Technical note: Wellbore water volume computation of tracer test in numerical modelling in a confined aquifer

A ***Technical Note*** Submitted to ***Hydrology and Earth System Sciences***

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Supplementary Materials

1. Changes of the original MT3DMS code

2. Figures S1-S2

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1. Changes of the original MT3DMS code

MT3DMS is a 3D numerical model used to describe the multispecies solute transport in both confined and unconfined aquifer (Zheng and Wang, 1999). As mentioned in Section 2.4, the traditional model may cause errors in modeling solute transport in a well-confined aquifer system. The main reason is that water in an open wellbore is unconfined, but is treated as confined, which is incorrect. Consequently, thickness of water in the wellbore is assumed to be constant and same as the aquifer thickness, which is not true. In this study, the MT3DMS code is revised to eliminate this error for numerical simulation.

The original computer program of MT3DMS consists a main program and many modules, such as ADV (Advection Package), DSP (Dispersion Package), SSM (Sink & Source Mixing Package), RCT (Chemical Reaction Package), BTN (Basic Transport Package), FMI (Flow Model Interface Package), GCG (Generalized Conjugate Gradient Package), and so on. The ADV, DSP, SSM, RCT packages are used to solve advective, dispersive, sink & source, and chemical term in the governing equation of the solute transport, respectively. As Eq. (13), Eq. (14), Eq. (15) are respectively formulated in the BTN, SSM and RCT packages, the changes of the code mainly happen in these two modules. The detailed information of the changes could be seen in the revised MT3DMS code.

In the BTN module of the original code of MT3MDS version 4, “RETA(N, ICOMP)” in the computing code means retardation factor. As for Cell 2 in Figure 1, the corresponding code is revised by

RETA(N, ICOMP)= RETA(N, ICOMP)× $B_{Cell2,w}$/DZ(N), (B1) where $B_{Cell2,w}$ is computed by MODFLOW, and DZ(N) is the vertical thickness of cell. When the water level in Cell 2 is equal to the vertical thickness of cell, the code (B1) reduces the original one.

In the SSM module of the original code of MT3MDS version 4, "RHS(N)" in the computing code represents Eq. (14). As for Cell 2, the corresponding code is revised by

RHS(N)= RHS(N)-QSS×CTMP×DELR(J)×DELC(I)×$B_{Cell2,w}$, (B2)

where QSS is pumping rate, CTMP is concentration, DELR(J) and DELC(I) are the horizontal dimensions of the cell. When $B_{Cell2,w}$= DH(J, I, K) which is the vertical thickness of cell, the code (B2) reduces the original one.

Similarly, the code DELR(J)×DELC(I)×DH(J, I, K) in the RCT module is revised into DELR(J)*DELC(I)* $B_{Cell2,w}$ for Cell 2 in Figure 1.

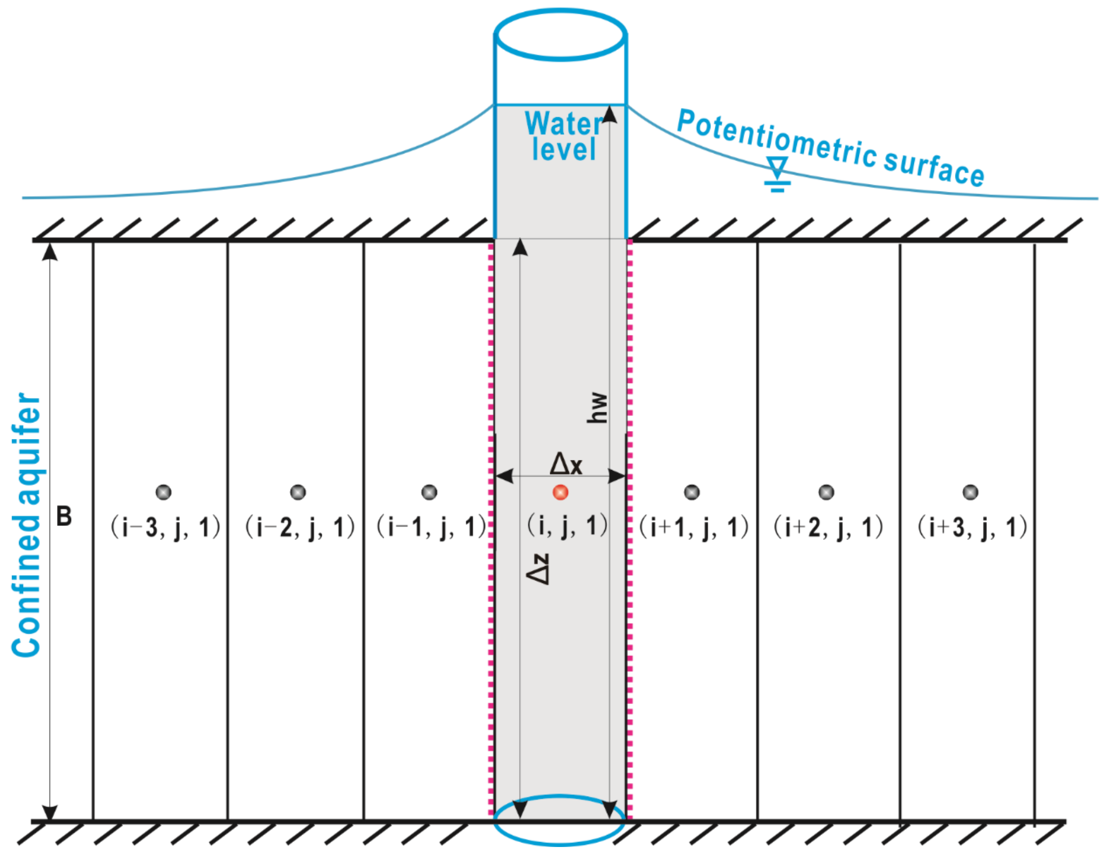

Figure S1. A grid system of 2D reactive transport model in a wellbore-confined aquifer system