Simulation of chaotic mixing dynamics in microdroplets

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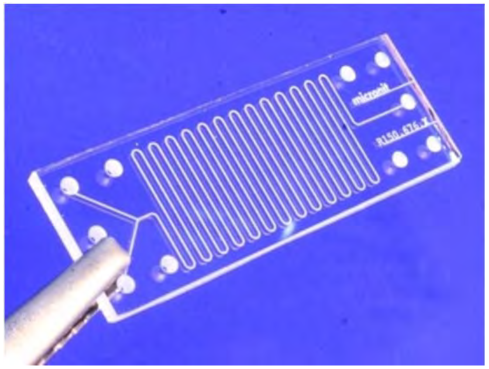
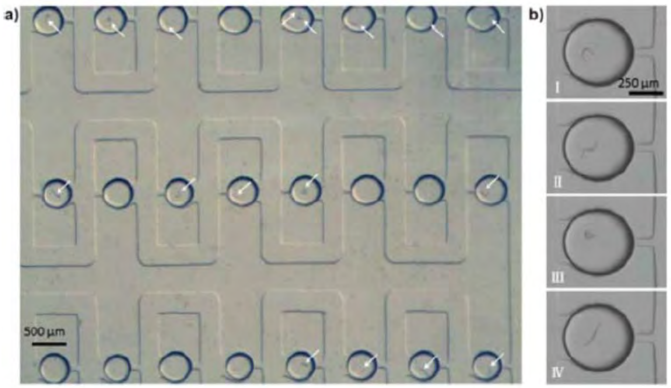
Microfluidics and Microdroplets

Microfluidics deals with the behavior, precise control and manipulation of fluids that are geometrically constrained to a small, typically sub-millimeter, scale.



----A definition from wikipedia

In microfluidics, microdroplets are widely used as discrete 'container' for forming isolated circumstance and precisely manipulating.



Instead Of

W. W. Shi, J. H. Qin, N. N. Ye, B. C. Lin, Lab Chip 2008, 8, 1432.

Rapid Mixing in droplets

Rapid mixing is of essential importance in many microfluidic applications such as chemical reactions, drug delivery, sequencing or synthesis of nucleic acids, protein crystallization, etc.

However, it is difficult to mix fluids in microchannels since flows in these channels are generally laminar and molecular diffusion is usually insufficient to mix fluids:

$$t_D = \frac{w^2}{D}$$

w is characteristic length, *D* is diffusivity (~10^{-9} m^2/s)

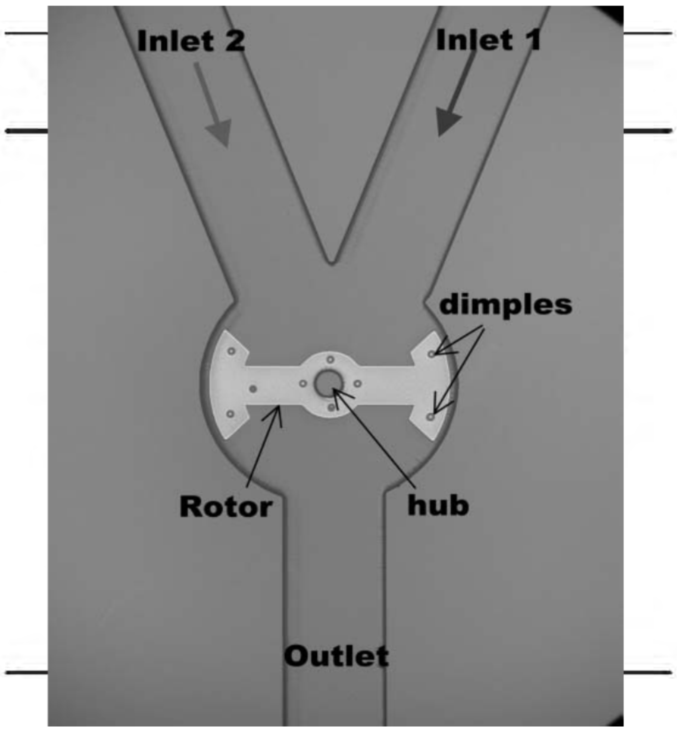
How ?

