Dear reviewer,

Thank you for your detailed comments. The following are our detailed responses to each of your comments. In the following, the reviewer's comments are highlighted in boldface and our responses are in normal text.

('Equation' refers to the equation in manuscript, while 'Eq' refers to the equations in this document.)

'Equation (1) is the water content-based Richards equation. It is well known that this kind of formulation cannot handle saturated problems and is not well posed at the interface between two layers, because water content is discontinuous. The mixed form of Richards equation should be used.'

We think Equation (1) in the manuscript is the mixed form (with combination of Equation (3)). We wrote this as the general governing equation. However, our MATLAB code solves the head-based Richards equation, not the water-content based equation.

The head-based form and the mixed form of Richards equation are both commonly used for modeling water flow in porous media. We choose the head-based form because the head is continuous across the soil interface (especially for 3 or more layered soils) (Zha et al., 2019). In addition, many popular models, such as SWAP (van Dam and Feddes, 2000), are also based on head-based Richards' equation:

$$c(\varphi)\frac{\partial \varphi}{\partial t} - \frac{\partial}{\partial z}(K(\varphi)(\frac{\partial \varphi}{\partial z} - 1)) = 0 \quad (1)$$

where $c(\varphi)$ equals $\frac{\partial \theta}{\partial \varphi}$, and known as moisture capacity.

The mixed form of Richards' equation is no doubt a better choice. Because $c(\varphi)\frac{\partial \varphi}{\partial t}$ may not numerically equal $\frac{\partial \theta}{\partial t}$ (Celia et al., 1990; Clark et al., 2021), *c* (from Eq. (1)), could introduce mass balance errors. However, the mass balance of head-based form can be significantly improved by a second-order approximation to the time derivative (Celia et al., 1990) and effectively controlled by adaptive time-stepping schemes (Ireson et al., 2023). Given our solvers adopt adaptive time stepping schemes, our program meets the mass balance requirement.

To reduce confusion, we will change Equation (1) in the manuscript to a head-based equation in the revised manuscript, which will not affect the remaining part of the manuscript. We will also add the above to our discussion section.

'The heat transfer equation (2) is not correct. Csoil depends on the water content and should be embed in the time derivative.'

We think our equation (2) is correct. The proof is provided below. As you indicated that C_{soil} is a function of soil water content, and the heat transport equation can be written as:

$$\frac{\partial C_{soil}(\theta)T}{\partial t} = \frac{\partial}{\partial z}\left(k_H \frac{\partial T}{\partial z}\right) - C_w \frac{\partial qT}{\partial z} - C_w ST \tag{2}$$

However, this equation can be further rewritten as:

$$C_{soil}(\theta)\frac{\partial T}{\partial t} + TC_w \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(k_H \frac{\partial T}{\partial z}\right) - C_w q \frac{\partial T}{\partial z} - C_w T \frac{\partial q}{\partial z} - C_w ST \tag{3}$$

by combining:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - S \tag{4}$$

Eq. (3) can be simplified:

$$C_{soil}\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(\frac{k_H \partial T}{\partial z}\right) - C_w q \frac{\partial T}{\partial x} \tag{5}$$

Therefore, the heat transport equation in our manuscript is correct. It is just another form of the same expression.

'More information should be provided concerning the solvers (ode113, ode23tb).'

Thank you for your comments. Details about ode113 and ode23tb in the manuscript can be found on the MATLAB official website (https://www.mathworks.com/help/matlab/math/choose-an-ode-solver.html). To address your comment, we will add a brief description about the two solvers in the revised manuscript, put citation and the internet link to help readers understand the solvers.

'The tests 1 to 6 are very qualitatively discussed. Only different types of processes are checked. Physical processes can be verified but it does not mean that the computed variables and the process kinetics are correct. Moreover, these tests are development tests. They do not provide any new information on processes and therefore, should not be part of the manuscript. It is expected that models overcome these kinds of tests before publication.'

Thank you for your comments. These theoretical test results are included to keep consistency with previous isotope modelling studies. As mentioned in the manuscript, these tests are necessary for an isotope model because they can validate the accuracy and stability of the numerical model. Besides, these tests are included in the Sispat (Braud et al., 2005) and recent updated HYDRUS (Zhou et al., 2021). However, we also agree to your opinion, these tests do not provide any new information and the model should pass these tests before publication. Therefore, we will put them to appendix as necessary.

