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A relevant coupled particle-tracking solution for network reaction and multirate mass transfer under heterogeneous conditions

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Considering complex physical and reactive processes is necessary to a trustable plume behavior prediction. However, complexity is often synonym of inefficiency and numerical problem for existing model.

We present an efficient particle method to simulate plumes evolution moved by advection-dispersion and affected by network reactions and multirate-mass transfer processes under heterogeneous spatial conditions. The stochastic approach is based on the derivation of the probability that a particle being at a certain position, specie and mobility zone will move into another specie and/or zone. Transport processes are fully coupled with reactions. The particle method is free of numerical dispersion and overcomes the inherent numerical problems stemming from the incorporation of heterogeneities into reactive transport codes based on Eulerian approaches. Even if the method aims to be universal, we show that analytical solutions can be provided for the simpler cases, which may improve consequently the model efficiency.

Illustratively, we apply our method to model the sequential degradation of chlorinated solvents (PCE $\Rightarrow$ TCE $\Rightarrow$ DCE $\Rightarrow$ VC $\Rightarrow$ 0) into a finely discretized field and show how spatially variable coefficients of hydraulic permeability, bio-decay and mass transfer affect the spatial and temporal behavior of the four reactive plumes.