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Microscale modeling studies of chemical transport from petroleum contaminant sources

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Thirty years after the earlier studies of groundwater pollution by petroleum hydrocarbons, the dominant mechanisms and the uncertainties that arise in real field behaviors of nonaqueous phase liquid (NAPL) are still largely unresolved. The relevant literature has emphasized numerical modeling of multiphase flow using continuum approaches. These approaches do not consider chemical component transport following NAPL release into the subsurface and at the later time, both of which are of interest in the cleanup of contaminated sites. In current studies of natural attenuation, the release of chemicals tended to be overestimated by general continuum-concentration-gradient approaches. In this work, we propose using the Lattice Boltzmann method to simulate the dissolution of chemicals out of the NAPL source to quantify the release of dissolved chemicals into the water. The findings from these simulations would add insight to the multiphase flow and partitioning of contaminants from contaminated sources.