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Interactive comment on "New Model of Reactive Transport in Single-Well Injection-Withdrawal Test with Aquitard Effect" *by* Quanrong Wang et al.

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General comments 1. The present work presents a novel analytical treatment of single-well injection withdrawal (SWIW) tests, whereas the impact of mixing in the well and the presence of confining aquitards are considered. I applaud the Authors for the efforts in the derivation of the solution (math not checked) and the commitment to introduce more flexibility in the conceptual model. Yet, I am not sure about its usefulness to other researchers, it is very complicated! Maybe, if the Authors made available a script for the calibration against data it could be beneficial to the usage among practitioners. Regarding the quality of the paper, I see many unclear points or unclear parts. I listed below a series of comments which I hope will make the paper more clear. Moreover, I have some criticisms about the employed sensitivity analysis, which it seems to be

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Discussion paper

a weak one in my personal opinion. Reply: Thanks. We have carefully revised the manuscript after considering all the comments.

Specific comments 1. line 15: why put emphasis on the use of Green' function for the extraction phase in the abstract? This leads to think 'what about the other phases?'. I would remove this comment. Reply: Implemented. We have removed it. See Line 14.

2. line 17: I would replace 'tested by' with 'tested against results grounded on numerical simulations', or something similar, i.e., the numerical simulations results serve as reference values to be matched and do not verify the validity of the assumptions directly. Reply: Implemented. "tested by a numerical solution" has been changed into "against results grounded on numerical simulations". See Lines 18-19.

3. lines 17-19 'The sensitivity analysis demonstrates that the influence of vertical flow velocity and porosity in the aquitards, and radial dispersion of the aquifer is more sensitive to the SWIW test than other parameters.'. Which sensitivity analysis? The fact that the latter has been conducted is not specify earlier in the text. Moreover, specify which kind of sensitivity analysis you are using. Furthermore, the sentence is rather confusing: it says that the influence of three-parameter is more sensitive to the SWIW test, than other. What is the difference between influence and sensitivity? Is it the influence that varies as a function of the SWIW test? . . . I was thinking that are the results of the SWIW (i.e., model output) to be largely sensitive (i.e., influenced by) to the three mentioned parameters (i.e., model inputs), but maybe I am biased by my previous experiences with sensitivity analysis. Please clarify. Reply: Implemented. See Lines 19-20.

4. line 23 'The new model of this study performs better than previous studies excluding the aquitard effect for interpreting data of the field SWIW test' too general. Please specify which field test you are referring to, since the quality of the novel solution can be worse than previous ones in case the system do not have an aquitard, for example. Reply: Implemented. See Lines 24-25, and Lines 277-283.

5. lines 49-50 ‘Another assumption included in many previous models of radial dispersion is that the concentration of the mixing water with the injected tracer is equal to the injected tracer concentration during the injection phase’ the sentence is not very clear. What is the mixing water? ‘is equal to the injected tracer concentration’ of what? Please revise the sentence. Moreover, lines 53-55 ‘This assumption implies that the mixing effect in the wellbore is not considered, where the mixing effect refers to the mixture between the original (or native) water and the injected tracer in the well.’ ow there is the native water which is not mentioned earlier. . . . I can grasp the general idea that there is a difference between the concentration of tracer between the resident water, injected water and water within the well where mixing occurs, but not in a standalone manner from these lines (i.e., I need to think about them and deduce that this the implied message). Please clarify, maybe with an additional figure. Reply: Implemented. See Lines 51-62.

6. line 61 ‘mostly because ADE could not adequately interpret anomalous reactive transport,’ this true when the ADE is used to capture the whole behavior of the system, i.e., as an effective model for all the system behavior to be characterized by a single representative value of advection, dispersion and reaction. Instead, if ADE is finely discretized (i.e., the system heterogeneity is properly detailed) and then (numerically) solved it can fairly well capture anomalous behaviors. Please clarify this point. This is in line with the mentioned superior capacity of effective transport models mentioned afterward (e.g., MMT,CTRW, fADE, MIM) to have a superior capacity in rendering anomalous behaviors of heterogeneous system when viewed as a whole (e.g., spatially integrated BTCs). Reply: Implemented. See Lines 63-79.

7. line 74 ‘anonymous’ I suppose anomalous. Reply: Implemented. “anonymous” has been changed into “anomalous”. See Line 76.

8. line 86 ‘Some examples of weak heterogeneity include the Borden Site of Canada (Sudicky, 1988)’ this is just one example, either add others or modify the sentence. Reply: Implemented. The Borden Site of Canada (Sudicky, 1988) is one example of

weak aquifer heterogeneity. See Lines 104-105.

