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Journal of Hydrology 309 (2005) 301–320
Journal of Hydrology
www.elsevier.com/locate/jhydrol

SiSPAT-Isotope, a coupled heat, water and stable isotope (HDO and $H_2^{18}O$) transport model for bare soil. Part II. Evaluation and sensitivity tests using two laboratory data sets

I. Braud[a,d,*], T. Bariac[b], M. Vauclin[a], Z. Boujamlaoui[c], J.P. Gaudet[a], Ph. Biron[b], P. Richard[b]

[a]*LTHE (UMR 5564 CNRS, INPG, IRD, UJF), BP 53, 38041 Grenoble Cédex 9, France*
[b]*BIOMCO (UMR 7618, CNRS, INRA-INAPG, UPMC), Bâtiment EGER, 78850 Thiverval-Grignon, France*
[c]*Institut Agronomique et Vétérinaire Hassan II B.P. 6202 Rabat-Institute, Rabat, Morocco*
[d]*Cemagref UR Hydrologie-Hydraulique, 3 bis Quai Chauveau, 69336 Lyon Cédex 9, CP 220, France*

Received 20 November 2003; revised 6 December 2004; accepted 21 December 2004

Abstract

Stable water isotopes are tracers of water movement within the soil–vegetation–atmosphere system. They have the potential for a better understanding of water vapour transport within soils, evaporation and transpiration processes. To better understand those potentialities and possible lack of knowledge, a coupled heat-water and stable isotope transport model, called SiSPAT-Isotope was developed for bare soil. We presented the theoretical basis of the model in the first part of the paper, including a first validation of the likelihood of model results and a comparison with existing analytical solutions. In this companion paper, we go a step further by comparing the model results with two data sets collected on laboratory columns. In both cases, five soil columns were saturated and let drying during 173 and 253 days, respectively. At selected dates, one of the column was cut into slices and analysed to determine the volumetric water content, the deuterium and oxygen 18 concentrations profiles. The first data set was acquired on disturbed soil columns. The second one was collected on non-disturbed soil columns and it included a complete monitoring of atmospheric variables. It was not the case for the first one and a sensitivity analysis of model results to the air humidity was performed, showing its large influence on surface isotope concentrations. For both data sets, we also conducted a sensitivity analysis to the formulation of the kinetic fractionation factor, conditioning the resistance to isotope transport between the soil surface and the atmosphere, and to the value of soil tortuosity. The results showed that the model was able to reproduce the behaviour of the observed concentration profiles. A fair agreement between measured and calculated values was obtained for all profiles for the disturbed soil. Near surface concentrations were in general overestimated for the undisturbed soil, raising the question of possible influence of immobile water on concentrations values. We showed that soil tortuosity was mostly influential on the depth of the peak isotope concentration, which opens perspectives for its retrieval from the measurement of isotope concentration profiles. When only molecular diffusion was considered, the model was not able to

* Corresponding author. Address: Cemagref UR Hydrologie-Hydraulique, 3 bis Quai Chauveau, 69336 Lyon Cédex 9, CP 220, France. Tel.: +33 4 72 20 78 87; fax: +33 4 78 47 78 75.
E-mail address: braud@lyon.cemagref.fr (I. Braud).

doi:10.1016/j.jhydrol.2004.12.012

reproduce the liquid slopes of the deuterium/oxygen 18 relationships at the beginning of the drying process. Results were more in agreement with the data when molecular diffusion combined with turbulent transfer were considered. Further laboratory and field experiments are, however, still required to derive a formulation of the kinetic fractionation factor adapted to drying soils and non-saturated conditions.

Keywords: Coupled heat; Water and stable isotope transport model; Resistance to isotope transfer; Laboratory soil columns; Kinetic fractionation factor

1. Introduction

A modelling effort was undertaken in order to develop a coupled heat, water and stable isotope transfer model (SiSPAT-Isotope) in the soil–vegetation–atmosphere continuum. A physically based model, representing the full interactions between the atmosphere, the soil, the vegetation and stable isotope species can provide a powerful tool for testing various hypotheses about active processes. As it also provides a synthesis of the current understanding of these processes, it can help, when compared with observed data, to identify the gaps in knowledge and the points requiring further investigations. The proper simulation of oxygen 18 concentration in transpiring leaves has also been shown to be important for the determination of the isotope signature of CO_2 and the identification of the sources of CO_2 encountered in the atmosphere (Helliker and Ehleringer, 2000; Ferretti et al., 2003).

The first step of our modelling effort led to the development of a first version of the model, operating on bare soil (Braud et al., 2004). In the first paper, we performed a verification of the code using "likelihood" tests proposed by Mathieu and Bariac (1996) and a comparison with existing analytical solutions under steady state conditions (Barnes and Allison, 1983, 1984). However, a full validation of the hypotheses and formulations was required, especially under non-steady state regime. To achieve that goal, we use here two existing data sets, collected on drying soil columns. Those data sets do not allow a full validation of the model, because the soil evaporation flux was prescribed from the potential evaporation and not from the surface energy budget. However, it was a necessary step in simplified conditions. The first data set was obtained on disturbed homogeneous soil columns. The second data set was collected on undisturbed heterogeneous soil columns. The assessment of SiSPAT-Isotope (Braud et al., 2004) required two steps: (i) first an evaluation/calibration of the heat and water flow components against data (ii) second an evaluation of the model results in terms of isotope concentrations profiles and deuterium/oxygen 18 relationships. Because all the data required to run the model were not always available with the required accuracy, we performed sensitivity tests to complement the analysis. Special attention was also given to the formulation of the resistance to isotope transport between the soil surface and the atmosphere, which depends on the kinetic fractionation factor, by comparing various formulations encountered in the literature. The data sets used in this study were not designed for the validation of a model such as the SiSPAT-Isotope model and all the required information was not monitored. However, we considered that their use was valuable in order (i) to assess if the model was able to reproduce the main feature of these data sets, and (ii) to prepare the design of future experiments by identifying the most sensitive variables and parameters for accurate monitoring. Therefore the study provides an example of synergy between model building, model sensitivity study and experimental design for the study of particular processes and the validation of modelling approaches.

The physically based model and the data sets are briefly described in Sections 2 and 3, respectively. Sections 4 and 5 present the model set up, the results and the sensitivity tests for the disturbed and undisturbed soils, respectively. Eventually Section 6 presents a general discussion and draw some conclusions and guidelines for further studies.