

Reply to comments on interactive discussion "Functional test of pedotransfer functions to predict water flow and solute transport with the dual-permeability model MACRO" by J. Moeys et al.

1 Notable changes to the article

1.1 Text and results presented

No changes have been made to the results presented, as no new modelling has been done. We have not followed the suggestion of reviewer 1 to test a new calibration method, but we explain why in the reply to comments. We have added several clarifications and additions in the text, described in the reply to comments. We have also added a table in the supplementary materials with the modelled water balance components of each lysimeter included in this study.

1.2 Figures

Many figures have been changed in order to improve their readability. Fig. 1 is now provided in a higher resolution. Fig. 3, as well as all the 16 figures of the supplementary materials, have been totally changed in order to make them more readable, and to better reflect the way measurements were done (*line plot replaced by a step-line plot*). Figs. 4 and 5 have been totally changed too, to improve the readability, and they are now merged into a single figure (with 4 subfigures), now referred to as fig. 4. Figs. 6 and 7 have been left unchanged, as we think they are already very readable, but they are now referred to as Figs. 5 and 6, respectively.

2 Anonymous Referee #1

2.1 General comments

[NB: the comments numbering was added by the article's authors after the review]

Com. 1: This paper presents a test of pedotransfer functions for predicting water flow and solute transport for a model with preferential flow. The development of pedotransfer functions for preferential flow models is an important issue and not many studies are available. For this reason, publication of this paper in HESS is justified. However, there are some concerns which need to be addressed before the paper can be published.

Com. 2: My most important concern is about the calibration procedure used to compare the blind simulations with simulation with calibrated model parameters. The authors have not used a comprehensive calibration procedure, but instead used a

limited calibration procedure in which first the water flow component and then the solute transport model was calibrated. The calibration parameters chosen appear to be quite arbitrary, for example the water uptake and anion exclusion factors are calibrated to mimic faster transport in the soil matrix.

The main focus of the paper is on blind predictive capability, so our objective with the calibration was not at all to do a comprehensive procedure, but rather just to see if a limited calibration would improve upon blind predictions and compensate for the failure to account for macropore flow. See below for a more detailed argumentation.

Com. 3: An increase of the dispersion length would have been a more appropriate choice, and would probably have given dispersion lengths that are more in line with the median value of 5 cm as suggested by Vanderborght and Vereecken themselves.

The dispersivity could have been calibrated instead of the anion exclusion factor. But, as explained in the article (p 2256 l 10: "*for experiments carried out at steady flow rates of less than 1 mm h^{-1} , which should exclude the influence of dispersion due to macropore flow*") we think that the 5 cm value obtained by Vanderborght and Vereecken (2007) encompass both dispersion and some forms of preferential flow (in their abstract "*The activation of large interaggregate pores may explain the increase in dispersivity with increasing flow rate in fine-textured soils, which was not observed in soils with a coarser texture*"). We therefore thought it would be better to calibrate another parameter, anion exclusion, that was not already accounted by MACRO macropores or dispersion parameters.

Instead of writing "In a second step, we investigated the potential for improving the simulation results by calibrating...", we have now written "In a second step, we used a *simple procedure* to investigate the potential for improving the simulation results by calibrating..."

Com. 4: I would suggest carrying out a more detailed calibration exercise for a subset of lysimeters to test if this limited procedure is adequate.

We realize that the calibration exercise we have conducted is inadequate to fully encompass all the possible uncertainties of the parameterisation scheme we present in this article. The primary objective of this article is to test whether blind-parameterisation of MACRO is feasible for simulations at the regional scale. The calibration procedure was therefore only a minor objective, to highlight a few possible improvements in the parameterisation routines. It is unfortunately out of the scope of this article to test a more detailed calibration procedure.

Com. 5: Another concern pertains to the modelling experiment. The authors have selected a zero tension lower boundary condition for the water flow model. This is not an appropriate boundary condition for plant-covered lysimeters. The soil will often be unsaturated throughout, and in this case the zero tension boundary condition will give completely wrong modelling results. I suggest redoing the simulation with a free drainage boundary condition, in which the outflow stops if the soil is unsaturated (a lysimeters boundary condition).

We are not sure we understand what the reviewer means by "in this case the zero tension boundary condition will give completely wrong modelling results". Does the reviewer mean that if we set a zero tension at the bottom of the soil profile, then the model will simulate upward water flow by capillary rise, and thus bias the water balance if additionally water is taken up by a plant growing in the profile? This is not the case. It was maybe a little unclear in our article, but the lower boundary condition for a lysimeter in MACRO uses a zero pressure head at the bottom boundary, but no upward flow is allowed. We have now clarified the text regarding this point.

