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Interactive Comment

Interactive comment on "A parsimonious analytical model for simulating multispecies plume migration" *by* J.-S. Chen et al.

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Please note. Authors' responses follow immediately below the reviewers' comments.

This manuscript summarizes a new analytical model that simulates the reactive transport of multiple interacting species in a 2D groundwater flow system. The authors describe the model (with derivations in the appendices), and then provide several examples showing model output, comparison with a numerical model, and a short sensitivity analysis to identify influential transport parameters. Overall, the manuscript is organized well and covers an important topic. However, before recommending publication the following points must be addressed:

- One of the main concerns is the lack of connection with real-world systems. The authors compare their model with other models, but the actual behavior of the chemical species (particularly the sequential first-order decay reactions) in actual aquifer systems is not discussed, nor is it discussed in the Methods, Results, or Discussion sections. Without this connection, it is difficult for the reader to have confidence that modeling results (and the model itself) can be useful if applied to real-world systems.

Response: Analytical multispecies models are widely used to evaluate natural attenuation of plumes at chlorinated solvent sites. A study of 45 chlorinated solvent sites by McGuire et al. (2014) found that mathematical models were used at 60% of these sites and that the public domain model BIOCHLOR (Aziz et al., 2000) provided by the Center for Subsurface Modeling Support (CSMoS) of USEPA was the most commonly used model. The utility of the BIOCHLOR model to the real-world problems has been demonstrated by an example application that it can reproduce plume movement from 1965 to 1998 at the contaminated site of Cape Canaveral Air Station, Florida. The illustrative example of the developed analytical solution in our study considered the example reported in the BIOCHLOR. BIOCHLOR model uses analytical solutions to a set of advection-dispersion equations coupled by sequential first-order decay reactions. The BIOCHLOR analytical solution is valid for the case of having identical retardation coefficients for all species. The same equations were considered in our study to develop new analytical solutions. Our new solutions can consider the case that each species has its own retardation coefficients. Thus, we assure that our analytical solutions have more practical applications than the BIOCHLOR model to the real-world system.

References: McGuire, T. M., Newell, C. J., Looney, B. B., Vangeas, K. M., Sink, C. H., 2004: Historical analysis of monitored natural attenuation: A survey of 191 chlorinated solvent site and 45 solvent plumes. Remiat. J. 15: 99-122. Aziz, C. E., Newell, C. J., Gonzales, J. R., Haas, P., Clement, T. P., Sun, Y., 2000: BIOCHLOR– Natural attenuation decision support system v1.0, User's Manual, US EPA Report, EPA 600/R-00/008, EPA Center for Subsurface Modeling Support (CSMOS), Ada, Oklahoma.

- In relation to the previous comment, the authors need to discuss limitations of their model. For example, I assume that the flow field used in the analytical model is steady state, and that sources and sinks within the groundwater system are ignored. When do these conditions actually occur? Under what field conditions can the model actually be applied? Again, without relating the model to reality, much of this is ignored by the authors.

Response: All models have their limitations because they used physically-based mathematical equations to describe the transport processes in the subsurface system. The appropriateness of model depends on if transport behavior follows the basic assumptions of the physically-based mathematical equation. The analytical model in our study considers a steady uniform flow field and a boundary source. Thus, our model can be applied to a field site that has a steady uniform flow field and the contaminant source can be treated as a boundary source. Analytical model considers the same flow and source condition such as the BIOCHLOR model are widely used to assess many real-world problems. Detailed contaminated site applications were illustrated in the BIOCHLOR User's manual. We have elaborated a discussion on limitation of our analytical model in the revised manuscript for better readership.

- The use of the model requires a number of complicated numerical methods (correct?). So, at what point does the analytical solution actually become a numerical solution? Also, the authors never report the run-time of the model simulations in comparison with those of the numerical model (LTFD). Due to the complicated nature of the analytical model, I would assume that the run-times are substantial. Without this reported, it is hard to assess whether the newly developed analytical model is an improvement over numerical models. This must be reported and discussed.

Response: The developed analytical model is straightforwardly evaluated by two series summations and does not require any complicated numerical method. The only numerical method involved in the code development is the determination of the eigenvalues which need to be obtained from the eigenvalues equation in Eq. (A19). The numerical method to solve the eigen-value equation is quite easy and can be found in

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van Genuchten (1982). The computation is not time-consuming. The computational time for evaluation of the solutions at 50 different observations only takes 0.140 second computer clock time on an Intel Core i7-2600 3.40 MHz PC for species 1. We have added the discussions on the computational time in the revised manuscript.

Reference: van Genuchten, M. Th., Alves, W. J., 1982: Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation, US Department of Agriculture, Washington, DC, Technical Bulletin No. 1661, 151 pp.

- The derivations are very hard to sort through as a reader, particularly if the reader is not well versed in the intricacies of the numerous transformations, etc... that are being performed. Please narrate the derivations in clear, concise language, with clear definitions and explanations. As written, most readers will skip over the derivations.
- The first few sub-sections of the "Results and Discussion" section in fact seem like Methods. For example, 3.1 and 3.2 should be in the Methods section, since derivations are presented.

Response: Thanks for the constructive comment. We elaborate on the detailed mathematical manipulations and procedures to obtain the final solutions in the revised manuscript for better readership. Moreover, Sections 3.1 and 3.2 are moved to Section 2 “Governing equations and analytical solutions”.

- Overall, there are too many tables and figures. The large amount of model output shown in the tables probably is not needed, and instead can be replaced by metrics in several tables. The large amount of results is very tedious for a reader to sort through, and in the end discourages the reader from analyzing the model data and results critically.

Response: Thanks for the helpful comments. Actually we have moved most of tables to the appendix. These figures and tables in the main text are important to illustrate the investigation of the convergence the derived solution, the accuracy of the computer code as well the transport processes affecting the transport behaviors.

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Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 12, 8675, 2015.

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