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Sunyoung Bu* (agatha@email.unc.edu), Department of Mathematics, University of North Carolina, Chapel Hill, NC 27599-3250, Chapel hill, NC 27514, and Jingfang Huang, Treavor H Boyer and Cass T Miller. An Evaluation of Solution Algorithms and Numerical Approximation Methods for Modeling an Ion Exchange Process.

In this work, we discuss the modeling and numerical simulations of the dissolved organic carbon (DOC) removal process in water treatment studies. We first introduce a new age-averaged model (AAM) that averages all ion exchange particle ages for a given size particle to avoid the expensive Monte-Carlo simulation associated with previous modeling applications. To approximate both the original Monte Carlo algorithm and the new AAM for this two-scale problem, we introduce a scheme using an integral equation based Krylov deferred correction (KDC) method and a fast elliptic solver (FES) for the resulting elliptic equations. Numerical results are presented to validate the new AAM algorithm, which is shown to be more computationally efficient than the original Monte Carlo algorithm. We also demonstrate that the higher-order KDC scheme is more efficient than the traditional finite element solution approach and this advantage becomes increasingly important as the accuracy of the solution desired increases. We also discuss issues of smoothness, which affect the efficiency of the KDC-FES approach, and outline additional algorithmic changes that would further improve the efficiency of these developing methods for a wide range of applications. (Received September 21, 2010)