9. lines 89-96 'Second, for moderate or even strong heterogeneous media such as Cape Code site (Hess, 1989) or MADE site (Bohling et al., 2012), the analytical model developed under the homogeneity assumption is also valuable, but in a statistical sense, as long as the media heterogeneity can be regarded as spatially stationary, meaning that the statistical structure of the media heterogeneity does not vary in space. In this setting, the analytical model developed under the homogeneity assumption is used to describe the (ensemble) average characteristics of an ensemble of heterogeneous media which are statistically identical but individually different. In another word, such an analytical model will provide a statistically average description of many realizations (an ensemble) which are similar to the heterogeneous media of concern, but it cannot provide an exact description for the particular heterogeneous media under investigation' .. . . this made me think that the validation strategy based on the direct numerical simulations is not valid: those simulations are considering directly an homogenous media (with deterministic properties) and NOT the statistical average of the SWIW results across a set of Monte Carlo realizations of the conductivity fields, characterized by either small, middle or large variance. Please clarify this point. Reply: Implemented. See Lines 95-99. The description of 'Second, for moderate or even strong heterogeneous. . ." in the original manuscript has been deleted. Such assumptions might be oversimplified for cases in reality, while they are inevitable for the derivation of the analytical solution, especially for the aquifer homogeneity. For a heterogeneity aquifer, the solution presented here may be regarded as an ensemble-averaged approximation if the heterogeneity is spatially stationary. If the heterogeneity is spatially non-stationary, then one can apply non-stationary stochastic approach and/or Monte Carlo simulations to deal with the issue, which is out of the scope of this investigation.

10. line 99 'A schematic diagram of the model investigated by this study is similar to Figure 1 of Wang and Zhan (2013)' please add this figure and incorporate what mentioned above in comment 5. Reply: Implemented. A new figure has been added,

See Figure 1.

11. Eq.s (1)-(3) I didn't quite understand the + notation: I would say that the fact that the velocity component is pointing towards the well or in the opposite direction is in the value of (for example) va considering (1), similar for the others velocity components in (2) and (3). I would say that the value of va (and others advective velocities) varies as a function of the SWIW phase. If not va should be the module of the advective component, no? Maybe I am wrong. Reply: Implemented. Eqs. (1) - (3) have been revised.

12. Eq. (12a) what's C0? (12d) there is a without subscript, what's that? Reply: Implemented. See Lines 159-161. ξ=2πr_w θ_m 2B, (12d) where h_(w,inj) is the wellbore water depth [L] in the injection phase, C_0 is concentration [ML-3] of prepared tracer.

13. Eq.s (8)-(11) Highlight that in the imposition of the continuity of flux across the well and the formation only the mobile fractions are considered, for who are not familiar with the MIM model? Reply: Implemented. See Lines 152-154. Eqs. (8) - (11) indicate that the flux continuity across the interface between well and the formation is only considered for the mobile continuum (or mobile domain).

14. 'For instance, if the characteristic length of SWIW test is l and the aquifer hydraulic diffusivity is D=Ka/Sa, where Ka are Sa are the radial hydraulic conductivity and specific storage, then the typical characteristic time of unsteady state flow is around tc = lËĘ2/2D. For instance, for a typical lc=10 m, Ka=10 m/day and Sa=10-5 (m-1) (which are representative of an aquifer consisting of medium sands), the value of tc is found to be 5x10ËĘ-5 day.' How do the authors determine the characteristic length lc? In my experience this length is typically a function of the aquifer diffusivity, e.g., for tidal fluctuations is idealized coastal aquifer (e.g., homogeneous, infinite lateral extension) there is a proportionality of the kind lc = sqrt(K/S) (see e.g., Guarracino et al., 2012). Moreover, the proposed estimate of 10 m disagree with the results presented in fig-