increase the interfacial surface area and reduce the striation length

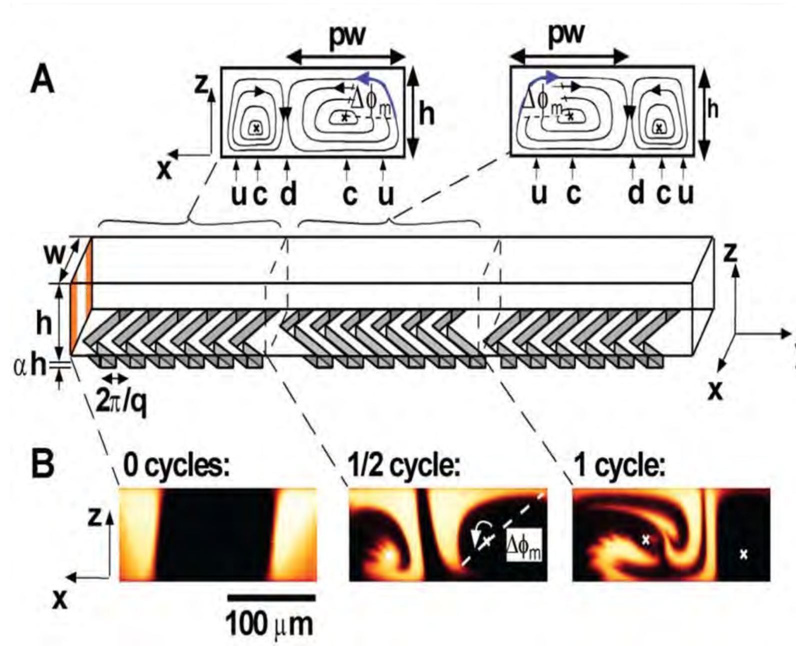
chaotic mixing

Existing Methods

The mixing principles can be divided in two classes: passive and active mixing, relying either on the pumping energy or provision of other external energy to achieve mixing.



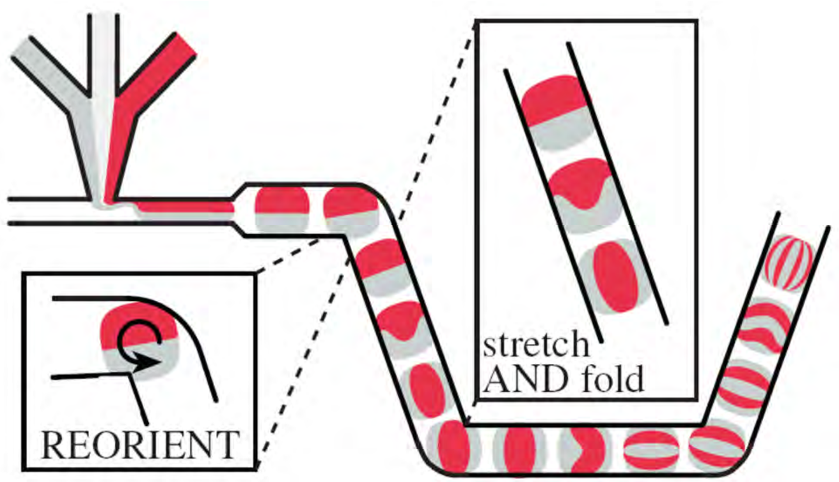
active mixing



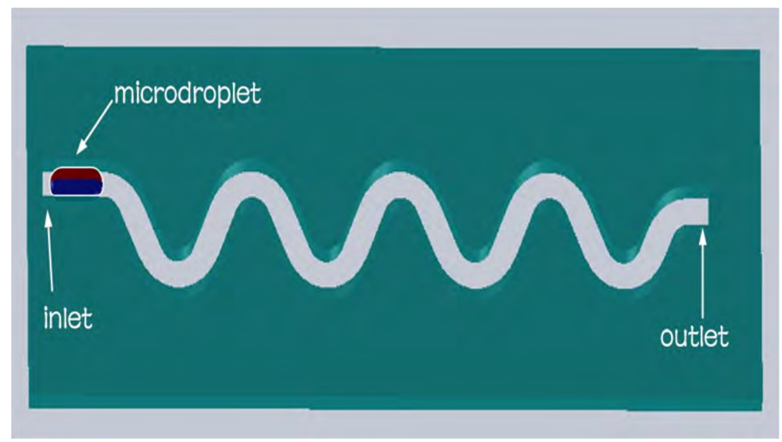
passive mixing

Serpentine microchannels

Using a combination of turns and straight sections, serpentine microfluidic channels could create unsteady fluid flows that rapidly mix the multiple reagents contained within droplets (through decreasing striation thickness).



