Review of "Multi-response modeling of an unsaturated zone isotope tracer experiment at the Landscape Evolution Observatory" (HESS-2016-228)

Summary:

This manuscript deals with the modeling of an unsaturated flow and isotope tracer experiment. The experiment, conducted at the Landscape Evolution Observatory (LEO), involved successive injections of water and deuterium-enriched water into an initially very dry hillslope. Multivariate observations were presented for flow and transport: soil moisture, water and tracer outflow, breakthrough curves and total water storage. Simulations were performed with the physically-based distributed numerical model CATHY that solves the 3D Richards and advection-dispersion equations and includes coupling with surface routing equations. The modeling approach succeeded in simulating the integrated flow and transport responses. However, with the same parameterization it failed to restitute the point measurements of the water contents and the tracer concentrations.

Overall quality:

This manuscript is clear, well structured, and pleasant to read. The experimental results are new. However, they should be better described and discussed. It is surprising to see that these well-calibrated experiments are so difficult to model. Some of the numerous parameterizations added in the successive simulations look arbitrary and their choice should be better justified. Furthermore, the cumulative mass balance error of tracer in the CATHY simulations is relatively large (~2% with respect to the total mass injected) and this fact should therefore be discussed. The conclusions of the manuscript would be more convincing if more than one numerical code were used. But this task could be further accomplished in a future publication. Very surely, these experiments and their first simulations could serve as a nice benchmark for physically-based distributed numerical models provided the full dataset is rendered available.

In my opinion, the experimental results and the corresponding simulations are very interesting and deserve to be published in HESS. However, some corrections and/or clarifications should be accomplished prior to publication. The authors will find below some remarks to correct or complete their manuscript.

Major Comments:

(1) The experimental results are new and interesting. However, the description and discussion of the water contents and concentrations measured should be improved. You will find below some examples of questions that arise about the experimental results.

> (1a) Page 4, Figure 1: Please comment the peak of δ^2H during the first irrigation event.
>
> (1b) Page 18, line 7: You are using the soil water content at 4 different depths averaged over 496 sensors. Can you quantify the soil heterogeneity from a statistical analysis of these 496 experimental vertical profiles?
>
> The landscape geometry is symmetric. All parameter heterogeneities included in the simulations are symmetrical as well. Does one observe this symmetry also in the experimental results? For example, are the θ vertical profiles measured along two vertical lines that are located at the same distance from the seepage face but on either side of the landscape similar?
>
> Is the variability of the profiles correlated with the rainfall variability?

(1c) Page 20, Figure 11: The time evolutions of θ measured at the points located at the centre of the hillslope (points a, b, and c) clearly show that the bottom of the hillslope has become water-saturated after the 2nd rainfall event. This point should be discussed in the paper. CATHY has clearly failed to simulate this saturated zone. More generally, practically all θ values obtained from the simulation, presented in Fig.11 are lower than the corresponding values obtained from the measurements. Do you have an explanation for this lack of water in the CATHY simulations? I think it would be better to calibrate some parameters (e.g., n_{VG}) from distributed θ profiles instead of calibrating parameters from averaged θ profiles. As a matter of fact, the vertical evolution of the wetting front varies depending on whether it is observed at the top of the landscape or in the zone of flow convergence.

(2) Some hypotheses and some results of the modeling approach require further argumentation and discussion.

(2a) Page 8, line 16: Several parameterizations in the simulations are arbitrary and not justified. For example, why did you choose a depth of 38 cm? Did you perform a calibration? Evaporation is often assumed to be active only over the first few centimeters.

(2b) Page 8, line 21: Same as remark (2a): Why did you choose λ=1 m^{-1}?

(2c) Page 8, line 20: There is no moisture content dependence term in the sink term given by Eq. (15). What happens if there is not enough water for evaporation in the upper 38 cm of soil?

(2d) Page 9, lines 3-5: Same as remarks (2a) and (2b): the choice of f_c looks very arbitrary. Please justify it.

(2e) Page 11, Table 3: Same as remarks (2a), (2b), and (2d): how did you choose the k values? Did you perform a calibration?

