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Reactive transport with wellbore storages in a single-well push–pull test

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Supplemental Materials:

MODFLOW/MT3DMS has been widely used to simulate the groundwater flow and reactive solute transport, including the solute transport in the SWPP test with the transient flow field. However, we found that the mathematic models of the reactive transport in MT3DMS might cause great errors (Wang et al. 2018, WRR, Wang et al., 2018, JH). The reason could be explained as follows.

The governing equation of the reactive transport in MT3DMS is (Wang et al. 2018, WRR, Wang et al., 2018, JH):

$$\frac{\partial(\theta C^k)}{\partial t} = L_{DSP}(C^k)+L_{ADV}(C^k)+L_{SSM}(C^k)+L_{RCT}(\theta C^k) + q_s C_s^k, \; t > 0, \quad \text{(S1)}$$

where C^k is the dissolved concentration of species k [ML^{-3}]; k is an positive integral to account for the number of species [dimensionless]; t is time [T]; r is radial distance from the wellbore [L]; θ is porosity of the porous media [dimensionless]; r_w is well radius [L]; α_r and v are the radial dispersivity [L^{2}T^{-1}] and flow velocity [LT^{-1}]; $L_{DSP}(\cdot)$, $L_{ADV}(\cdot)$, $L_{SSM}(\cdot)$, and $L_{RCT}(\cdot)$ are the operators for the dispersion, advection, other sink/sources excluding the wellbore, and chemical reaction terms, respectively; q_s is volumetric flow rate per unit volume of aquifer [T^{-1}], and it is positive for the injection well, and negative for the pumping well. C_s^k is the concentration of species k [ML^{-3}] in the injection solute, and it is equal to C^k for the pumping well.

Eq. (S1) is applicable for both aquifer and wellbore REVs, and it can be expressed using the mass balance principle as follows (Zheng and Wang, 1999):

$$(\text{Mass Accumulation})_{Cell} =$$

$$(\text{Net Mass Flux})_x+(\text{Net Mass Flux})_y+(\text{Net Mass Flux})_z +$$

$$(\text{Net Mass Flux by Source or Sink})_{Cell} + (\text{Net Mass Flux by Reactions})_{Cell}, \quad \text{(S2)}$$

where the subscripts x, y, and z represent the x, y, and z axes, and

$$(\text{Net Mass Flux})_x = -\frac{\partial}{\partial x}(C^k \theta v_x^* \Delta y \Delta z)\Delta x, \quad \text{(S3a)}$$

$$(\text{Net Mass Flux})_y = -\frac{\partial}{\partial y}\left(C^k \theta v_y^* \Delta x \Delta z\right)\Delta y, \quad \text{(S3b)}$$

$$(\text{Net Mass Flux})_z = -\frac{\partial}{\partial z}(C^k \theta v_z^* \Delta x \Delta y)\Delta z, \quad \text{(S3c)}$$

$$(\text{Net Mass Flux by Source or Sink})_{Cell} = W_s C_s^k \Delta x \Delta y \Delta z, \quad \text{(S3d)}$$

$$(\text{Net Mass Flux by Reactions})_{Cell} = \theta \Delta x \Delta y \Delta z \sum R_k, \quad \text{(S3e)}$$

$$(\text{Mass Accumulation})_{Cell} = \frac{\partial}{\partial t}(C^k \theta \Delta x \Delta y \Delta z), \quad \text{(S3f)}$$

where v_x^*, v_y^*, and v_z^* are the instantaneous mass velocities [ML^{-3}] along the x, y, and z axes, respectively. Δx, Δy, and Δz are the dimensions of the REV along the x, y, and z axes, respectively. Δz is constant for a confined aquifer. The detailed explanations of parameters in Eqs. (S1) - (S3) could be seen in Zheng and Wang (1999).

We need to point out that the present modeling practice of applying above Eqs. (S1) - (S3) for a well-aquifer system has a few problems that must be recognized. For example, the porosity of the wellbore is unity, and the water level in the wellbore is time-dependent in a confined aquifer, while is not constant (e.g. Δz). However, such features have not been adequately dealt with in using above Eqs. (S1) - (S3), which assumes that the porosity of the wellbore is the same as the porosity of the surrounding aquifer, and the volume of the water in the wellbore is constant, e.g. it is $\theta \Delta x \Delta y \Delta z$ in Eq. (S3f).

