Simulation of Microscale Chemical Separation Processes Using the Lattice-Boltzmann Method

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MICRO-CATS ™

Introduction

■ The efficiency of chemical separation processes is enhanced in microscale systems due to the reduced diffusion length scales.

■ Phase interfaces (liquid-liquid, liquid-vapor, fluid-solid) play an important role in many of these processes. Surface tension and wettability can dominate flow behavior at micron length scales.

■ The objective of this work is to develop a simulation capability which can model microseparation processes, including interface behavior.

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Lattice-Boltzmann (cont)

- The density and velocity are calculated by

$$\rho = \sum_{i=0}^{b} f_i \qquad \rho u = \sum_{i=1}^{b} e_i f_i \qquad \rho_k = \sum_{i=0}^{b} g_i^{(k)}$$

- The equations of motion are

$$f_i(r + e_i, t + 1) = f_i(r,t) - \frac{1}{\tau_\rho} (f_i(r,t) - f_i^{eq}(r,t))$$

$$g_i^{(k)}(r + e_i, t + 1) = g_i^{(k)}(r,t) - \frac{1}{\tau_k} (g_i^{(k)}(r,t) - g_i^{(k)eq}(r,t))$$

where τ_ρ and τ_k are relaxation times.

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Equilibrium Distributions

■ **The equilibrium distributions f_i^{eq} and $g_i^{(k)eq}$ are given by**

$$f_i^{eq} = A + \frac{\rho D}{bc^2} e_i \cdot u + \frac{\rho D(D+2)}{2bc^4} u \cdot e_i e_i \cdot u - \frac{\rho D}{2bc} u \cdot u + G_{\alpha\beta} e_{i\alpha} e_{i\beta}$$

$$f_0^{eq} = A_0 - \frac{\rho}{c^2} u \cdot u$$

$$g_i^{(k)eq} = B^{(k)} + \frac{\rho_k D}{bc^2} e_i \cdot u + J_\alpha^{(k)} e_{i\alpha} + \frac{\rho_k D(D+2)}{2bc^4} u \cdot e_i e_i \cdot u - \frac{\rho_k D}{2bc} u \cdot u + H_{\alpha\beta}^{(k)} e_{i\alpha} e_{i\beta}$$

