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Interpretation of a transport experiment with bimolecular reaction using a single-rate mass-transfer model with a temporally variable coefficient

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Recently there have been a number of approaches to interpret the column experiments of Gramling et al. (2002) involving the formation and transport of CuEDTA2- in an irreversible reaction. The experimental data could not be properly fitted with an advection-dispersion equation assuming instantaneous reaction. Alternative approaches have been used to model the experiments using upscaled models, where instantaneous reactions are substituted by models based on incomplete mixing or in non-instantaneous reactions including some upscaled coefficients. Here we explore another possibility for an upscaled model, where reaction is again assumed as instantaneous and irreversible, and incomplete mixing is modeled by means of a single-rate mass-transfer model where the transfer coefficient varies with time (t-SRMT). This model is the extension to reactive transport of the model presented recently by Fernàndez-Garcia and Sanchez-Vila [2015], being a proxy for a general multi-rate mass-transfer model. The evaluation of the model performance allows getting insight about the physical meaning of the parameters in the t-SRMT model, explaining some observations regarding the apparent mass-transfer coefficients registered in the literature.