Figure S1 shows comparison between the analytical solutions and numerical solutions by MODFLOW/MT3DMS. The parameters used in this case are: The aquifer dimensions are 100m$\times$ 100m $\times$ 6m, the horizontal hydraulic conductivity is 10 m/day, the horizontal anisotropy is 1.0, the injection flow rate is 20 m^3/day, the porosity is 0.3, the longitudinal dispersivity is 0.5m, the ratio of horizontal transverse dispersivity to longitudinal dispersivity is 0.1, and the ratio of vertical transverse dispersivity to longitudinal dispersivity is 0.01. The well is located in the center of the aquifer and fully penetrates the aquifer. To test the influence of water level on the mixing effect, three sets of initial conditions of the hydraulic head are employed: h_0 =6m, h_0 =30m, and h_0 =60m. A greater initial head implies a greater water level in the wellbore. As the flow is assumed to be in steady state, the information of the specific yield and the specific storage are not needed. The spatial discretization is $\Delta x = 0.4m$, $\Delta y = 0.4m$, and Δz=6m. The aquifer is vertically discretized into one layer. This is because the flow direction is radially horizontal for a well fully penetrating a homogeneous aquifer. The drawdowns in the wellbore are set as -0.346m for all cases.

Figure S1 shows the comparison between the analytical solution and numerical solution by the MT3DMS code is obvious, and numerical solution is independent on the water level in the wellbore, which is not accurate.

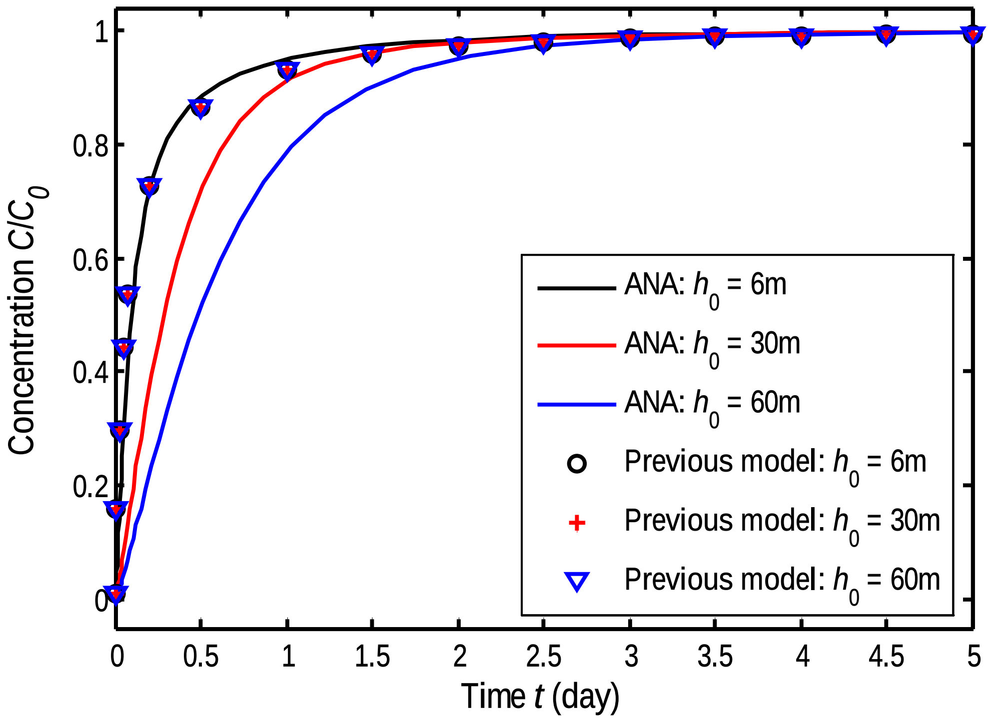

Figure S1. Comparison between BTCs by the analytical and numerical methods in the wellbore in the injection test (from Figure 3A of Wang et al., 2018, JH). "ANA" represents the analytical solutions. "Previous model" represents the numerical solutions by MODFLOW/MT3DMS. "h_0" represents the initial water level in the wellbore,

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