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Interactive comment on "Tracer test modeling for local scale residence time distribution characterization in an artificial recharge site" *by* C. Valhondo et al.

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Comments on "Tracer test modeling for local scale residence time distribution characterization in an artificial recharge site" submitted to HESS by Valhondo et al.

The manuscript features investigations on a tracer test in an artificial recharge site by utilizing a simulation approach. Different implementations of the study area are realized with homogeneous and heterogeneous hydrogeological setups. The motivation is to understand the relevance to implement different (heterogeneous) layers in order to represent correct flow and mixing behaviour of juvenile and upstream recharge waters to evaluate the performance of AR for contaminant removal. A key factor for this is the residence time distribution which was measured in a field campaign by break-

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through curves of a tracer test. The submitted manuscript is structured in a logical way, giving a comprehensive introduction and motivation, before presenting materials and methods, showing and discussing results, and finally, drawing some short conclusions. The work is of high quality, written in a clear and understandable way, while some figures and tables support the text, and relevant references are cited appropriately. The authors manage to resemble the measurements with the model software remarkably well, albeit the relatively complex study area. By comparing results from homogeneous and heterogeneous setups, conclusions clearly show deficits of a homogeneous setup. Yet, still some questions remain open for further investigation (e.g. uniqueness of two calibrated heterogeneous setups). Already with these two aspects, I think that the manuscript is of high relevance for current research. Nevertheless, the manuscript also can be improved, especially in the following major points: a) The description and motivation of the used "tracers" (amino-G, TCE, EC) should be given in a clearer way for the reader to understand which is used for what purpose. This may be done by giving a short overview in the beginning of the methods section. b) The information given on the modeling tool are too scarce. A very short description on the type of the tool, and its features should help to understand the decision to use this tool. Furthermore, the description on the modeling strategy, and the implementation of the model (model setup) could need some more structuring (clear description of all boundary conditions, section 2.3, and full list of calibrated parameters). Also, information on the calibration strategy should be provided. c) Finally, I would like to encourage the authors to state a more profound argumentation why they set up the heterogenous models in the way they did. For example, why were 9 layers chosen and not 5, 15, or 40? I think that this can aid to support their conclusions, ie. to highlight relevance of a layered model structure in the study area.

With these general comments, I enclosed a list of more specific ones. If the authors decide to reply to these comments, I would be available for a second revision, if the authors think that my comments gave a valuable input.

I think, that this manuscript is already of high quality and tackles an important topic. I, therefore, suggest to consider the submission for publication after revision.

Abstract: Page 2, Line 8: You say that you used the numerical model to "...extend characterization to other flow conditions...", but I could not find any scenario simulations that are different from the observation times in the manuscript. Could you please rephrase this?

Page 3, Line 24: You write "Characterizing heterogeneity in such systems at the recharge basin scale is required for proper representation of RTDs. But it is hard because the head differences are small and detailed hydraulic testing difficult to perform." - While the mentioned issues are problematic indeed (ie. difficulties with small head differences, and to get detailed information of hydraulic properties), I would also add, that measuring hydraulic properties and the distribution of the heterogeneity (micro and makro scale) is unfeasible, as you would never be able to cover the whole basin in the full resolution.

P4, L7: "The objective of this paper is to describe the tracer test and its interpretation using both heterogeneous and homogeneous models to assess the need for model complexity." - The objective of paper you describe here is somewhat different from the one you give in the title: here, it sounds as if you wanted to evaluate the necessity of complexity in a numerical model, while the title leads to the intention that you want to model RTD in an AR site. Can you please synchronize these locations (ie. add the missing part in the text or rephrase the title)?

Figure 1: * (C) - Can you please add the location of the cross-section in (A) and/or (B)? - I do not understand what the blue arrows indicate - can you please explain these? - What are "thick" and "fine" sediments? - Can you please add a legend to the statigraphic log (or add the description of the layers right next to it)?