$$g_0^{(k)eq} = B_0^{(k)} - \frac{\rho_k}{c^2} u \cdot u$$

**where D is the dimension, b the number of lattice vectors and
c is the lattice constant.**

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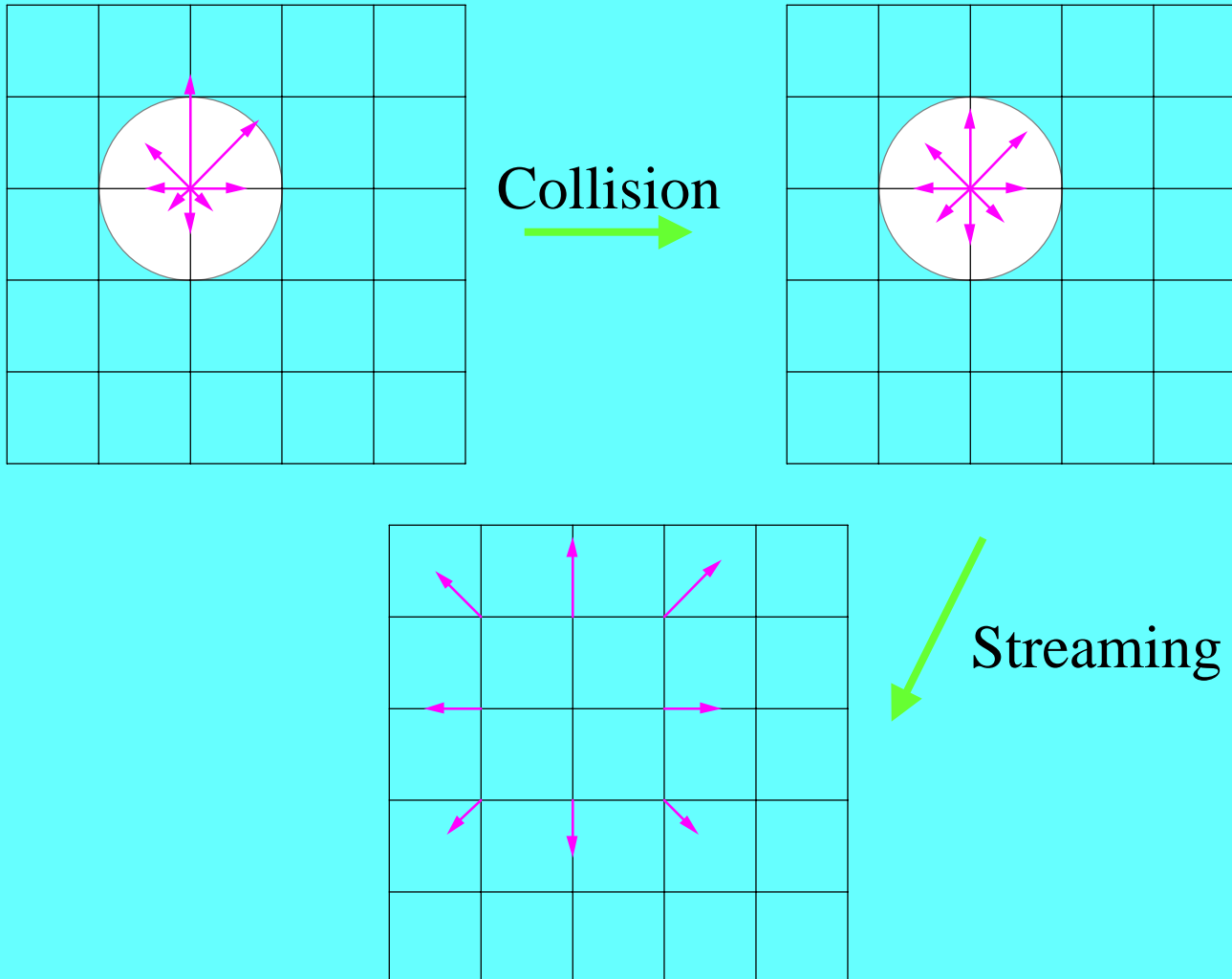**Pacific Northwest National Laboratory**

Solution Procedure

At each time step:

■ Stream particles from adjacent lattice points.

■ Calculate equilibrium particle distribution at each lattice point.

■ Collision - relax the distribution toward equilibrium values. The rate of relaxation is determined by the time step / viscosity.

Additional steps are required for boundary conditions, body forces, gradient terms, output processing, etc.

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Solution Procedure

Collision

Streaming

Model Features

- For single-phase, single-fluid systems:
  - 2nd order solution to the Navier-Stokes equation
  - Diffusion transport based on gradient of chemical potential

- For multi-phase, multi-component systems:
  - liquid-liquid and liquid-vapor interfaces are represented by a continuous density profiles which freely moves through the lattice grid.

- The wettability and adsorption of individual chemical species on solid surfaces are specified using surface-fluid potential gradients..