Com. 6: In some cases, the pedotransfer functions appear to be unnecessarily simple, giving only four classes. As an alternative, Jarvis et al. (2007) presented a continuous pedotransfer function for the effective diffusion path length based on organic matter and clay content. The authors should justify why this more sophisticated pedotransfer function was not used in this study and how these two estimation procedures relate to each other.

Indeed, the work presented by Jarvis *et al.* (2007) presents a continuous pedotransfer function for the effective diffusion pathlength. It has however only been calibrated (and tested) on a few Swedish tilled topsoils. It therefore cannot be expected to have relevance for subsoils or uncultivated topsoils (e.g. grassland), and may have little geographical generality: Swedish soils are generally very young (i.e. have undergone little pedogenesis) as compared to some other soils in Europe, so their structure might be quite different from other European soils (Luvisols for instance). In contrast, the scheme used in our paper to support the class pedotransfer function for the diffusion pathlength (and other parameters related to soil structure) was designed to be generally applicable to all soils of Europe (including subsoils) and has been tested on much larger datasets (see Jarvis et al., 2009).

2.2 Specific comments

Com. 7: Page 2246 – line 15 and 21: I don't agree with the statement that water flow is reasonably well simulated. A modelling efficiency of 46% does not justify this.

Our statement "water flow was generally reasonably well predicted (median model efficiency, ME, of 0.42)" is of course very subjective. If the model had been calibrated, a value of 0.42 would not be very satisfactory. But in our case, we present result of simulations with 'blind'-parameterisation of the model, and we think 0.42 is satisfactory (as it could be much worse).

Com. 8: Page 2251 – line 8: There is no relation between the organic carbon content mentioned in the text and the values presented in table 2. The median value is lower than the lowest value in the table!

Only average values for topsoil horizons are presented in the table. The median value given in section 2.1 concerns all horizons, including subsoil horizons. We have now made the text clearer, and included a median value for topsoil horizons only.

Com. 9: Please replace T/m³ by kg dm⁻³.

Done

Com. 10: Page 2252 – line 5: please give the model version here, and discard it at page 2253

Done

Com. 11: Page 2253 – line 6: pH water, pH CaCl₂ or pH KCL?

pH is only used as a potential limiting factor for earthworms abundance (if it is lower than a threshold), in the “earthworms” sub-part of the decision tree used to define the horizon’s preferential flow class. We have not chosen a specific pH measurement method as a reference for this part of the decision tree, despite the fact that measured pH will vary with the measurement method. This tree is designed to be used on soil survey data, where pH is one of many *estimated* soil properties, and only one measurement method is generally available. Additionally, we don’t think the tree is accurate enough to justify the preference for one particular method (it would be a false accuracy).

There could also be methodological concerns for the measurements methods employed for bulk density, organic matter and texture, but it depend in this case of the characteristics of the HYPRES database employed by Wösten *et al.* (1999).

Com. 12: Page 2253 – line 15: It is not clear from the text how the entire $\theta(h)$ relationship is build. The authors describe the estimation procedure for the saturated water content and the water content at wilting point, but not for the water contents in between.

As explained in the paper, MACRO 5.2 uses the van Genuchten water retention function in the soil matrix. The parameters of this function are used to calculate water content at any pressure head. We have slightly modified the text to make that clearer.

Com. 13: Page 2254 – line 8: Is there an explanation for the systematic difference of the data from the three authors?

No, we don’t have one.

Com. 14: Page 2255 – line 16: As this relates to a crop, this is not a PTF.

We have now replaced the abbreviation "PTF" by "estimation algorithms" (when referring to both soil and crop parameters) or "lookup tables" (when referring to crop parameters only).

Com. 15: Page 2256 – line 10: The choice for the 3.4 cm needs to be justified in more detail. According to the author of this paper, not all experiments with high flow rates exhibited preferential flow, so eliminating these experiments is rather arbitrarily. As mentioned in the general remarks, a higher value of the dispersion length would be more logical.

It is true that not all experiments with high flow rates exhibit preferential flow, but the only way to remove the effect of preferential flow from the dispersivity parameter (which we must do) is to consider only experiments with lower flow rates, even if that

may also exclude some experiments that do not have preferential flow (because they are sandy soils of high matrix conductivity, for example).

If we would have set the *effective* dispersivity to a higher value, then we would overestimate dispersion, as preferential flow is explicitly modelled in MACRO and results in a higher *apparent* dispersivity.

We have added a sentence to clarify this.