ures 2-3 where the solute travels up to 100 m, suggesting that the influence of the SWIW test is at least reaching that distance. I am not entirely convinced about the fact that push-pull tests can be seen as steady state tests and with the justification provided by the Authors, I leave to the Editor the judgment here. Nevertheless, I agree on the need to simplify the (already complex) analysis choosing the steady state! Reply: Implemented. See Lines 178-190. In the comment by reviewer: "In my experience this length is typically a function of the aquifer diffusivity, e.g., for tidal fluctuations is idealized coastal aquifer (e.g., homogeneous, infinite lateral extension) there is a proportionality of the kind lc = sqrt(K/S) (see e.g., Guarracino et al., 2012)", the formula of computing the characteristic length lc may be not right, since the dimension of sqrt(K/S) is L/sqrt(T), while the dimension of lc is L. By checking Guarracino et al. (2012), we found that authors employed "sqrt(K/(ωS))" to calculate the characteristic dampening distance, where ω is tidal angular velocity (T-1). This approximation is generally acceptable given the very limited spatial range of influence of most SWPP tests. For instance, if the characteristic length of SWPP test is l and the aquifer hydraulic diffusivity is D=Ka/Sa, where Ka are Sa are respectively the radial hydraulic conductivity and specific storage, then the typical characteristic time of unsteady-state flow is around t_c≈lˆ2/2D. The typical characteristic time refers to the time of the flow changing from transient state to quasi-steady state, where the spatial distribution of flow velocity does not change while the drawdown varies with time. This model is similar to the model used to calculate the typical characteristic length of the tide-induced head fluctuation in a coastal aquifer system (Guarracino et al., 2012). For Ka=1m/day, Sa=10-5m-1 and l=10m (which are representative of an aquifer consisting of medium sands), one has t_c≈lˆ2/2D=5.0×10ˆ(-3) day, which is a very small value. To test the model in computing t_c, the numerical simulation has been conducted, where the other parameters used in the model are the same as ones used in Figures 2 and 3. Figure S2 shows the flow is in quasi-steady state when time is greater than t_c, since two curves of t =5.0×10ˆ(-3) day and t =10.0×10ˆ(-3) day overlap. As for the typical characteristic length, if the values of Ka, Sa, and B have been estimated by the pumping tests before the SWPP test, it could be calculated by numerical modelling exercises using different simulation times.

15. line 289, in the comparison against the numerical solution the porosity of the immobile region of the aquifer is zero, why? There is also a general ω =0, to which mass transfer makes it reference? Why zero? Aren't these choices limiting the testing of the proposed solution? Reply: Implemented. We have revised it: θ_im=0.05, and ω=0.01d-1. See Line 308.

16. lines 309-310 'As mentioned in Section 3.1, the new model is a generalization of many previous models, and the conceptual model is more close to reality.' Again, too general. This novel solution could or not be closer to reality depending on the specific case. Reply: Implemented. See Lines 24-25, and Lines 277-283.

17. line 323 'To prioritize the sensitivity of parameters involved the new model' an in is missing (i.e., 'in the new model'). Moreover, the sensitivity is not a property of the parameters (or model inputs), but it is of the output with respect to the parameters. You want to quantify/evaluate the sensitivity of predictions with respect to the diverse parameters. Sensitivity cannot be prioritized, it is what it is and it is dictated by the way a model builds relationship between input(s) and output(s). Then you can prioritize the estimate of those parameters that influence the most the output. Reply: Implemented. "in" has been added. See Line 339. To prioritize the sensitivity of predictions with respect to the diverse parameters involved in the new model, a sensitivity analysis is conducted in Section 5.2. See Lines 354-372.

18. Eq. (29), the definition and explanation is quite obscure. The only clar thing is that it sensitivity is grounded here on the concept of derivative. Then, what is ci? Moreover, the subscript i does not vary at all, what is it? Why there is Ij before the derivative?. Furthermore, this equation implies (i) that only variation of a single parameter at time are considered and (ii) it seems that the index associated with a parameter is evaluated around only one value of that parameter. These features prevent the identification

of non-linearities and parameters interactions, which are quite likely to occur for the present model. The proposed method is a quite restricted characterization of sensitivity to me, if the model is not expensive I would suggest using a global sensitivity method: Sobol' indices (see Sobol, 2001) or DELSA (see Rakovec et al., 2014). On this point I leave the final decision to the Editor. Reply: Implemented. See Lines 355-372. The model of Eq. (29) in the original manuscript is for the local sensitivity analysis, and it has been deleted. Instead, a global sensitivity analysis is conducted using the model of Morris (1991) to investigate the importance of the input parameters on the output concentration.

19. lines 389-390 'The new model is most sensitive to the aquitard porosity and aquifer radial dispersivity' the model results are... 'after a comprehensive sensitivity analysis' you discover the previous thing after performing the sensitivity analysis, and it is not the latter that implies the former results; the sensitivity analysis is just a way to quantify the former aspect. Moreover, I would avoid comprehensive, see comment 18. Reply: Implemented. See Lines 354-372. A global sensitivity analysis is conducted using the model of Morris (1991). The description of the sensitivity is also revised.

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