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Model Equation of State
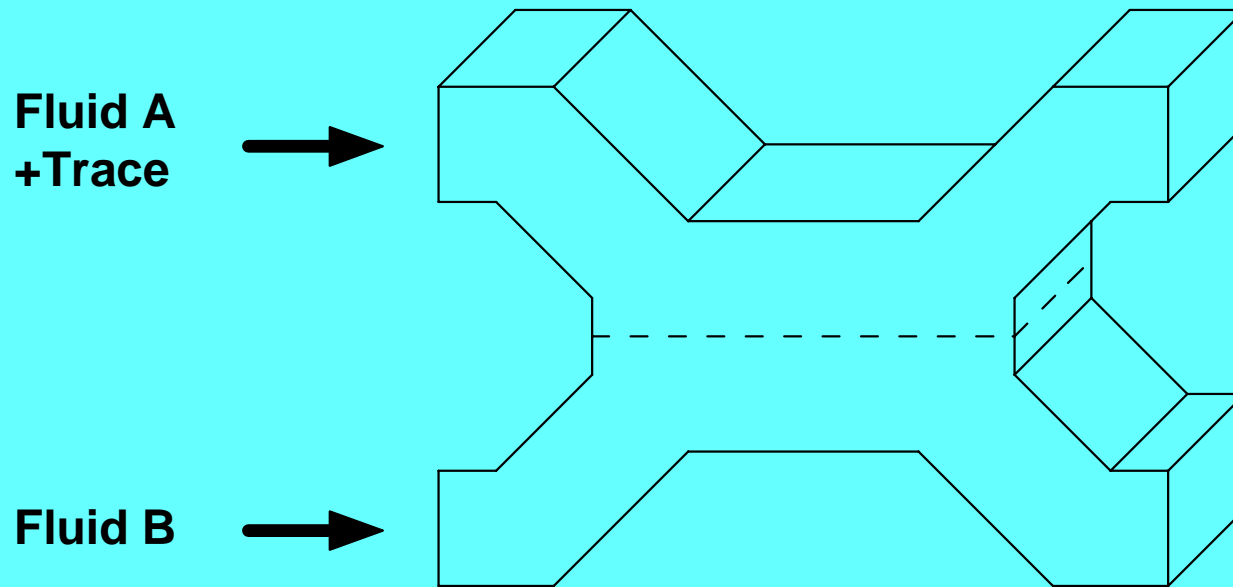
- The free energy functional has the Cahn-Hilliard form

$$\Psi = \int (\psi(T,\rho,\{\rho_k\}) + \kappa(\nabla\rho_1)^2 + \kappa(\nabla\rho_2)^2)dr$$
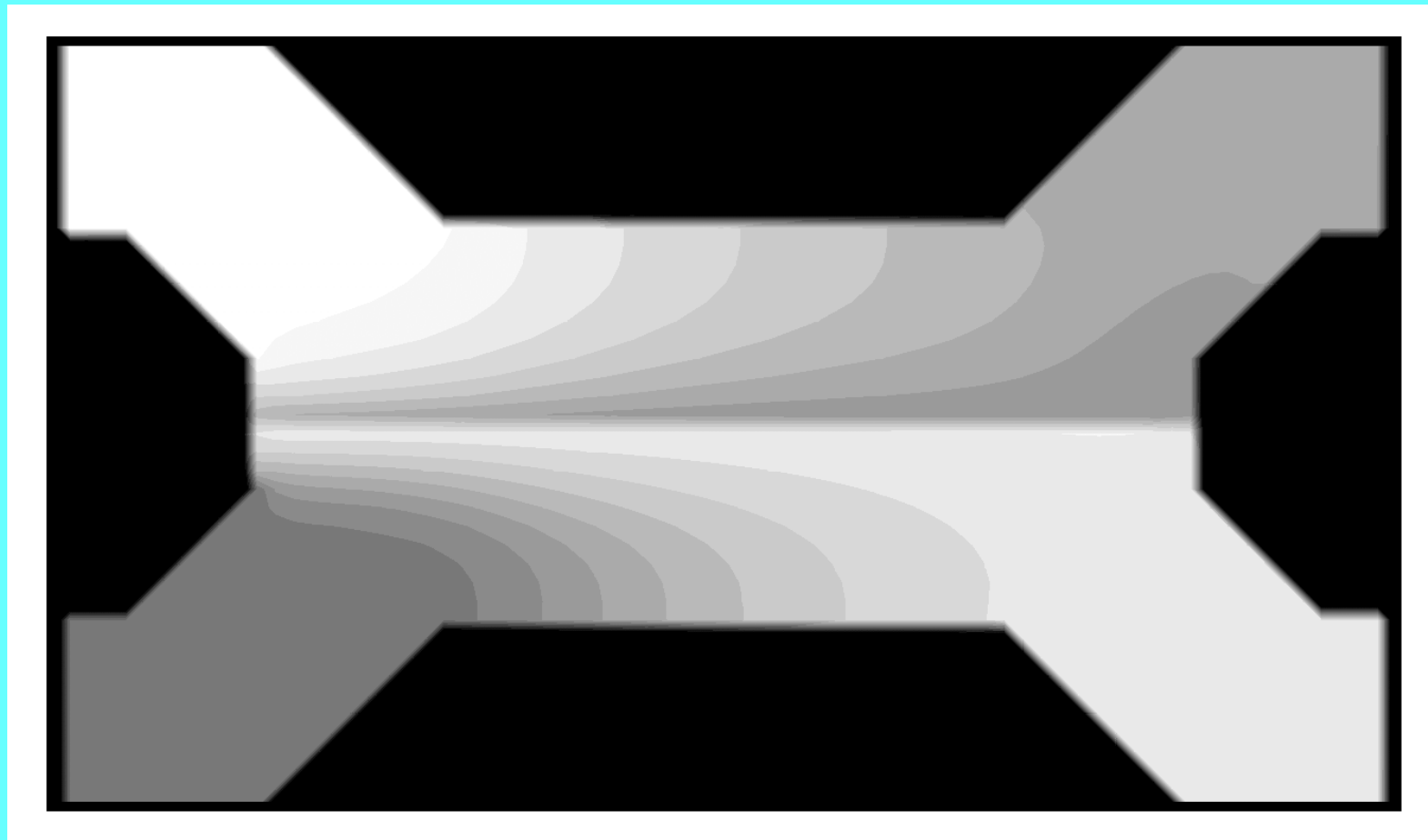
- The chemical potential for species k>2 is given by

