

Responses to Referee Review 2

We thank the referee reviewer Prof. Dr. Erwin Zehe for his comprehensive and insightful comments. Our responses to the reviewers' comments are given below. The original comments from referee reviewer 1 were marked with blue color, and our response in black.

Summary:

The proposed study explores controls on residence and travel time distributions in a forward coupled model exercise, using a coupled version of the mHm and OpenGeoSys models. Study area is the Naegelstaedt catchment in Germany. The authors explore 8 different recharge scenarios from the mHm which serve as input to the ground water model and which are marked by tracer to tag the path and the age recharge water when it travels through the aquifer to the stream. To this end they generate several realizations of random hydraulic conductivity fields which are constrained to fit a set of distributed head data. The authors compare their simulated travel time distributions to an exponential travel time distribution which is based on an analytical solution, which reveals stronger skewness in the simulated ones. The author do furthermore quantify the uncertainty in average travel time, shed light on the fraction of active to total storage and discuss the age selection of the catchment.

Evaluation: The proposed study has a high scientific significance and I very much like the general approach. Nevertheless, it is in the present form not acceptable, because quite a few important points need further clarification and the presentation quality is up to the standard of HESS.

Response: Thank you very much for your overall assessment to our manuscript as well as for your insightful suggestions. We have revised the manuscript carefully following your suggestions. A revised manuscript will be uploaded soon.

Major points:

- Eq. 9 (the master equation) assumes that storage components of an age $\tau < T$ are well mixed. I wonder whether this can be assumed for the selected random fields. This depends strongly on the correlation lengths and the total extent of the domain and maybe even more on the question whether preferential flow paths are present here?

Response: Thank you for the comments. Eq. 9 (the master equation) is the fundamental formula for connecting conservation of mass and water age. In general, it does not rely on any presumed mixing hypothesis (Botter et al. 2011). Nevertheless, we agree with the reviewer that the well-mixed assumption needs to be made to derive the analytical solution.

We agree with the reviewer that the random K_s fields used in this study do not guarantee a well-mixed storage. Actually, our study is designed to investigate that in a real-world catchment, how skewed is the shape of the simulated TTD compared to the well-mixed TTD, and how the waters particles with different ages are discharged into streams.

The well-mixed assumption is valid when the aquifer is homogeneous, and the drop in the water table between the maximum and minimum head is small compared with the aquifer total depth. Otherwise, the SAS function can deviate from the well-mixed scheme and take on complex shapes even in the saturated region of a homogeneous aquifer depending on the bed form (Van Der Velde et al. 2012).

Are they present? And what is the correlation length of the generated random fields, and the nugget to sill ratios? How did you assess this information and did you vary them between the realizations? Or this is uncorrelated noise?

Response: This is a misunderstanding in the K_s fields. We apologize for the unclear description of the random fields in the original manuscript. We would like to elaborate more on the hydraulic conductivity (K_s) fields used in this study. The K_s fields are not based on geostatistical interpolation. They are based on zonation, whereby parameter values are assigned as piecewise constant values to defined areas (zones) in the model domain (Anderson P. 2002). Spatial changes in parameter values occur only among zones. Delineation of zones relies on information contained in the hydrogeological investigation that identifies areas where parameters are likely to be the same. The geometric mean of expected values of a given parameter within the zone is assigned to the zone if heterogeneity is thought to be random, which means the variance and correlation length are not included in this approach (Anderson P. 2002). This zoned aquifer system indicates that water particles can go through more-permeable zones (i.e. layers with high K_s values) more easily than low-permeable zones, thus forming preferential flow pathways in more-permeable layers. To avoid this misunderstanding, we revised the manuscript accordingly. Please check out the revised manuscript.

On the basis of the points stated above, the random fields do not follow the well-mixed assumption. Alternatively speaking, the well-mixed scheme is a baseline scenario for quantifying the transport dynamics in a complex real-world catchment. The influence of spatial variability of input forcings in the systematic preference for waters with different ages is also investigated in this study, which has not been investigated in a real-world catchment before based on our knowledge.

- There might be a conceptual problem, depending on what your particles shall actually represent. In case the particles shall mark the travel path of water (not of a solute) I think they should move in a purely advective manner, which means that eq. 6-8 need to be different. There is not diffusive mixing among water molecules (as long as we neglect different isotopic compositions). Or do they mark the fraction of different water

isotopes, than this should be stated? But in this case I wonder where the dispersivity does stem from? Other tracers?

Response: Thank you again for this comment. We fully agree with the reviewer that in the case that particle tracer represents the water rather than the solute, the dispersion process should be ignored. The random walk particle tracking algorithm is capable to deal with reactive transport problems. Therefore in the original manuscript, Eq. 6-8 are written in their full form to incorporate both diffusion and advection processes, but we only consider the advection process in this study. Actually, we clarified this point already in the original manuscript: *“In this study, we focus on the predictive uncertainty within the convection process. Therefore, the molecular diffusion coefficients are universally set to 0 for all ensemble simulations.”* (Page 11, Line 5-7 in the original manuscript).

The particle tracking scheme used in this study is capable to simulate both diffusion and advection processes, therefore Eq. 6-8 were written in a complete form to incorporate both processes. The velocity component in these three equations, namely V_x , V_y , and V_z , are essentially different.

