Interactive comment on "Caffeine vs Carbamazepine as indicators for wastewater pollution in a karst aquifer" *by* Noam Zach Dvory et al.

Anonymous Referee #2

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In its current form I would recommend publication with minor corrections.

The authors studied transport dynamics of two tracers, carbamazepine CBZ and caffeine CAF, using a dual-continuum saturated/unsaturated flow and transport model including a coupled 1D model to simulate the vadose zone. The topic can be considered highly challenging, both from a conceptual point of view and the difficulties associated with the highly contrasting continua. The authors demonstrate the limitation and benefits of each substance. While CBZ due to its conservative nature can be used to delineate the extent of contamination it is affected by background concentrations. CAF on the other hand is affected by degradation but can be employed to identify short-term

contamination events. The paper is short but concise. In addition to the results from the Water Research paper the authors have addressed the transport of caffeine and compare it to the transport of carbamazepine and associated processes. Some of my comments target the specifics of the signal transformation, and if the authors address them, I believe the paper will stand out more compared to the WR paper.

I agree with the comments of the editor that the paper in parts resembles the paper published in Water Resources. Both manuscripts use the same (in most aspects) underlying flow and transport model and in that sense it is understandable that the authors use the model for various application cases (here most of the model description is omitted and the respective paper is cited for reference).

Figures 1,2 and 3b are taken from the previous manuscript with no or very little modification. In addition to the overlap as indicated by the editor this should be fixed (Figure 1 is probably the most critical one and should be slightly modified, also to avoid any copyright issues).

Content-related comments:

1. (p6): For the sake of completeness please add units to the description of the equations.

2. (p5): The section "Numerical model" would greatly benefit from a conceptual sketch of the model framework (the Water Research paper provides a conceptual model of the hydrogeological system only). The model is quite complex and as the authors have already limited the model description here. A conceptual sketch would also allow readers to understand more aspects of the model without first having to read another paper. This would also help to make the paper stand out slightly more compared to the WR paper.

3. (p5, line 28): From the description here it is not entirely clear to me if both the 1D and 3D part of the domain are subject to a multi-continuum coupling. In this sense also the terms high and low permeable region are (from a conceptual point of view) associated with different compartments of the aquifer. High permeable regions in the vadose zone are possibly (enlarged) fractures and to a limited degree former conduit systems depending on the longterm evolution of the system, while in the 3D part the high permeable regions are commonly the conduits. This should be clarified, possibly also in conjunction with my previous comment to add a conceptual sketch.

4. (p6): In addition to the conceptual sketch I think a figure showing the discretized model domain including boundary conditions (both for the large and small model) would be adequate to be added to the section "Mathematical model setup".

5. (p7, line 15-19): To what extent does the vadose zone possibly affect the (bulk) dispersivity? The chosen approach is common for saturated systems but may be affected by the vadose zone which imposes an additional transformation/dispersion of the signal. I understand that this is a very difficult topic and would only ask for a brief comment if this might be the case (or not if the authors can clearly rule this out). In this context the authors mention that CBZ is stored in the vadose zone (on page 14, line 11), hence I would expect an influence.

6. (p12): Are the parameters λ and K_d defined for both the 3D section and the 1D vadose zone? This information should be added. Please also see my comment 3.

   Is the degradation of caffeine affected by the presence of an airphase? If this is the case then this should be briefly discussed either here or in the discussion section.

7. (p13, Fig 4): I am a bit confused by both sensitivity analyses but may have missed some information in the manuscript. I would expect an opposite behavior for

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λ as well as K_d. I would expect lower peaks (and low tailing, i.e. generally a decline in mass) for higher values of degradation. The same applies for the distribution coefficient (which to my knowledge is commonly defined as activity of solid/aqueous phase). Here I would expect lower peaks for higher values of Kd as CAF tends to be in an sorped state.

In Figure 4a it is difficult to see where the peak of parameter combination 6 is (only the tailing is clearly visible). A different color (gray or colored) for the fitted values (both in A/B) could help to enhance visual clarity.

8. (p14, line 5): Is this correct? I would expect low background concentrations to be beneficial for the detection of a new signal.

Typographic corrections:

I am not a native speaker and can only partially comment on proper grammar. The following are mostly typographic corrections and recommendations to enhance the comprehensibility.

1. (p3, line 6): Maybe rephrase. Do the authors mean that Sorek creek watershed accounts for 88km^2 within the study area or that the Sorek creek study area is 88km^2 in size?

2. (p3, line 19, 20): This may be journal-specific but commonly only numbers exceeding 12 are spelled out.

3. (p6-7, line 28/1): I assume the authors mean main memory not the CPU cache. Possibly rephrase as "owing to a lack of main memory".

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4. (p7, line 4): Is the grid becoming finer towards the top or the bottom of the domain? Possibly rephrase to clarify.

5. (p12, line 11): "...assigning $\lambda = 0$ in the matrix,..."

6. (p13, Fig. 4): Please match the font/fontsize of the insets in A and B (lambda and Kd values)

7. (p14, line 23): "A quasi 3D dual permeability..."

8. (p14, line 25): I think it should be "calibration with monitoring data..."