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

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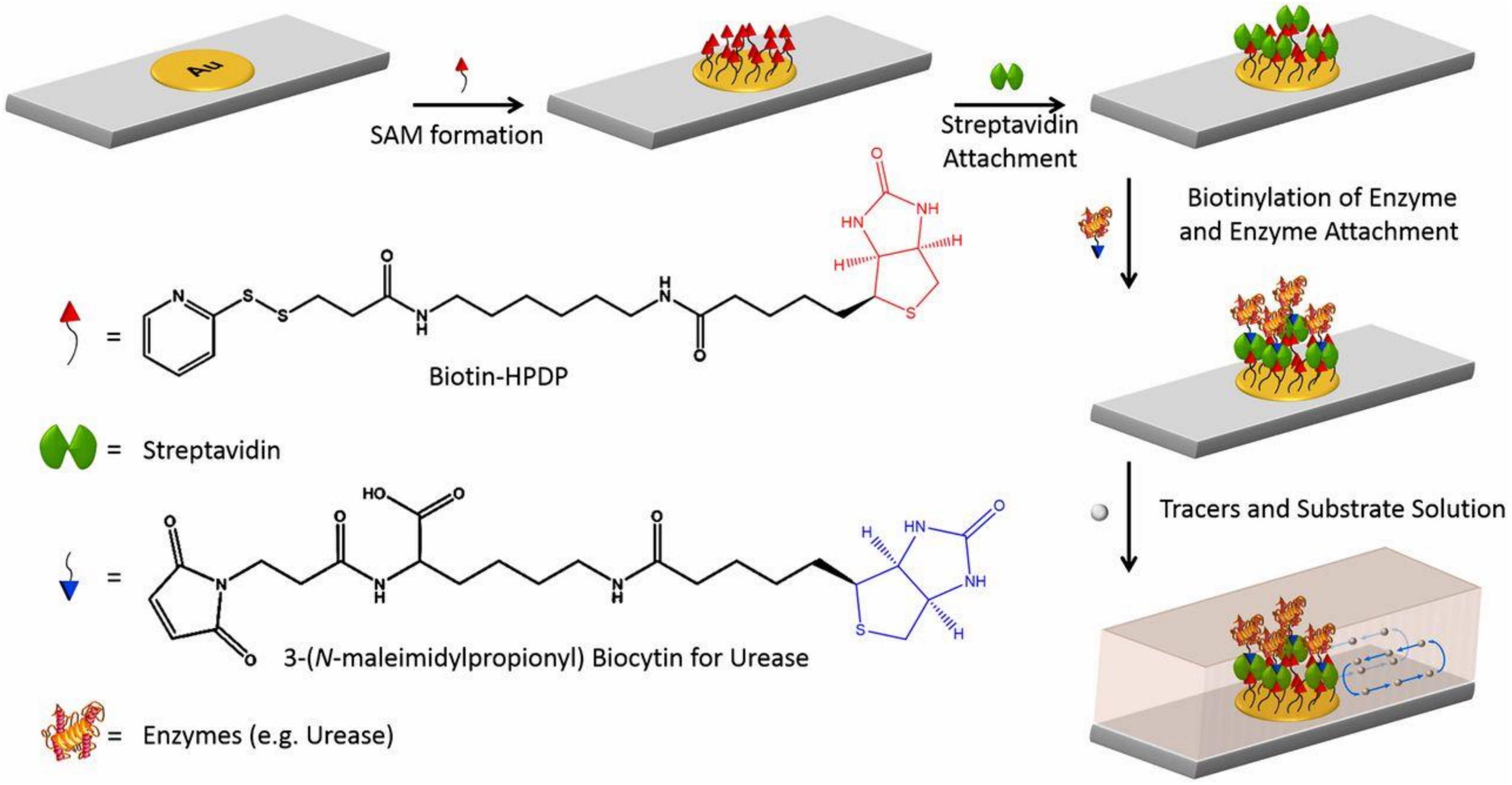
Introduction