We revised the manuscript according to the reviewer’s comments. In the revised manuscript, these equations were moved to the appendix in order to make the structure clear and avoid misunderstanding.

- The recharge amount, the generated parameter fields and base-flow production are not independent. I see that the k_s parameter field is adjusted such that the generated parameter sets match the head data (which is by the way not so difficult). But to have a consistent model the simulated base-flow production from OpenGeoSys needs to match the simulated base-flow of the mHM (which is calibrated to stream flow). A consistent match of both the head and the base-flow is crucial for credibility of the model structure and it’s ability to simulate travel time distributions for the selected system.

Response: Thank you again for this important observation. We completely agree with the reviewer that the recharge, the generated parameter fields and the baseflow production are not independent. As the reviewer pointed out, both baseflow and groundwater heads should be matched to close the water budget and achieve realistic parameter values. This is also what we did in this study. Because for the steady-state system, the total amount of inflow (i.e. groundwater recharge) equals to the total amount of outflow (baseflow in this case) for the OGS groundwater model. Given that the recharge is directly taken from mHM, the baseflow is also consistent with the one estimated by mHM. The water budget is naturally closed. We addressed and discussed in more detail in our previous study (Jing et al. 2018).

Following the reviewer’s advice, we also clarified this point in the revised manuscript: *“For the steady-state system and the one-way coupled model, outflow from aquifer to the streams (i.e. baseflow) proves to be consistent with the baseflow originally estimated*

by mHM, implying that the water budget in the subsurface system is essentially closed (Jing et al. 2018)."

We also agree with the reviewer that the K_s fields also have an impact on the recharge. We admit this influence was not considered in this study, because the one-way coupled model is not capable to include such a two-way interaction. We fully acknowledge this limitation in our previous paper, where we also discuss some of its ramifications (Jing et al. 2018).

Technical details

- The control for contamination is in fact the Damkohler number, which relates residence times and degradation time scales.

Response: We fully agree that the Damkohler number is the relevant scaling number for reactive transport processes. However, in this study, we deal with water flow only. As a result, we do not consider it to be necessary to include this number in our discussion.

- Eq. 9: $P_Q(T,t)$ is a exceedance probability (otherwise this does not make sense).

Response: Agreed. $P_Q(T,t)$ is the exceedance probability.

- Eq. 9 What is Q_j and what is N - the number of different "outlets"?

Response: Exactly. Q_j is the j -th outflux, and N is the total number of outfluxes.

- I have problems with the terminology of a "StorAge selection" function (even if it is established), as the stream doesn't do an active select water of different ages.

Response: As this term has been widely used by many other researchers, we simply apply the same name with them. Maybe this terminology is tricky, it is beyond our capability to judge whether this name is reasonable or not.

- Preferential flow does not necessarily mean that Peclet number is large, if the flow is still in the near field and mixing among the flow paths is small. There is literature evidence for this.

Response: Agreed. We also found out that this statement is not directly relevant to the main idea of this paper, so we deleted this sentence in the revised manuscript.

- Eq. 6 - 8: Z is a Gaussian random number, otherwise the coefficient in below the root is $1/6$.

Response: Agreed. We changed it as proposed.

- Parts of the section 4.1 should be shifted into the methods section!

Response: Thank you for this observation. We changed it as proposed.

- Page 14: Figure 5 is a scatter plot of heads (simulated and observed) not of the head residuals.

Response: Changed as proposed.

- Page 6 line 5: Repetitive statement on the TTD of the soil?

Response: We deleted the repetitive statement as proposed by the reviewer.

- Not sure what is meant with "backward travel time distribution"?

Response: The backward travel time distribution complies with the problem of how a sample of water taken at a time t is the result of transport processes that involve inputs generated from all previous times (Benettin, Rinaldo, et al. 2015).

TTDs can be interpreted in two different ways, depending on whether they track ages forward or backward in time. In "forward" tracking, one selects a given particle injection at a fixed time t_i and follows the subsequent exit times. In "backward" tracking, instead, one focuses on a given exit time t_{ex} , considers the particles that leave the system at t_{ex} and then tracks their various entrance times backward in time (Benettin, Kirchner, et al. 2015). In this study, we only use backward distributions.

- Page 8 line 20: how are they interpolated?

Response: We use a bilinear interpolation approach. Following the reviewer's suggestion, we modified the manuscript as follows: *"The gridded recharges estimated by mHM are interpolated and then assigned to each grid nodes on the upper surface of OGS mesh using a bilinear interpolation approach."*

- Figure 1: Caption is not self-explaining: what is mo, mu, mm etc?

Table 1: Please explain km and ku.

Response: Thank you again for this observation. Mo, mu, and mm stand for three geological zones -- Upper Muschelkalk, Middle Muschelkalk, and Lower Muschelkalk, respectively. Km and ku stand for the Middle Keuper and Lower Keuper. We added the full name of these geological zones into the Figure 1 and Table 1 as you suggested.

-What is the estimation variance of the mean you calculated (based on the standard deviation and the sample size), might be nice to add this to Figure 8.

Response: Thank you for this suggestion. Following this suggestion, we added the variance of the mean travel time (MTT) into the Figure 8 b). Please check it out in the updated manuscript.

- I think the paper would greatly benefit from a thorough proof reading.

Response: We did a thorough proofreading already together with a native speaker. Please check out the revised manuscript, which will be uploaded soon to HESS.

References:

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