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

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Introduction: The use of catalysts to create motion on the microscale has been studied extensively (1,2). Enzyme micro-pumps function through a unique mechanism studied using COMSOL Multiphysics. In this particular model, multi-pump systems were studied over different parametric values.

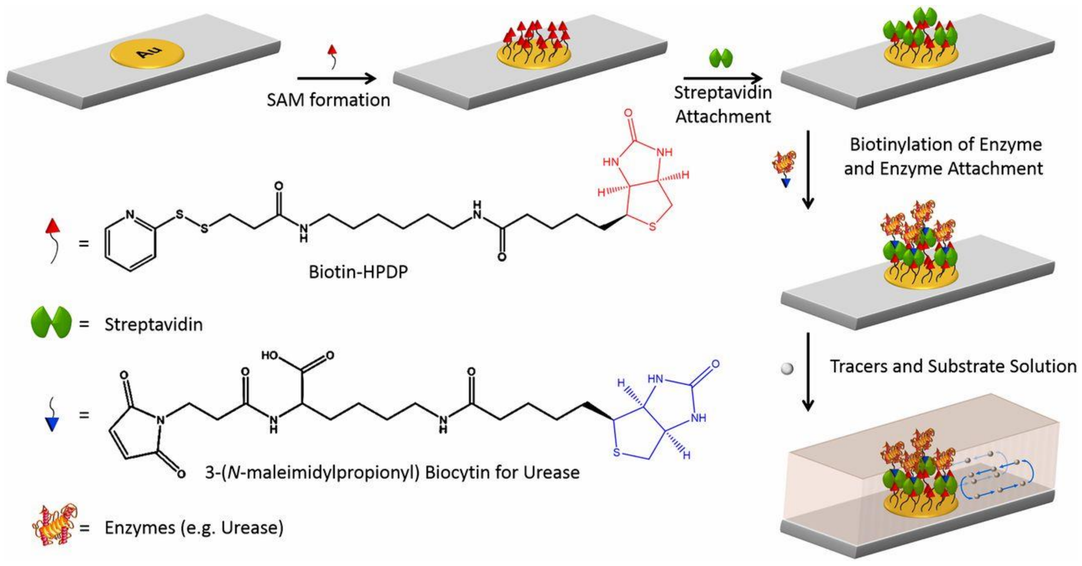

Figure 1. Schematic showing enzyme immobilization on a surface (1).

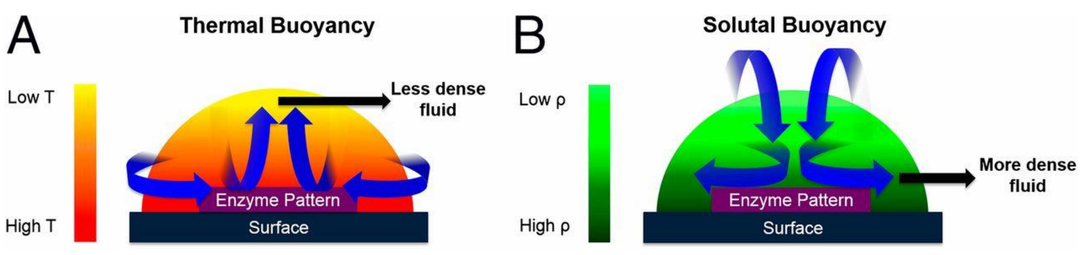

Figure 2. Detailed description of pump mechanism (1).

Computational Methods: Using the chemical reaction engineering module of COMSOL Multiphysics, a spatio-temporal study was constructed that analyzes the fluid flow profile of a multi-pump system as a function of the inter-pump distance (d), the ratio of the pump reaction rates (R), and the chemical species' coefficients of volumetric expansion (β).