$$\mu_k = kT\ln(\rho_k) - \alpha_k \frac{\rho_1}{\rho_1+\rho_2} - \beta_k \frac{\rho_2}{\rho_1+\rho_2}$$

where α and β control the affinity of the species for the two fluids.
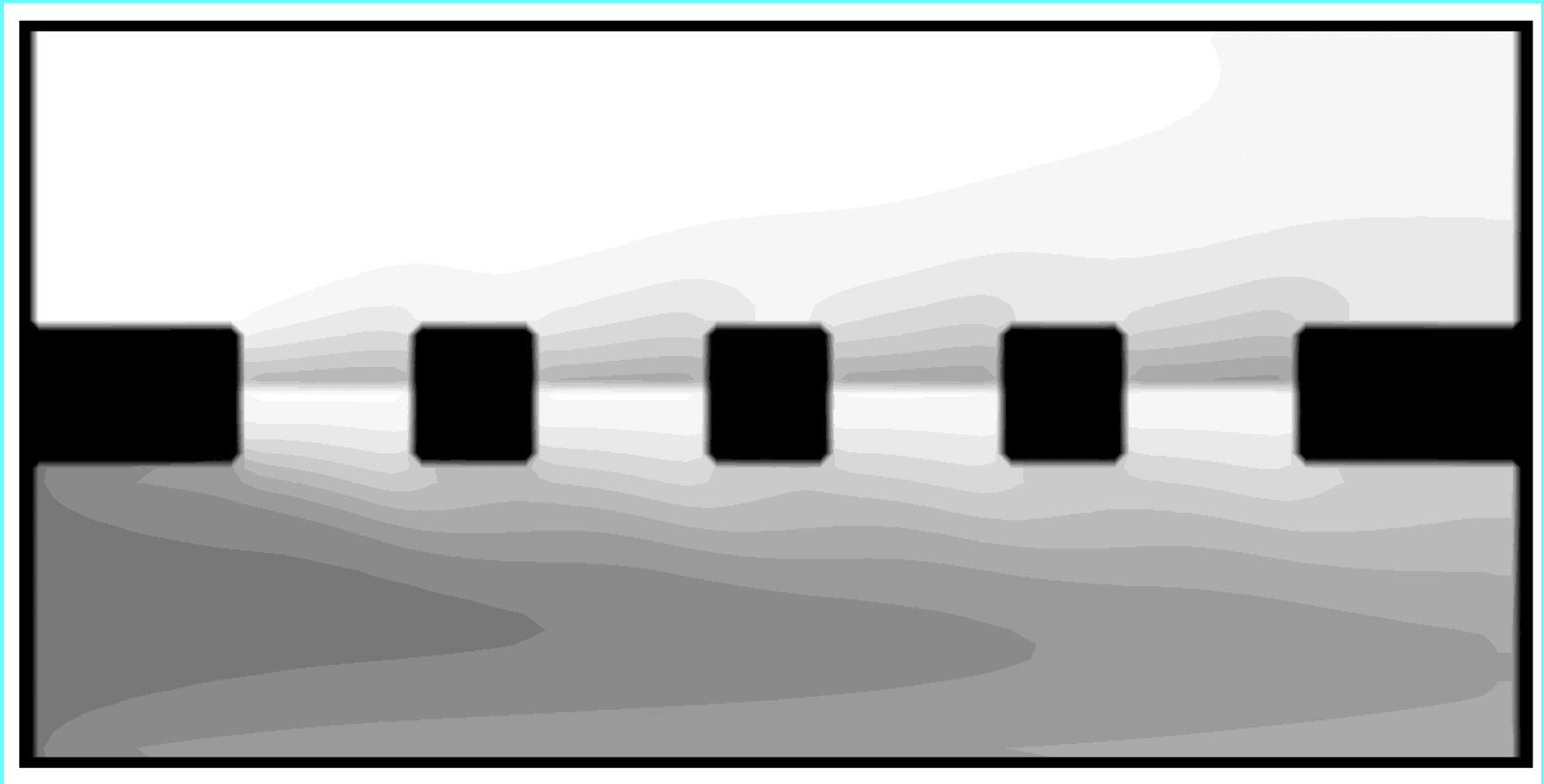
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Fluid-fluid