P6, L2: You write that "The Llobregat River was disconnected from the aquifer...", but the arrow in fig 1B shows a groundwater flow direction parallel to the river; can you

please explain how you came to the conclusion of a disconnected river?

P6, L3: A question out of curiosity on the operation of the AR: what is the reason to divert the river water firstly to a "settlement basin" - is this due to high turbidity of the river water? Can you please provide an estimate of the volume of the basins (you only give an area here)?

P6, L5: How was the flow rate measured?

P7, L6: By writing "depths of 7 m" etc, you mean "meter below ground surface" or "meter below groundwater level"?

P7, L7: Can you please tell in which layers or depth the piezometers P2, 5, 9, and 10 are filtered?

P7, L12: Can you please add the location of the addition CTD-diver to the map (fig 1)?

I like the detailed description of the measuring campaign; this provides a solid information for the interpretation of the results!

Seciont 2.3.1 needs to be clearer. In the first paragraph, it is not obvious, which combination of boundary conditions you used to acquire information for the local domain BCs, and which type of BCs you implemented. Eg: P8, L23: You describe that you added inflow from "eastern and western local creeks". - I cannot find them in figure 1; can you please consider adding them in figure 1 for a better overview? - I assume, you used a Neumann-type boundary condition for implementing the creeks (as you write "inflow"). What type of BC did you use in the regional model? Did you also include the abstraction of the drinking water wells in the regional model to get the values for the creeks' inflow? - Why did you model the eastern part from the Llobregat river? Is this part of the domain relevant for the western model domain?

Why did you choose a triangular local model area? Wouldn't an area that is limited on the lateral sides by flow paths that provide a no-flow boundary be a better solution?

P9, L4: Add comma in "(local domain ≈0.5 x 1.5 km2, yellow triangle in Figure 1 A),"

Section 2.3.2 is a little confusing: I expected that you talk about the model setup of the local scale model (yellow triangle in fig 1), as you motivated the setup of this smaller model from an existing regional scale model in 2.3. Section 2.3.1 then gives BCs etc for the small scale model, as 2.3.3 give more details on it. In between, section 2.3.2 feels a little lost. Maybe, the information you provide there (hydraulic parameters, head data), could be given before 2.3.1? Besides this, the heading of 2.3.2 does only suspect info on the large scale model, while there is actually also some info on the local domain.

P9, L8: You say that there is a strong local heterogeneity (layering due to fluvial deposition). Can you please motivate your decision to use exactly 9 layers? How many hydrogeological layers can you find in the domain? Do these 9 model layers represent major (important) hydrogeological layers at the site? What would happen, if you used 100 layers (ie. using more than one grid layer per hydrogeol. layer)? Can these 9 layers represent vertical distribution of a tracer within one hydrogeol. layer?

P9, L8: You write, that the nine layers "overlapped in the local domain". Do you mean vertically overlapping of the elements (ie. you get prism elements) or elements overlapping in the way of "being at the same location"?

P9, L9: You state, that you "linked" the layers "by one-dimensional elements". - What is the motivation to do so? Are the layers you introduced in the 3d part of the model domain disconnected initially? Do these linking elements exist for the communication of the layers? - Did you link at nodes or elements? - How many 1d elements did you use to link two layer's nodes/elements (only one line)?

P9, L10: You describe, that you introduced two top layers (8 & 9) for the reactive barrier. Assuming, that the preferential flow direction is vertical, and considering that you use linear elements for vertical exchange, why is it necessary to use a second layer for this feature - wouldn't one be enough? Besides that, can you say, that this top reactive barrier layer is having homogeneous properties in horizontal extent? Could it be clogged

preferably at the inflow zone due to stronger biological activity and availability of nutrients? (Later, you also distribute the tracer along the infiltration bed, based on a similar assumption.) What would be the influence of such reactive barrier heterogeneity on the distribution of the infiltrating water/tracer?