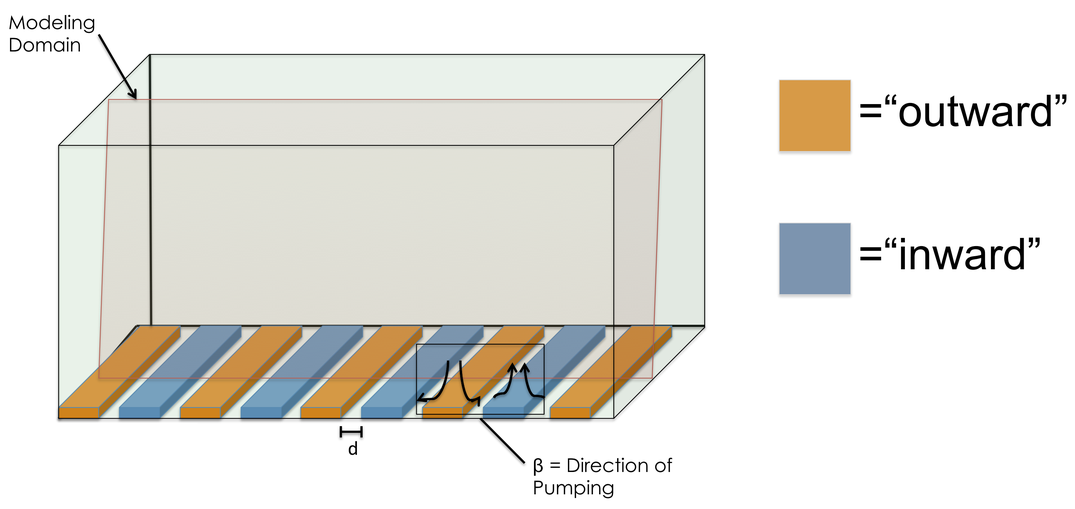

Figure 3. 3-D view of the physical modeling domain and parameters. "d" is the distance between pumps, and "β" is the parameter that governs the individual pumps' direction of pumping. The model is studied in the 2-D plane (red outline).

A fluid force is defined over the entire domain by using the Boussinesq Approximation of the non-inertial Navier-Stokes equation.

$$\rho\frac{\partial \mathbf{u}}{\partial t} = \nabla\cdot\left[-p\mathrm{I}+\mu\left(\nabla\mathbf{u}+\left(\nabla\mathbf{u}\right)^{T}\right)\right]+F,$$

$$\nabla\cdot\mathbf{u} = 0, F = -\rho_0\tilde{g}\left(\sum\beta_{species}c_{species}\right)$$

The parameters are defined as follows:

$d = Interpump\ distance$

$\beta = Volumetric\ Coefficient\ of\ Expansion$

$$R = \frac{Reaction\ rate\ of\ outward\ pump}{Reaction\ rate\ of\ inward\ pump}$$

Results: Shown below are different velocity profiles defined on a 1-D cutplot of the data set. The data for the time-lapse comes from a video analyzing a 2-D cutplot of the domain.

