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Mitigating Numerical Dispersion for High-Fidelity Back Diffusion Modeling in Low-Permeability Zones: Validation Against Laboratory Experiments

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Back diffusion from low-permeability zones is a critical driver of sustained groundwater contamination even after source depletion. While its physical mechanisms have been identified through various studies, such as Yang et al. (2015), precise numerical modeling is essential for predictive applications. However, numerical dispersion—a common issue in diffusion-dominated transport modeling—often distorts concentration profiles and compromises accuracy. This study validates back diffusion processes using numerical modeling and addresses numerical dispersion through grid refinement and optimized time-discretization. Using HydroGeoSphere (HGS), we replicated the chamber experiments of Yang et al. (2015), simulating solute diffusion from a sand layer into a clay layer followed by the subsequent back diffusion. Experimental parameters, including boundary conditions, diffusion coefficients, and retardation factors, were rigorously incorporated. To mitigate artificial dispersion at the clay-sand interface where sharp concentration gradients occur, local grid refinement was implemented, while adaptive time-stepping was applied to ensure temporal precision. The results indicated that variations in grid size did not lead to significant differences in accuracy, suggesting that the tested resolutions were already sufficient to suppress numerical dispersion to negligible levels. This implies a need for future investigations using larger grid scales to explicitly identify the threshold where numerical dispersion begins to distort back diffusion profiles. Adaptive time-stepping was found to be instrumental in ensuring numerical stability and high resolution during the critical transition period from forward diffusion to back diffusion. This research demonstrates that back diffusion can be effectively validated through numerical simulations when artificial dispersion is minimized. The proposed optimization framework not only accurately replicates laboratory findings but also provides a robust basis for extending back diffusion analysis to field-scale groundwater systems. Future efforts to calculate optimized numerical parameters through additional experiments are expected to provide practical contributions to the understanding and remediation of back diffusion-driven contamination.