P9, L15: I do not understand, why you used the TCA for validation - I thought that you wanted to use the amino-G tracer for this? How did you probe for and measure TCA? Some TCA information is partly given in 2.4, but at this section it is not clear to me, why TCA is used. Maybe, you can write a short overview-like, introductory information on the intended usage of TCA and amino-G in 2.3 (or even 2.2)?

P9, L17: What is "Transdens"? A modeling tool? Can you please give a little more information on this?

P10, L9: "...whole basin water volume, as a consequence the maximum..." - I suggest to divide this sentence (and add a comma): "...whole basin water volume. As a consequence, the maximum..."

P10, L6 - L15: The reason to divide the basin into nine zones was hard to understand in the first place, as you state some results where the reader expects the model setup (which it indeed still is). Yet, there are some questions: What is the "amino-G acid concentration function"? Is this the concentration you measured at P8.3 (probably not)? Or is it defined through the input of amino-G at point A? How did you measure this function? Also, it is unclear to me, how you defined the different zones i-ix and on what basis you set values for the distribution parameters within the zones? Can you plot or state the distribution parameters in a table?

P10, L16: I don't think it is important to state that "time discretization was quite irregular". It is common to have a variable time stepping in a numerical model. The relevant questions for time step sizes would be, how you defined the different time step sizes (usually based on the error of an iteration, but here probably defined through the measurement time steps?), and whether large time steps still yield valid Courant numbers

(if applicable for your model).

P10, L21: Ly = Layer? Why didn't you distribute the inflow also on Layer 8? Did you distribute the inflow equally or weighted?

P10, L22: "The standard deviation assigned to all concentration measurements at each observation point was 1% of the maximum concentration at each point, which was to ensure that a comparable weight was given to each point during calibration (maximum concentration varied 25 by ≈2 orders of magnitude)" - I think this is an unfortunate decision. With this assumption, if an observation point has a low concentration, it must show a much more accurate measurement than a high concentration point. Thus, the points would be biased and low concentration points would be forced to perform much better. Wouldn't it have been better to use the standard deviations from the calibration/regression line of the fluoresence meters?

P11, L1: "...two different convergence points of the calibration process..." - Where there more than those two convergence points? - You say, that you defined two heterogeneous property distributions from the calibration. Could it also be, that the conceptual model has a fault, if the calibration does not produce a unique result? Did you consider other setups?

P11, 2.4 Validation: - At this point of the manuscript, I do not understand, how you use TCA and EC data for validation. Do you try to calibrate porosity, dispersivity, retention or decay coefficients? Why do you need two parameters for this? Maybe, you can give a short, comprised overview of what tracers you use for what purpose in the introduction? - Because of the first point here, it is also hard to understand the usage of the boundary conditions: + Why do you set TCA to the maximum value but EC to the mean? + Why do you use measured EC time series as the recharge BC? + What are the "lateral inflows"? Can you show that in fig 1? + Did you simulate decay of the TCA? + I am sorry, but I do not understand this sentence: "TCA and EC concentrations in the northern border of the local domain were prescribed based on the TCA and EC

measured at P1 and adjusted for the travel time from the northern border to P1."

Figure 2: - Time unit of head series is probably not days (looks like months with years as axis).

P13, L2: "...surface (Fig. 2). Figure2 displays..." - Please add a space in Figure2. - I think, you should also decide on using either "Fig." or "Figure".

P13, L2: "...piezometers located around local domain." - I think, it was better to write something like "...piezometers located around the local domain.", or even "...piezometers located within the local domain."

P13, L3: "The fit was good,..." - Can you please give a quantitative measure (regression coefficient, RMSE, Nash-Sutcliff or similar)?

P13, L4: "The fit was good, which suggests that the size of the multilayer local domain was sufficient to reproduce head variations at the monitoring piezometers close to the basin where the gradient is mainly vertical ($\approx$ 10%)." - Before, you said, that you produced three model variations; which one is used here to show fig 2? I would also argue, that if you have more than one unique solution (if the amount of measured data is enough), a good fit does not necessarily mean a sufficient model setup. - A gradient of 10% is a large value (10 cm head difference in 1 m, understandably for the AR), but not "mainly vertical". I suggest to rephrase this sentence to highlight the influence of the AR on the head distribution. - After reading explanations on fig 3, I undertand, that you are referring to the vertical gradient itself. Please clarify this.

