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Chaotic Advection-Driven Mixing in Unsteady Three-Dimensional MHD Flows in Microfluidic Devices

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229th ECS Meeting, San Diego, May 29-Jun 2, 2016



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Outline

- Motivation
- Problem Description
- Technical Highlights
- Results
- Discussion
- Conclusions
- Ongoing and Future Work





Motivation

- Speed of chemical reactions is dictated by mixing efficiency
- Low Reynolds number (~1) makes mixing a challenge
- Introducing Turbulent-like features can enhance mixing
- Chaotic advection provides foundation for analysis and control
- Simulations based on Navier-Stokes equations provide many insights
- Powerful post-processing tools help understand underlying mixing phenomena
- Simulation results can help develop new mixing and flow control strategies



- Stirring vs. mixing: An important distinction
- Stirring increases the mean value of gradients
- Mixing decrease the mean value of gradients
- Stirring leads to stretching and folding of the interface
- Chaotic advection is an efficient way of stirring
- Mixing is complete when the gradients disappear



- MHD can introduce a non-intrusive driving force
- Lorentz force $\overline{j} \times \overline{B}$ for MHD is due to ionic currentmagnetic field cross product
- Flow field and species concentration fields are obtained by solving unsteady, 3D Navier-Stokes equations
- Extensive post-processing is performed to visualize the results and obtain mixing quality
- Passive numerical particles are tracked by integrating the

advection equation

$$\frac{dX}{dt} = \overline{V}(\overline{X}, t)$$



Cell geometry

Shallow open cell $r_1 = 3mm$ $r_2 = 2.4 mm$ $r_3 = 2mm$ $r_d = 0.16 mm$ H = 0.5 mm



NaCl solution: ρ = 1000 kg/m³, μ = 0.001 kg/(m.s), C^{*} = 0.1M, ϕ = 0.04 V, σ = 1.29 S/m. Magnetic field: B_z = 0.36 Tesla



Problem Description Governing Equations

Continuity: $\nabla \cdot \mathbf{V} = 0$

Momentum:

$$\rho \frac{D\mathbf{V}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{V} + \mathbf{F}_{\mathrm{L}}$$

Lorenz Force: $\mathbf{F}_{\mathrm{L}} = -\sigma \nabla \phi \times \mathbf{B}$

Electric Field Outside Double Layer:

$$\nabla^2 \phi = 0$$

Auxiliary Equations

Passive Particle Trajectory:

etory:
$$\frac{d\mathbf{X}(t)}{dt} = \mathbf{V}(\mathbf{X}, t)$$

 $\alpha(t) = 1 - \frac{\delta^2(t)}{\delta^2(0)}$

MixingPerformance:

$$\delta^{2}(t) = \iiint \left[C(x, y, z, t) - \overline{C} \right]^{2} dx dy dz$$

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 $3^{+10^{+}}$

2nd order, implicit

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = F(\phi^{n+1})$$



Gouy-Chapman Model for Double Layer







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Switching Scheme 1

$$\phi_{A} = 0.04V \quad \phi_{C} = 0 \quad kT < t < kT + \frac{T}{2}$$
$$\phi_{A} = 0 \quad \phi_{C} = 0.04V \quad kT + \frac{T}{2} < t < (k+1)T$$



Switching Scheme 2

$$\phi_{A} = 0.04V \quad \phi_{C} = -0.04V \quad \nabla \phi_{B} = \nabla \phi_{D} = 0 \quad kT < t < kT + \frac{T}{2}$$
$$\nabla \phi_{A} = \nabla \phi_{C} = 0 \quad \phi_{B} = 0.04V \quad \phi_{D} = -0.04V \quad kT + \frac{T}{2} < t < (k+1)T$$

$$k = 0, 1, 2, 3, \dots$$



• Scheme 1, Scheme 2

Velocity vectors Velocity profiles Potential contours Current lines Poincaré maps Mixing performance

• Scheme 2

...+

Particle concentration maps Species concentration contours Material line deformation

Observations





(d)

Scheme 1

(a) Velocity vectors
(b) Velocity profile
(c), (d) Potential contours and current flux lines
(c: z = 0.4 mm plane,
d: y = 0 plane)





Scheme 1 Poincaré maps z = 0.4 mm

Number of periods are shown in parentheses



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Scheme 1

Evolution of mixing quality vs. time *t* for 5 values of T in plane z = 0.4 mm





Scheme 2

- (a) Velocity vectors
- (b) Velocity vectors
- (c), (d) Potential contours and current flux vectors and lines (c: z = 0.4 mm plane, d: y = 0 plane)





 \mathbf{a}



Scheme 2. *T* = 4s, *t* = 200s z = 0.4 mm plane.

- (a) Poincaré map
- (b) particle concentration map
- (c) species concentration contours
- (d) Stretching and deformation of two material lines.



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Scheme 2

Temporal evolution of mixing quality α and degree of mixing ϵ . T = 4s.



- Switching Scheme1 is a practical way to create the blinking vortex model
- Scheme 1 results are similar to those from the Stokes flow model
- Results from particles and material lines show that α increases with period T
- Switching Scheme 2 improves α over Switching Scheme 1
- The islands disappear faster in Scheme 2 compared to Scheme 1
- Each pair of disks is insulated during part of the cycle. No current on the disk, no vortical flow around the disk to isolate it



Conclusions and Future Work

- Even better mixing may be possible with more number of electrodes
- Optimal geometric placement and judicious choice of switching schemes may further improve mixing.
- Islands disappear faster with the electrodes insulated during part of the cycle
- The Navier-Stokes simulations show differences compared to the Stokes flow model for $Re_{H} >> 1$
- Good post-processing tools are necessary for analysis



Conclusions and Future Work

- Chaotic advection increases with increase with the dimension of the problem (no chaotic advection in 2D, and increases in the order: unsteady 2D and steady 3D, unsteady 3D
- Length scales and time scales have an influence on chaotic advection
- CFD simulations advance the modeling over potential flow and stokes flow
- Work on Transmission Line Equivalent Circuit (TLEC) model is in progress