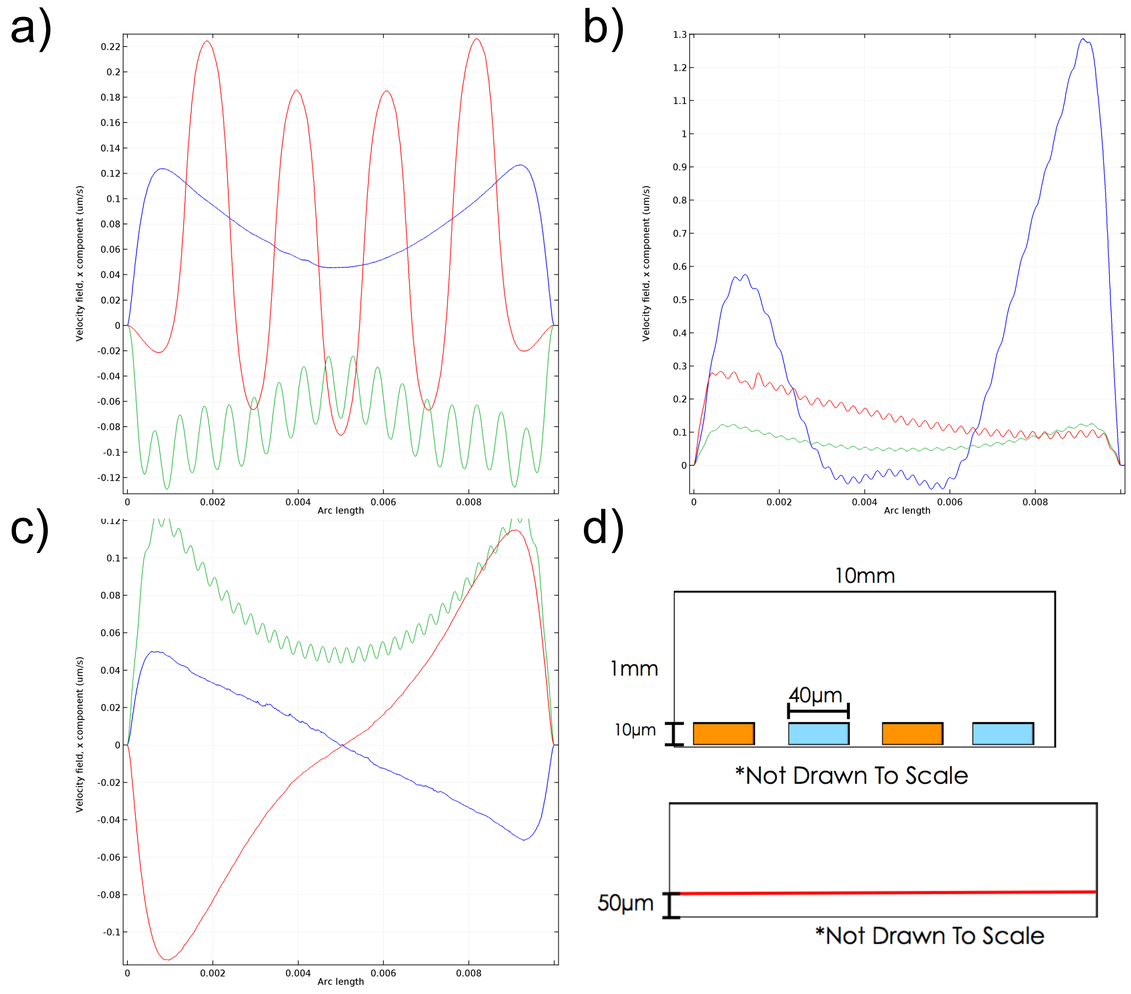

Figure 4 (a-d). Graphs of the velocity profiles over the 1-D cutplot in three parametric sweeps: (a) spacing, (b) ratio of reaction rates, (c) β or the direction of pumping. Visual representation of 1-D and 2-D cutplots of the data is shown in (d).

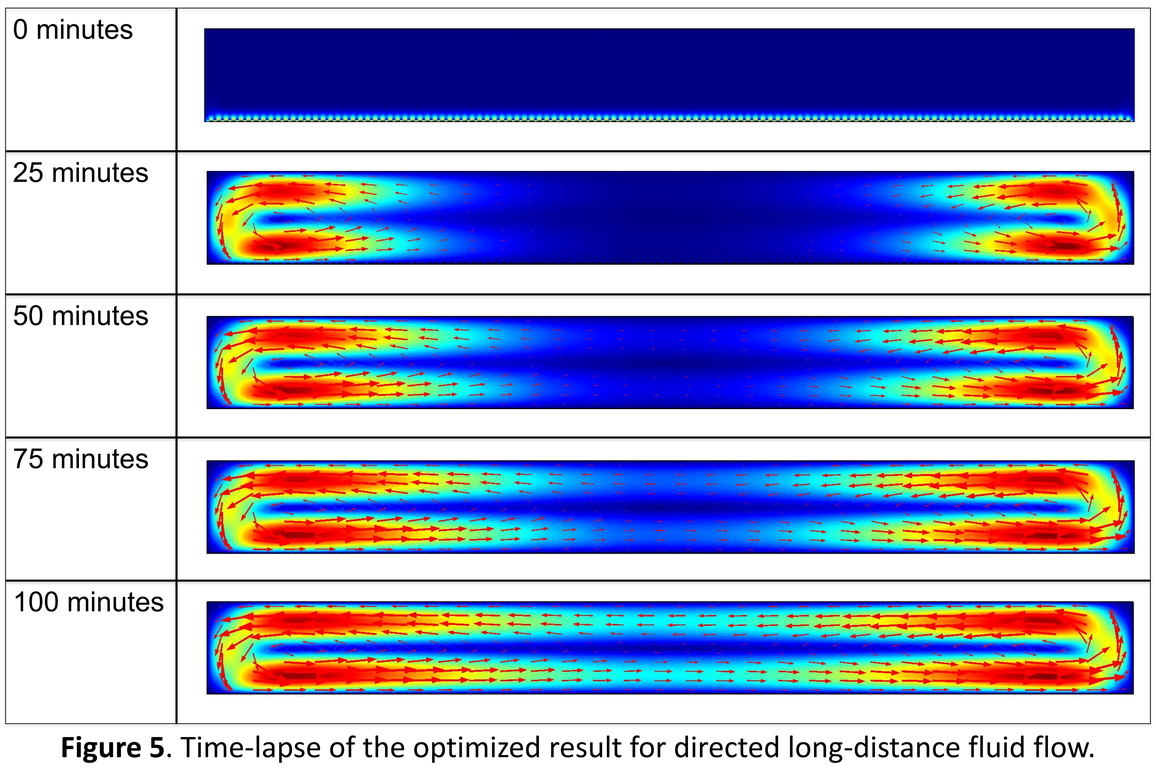

Figure 5. Time-lapse of the optimized result for directed long-distance fluid flow.

Conclusions: Achieving a directed, long-distance fluid flow in our modeling domain was shown to be possible. With the three parameters optimized at d = 40 μm spacing, equal reaction rates of inward and outward pumps, and alternating inward and outward pumping, one convective loop formed.

References:

1. I. Ortiz-Rivera, et al., Convective flow reversal in self-powered enzyme micropumps, *PNAS,* **113**, 2585–2590 (2016).
2. S. Sengupta, et al., Self-powered enzyme micropumps, *Nat. Chem.*, **6,** 415-422 (2014).