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

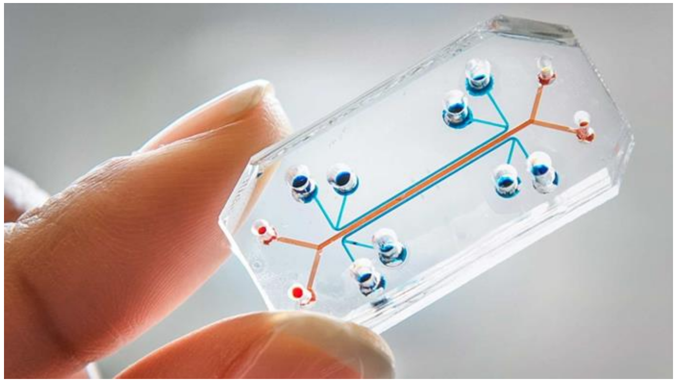
Motivation

Use for micropumps

- Microfluidic devices
- Non-pressurized fluid flow

Future direction (multi-pumps)

- Imitation of biological systems
- Sensors
- Stimuli-response systems



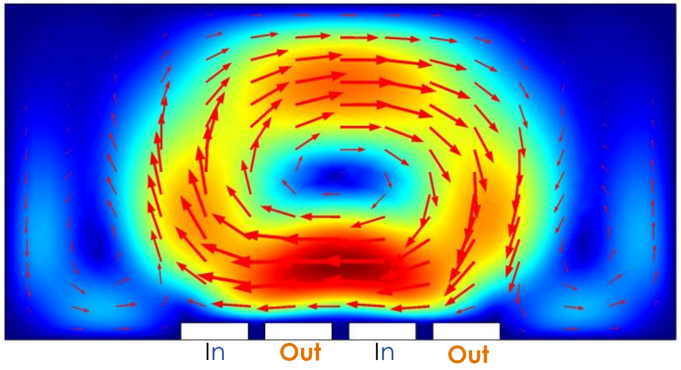


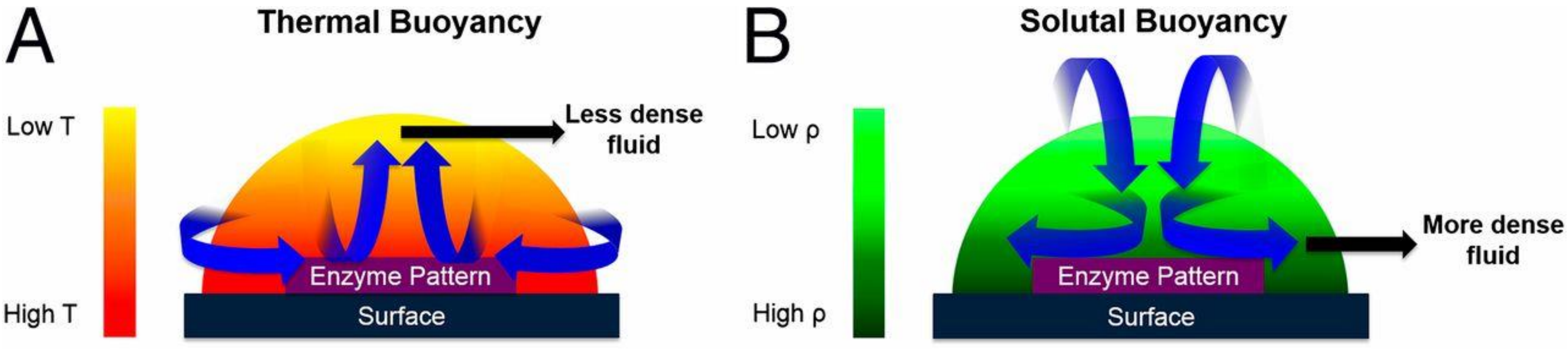
Image Source: http://discovermagazine.com/media/Images/Issues/2015/june/organ-chip.jpg

Enzymes as Micro-pumps

Thermally driven pumps

- Thermal coefficient of expansion
- Inward/outward

- Molar coefficient of expansion
- Inward/outward



Ortiz-Rivera, et al., Convective flow reversal in self-powered enzyme micropumps, PNAS, 113, 2585–2590 (2016).