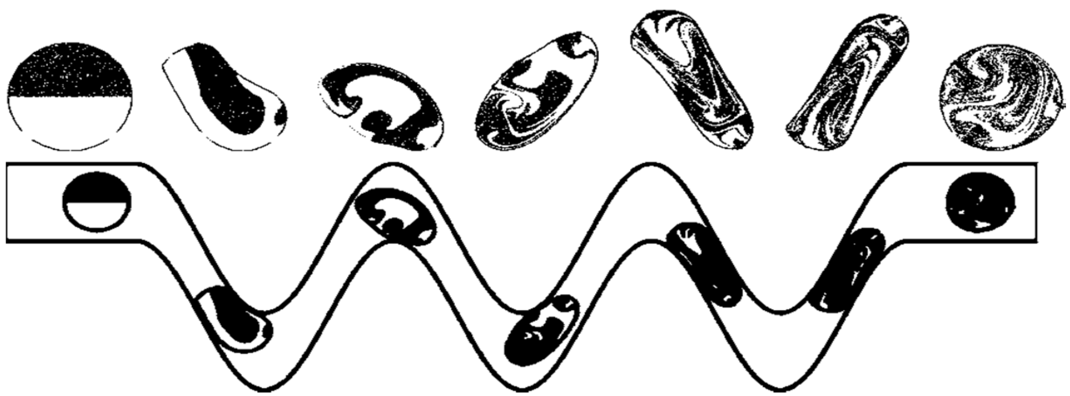
baker's transformation



Serpentine microchannel that we studied

Current Progress

Most of related works used particles tracing method and molecular diffusion effect were omitted.



Metin Muradoglu, Howard A. Stone,PHYSICS OF FLUIDS 17, 073305 2005

Until now, reports that directly compare simulation with experimental results in microdroplets have not been found.

Physical models

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{u} \right) = 0$$

continuous equations

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho(\vec{u} \cdot \nabla)\vec{u} = -\nabla p + \nabla \cdot (\mu \nabla \vec{u}) + \vec{F}_{st} \qquad F_{st} = \sigma \kappa \delta_{\text{int}\,erface} \vec{n}$$

NS equations

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = \gamma \nabla \cdot (\varepsilon \nabla \phi - \phi(1-\phi)\frac{\nabla \phi}{\left|\nabla \phi\right|})$$

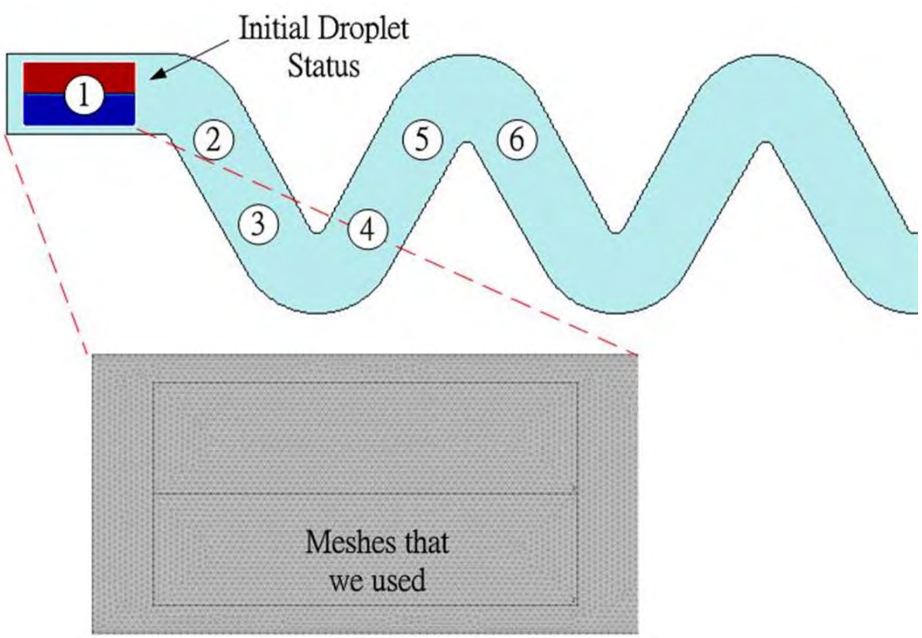
transport and reinitialization

$$\frac{\partial c_i}{\partial t} + \vec{u} \cdot \nabla c_i = \nabla \cdot \left(D_i \nabla c_i \right)$$

convection and diffusion equation

In COMSOL Multiphysics 4.1, Laminar two-phase flow level set model and transport of diluted species model could express the above equations.

Meshes and solving



Geometry and Meshes of the model

During mesh process, triangular meshes (with maximum size of 1.2 um) are adopted and boundary layer mesh is added to refine the grids near the walls.

