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An Embedding Method for Simulation of Immobilized Enzyme Kinetics and Transport in Sessile Hydrogel Drops

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Abstract

We present a new numerical method, termed the embedding method, to solve a system of nonlinear PDEs for multi-phase problems in asymmetric 3-D domains. The main feature of this method is its ability to perform interface calculation and account for conditions relating solution properties across phase interface using a finite difference / volume-fraction-based front-capturing hybrid technique. The approach begins by considering the computational domain as physically separated phases. A finite difference method with a Cartesian grid is employed on the whole domain while modifications are applied to correct boundary conditions at the interfaces. The volume-fraction-based front-capturing algorithm is used to capture each interface in terms of the volume fraction in each cell. The major aspect of this method is its implementation simplicity, which results in code generation that can be highly optimized. To highlight this method, an application is presented for simulation and investigation of enzyme reactions within a sessile hydrogel drop, where the Michaelis-Menten kinetics is used to model the reaction mechanism.