Current Studies

Three parametric sweeps:

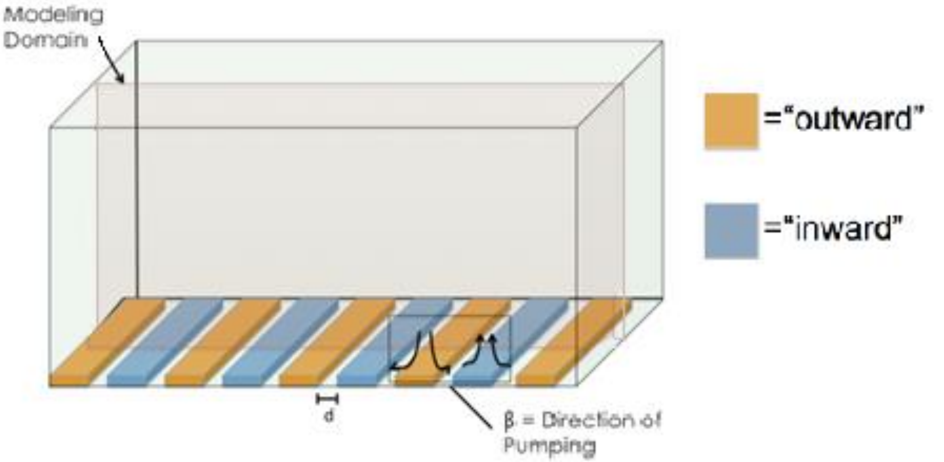
- Distance between pumps (d)
- Ratio of reaction rates (R)
- Direction of individual pumping (β)

$$d = Interpump\ distance$$

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

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

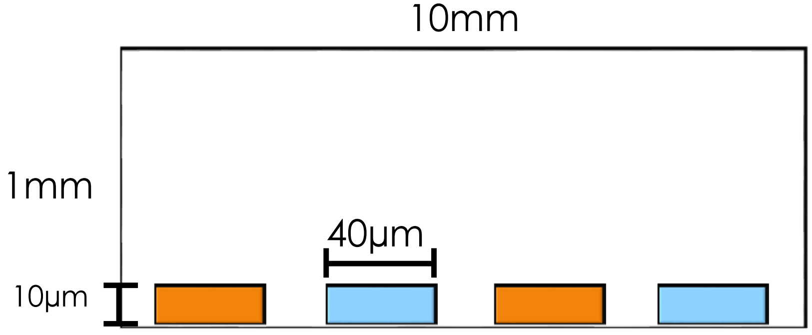
The goal is to create a directed flow within the multi-pump system.



Modeling Procedures

Physics modules used:

- 0-Dimensional chemical engineering to space dependent model in a simplified 2-dimensional system
- Chemistry
- Transport of diluted species
- Laminar (creeping) flow



