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Efficient random walk particle tracking algorithm for modeling advection-dispersion transport in highly heterogeneous porous media

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The random walk particle tracking (RWPT) method is a well established alternative to grid-based Eulerian approaches when simulating the advection-dispersion transport problem in highly heterogeneous porous media. A difficulty of the method is the loss of accuracy of the dispersive displacements when the dispersion tensor or the water content is spatially discontinuous, which is common in heterogeneous unsaturated soils. The interpolation method is mostly used to smooth the variables in the vicinity of the discontinuity (e.g., velocity, dispersion tensor, water content), and to apply the smoothed variables to the calculation of the dispersive terms. Convergence is achieved by refining the interpolation grid and the time step size simultaneously, which is computational inefficient. An alternative method which does not need the refinement of the interpolation grid is the partially reflecting barrier method. However, this method has been outperformed by other RWPT methods in previous studies. In this contribution, we present three corrections to the partially reflecting barrier method that improve its accuracy and efficiency so that, especially for large grid sizes, it outperforms other methods: i) The systematic overestimation of the second dispersion displacement across an element interface when a linear time splitting is used was corrected for using a non-linear time splitting. ii) The two-sided reflection coefficient was replaced by a one-sided reflection coefficient that represents the effect of discontinuous dispersion coefficients correctly for $\Delta t \rightarrow 0$ but eliminates redundant reflections and thereby reduces the error for discrete Δt. iii) The transformation of the dispersive displacement across the element boundary for complex multidimensional transport problems. The proposed corrections are verified numerically by comparison with analytical solutions and by a detailed comparison with the interpolation method for a three-dimensional test scenario. We demonstrate the general applicability of the reflection barrier method to complex multidimensional transport problems. The results indicate that the improved RWPT algorithm is a very efficient approach for transport problems with highly heterogeneous dispersion tensors and water contents. Because the new algorithm efficiently simulates both advection- and dispersion-dominated transport conditions, it enhances the applicability of RWPT to scenarios in which both conditions occur, as for example in the highly-transient unsaturated zone.