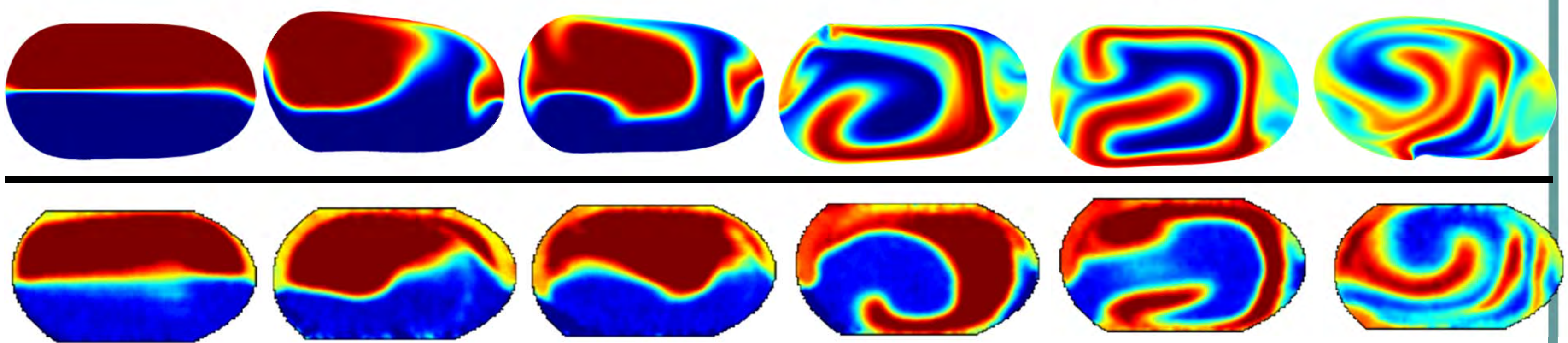
Then, the model with about 2e6 degrees of freedom were solved.

The model is sent to the computer server (HP ML370 G6) and assigned 20G RAM and 5 cores. The whole calculation process lasts 4 days.

Results and discussion

Simulation Results

Location: 1 2 3 4 5 6



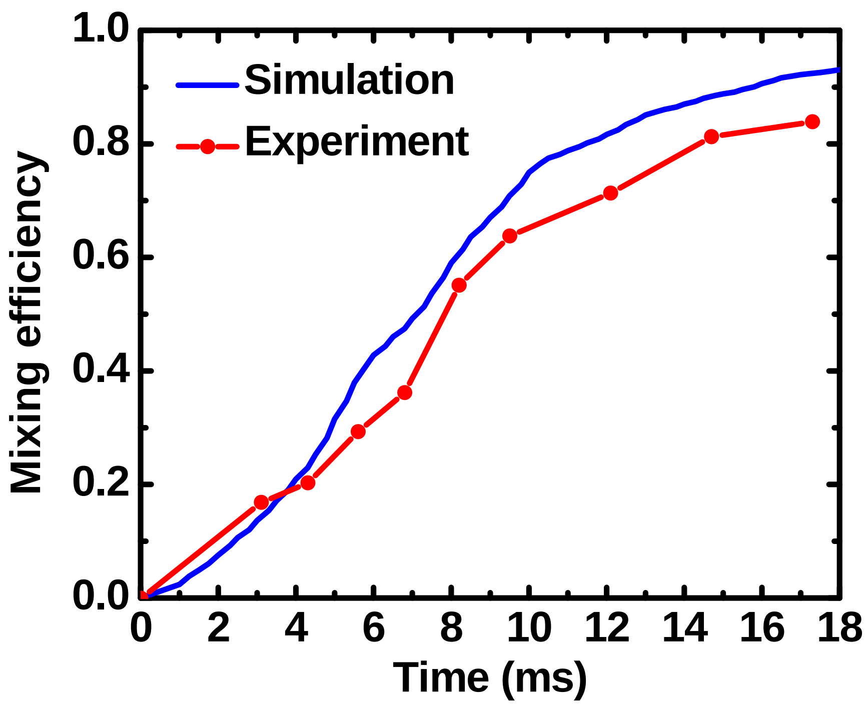
1 2 3 4 5 6

Experimental Results *Jiang et al. 2011 submitted*

Baker's transformation could be observed in the simulation results.
The simulation and experimental results matches well.

Results and discussion

In order to characterize the mixing efficiency in droplet more precisely, we calculate the mixing efficiency during droplet along the serpentine channel,



Mixing efficiency within a droplet along the serpentine channel

Mixing efficiency is defined as:

$$M_i = \left(1 - \frac{\int_A |c_i - c_\infty| dA}{\int_A |c_0 - c_\infty| dA}\right)$$

where c_i is the concentration distribution of species i, c_0 is the initial concentration, c_∞ is the concentration of complete mixing

Conclusion

➢We performed 2D numerical simulation to directly visualize millisecond chaotic mixing dynamics inside microdroplets moving through a serpentine channel.

➢The simulated patterns clearly indicate the internal mixing process within droplets moving along serpentine channels. The mixing efficiencies of chaotic mixing, calculated from both experimental and simulation results, also show good agreement.

➢This work provides insight into mixing dynamics in droplet-based microfluidic devices, and will serve as a promising diagnose tool for real-time monitoring of biochemical reactions in lab-on-a-chip systems.

Thanks

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Thanks for your attention!