Extraction (continuous film)
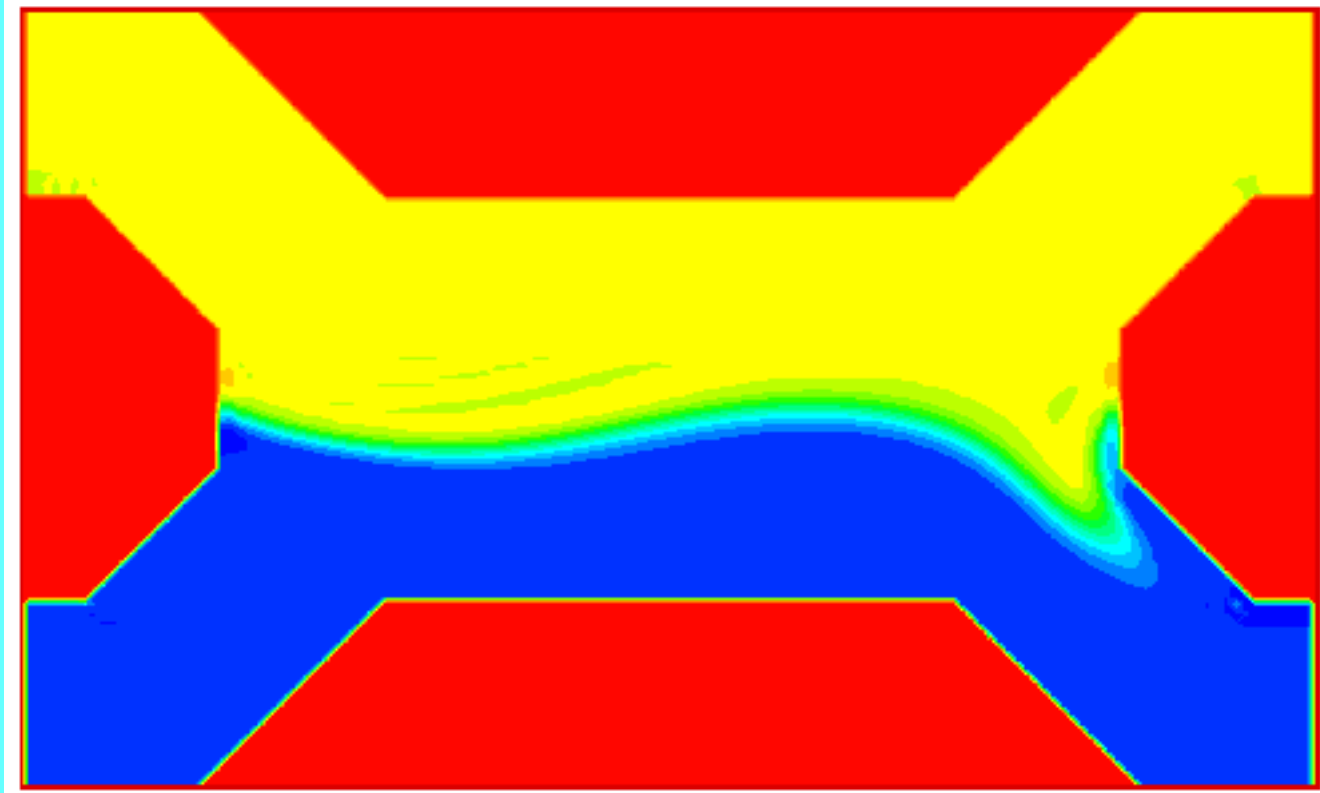
**Fluid A
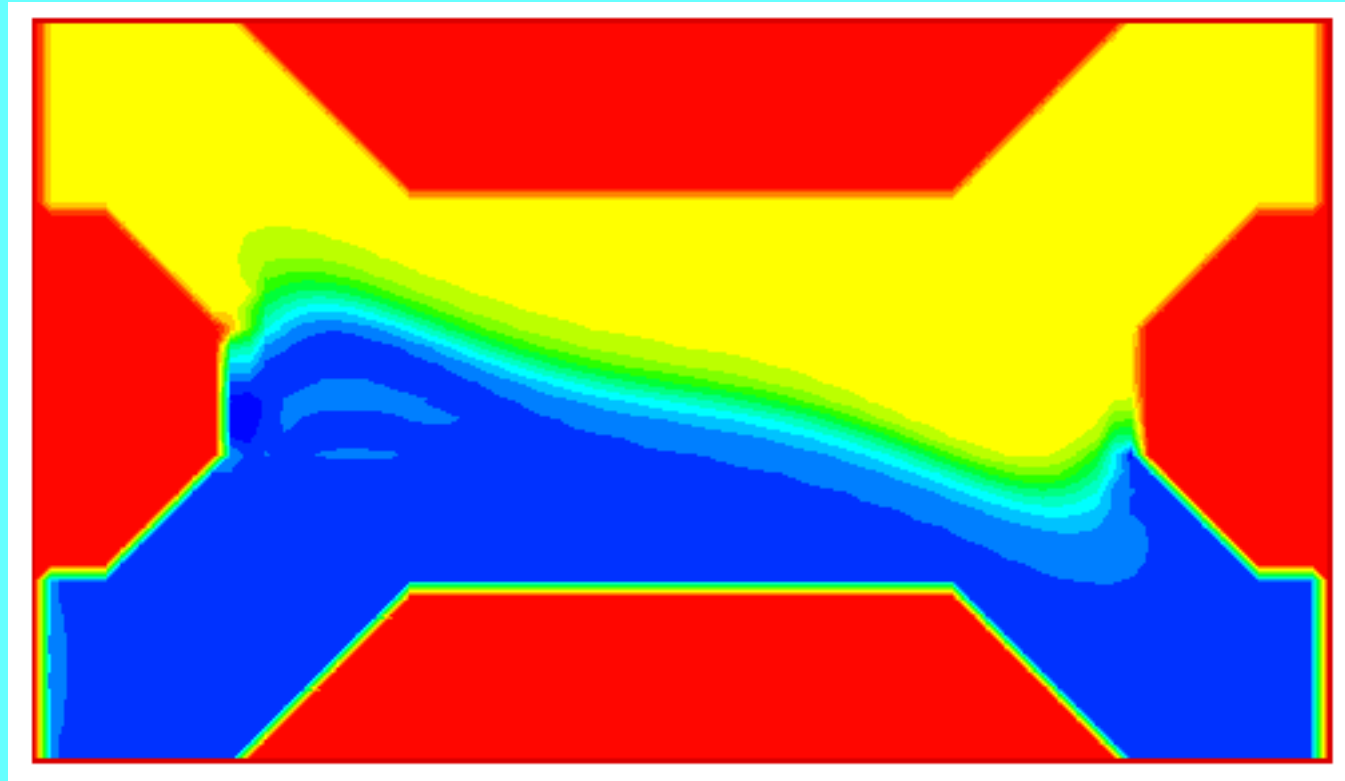+Trace** →

