Modeling porous or reactive surfaces under strong shear: Beyond Damkohler

Preyas Shah and Eric S. G. Shaqfeh
preyas@stanford.edu, esgs@stanford.edu

Abstract.

Surfaces which include heterogeneous mass transfer at the microscale are ubiquitous in nature and engineering. Many such media are modeled as via an effective surface reaction rate or mass transfer coefficient employing the original ansatz of Damkohler Ð i.e. reaction limited transport at the microscale. However, this assumption is limiting, particularly when there is strong flow. We are interested in modeling porous surfaces that occur naturally in biological systems such as leaky tumor vasculature where the effective Dahmkohler number at the microscale can be O(1) and the local Peclet number may be large. In order to expand the range of the effective mass transfer surface coefficient, we study transport in a uniform bath of a species in an unbound shear flow over a wall. The wall has a heterogeneous distribution of first order surface reactive circular patches (or pores). To understand the physics at the length scale of the pore size, we first analyze the flux through a single pore. We use both analytic and boundary element simulations for this purpose. The shear flow induces a 3-D wake structure downstream of the patch. When two pores are aligned in the shear direction, the wakes interact to reduce the per pore flux compared to the single pore case. Having determined the length scale of interaction between two pores, we study the transport to a periodic and disordered distribution of pores Ð again using analytic and boundary integral techniques. We obtain, up to non-dilute pore area fractions, an effective boundary condition for the transport through pores that depends on local mass transfer coefficient (or reaction rate) and shear rate. We demonstrate that this boundary condition replaces the details of the heterogeneous surfaces at a wall-normal effective slip distance also determined for up to non-dilute pore area fractions. The slip distance again depends on the shear rate, and weakly on the reaction rate and scales with the pore size. These effective boundary conditions can be used directly in large scale physics simulations as long as the local shear rate, reaction rate and pore area fraction are known.

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