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COMMENT

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This article is a comment on *Fiori et al.* [2015], doi:10.1002/2015WR017118.

Key Points:
- Authors find proxy transport models to be good predictors
- Their finding applies to Markovian flow/transport processes
- I show that their conclusions do not extend to more realistic non-Markovian conditions

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Comment on "Advective transport in heterogeneous aquifers: Are proxy models predictive?" by A. Fiori, A. Zarlenga, H. Gotovac, I. Jankovic, E. Volpi, V. Cvetkovic, and G. Dagan

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Abstract Fiori et al. (2015) examine the predictive capabilities of (among others) two "proxy" non-Fickian transport models, MRMT (Multi-Rate Mass Transfer) and CTRW (Continuous-Time Random Walk). In particular, they compare proxy model predictions of mean breakthrough curves (BTCs) at a sequence of control planes with near-ergodic BTCs generated through two- and three-dimensional simulations of nonreactive, mean-uniform advective transport in single realizations of stationary, randomly heterogeneous porous media. The authors find fitted proxy model parameters to be nonunique and devoid of clear physical meaning. This notwithstanding, they conclude optimistically that "i. Fitting the proxy models to match the BTC at [one control plane] automatically ensures prediction at downstream control planes [and thus] ii. . . . the measured BTC can be used directly for prediction, with no need to use models underlain by fitting." I show that (a) the authors' findings follow directly from (and thus confirm) theoretical considerations discussed earlier by Neuman and Tartakovsky (2009), which (b) additionally demonstrate that proxy models will lack similar predictive capabilities under more realistic, non-Markovian flow and transport conditions that prevail under flow through nonstationary (e.g., multiscale) media in the presence of boundaries and/or nonuniformly distributed sources, and/or when flow/transport are conditioned on measurements.

Fiori et al. [2015] examine the predictive capabilities of (among others) two "proxy" non-Fickian transport models, MRMT (Multi-Rate MassTransfer) and CTRW (Continuous-Time Random Walk). Proxy model predictions of mean breakthrough curves (BTCs) at a sequence of control planes are compared with near-ergodic BTCs generated through two- and three-dimensional simulations of nonreactive, mean-uniform advective transport in single realizations of stationary, randomly heterogeneous porous media. Fitting MRMT and CTRW to simulated BTCs at one control plane yields correlated, nonunique parameter estimates for each proxy model. Notwithstanding this lack of uniqueness, the three models yield comparable BTC predictions at control planes further downstream. The authors attribute this good agreement between model predictions to their Markovian nature, which allows representing all three time-nonlocal solutions (mathematically and/or in principle) by means of temporal convolution integrals. They conclude optimistically that "i. Fitting the proxy models to match the BTC at [one control plane] automatically ensures prediction at downstream control planes [and thus] ii. . . . the measured BTC can be used directly for prediction, with no need to use models underlain by fitting."

Fiori et al. [2015] note in passing that "Some aspects of the Markovianity of transit times have been discussed in *Neuman and Tartakovsky* [2009]." I consider it important for WRR readers to be aware that, in this latter paper, we compared theoretically four nonlocal models of advective and dispersive transport in randomly heterogeneous media, including CTRW. One of the four approaches [*Neuman*, 1993; *Morales-Casique et al*., 2006a, 2006b] "describes transport at some reference support scale by a classical (Fickian) advection–dispersion equation (ADE) in which velocity is a spatially (and possibly temporally) correlated random field. The randomness of the velocity, which is given by Darcy's law, stems from random fluctuations in hydraulic conductivity (and advective porosity though this is often disregarded). Averaging the stochastic ADE over an ensemble of velocity fields results in a space–time nonlocal representation of mean advective–dispersive flux." Neither the spatial nor the temporal integrals comprising these nonlocal expressions are convolutions in that they depend not merely on differences between values at two points in space and/or time but on the values themselves. They are therefore, generally, not Markovian in that one must know the system's history, not merely its present state, to predict its future.

Only in the special case of mean-uniform flow in an infinite, stationary domain do the nonlocal integrals of *Neuman* [1993] and *Morales-Casique et al*. [2006a, 2006b] become convolutions. Had *Fiori et al*. [2015] been aware of this, they would not have found it necessary to learn about it from numerical experiments (though such experiments do constitute a useful computational verification of our theoretical finding). The authors would likewise have anticipated, on the basis of our work [*Neuman and Tartakovsky*, 2009], that "no unique set of parameters could, in general, provide such predictions with any degree of reliability or confidence . . . there does not appear to be any formal link between such . . . parameters and measurable medium properties (e.g., hydraulic conductivity and advective porosity) or flow parameters (e.g., hydraulic gradients, fluxes and advective porosities)." I am nevertheless glad to see them confirming this numerically.

Under more realistic conditions of flow through nonstationary (e.g., multiscale) media in the presence of boundaries and/or nonuniformly distributed sources, and/or when flow/transport are conditioned on measurements, these phenomena are not Markovian. In contrast, CTRW "yields a representation of advective-dispersive flux that is nonlocal in time but local in space," with a nonlocal term that constitutes convolution in time [*Neuman and Tartakovsky*, 2009]. The same is true of MRMT. For this and other reasons Neuman and Tartakovsky concluded that "such models cannot be used to predict plume evolution . . . with any known degree of reliability." Correspondingly, the optimistic conclusions reached by *Fiori et al*. [2015] vis-à-vis the predictive capabilities of CTRW and MRMT under conditions of mean uniform flow do not extend to more realistic, non-Markovian flow and transport conditions of the kind just mentioned. This too the authors could/should have anticipated on the basis of our earlier theoretical analysis, and stated explicitly.

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