Fluid B →

Fluid-fluid Extraction (continuous film)

Fluid-fluid Extraction (contactor plate)

Pressure Differential (continuous film)

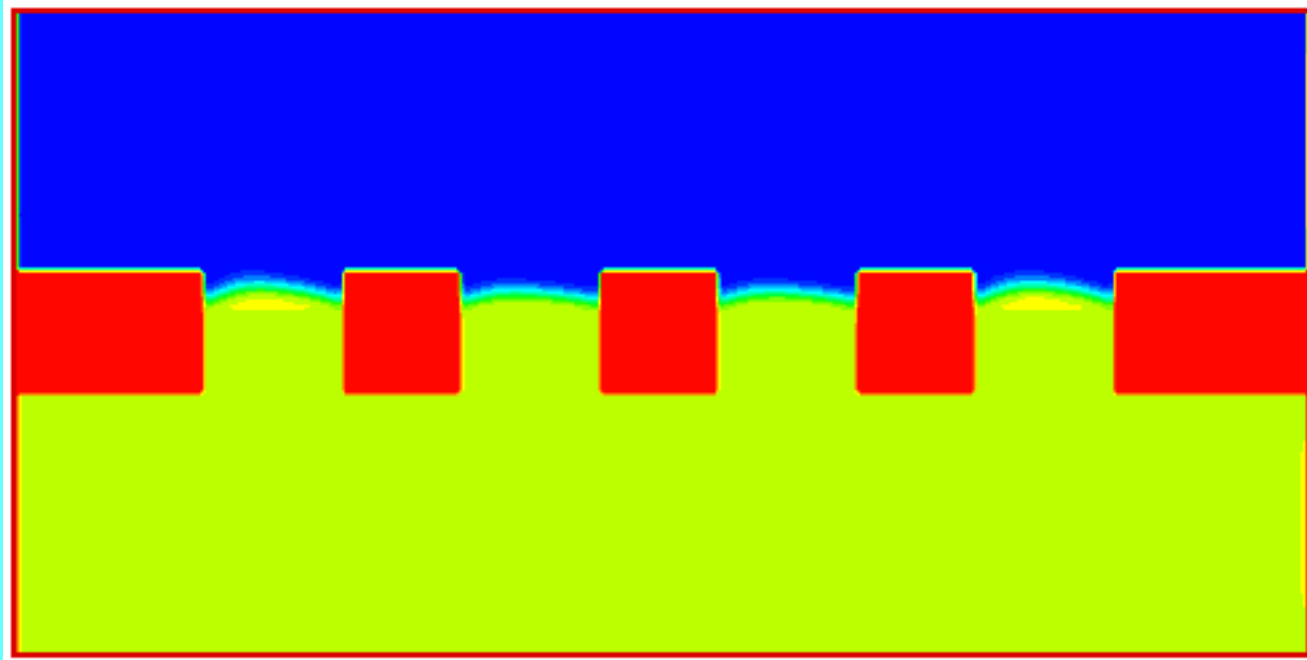# Countercurrent Flow (continuous film)

