

Interactive comment on “A general real-time formulation for multi-rate mass transfer problems” by O. Silva et al.

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The major contribution of this manuscript is presentation of a numerical implementation of the multi-rate mass transfer (MRMT) model that is widely used to represent non-equilibrium transfer processes in subsurface and surface hydrology. Some common applications of the MRMT model include fluid flow in fracture-matrix systems, and transport of solutes undergoing nonequilibrium sorption. In Sections 2 and 3, the authors have a succinct summary of the basic governing equations for the subsurface fluid flow and solute transport problems, and demonstrate how the discretized equations are modified to incorporate the MRMT model. In essence, only the storage and source/sink portions of the governing equations are affected, so MRMT only requires modification of the diagonal term and the right-hand-side of the discrete system. In

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Section 4, the manuscript then summarizes results from the literature showing how MRMT is mathematically equivalent to other nonequilibrium formulations (i.e., memory functions, fractional calculus, and continuous time random walk). The major new contribution is in Section 5 where the details of a Fortran 90 module are presented. The object-oriented programming paradigm is used to develop a general, flexible, and self-contained module that can be interfaced with any existing numerical flow and transport code. Finally, the new module is validated through comparison with other solutions in the literature.

My evaluation is that the module described in this manuscript will be a very useful and valuable tool that will enable scientists working in a variety of fields to modify their simulation codes to incorporate MRMT processes. The main contribution of the manuscript is presentation of the mathematical framework and Fortran 90 module that enable easy integration of MRMT into existing codes. The other sections of the manuscript summarize and synthesize existing results in the literature. So in this respect, the manuscript is more in the spirit of a “Computers in Geosciences” paper. Although I recommend that the manuscript is suitable for publication, it may have a more significant impact if it were to appear in a journal like “Computers in Geosciences” instead of “HESS.”

I have a few suggestions to improve the manuscript.

1. There are a couple of additional references that could be included. The Tsang and Tsang paper in Geophysical Research Letters is a classic reference that is relevant. Also, the paper by Sudicky in the March 1990 issue of Geoderma is relevant.
2. p. 2417, l. 17. I did not think that Barker or Acuna & Yortos used fractional calculus, but perhaps their flow dimension framework can be cast as fractional derivatives.
3. Section 4 showing the equivalence between MRMT and other methods could be better organized, perhaps using sub-sections. I also wonder if some of these results could be summarized in a table.

4. Figure 3. It is not clear what the numbers signify on the flowchart.

5. Section 5. The authors should explain a little about the advantages of using XML for the input files. These are not very many parameters needed in the input file, and I would like to understand the advantage of using XML.

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