Com. 16: Page 2260 – line 25: A perennial crop does not automatically imply that the Leaf Area Index is constant in time. Probably in FOOTPRINT, but not in reality. And a seasonal course of the LAI is also normal in temperate climates, so not limited to Nordic countries.

Yes, exactly. We can only account for the processes we are able to parameterise without measurements, and that sometimes implies severe simplifications compare to reality.

The reviewer is right to state that a seasonal course of LAI is expected even outside Scandinavia. Nonetheless the only grassed lysimeters of our dataset are located in Sweden, so we only commented on what happens in Sweden. We also meant that the non-constant course of LAI is more obvious in latitudes where frost and snowfall periods are longer.

Com. 17: Page 2274 - table 4: is the effective diffusion pathlength also set to 3 mm for macropore flow class I?

Yes. In this exercise we had no soil profile presenting a harrowed layer.

2.3 Technical comments

Com. 18: The quality of the figures is not acceptable for publication in HESS, please improve the quality of these figures.

We are not sure what the reviewer means by 'improve the quality of these figures', but we suppose it means improving their readability. We have made improvements to the figures to make them more readable. These changes are listed in the 1st part of this document.

3 Anonymous Referee #2

3.1 General comments

Com. 19: This study presents an evaluation of pedotransfer functions that are used to derive parameters of a model that considers preferential flow and transport. Simulations of the parameterized model were compared with data from lysimeter experiments. In order to evaluate the effect of preferential flow, also simulations were run in which the preferential flow process was 'turned off'.

Com. 20: The results indicate that the fraction of the leached tracer shortly after tracer application was considerably better predicted when preferential flow was taken into account and parameterized using the pedotransfer functions. Besides a direct comparison between simulated and measured leachate rates and leached solute fractions, also the measured and simulated ranking of the soils in terms of their vulnerability to leaching and preferential transport was compared.

Com. 21: The outcome of this study is of great relevance for risk assessment and risk management or mitigation that is related to diffuse pollution of groundwater by surface applied agrochemicals, which require regional scale evaluations of solute transport. So far, preferential flow processes have rarely been considered in regional scale assessments. It would be good though if some references are made to other studies in which regional scale modelling of e.g. pesticide leaching was carried out.

We did already cite regional scale modelling studies, but they were quite old (Wagenet and Hutson, 1996; Soutter and Pannatier, 1996). We have added a citation to Leterme *et al.* (2007) and Tiktak *et al.* (2002).

Com. 22: Although the paper is in general clear and sufficiently detailed, there are a few things that need clarification.

Com. 23: Firstly, leached mass fractions are evaluated after certain amounts of pore volumes were drained. It is however not clear how the pore volumes were defined. Since the water content varies over time, the definition of a pore volume is not straightforward.

Yes, good point, thank you. In this study, what we call "pore volume" is in fact the porosity multiplied by the profile depth. We know it is not the best way to "scale" water or solute transport time series, as a real pore volume (water-filled porosity) would be better. But this would require knowing the water content in each lysimeter (either time variable or average), and we don't have such information. We have added a definition of what we mean by pore volume in the paper.

Com. 24: Secondly, I assume that the lysimeters were not weighted neither that water contents in the lysimeters were measured. Therefore, it is not clear how pore volumes could have been derived directly from measurements.

The pore volume was derived from the bulk density of each layer and their thicknesses. This has now been clarified in the paper.

Com. 25: Secondly, it would be good if some more basic parameters of the water balance in the lysimeters were given. For instance, what was the amount of rainfall, potential crop ET, and leachate during the measurement period in the different lysimeters? This could give an impression about the importance of the root water uptake parameters such as the rooting depth and the root water uptake compensation factor. I guess that for situations where crop ET is close to the potential crop ET, root uptake parameters will not have a big impact on the water balance simulations.

Yes. We have added Table S1, in the supplementary materials, with the total rainfall amount, the total simulated evapotranspiration and the total simulated percolation of each lysimeter. Additionally, the measured amount of water percolated was added to figure 3, as well as all figures in the supplementary materials.

Com. 26: In the supplementary material, it would be good to show also the cumulative amount of leachate.

OK, we have done so (both for water and solute).

Com. 27: Given the length of the experimental period (one to two years) it is rather strange that less than 0.3 pore volumes leached out of some lysimeters. For a lysimeter of 1 m length, a volumetric water content of 0.25, 0.3 pore volumes corresponds to 75 mm of leachate which is rather low for a period of 1 to 2 years.

This is due to our unusual way to define the "pore volume". Our pore volume is calculated with the total porosity (see the modified article), so it represents more water than if it had been calculated on the water content. All the figures in the supplementary materials now also present the final accumulated water drainage, in addition to the pore volume(s) presented in the x-axis, so the reader can see how much water that represents.