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Pressure Differential (contactor plate)
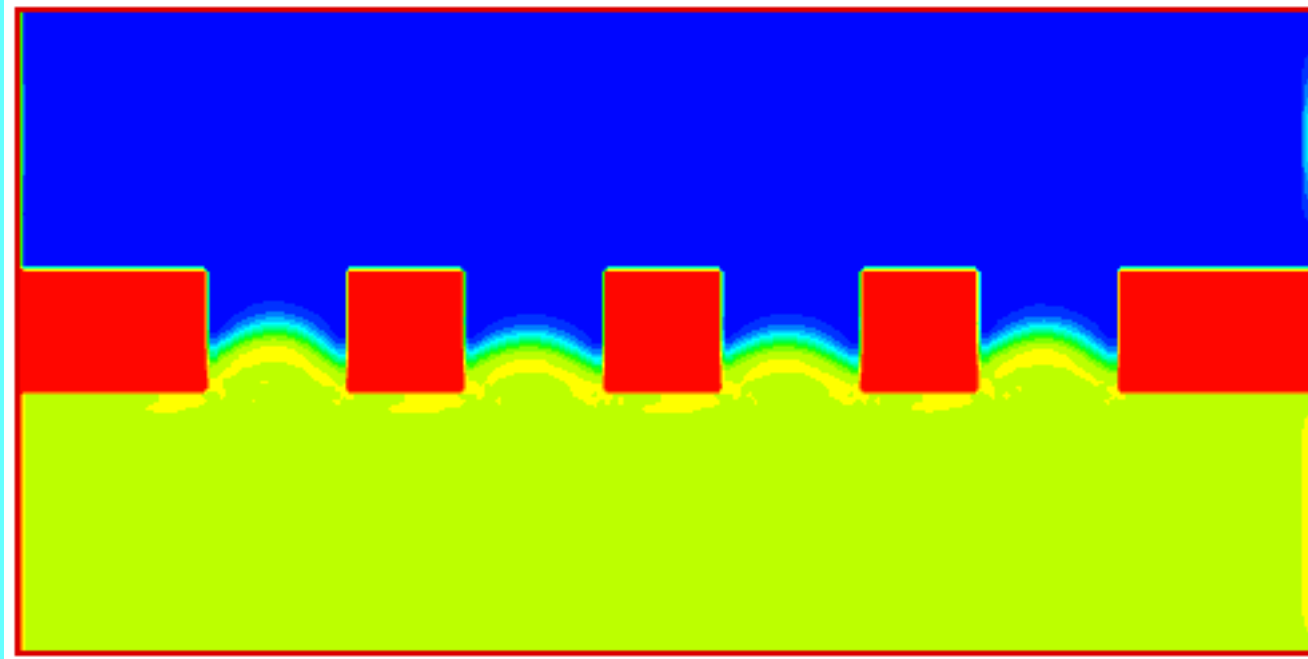
Breakthrough (contactor plate)

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Current Activities

- Simulation of other chemical separations processes
  - Distillation
  - Surface adsorption

- Verification and validation of lattice-Boltzmann simulation method

- Supporting the design of microseparation devices

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Conclusions

- A simulation capability has been developed which can model microseparation processes, including convection and diffusion transport.

- In addition, this method is used to model the dynamic interface behavior under different operating conditions. Issues such as interface stability and contactor plate breakthrough can be addressed using this approach.

- The usefulness of this method has been illustrated by simulating the behavior of model separation devices.