*Not Drawn To Scale

Equations

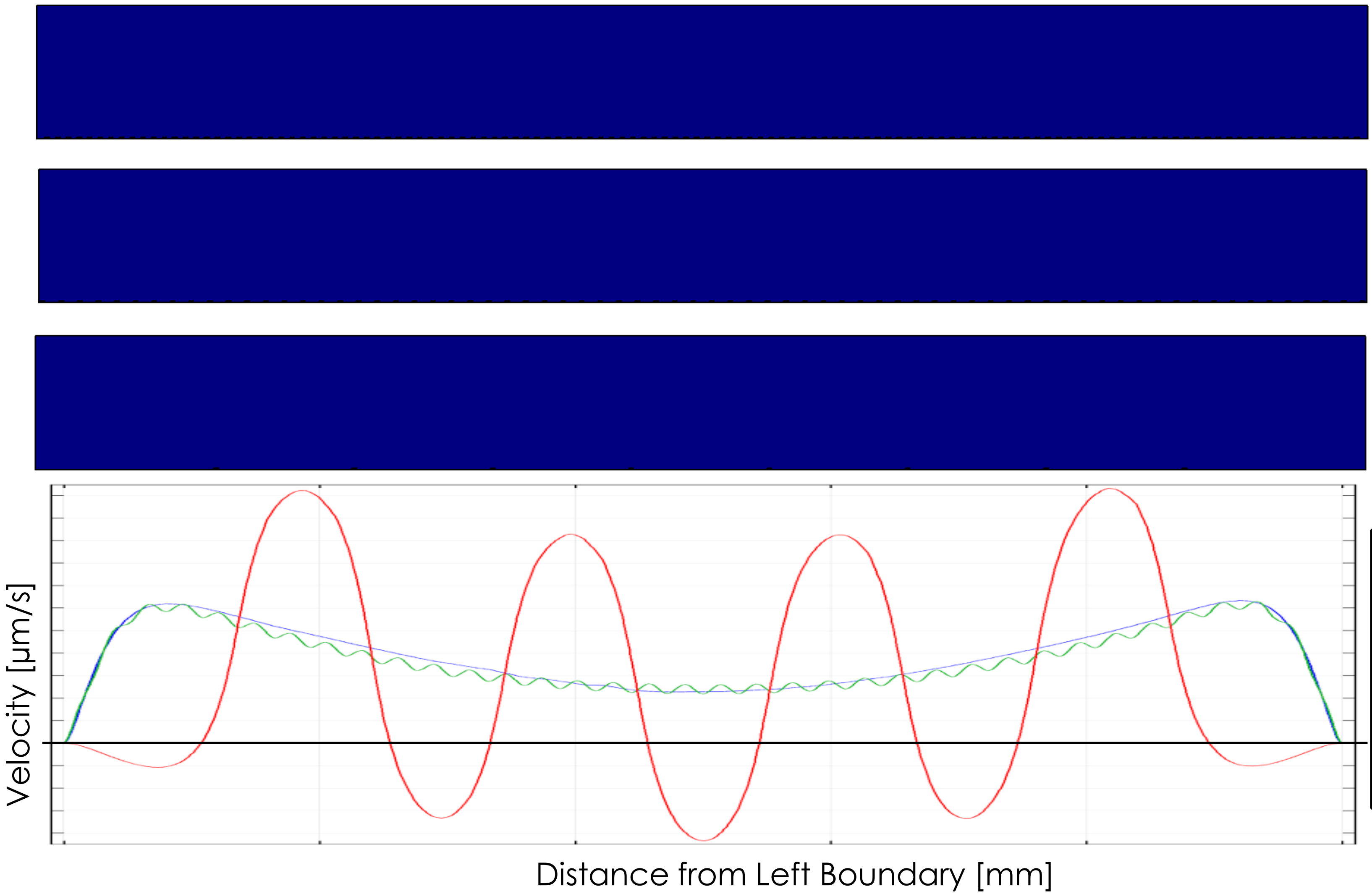
Boussinesq approximation of the Navier-Stokes equation:

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

$$F = -\rho_0 \bar{g} \left(\sum \beta_{species} c_{species} \right)$$

$$\nabla \cdot \mathbf{u} = 0 \qquad Re = \rho \mathbf{u} L / \mu$$

Results: Spacing



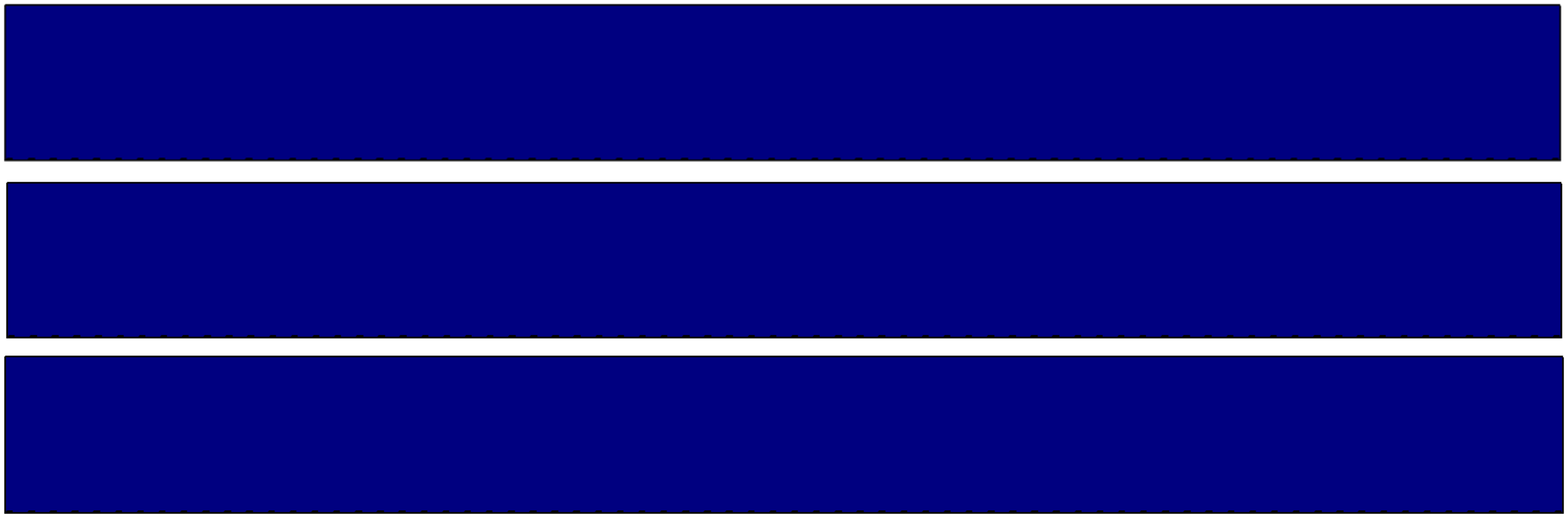
d = 40µm (Blue)

