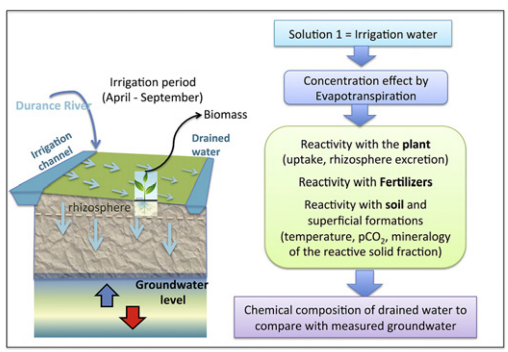
HIGHLIGHTS

- A new combination of crop–geochemical models studies agro-system sustainability.
- The stepwise modifications of soil solution are modelled during its path in soil.
- Measured composition fits very well with those computed validating the model.
- Irrigation water protects the soil minerals against natural tendency to acidification.
- P fixation in soil due to large Ca amount protects groundwater from eutrophication.

GRAPHICAL ABSTRACT



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ABSTRACT

By combining a crop model (STICS) and a geochemical model (PHREEQC), a new approach to assess the sustainability of agrosystems is proposed. It is based upon aqueous geochemistry and the stepwise modifications of soil solution during its transfer from the surface till aquifer. Meadows of Crau (SE France), irrigated since the 16th century, were field monitored (2012–2015) and modelled. Except for N, the mineral requirements of hay are largely covered by dissolved elements brought by irrigation water with only slight deficits in K and P, which are compensated by P-K fertilizers and the winter pasture by sheep. N cycle results in a very small nitrate leakage. The main determinants of the chemical composition changes of water are: concentration by evaporation, equilibration with soil pCO_2, mineral nutrition of plants, input of fertilizers, sheep grazing, mineral-solution interactions in superficial formations till the aquifer, including ion exchange. Inverse modelling with PHREEQC allows for quantifying these processes. For groundwater, measured composition fit statistically very well with those computed, validating thus this approach. This long-term established agrosystem protects both soil and water resources: soil nutritional status remains constant with even some P and (minor) K fixation in soils; long-term decarbonatation occurs but it is greatly slowed by saturation of irrigation water by carbonate; P fixation in soil protects groundwater from eutrophication.

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1. Introduction

In the circumstances of global changes, *i.e.* urban sprawl and climate change, risks of degradation of natural and agricultural environments increase and territories become more vulnerable (Pachauri et al., 2007; Zhang et al., 2007; Pageaud and Carré, 2009;

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Olioso et al., 2013; Baillieux et al., 2015; Trolard et al., 2016). Climate change may positively or negatively impact the services provided by ecosystems on which our social systems depend (Trolard and Dangeard, 2014).

To ensure the resilience of a territory face to these changes, we must start from the concepts of limited space, scarce resources especially soil and water and integrate information (Trolard et al., 2013b).

It is recognized that irrigated systems can regulate the local climate, water resources and food security but little attention has been spent to the influence of nutrients in irrigation water, except in the special case of the application of treated wastewater for agricultural irrigation, which could provide nutrients and provide economic benefits (Cromer et al., 1984; Burau et al., 1987; Asano, 1998; Shuval, 1991; Oron et al., 1995; Lubello et al., 2004; Bixio et al., 2006; Tsiridis et al., 2009; Angelakis and Bontoux, 2001). Water scarcity and increase of costs of fertilizers make a more rigorous evaluation of water use in agriculture necessary.

Groundwater and surface water are not isolated. Thereby, any development or contamination of one normally affects the other and the general composition of rivers (Livingstone, 1963; Sophocleous, 2002; Goren et al., 2014). Irrigation water directly influences groundwater quality: nutrient fluxes were paid a lot of attention to (Valett et al., 1996; Dahm et al., 1998; Bourg and Bertin, 1993; Gibert et al., 1997; Sophocleous, 2002).

The processes at the interface between surface water and groundwater affect solute retention in streams (Valett et al., 1996) and lateral nutrient fluxes between uplands and aquatic ecosystems (Dahm et al., 1998; Wallis et al., 1981; Grimm and Fisher, 1984).

In coastal areas, phreatic water exerts a pressure on sea water to prevent salt intrusion and protects resource for drinking water, agricultural and industrial needs, including tourism (Mayer et al., 2016).

Other studies revealed that plant activity enriches the upper part of soils with inorganic elements used during growth (*e.g.* Si, K, Ca, Mg) (Jobbágy and Jackson, 2001; Lucas, 2001; Barré et al., 2009). Some studies have provided evidence of plants accelerating silicate weathering and CO_2 consumption (Alexandre et al., 1997; Kelly et al., 1998; Moulton et al., 2000; Hinsinger et al., 2001; Song et al., 2011; Song et al., 2012).