P14, L2: "Conservative transport parameters were estimated for the nine layers of the local and basin domains using the tracer test data." - I would say, that this sentence should be given somewhere in 2.2 or 2.3, as it is more related to methodology than results. - Which "tracer test data" do you mean - TCA, EC or amino-G? - You never give a full list of transport parameters, please add this.

Table 1: - What is the thickness of the layers? Can you add this to the table? Then, you

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could also easily compare and evaluate the results to the hydrogeological and gamma logs you give before. - Layer 5 shows a hydraulic conductivity of ∼1000 m/d, which is ∼1e-2 m/s, a relatively high value - can you justify this (and the other values) from the hydrogeology? I cannot evaluate it, as you do not give exact information on the sediments (apart from being fluviatile). - Values for the reactive barrier seem relatively high, while I would expect them to be lower due to the finer material, clogging etc. Can you please explain this? - Also, in the reactive barrier layers, vertical conductivity is higher than horizontal - why? - Why are vertical porosity values so extremely low? Can you give an explanation within a physical meaning for such small values? - Do I understand it correctly, Layers 9 and 8 are only present at the infiltration basin? If yes, what happens to the vertical elements of Layer 7 where there is no layer above? - What is the meaning of the RMSWE values for hydraulic conductivity? I know, how to get RMS(W)E for hydraulic head or concentrations (or whatever primary variable you calculate) but not for a model parameter, if you do not have otherwise measured reference values. Can you please explain this, together with how you weighted the values? - Where is the "input mass in outcomes Het-1, Het-2, and Hom, after calibration"?

Figure 3: - Why does the tracer arrive earlier at P10 than P9, although the first lies behind the latter? I would expect the opposite. (You mention that in P19, L26ff, but do not explain the reason or state a possible explanation.) - It is hard to compare the breakthrough curves, as I could not find information on the filtered area of P2-P10. Please add this information. - Can you explain the unusual tailing of the measurements in P5? - Did you consider effects from double porosity to explain the long tailing of P8.1 and P9?

Figure 4: - The grey areas, should most likely show concentrations of ∼0 mg/l, but the legend does not show a grey value. I guess that this is due to lighting settings in Paraview (looks as if you were using this software to produce the figures). Can you please check this?

Figure 5: - From which year is the data you show here? - The legend says "Homo", in

the text you defined "Hom" to be the homogeneous case.

P20, L4: "...because the aquifer transmissivity in the local domain was ultimately the same." - I do not understand this; I thought, that your model had the same setup (i.e. layers have same size); now, if you use different hydr. conductivities, you should end up with different transmissivities. Can you please explain this (I am probably misunderstanding this)?

Questions on the model: - Do you define layer thickness through transmissivity of the layers? - What happens, when a solute in a top layer reaches the boundary of the local domain? Is it moving thÅŢough the outermost vertical elements to the lower layer? Does this vertical travel increase spreading of the plume? - Can you please provide a full list of parameters (eg dispersivity, diffusion coefficients...)?

Generell questions: - What is the distance to the groundwater table? I am asking to understand whether it would be important to include the passage through the unsaturated zone. - What was your calibration strategy? Did you conduct a manual or automatic calibration? Which parameters did you use for calibration (TCE, EC, amino-G, heads) and what was the target function (RMSE)? This is important to know in order to evaluate, for example, whether there could actually be more than two fitting calibrations (currently het-1 & het-2), and whether the current conceptual setup may be the reason for non-uniqueness. - The heterogeneous setup clearly shows a better performance (at least for the amino-G tracer). To what extent, do you think, should this heterogeneity be reproduced in the model? Would you think that 3 or 300 layers showed similar results? How could one determine the necessary degree of heterogeneity (or the "sensitivity" of heterogeneity)?

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