"L479-480: the reason for poor MAE value is unclear to me."

Figure 10a showed that the measured peak value of δ^2H does not match the simulation, which result in a large *MAE* at the top 0.1 m. Except this peak point, MOIST had good estimations on the remaining points.

The large *MAE* could be related to the heterogeneity of the soil column/flow paths. For example,

the sampling area on the 11th day participated less in the flow processes. Besides, evaporation results in the fractionation of deuterium at the top 0.1 m layer. Therefore, the simulated value does not match the measurement and lead to a large *MAE*.

"L521-540: The analysis of the difference between fully coupled or sequential approach (segregation) is convincing but it applies for an explicit time scheme discretization whereas HYDRUS and SiSPat use an implicit scheme. Moreover, the flow equation is written in terms of water content for MOIST, the other codes are using pressure based or a mixed form of Richards equation."

Thank you for your comments. The segregated method, either the implicit scheme or the explicit scheme, may introduce more errors than fully coupled method. The implicit scheme may have better performance than explicit one because the former is more stable. Both implicit and explicit schemes, solve PDEs numerically, therefore, there will be always errors accumulation in either of the two schemes, and therefore still can accumulate errors if a set of partial differential equations are solved sequentially. The coupled method, however, can reduce the error accumulation by solving a set of PDEs simultaneously. In out manuscript, an explicit example was used for easier understanding of the error difference between segregated and couple method.

Again, we used a head-based Richard equation, as can be seen from the MOIST source codes.

'L608-610: The discussion about boundary conditions and intermodal conductivity is very popular. There are key papers not cited in the manuscript that review some of the techniques (see for example Belfort et al.,. On equivalent hydraulic conductivity for oscillation–free solutions of Richards equation. Journal of Hydrology, 2013, 505, pp.202-217).'

Thank you for your suggestion. We will cite these key papers in our revised manuscript.

"MOIST was used to simulate two types of experiments and the authors concluded that MOIST is more accurate and reliable. This is not supported by the provided results. These results only show that MOIST might be better calibrated not that the numerical scheme – fully coupled- is better than other schemes. Parameters used by MOIST and the other models should be given."

We did not calibrate our model for both datasets. We used the parameters for the long-term experiment site that is provided by Stumpp et al. (2012) and also used by Zhou et al., (2021). Therefore, the model parameters are identical between our study and Stumpp et al. (2012) and Zhou et al. (2021). These parameters can be found in Table 4 from Stumpp et al. (2012) and the comparisons are showed in Figure 11 and Table 6 in the manuscript. We believe these comparisons support that MOIST has better performance mainly because the numerical scheme is different (segregated vs. coupled). However, in the revised manuscript, we will state the limitation that we only used two datasets for testing our model. More extensive verification is needed.

"The comparisons do not provide any information on the code accuracy and efficiency. To demonstrate the 'excellent performance of the MOIST,' the authors should compare their code with other existing codes (for example looking at breakthrough curves at

different locations) and check detailed mass balances, time and space discretization sensitivity and computer time."

Our tests are not exhaustive. But we do have most elements as you suggested for testing accuracy and efficiency. As mentioned above, we compared our code to different version of Hydrus under the long-term simulation (data come from Stumpp et al. (2012)). The simulated isotopic composition of outflow from a lysimeter is equivalent to the breakthrough curve simulation. In addition, the short-term experiment in EPFL has a spike treatment (irrigate water with a high concentration in a short time), then the simulated isotopic concentration at different depths can also be treated as breakthrough curves simulation, and the accuracy is checked by measured isotopic compositions at different soil depth.

Moreover, the first part of discussion (4.1) illustrated the sensitivity of MOIST on space discretization. As compared to Sispat, Soil-litter-ISO, and revised HYDRUS, MOIST can pass these theoretical tests by using a ten-times larger spatial step. The test 1 (Figure 12c and 12d in the manuscript) also showed that MOIST has a good mass balance performance and, the final isotope distribution being a straight line (test 1), especially at the top of the soil column (Braud et al., 2005).

We will state in the revised manuscript that our tests are not exhaustive, and more tests are needed.

Reference

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