3.2 Detailed comments:

Com. 28: p2247 In 20 and following: 'errors or uncertainties in the estimations of agro-environmental GIS' I would skip: 'the estimation of'

In our opinion a soil map is also a 'model' of reality, with some parameters, which are also uncertain, and impossible to know exactly. So a GIS results from estimations too.

Com. 29: 'errors in the parameter estimation algorithms used to estimate model parameters' I would skip 'used to estimate model parameters'

Ok, done.

Com. 30: p 2251 In 8 and 9: The organic carbon contents and bulk densities give here, are these parameters of the individual soil horizons? Are the median values calculated from the values of all soil horizons?

Yes, see above (+ clarification in the text).

Com. 31: p 2251: 'Daily weather data were available...' The generation of macropore flow is highly dependent on the rainfall intensity. Since the time scale of a rainfall event is considerably smaller than a day, daily rainfall data are not representative of the actual rainfall intensities. For simulating Hortonian surface runoff, aggregation of rainfall data on a daily time scale leads to a considerable underestimation of the runoff (Mertens, J., D. Raes, and J. Feyen. 2002. Incorporating rainfall intensity into daily rainfall records for simulating runoff and infiltration into soil profiles. *Hydrol. Process.* 16:731-739). Could this be discussed?

The way MACRO handles daily rainfall data was unclear in the article. We have improved that. Daily rainfall data are in fact internally converted into hourly rainfall data, using a constant (time invariable) rainfall intensity and starting the rainfall event (if rainfall there is) at midnight. This rainfall intensity was set to the same default value (2 mm h^{-1}) for all lysimeters in this article.

The reviewer is right in pointing out that this could have influenced of macropore flow in the studied lysimeters. Indeed, the average rainfall intensity we have used may be wrong, and the hypothesis that it is constant over time is of course wrong to. But we can't get better estimates of this rainfall intensity. Errors in the estimation of this parameter may well explain all or part of the observed systematic underestimation of preferential flow (if the hourly rainfall intensity is underestimated).

Thank you for pointing to us this interesting discussion point.

Com. 32: p 2252: In 22 and following. The length of the warm up period seems to depend on the time period between the installation of the lysimeter (or weather station) and the tracer application. The duration of a spin up period should be at least cover the time period that is necessary so that the system state at the start of the tracer application does not depend anymore on the initial conditions but on the weather conditions before the application and the soil properties. For most studies, the spin up period seems to be sufficiently long to fulfil this criterion. However, I am wondering whether this is also the case for the Brimstone study, for which only 14 days of spinup were considered.

The Brimstone experiment, though short, was carried out during winter when the soil should have been at or wetter than drainage equilibrium.

Com. 33: p 2253 In 21: '... the saturated water content in the soil matrix' Is this the water content of the soil when the water potential head is -10cm? Maybe add this definition here.

Yes. We have added that, when the matrix is saturated, $\psi = \psi_m$, as ψ_m is defined in the next sentence (and equal to -10 cm).

Com. 34: p 2254 In 5: Could some information be given about the method that is used to measure $K_{S(m)}$? I think differences in methods that were used to measure $K_{S(m)}$ are more relevant than the different researchers that carried out the measurements.

The same method was used by all 10 researchers. We have added a sentence in the article to mention this.

Com. 35: p 2254: In table 3, estimated macroporosities for different soil layers are given. The macroporosity decreases with depth.

Yes. This is due to the effect of tillage and soil structure.

Com. 36: p 2257 In 12: How was the pore volume of water drained calculated? The pore volume drained is the amount of water drained divided by the amount of water in the lysimeter. The water content in the lysimeters was not measured and it

changes over time. Therefore, the pore volumes must have been estimated making some assumptions about the water content.

See above.

Com. 37: p 2258: Eq. 5. I think the CCC is not correctly defined in Eq. 5. The squared deviation between the means should be added to (not subtracted from) the variances of the two variables.

Yes. This is a mistake we did in the transcription of the equation (not in the algorithm we used). Thank you for pointing out this mistake.

Com. 38: p 2259: In 19 and following. I think it is necessary to indicate briefly the effect of the compensation factor β on the water balance. I guess that a compensation factor β of 1 leads to more root water uptake than a compensation factor β of 0.

No, it is the other way round. 1 means no compensation, and zero complete compensation. We have clarified this in the paper.