(2f) Page 11, lines 1-6: The heterogeneity and anisotropy of k_s are justified by invoking the processes of clogging and compaction. Such modifications should induce a modification of the topography. Did you observe topographic changes caused by diffusive geomorphic processes such as rain splash during the rain events that lasted several hours? Pangle et al. (2015) affirm that "digital elevation models will be constructed at regular intervals and following all events with the potential to modify the topography", with a model surface precision of 0.002 m. Have you performed such measurements? If yes, did you observe some changes in the topography? Have you observed the formation of some crusts at the soil surface? The properties of the soil, e.g., its permeability, must be changed with time if crusts are forming.

(2g) Page 14, line 28: The best numerical results are obtained with the smallest value of the dispersivity. Can you discuss this result? Is it a proof that the soil is very homogeneous? It would be interesting to measure α_L for example from transport experiments in a column filled with the same porous media.

(2h) Page 16, line 5: Can you explain why the cumulative mass balance error is so large (~2%)?

MINOR COMMENTS:

(3) Page 4, line 3: Please clearly indicate the location of the seepage face. Is it the 11-m^2 boundary at the downslope end of the landscape?

(4) Page 4, line 9: The estimated evaporation rates are two times and ten times larger than the rates reported in Niu et al. (2014) and Pasetto et al. (2015), respectively, although the soil is drier. Can you explain this difference?

(5) Page 4, Figure 1: The irrigation rate is equal to 12 mm/h ~ 1.1×10^{-3} m^3/s. Please correct the y-scale for Q_r in Fig. 1.

(6) Page 4, Figure 1: Does the size of the symbols for $\delta^2H(t)$ correspond to the 0.5‰ analytical precision?

(7) Page 5, Equation (1): The CATHY model solves the coupling between surface and subsurface flows. Why do you not quote the surface flow equation?

(8) Page 5-6, section 3.2: How are the nonlinear terms in the equations being solved? Is it based on an iterative scheme with Picard iterations?

(9) Page 6, line 17: Please remove Eq.(6) because the effective saturation has already been defined in line 20.

(10) Page 6, line 19: Please replace the exponent in Eq.(8) with "-m" and add the definition of m:
$m = 1 - 1/n_{VG}$.

(11) Page 6-7, Eqs. (9)-(13): I am not convinced of the interest to present Equations (9)-(13). What is new in comparison with the schemes already described by Putti et al. (1998) or by Weill et al. (2011)?

(12) Page 7, section 3.3: How did you choose the horizontal and vertical discretizations? Did you verify the spatial convergence of the numerical simulations?

(13) Page 8, line 23: Please correct the values for the evaporation:
5 mm/d ≡ 5.8×10^{-8} m/s and 3.9 mm/ d ≡ 4.5×10^{-8} m/s

(14) Page 9, Caption of Table 1: z_i is the depth of the middle of the i^{th} layer.

(15) Page 9, Table 2: Please verify the values given in Table 2.
For example, for layer 5, $f_{c1i}=1.91\times10^{-8}\times c$, for layer 7, $f_{c1i}=2.36\times10^{-8}\times c$ and $f_{c2i}=1.41\times10^{-8}\times c$, for layer 11, $f_{c1i}=4.77\times10^{-8}\times c$, for layer 12, $f_{c1i}=6.75\times10^{-8}\times c$.

(16) Page 11, Table 3: Please correct the name of the last simulation: "f" instead of "e".

(17) Page 11, line 19: Please provide the definition of the coefficient of efficiency CE.

(18) Page 13, Figure 3: Figure 3 would be clearer if the time evolutions of the seepage face flow and of the total water storage for a given case were reported side by side instead of one above the other. Furthermore, the superposition of two simulated test cases in each figure is unnecessary.

(19) Page 14, lines 19-20 and line 26: Finally, which simulation (e or f) is used for the subsequent simulations? Please correct the text accordingly.

(20) Page 14, lines 30-32: I do not understand what you mean. In my opinion, in Fig.4, ^2H-labeled water appears in the measured outflow discharge and also in all simulated outflow discharges after the second pulse.

(21) Page 16, line 11: You cannot claim that a ~50% increase of the seepage face concentration after the third event is a slight increase.

(22) Page 16, line 17: The definition of c implies: $0<c<1$. What do you mean by a tracer concentration as high as 15? It would be interesting to show some vertical profiles of the water content and concentration.

(23) <u>Page 18, line 2</u>: In the first simulation, a part of the isotope tracer may evaporate but it is not all lost by evaporation.

(24) <u>Page 20, line 2, and Page 21, line 4</u>: Please add the name of the simulation: simulation l from Table 4. More generally, indicate in all figures the name of the simulations as specified in Table 4.