d = 100µm (Green)

d = 1000µm (Red)

Constant parameters:
- R=1
- First Pump= Outward
- Last Pump = Inward
- t=100min

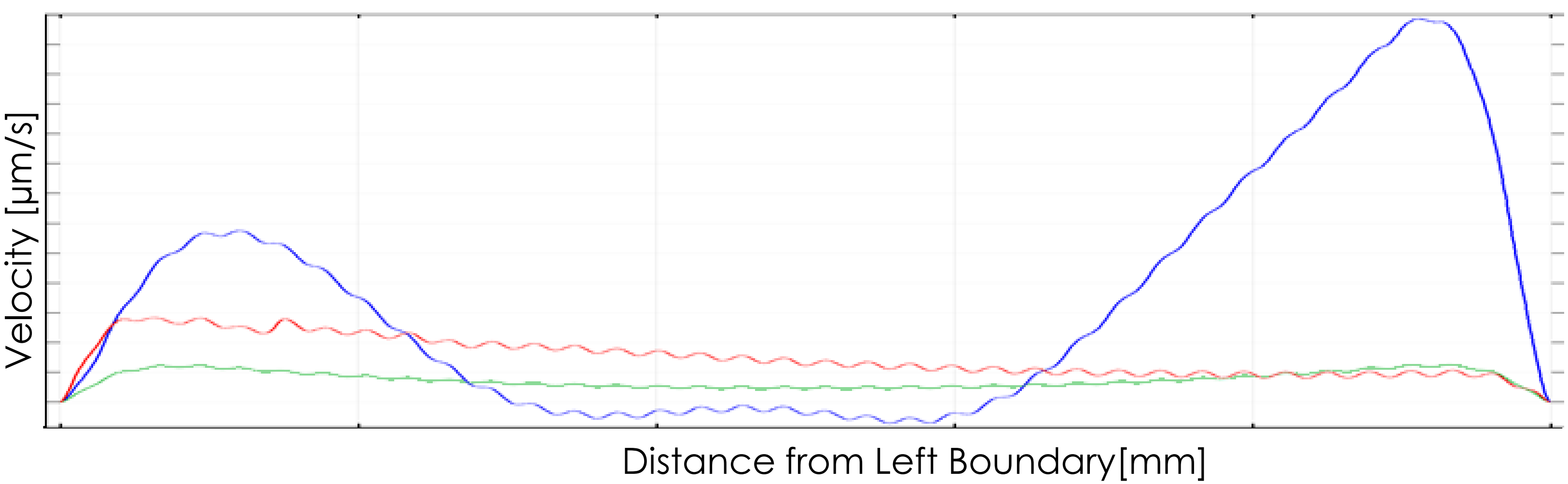
Results: Ratio of Reaction Rates



R = 0.2 (Blue)

R = 1 (Green)

