A Flow and Transport Model of Catalytic Multi-Pump Systems with Parametric Dependencies

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Abstract

The use of catalysts to create motion on the micro-scale has been studied in recent experiments(1,2,3). When a catalyst is submerged in a solution of its respective substrate or promoter, chemical energy derived from catalysis is converted to motion. More recently, these catalysts have been anchored to a surface creating fluid flow as pumps (1,3). Catalytic pumps could help overcome a crucial issue facing microfluidics in which fluid flow cannot be created without the use of pressurized systems. The mechanism by which the catalyst pumps work has been examined through both experiment and simulation (1,2,3). Using the COMSOL Multiphysics® software, the mechanism that drives micro-scale motion due to a catalytic reaction is studied. In previous simulations, a system that utilizes a single catalytic patch, or single pump, has been modeled (1,3). In this simulation, a multi-pump system is explored with both (a) varying the catalytic reactions used in the multi-pump system, and (b) changing the parameters that govern the magnitude and direction of the fluid flow, such as pump dimensions, diffusion coefficients, and volumetric expansion coefficients of the substrate and product.

Experimental setups of micropumps involve anchored catalysts in the center of a domain (Figure 1). The remainder of this domain is uniformly filled with the respective substrate for the catalyst, resulting in pumping. For computational simplicity, the geometry is assumed to be radially symmetric around the center of the patch in a 2-D model. The mechanism that drives the pumping is dependent upon density gradients as a result of the catalytic reaction. This model utilizes the Chemical Reaction Engineering and CFD Modules of the COMSOL Multiphysics® software, as well the 'Transport of Diluted Species' interface in order to properly define these density gradients and how they result in fluid flow. The boundary conditions, excluding the radially symmetric boundary, are defined as closed walls with no-slip and no-flux conditions. Through the Boussinesq approximation of the Navier-Stokes equation, a buoyancy force governed by the density gradient and gravitational forces is used to define the fluid flow. This physics is used in order to couple the transport of diluted species module with the laminar flow module. A free tetrahedral meshing is defined by the physics with fine properties in order to optimize computation time and quality of results. The time-dependent study is performed in two steps in which the first step solves the model for chemical reactions and species gradients, while the second uses the results from the first step in order to define the fluid flow. As a result of a parametric sweep across several parameters, different situations can be described in which the multi-pump system can reach optimal pumping speeds, reverse pumping direction, or act as a simple logic gate.

Reference

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Figures used in the abstract

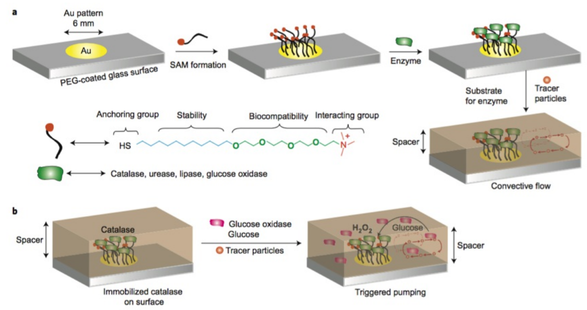

Figure 1: Figure 1 | Schematic that shows the enzyme immobilization on a surface and triggered fluid pumping by enzymatic micropumps. a, Au is patterned onto a PEG-coated glass surface using an e-beam evaporator. The patterned surface is functionalized with a quaternary ammonium thiol, which forms a self-assembled monolayer (SAM) on the Au surface. The negatively charged groups on the enzyme bind selectively to the SAM-functionalized Au patterned surface via electrostatic assembly, which results in enzyme immobilization on the surface. b, Catalase enzyme immobilized on the Au pattern causes fluid pumping as a result of the chemical decomposition of the hydrogen peroxide generated in situ from glucose in the presence of another enzyme glucose oxidase (3).