These studies point to the important role of plant to modify mineral balance of soil solution. Nevertheless, accounting for plant uptake is rather crude in biogeochemical modelling especially for daily uptake of inorganic elements by plants (Hartman et al., 2007).

In this context, the aim of this paper is to assess the sustainability of an intensive agricultural system under mediterranean to semi-arid climate.

The components of sustainability addressed here are: i) the short-term nutritional status of soils; ii) the long-term tendency of soils towards decarbonatation and acidification, and iii) the quality of phreatic groundwater as a regional resource. Our approach combines a crop model (STICS) and a geochemical model (PHREEQC) and is based upon aqueous geochemistry to simulate the stepwise modifications of soil solution during its transfer from the surface till aquifer. Though PHREEQC is basically a geochemical model, it is here extended for the first time to simulation of uptake of elements by plants, and use of proton balance allows for taking into account the rhizosphere effect of acidification of soil solution.

2. Modelling

2.1. State of the art on biogeochemical models

Different models combine geochemical processes in agroecosystems, as illustrated in Table 1. Most models have been developed for specific purposes: *e.g.* N and C cycles, acid rain or stress effects on forests.

Heat, water, nitrogen (N) and carbon (C) fluxes are simulated in many models of soil-plant-atmosphere system (Cramer et al., 2001; Morales et al., 2005; Yu et al., 2006; De Kauwe et al., 2013; Forster et al., 2013; Friedlingstein et al., 2016; Walker et al., 2014; Wenzel et al., 2014; Sándor et al., 2016; Senapati et al., 2016; Zhang et al., 2016) but do not pay attention to inorganic elements.

Nitrogen transport is studied through linking the hydrological flowpath and biogeochemical pathway in saturated/near-stream zones: this shows that surface/groundwater exchanges change rapidly on the timescale of hydrologic events, which controls the fate of N (Cirmo and McDonnell, 1997).

Solute retention in streams and lateral nutrient fluxes are modelled by linking hydrologic retention, biological nutrient cycling and chemical processes at the surface water/groundwater interface (Valett et al., 1996; Dahm et al., 1998).

Two models, PaSim and Biome-BGC MuSo, linking climate, soil, vegetation and management to ecosystem biogeochemical cycles were compared to simulate C cycle (Sándor et al., 2016), and fluxes between the terrestrial biosphere and the atmosphere in the context of the global change (Xiao et al., 2012; Cramer et al., 1999; Jung et al., 2007; Huntzinger et al., 2012).

Soil chemical and biological properties are combined to assess how nutrients cycling could be affected by wildfire (Fultz et al., 2016). The alpine hydrochemical model (AHM) gathered hydrological, geochemical, climatic and biogeochemical data sets to simulate daily stream chemical composition and its reaction to N deposition, but it cannot reflect terrestrial nutrient cycling (Meixner et al., 2000). SOILVEG and the combined FORGRO/NUCSAM gather biogeochemical and canopy processes to study effects of multiple stressors on forest stands, but they do not simulate stream chemistry (van Heerden et al., 1995; Mohren and van de Veen, 1995).

To capture ecosystem and surface water chemical response to atmospheric deposition and climate, biogeochemical model is established to simulate soil and surface water chemistry by linking ecosystem model (DayCent) with geochemical model (PHREEQC), nevertheless this model simulates only C, N, P, and S dynamics, there is no assimilation of cations (Ca^{2+}, Mg^{2+}, K^+) by plants (Hartman et al., 2007).

None of the preceding combination of models include both crop models for grassland ecosystems and biogeochemical models with their influence on soil solution and water quality.

Crop models can provide daily simulations of growth, but daily plant chemical analyses are very complicated and expensive to obtain.

2.2. Biogeochemical processes

Many processes influence the chemical composition of soil solution (Fig. 1): evapotranspiration, exchange of matter with soil and plants, inputs of fertilizers and manure (Mohammed et al., 2016b) and ion exchange. Thus it is necessary to acquire data on: i) the chemical composition of irrigation water and groundwater; ii) the nature and quantities of fertilizers and manure input on grassland soils; iii) the quantities of chemical elements harvested and exported during the various cuts of hay; iv) the effect of winter grazing meadows by sheeps, and v) pCO_2 and temperature conditions in the soil.

The approach is based on combination of existing models, namely the crop model STICS, (Simulateur mulTIdisciplinaire pour les Cultures Standard) (Brisson et al., 2008) and the geochemical model PHREEQC (pH-REdox-EQuilibrium written in C language) (Parkhurst and Appelo, 2013) (Fig. 2). This interface is a part included in the general PRECOS framework approach (Trolard et al., 2016). Basic principles of both models are given below.

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