Com. 39: On the other hand, I guess that increasing R_{max} leads to more root water uptake and decreasing it to less root water uptake. Therefore, the same amount of root water uptake (and consequently leachate) may be obtained when R_{max} is decreased and β is increased. Is it possible to disentangle R_{max} and β can not be disentangled from measured leachate without measured depth profiles of water content?

Yes, this may be the case, although we have not tested it. They are probably functionally correlated anyway. We have added a sentence in the article to point out this fact.

Com. 40: p 2260 In 21. I propose defining the anion exclusion factor here since it may be defined in different ways. I am familiar with a definition using a retardation factor that is smaller than 1.

Internally, MACRO defines a "mobile water content", $\theta_{mi(m)}$ that is calculated as $\theta_{mi(m)} = \theta_{mi} - \theta_{ae}$ if $\theta_{ae} < \theta_{mi}$, and $\theta_{mi(m)} = 0$ if $\theta_{ae} \geq \theta_{mi}$. See (Larsbo and Jarvis, 2003) p 29. We have added the definition in the article.

Com. 41: p 2261 In 1: Solute transport parameters were optimized based on the accumulated solute leaching. I propose including here that the parameters were optimized based on the accumulated solute leaching versus the cumulative leaching. Later in the text, it is mentioned that the entire breakthrough was used to calibrate the solute transport parameters.

We don't really understand the point. We have now written 'the best model efficiency on time series of accumulated solute leaching' to make this point clearer (if that was what the reviewer meant?).

Com. 42: p 2263: In the discussion on the calibrated R_{max} and b parameters, I think it should be mentioned that when these parameters are calibrated based on leachate measurements only, their estimates will be (negatively) correlated. Therefore, I am wondering whether the calibrated parameters have a physical meaning.

The parameters have physical meaning, but their correlation may make it difficult to identify their 'true' values. With only 16 samples (lysimeters), it is not surprising that correlations are unclear, so we have chosen not to comment on this in the article. When looking at the results for individual lysimeters, no clear tendency to equifinality could be identified, but with only 5 values tested for R_{max} and 5 for Beta, it is not very clear too.

Com. 43: p 2263: In 16. The excluded water content is expressed as a percentage. But it is not clear of what this percentage is taken? Is it a percentage of the total bulk soil volume (i.e. in line with the definition of a volumetric water content)? Or, is it a percentage of the saturated water content (i.e. in line with the definition of a degree of water saturation)?

See definition above and in the new version of the article.

Com. 44: p2264 In 4-7. It is not clear to me what the authors mean exactly with this sentence. Is the result remarkable because preferential flow also plays a role in soils and weather series for which no preferential flow is expected? Or is the result remarkable because despite the fact that in a number of soils and weather series no important preferential flow was simulated, the effect of preferential flow was nevertheless large when all soils were considered?

The latter. We have made this clearer. We have also replaced the word 'remarkable' by 'worth noting', as the latter is maybe less ambiguous (we did not mean 'exceptional').

Com. 45: p 2270 table 1: I propose including the dates when the tracers were applied. Breakthrough of tracers that are applied in autumn will not be influenced by the parameterisation of the root water uptake whereas breakthrough of tracers that are applied in spring will be more sensitive to root water uptake parameterisation.

Good point. We have done so. The time series presented in the graphs are / were actually starting at the application date. We have now added an arrow and text label on the graphs to make that clear. We have also added the application day on Table S1 of the supplementary materials.

Com. 46: p 2271 table 2: I propose to use besides the original classification of the soil types also a common classification for all different soils that are used.

It would be very relevant, but difficult, as there are no direct translation between USDA soil classification and the WRB. The 'simplest' would be to convert USDA classification into WRB reference, as the latter is simpler, but as none of the co-authors have actually described the soil profiles, it would be too approximate.

Com. 47: Supplementary material: I guess that the simulation results are those from the uncalibrated model? I would be good if this was mentioned.

Yes. We now mention it.

Com. 48: Why aren't also the simulation results of the calibrated models shown? I think it would also be useful to show the cumulated amounts of drainage that are

divided by the lysimeter lengths. This gives an overall impression of the amount of water leached during the experimental period relative to the length of the lysimeters.

We prefer not to do so. But we have added the final amount of water drained on the figures, to give a reference complementing the "pore volume" x-axis.

Com. 49: Supplementary material: In 14-15 water flow and solute transport are switched.

We have corrected this.

Com. 50: Supplementary material In 16: 'modelled water and solute flow have been downscaled ...' I would say that a temporal downscaling results in a higher temporal resolution.

This is a mistake, we meant *up*-scaled, as the temporal resolution of measured percolation is at a coarser resolution than the simulated one. We have corrected this.

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