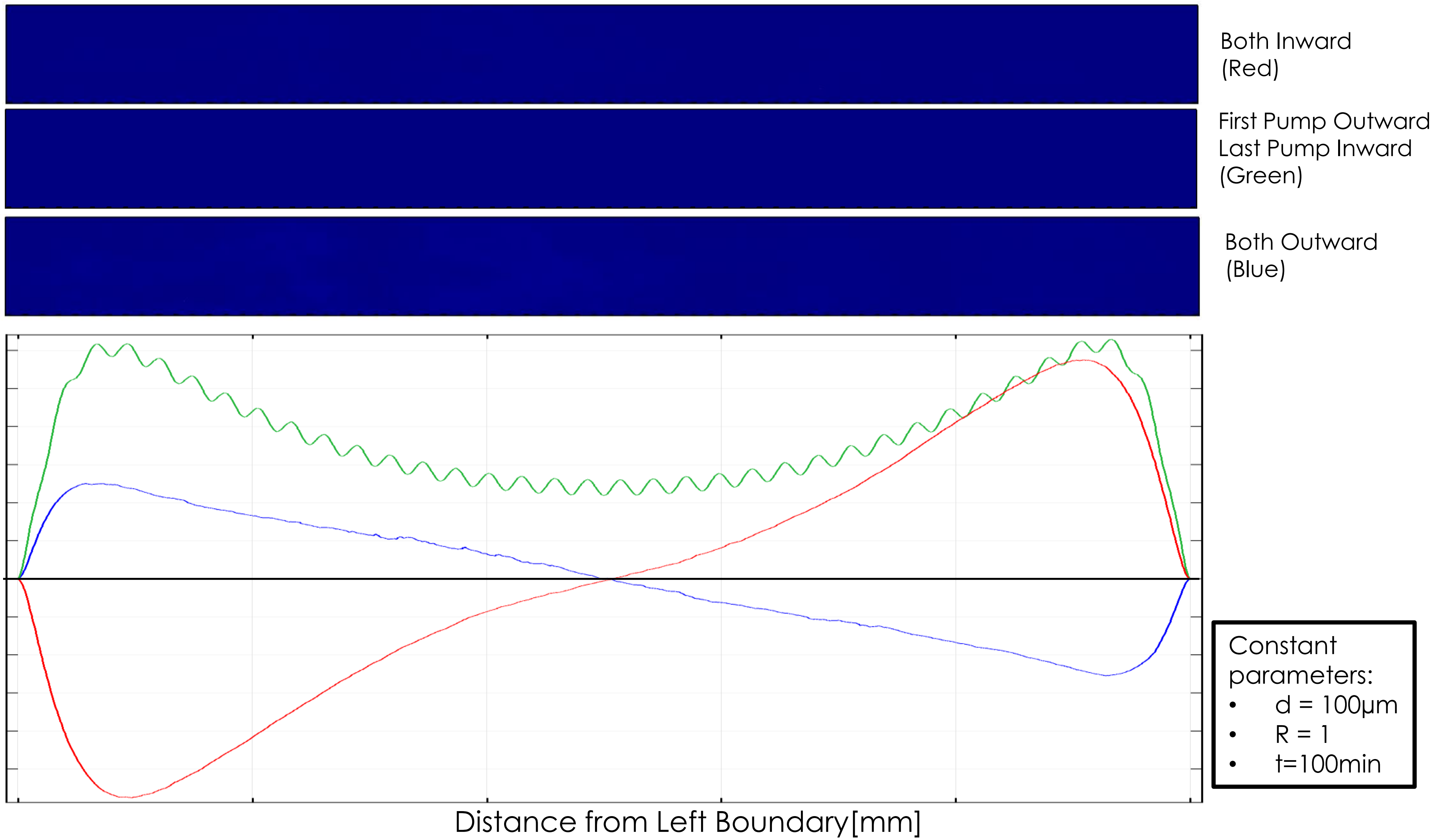
R = 5 (Red)



Constant parameters:

- d = 100µm
- First Pump= Outward
- Last Pump = Inward
- t=100min

Results: Direction of Pumping



Constant parameters:

- d = 100µm
- R = 1
- t=100min

Conclusions

Multi-pump system shows continuous long-distance flows under the following conditions:

- Small spacing between pumps
- Reaction rate ratio of 1
- Alternating inward/outward pumps

Acknowledgements

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Thanks to:

- Dr. Ayusman Sen and Dr. Thomas Mallouk
- Alicia Altemose, Erik Jewell, and Allan Brooks

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More Equations

Transport of dilute species:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) + \vec{u} \cdot \nabla c_i = R_i$$
$$N_i = -D_i \nabla c_i + \vec{u} c_i$$

