New Mixed Lagrangian-Eulerian Method on Cauchy Boundary in the Numerical Framework of MT3DMS

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Introduction

In the field of groundwater, MT3DMS has been a popular commercial software in research projects and practical field applications and has been significantly expanded to many areas including variable-density transport, non-aqueous phase liquid dissolution, and solute transport in unsaturated zone [1,2,3]. However, MOC, MMOC, and HMOC included in MT3DMS didn't treat straightforwardly or rigorously Cauchy boundary condition from the mathematical or numerical points of view. The objectives of this study are to (1) evaluate limitation and applicability of MOC, MMOC, and HMOC in MT3DMS on the Cauchy boundary conditions for the all flow regimes, and (2) propose a modified mixed Lagrangian-Eulerian method based on the numerical framework of ELM of MT3DMS for accurately solving solute transport problems with Cauchy boundary conditions in all flow regimes including both advection-dominated and dispersion-dominated.

Numerical Results

The example is identical to example 2 of Neuman [4], except that the constant concentration boundary condition of Neuman [4] is replaced here with a constant flux condition, i.e., $f(t)=1$ mg/l. The input parameters in Case 1A in Table 1 are the same as those described previously by Neuman [4]. The dispersion coefficients in Case 1B, 1C, and 1D were increased from that of Case 1A as shown in Table 1 to cover the spectrum from dispersion-dominated problems to advection-dominated problems associated with mesh Peclet numbers ranging from 0.04 to 200. The analytical solution is obtained following Van Genuchten and Alves [5].

For the implementation of Case 1A to Case 1D using the Neuman method, the spatial increment of the dispersion grid is the same as spatial increment in Table 1, keeping the spatial increment of the convection grid to be smaller than the dispersion grid by a factor of 11. The temporal increment of the convection grid and the temporal increment of the dispersion grid are identical to the temporal increment in Table 1. The LEZOOMPC approach and the proposed method set the advection zooming factor to 11 to achieve the same level of spatial refinement as the Neuman approach. The LEZOOMPC approach and the proposed method perform peak capturing. Additionally, in order to show the necessities of local grid refinement (LGR) schemes for accurate solution, the proposed method without any refinement were used for comparison with that with local grid refinement scheme. In addition, in the MOC and HMOC, the numbers of particles placed at each cell are set either 4 or 25 according to the relative cell concentration gradient. Time step sizes for all schemes in MT3DMS are same as temporal increment in Table 1. In addition, all schemes in MT3DMS use generalized conjugate gradient (GCG) solver.

Cases	V (m/day)	D (m^2/day)	Δt (days)	Δx (m)	Mesh Peclet No.	Mesh Courant No.
Case 1A	10,000	1	10^{-6}	0.02	200.0	0.5
Case 1B	10,000	50	10^{-6}	0.02	4.0	0.5
Case 1C	10,000	1,000	10^{-6}	0.02	0.2	0.5
Case 1D	10,000	5,000	10^{-6}	0.02	0.04	0.5

Table 1: List of input parameters, mesh Peclet numbers, and mesh Courant numbers for various cases.

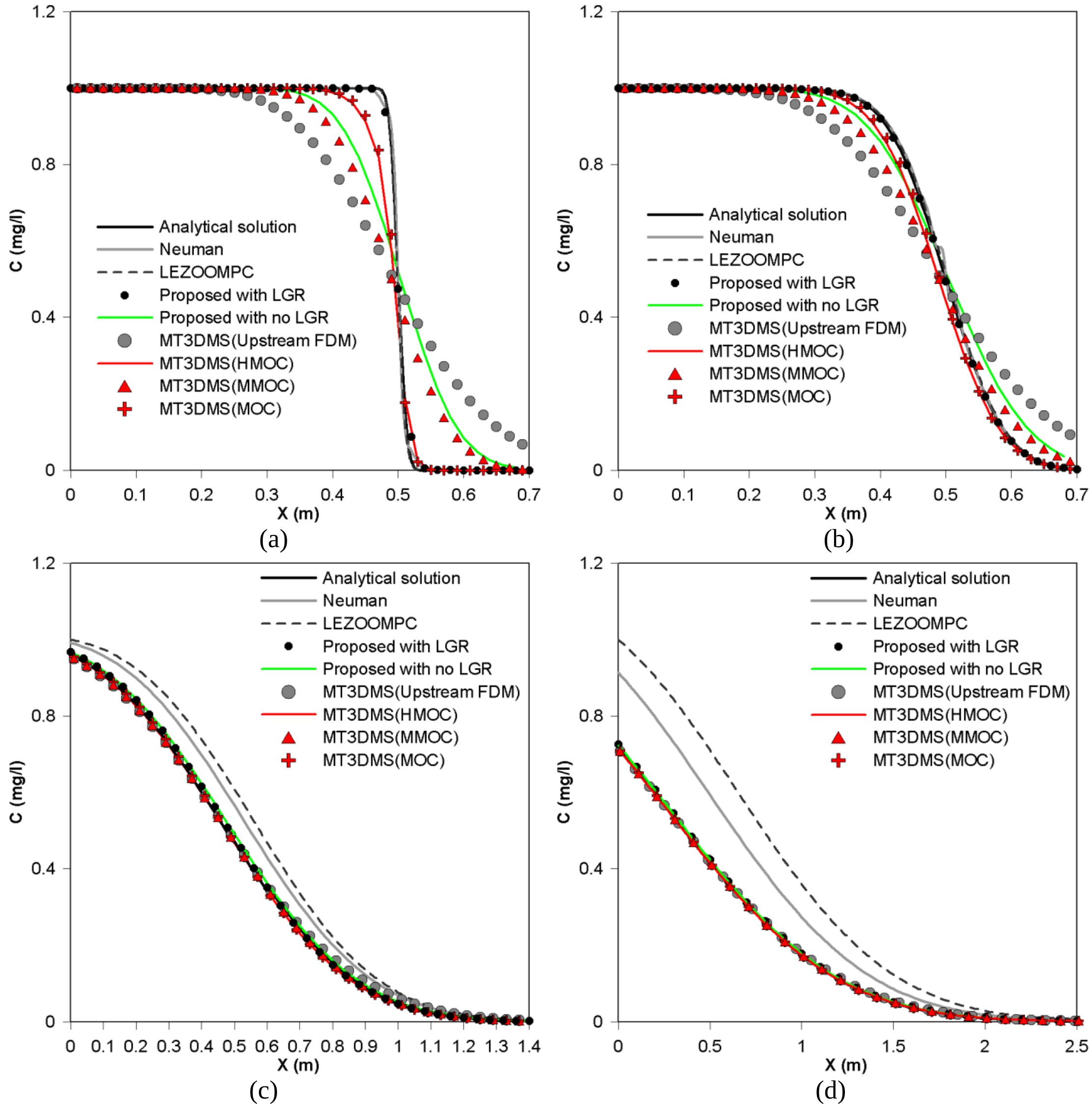

Figure 1: Results of Example of (a) Case 1A, (b) Case 1B, (c) Case 1C, and (d) Case 1D

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