Reaction rate calculations:

$$R_i = \frac{r_{max,i} c_i}{(K_{m,i} + c_i)} \ where \ K_{m,i} = 1000[um]$$
$$r_{max,i} = E k_{cat,i} M$$
$$where \ E = Concentration \ of \ Enzymes \ on \ Patch,$$
$$M = Number \ of \ Active \ Sites \ per \ Enzyme$$
$$k_{cat,A} = 5E6 \left[\frac{1}{s}\right] * R$$
$$k_{cat,B} = 5E6 \left[\frac{1}{s}\right] * \left(\frac{1}{R}\right)$$

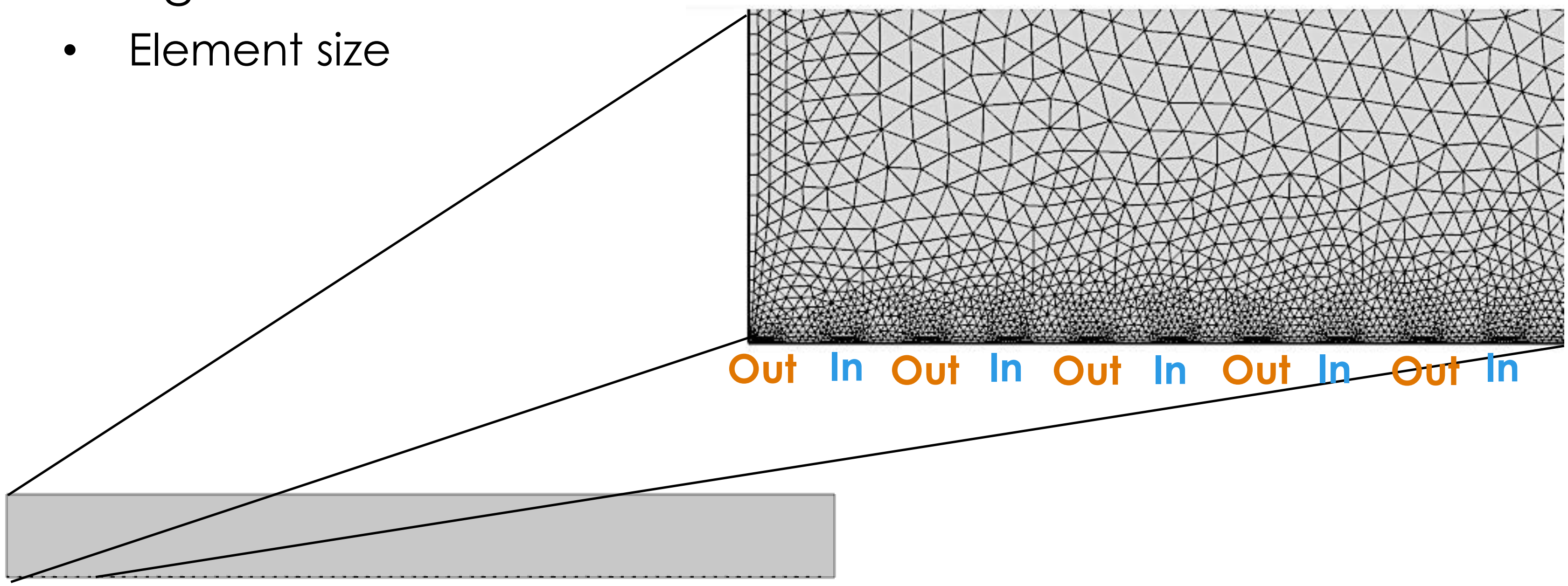
More Modeling Procedures

Geometry

- Dimensions
- Even number of pumps

Meshing

- Element size



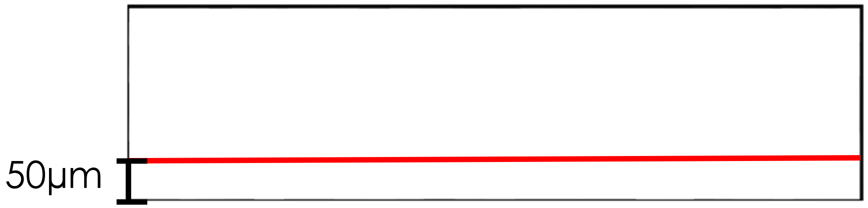
Post-Processing

Arrow surface

- Direction vectors of velocity
- Scaled by a factor of ~2000

Constant parameters

- Distance between pumps (d)=100μm
- Pump A outward/pump B inward
- Ratio of reaction rates (R)=1



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