Numerical Studies of Segmented Flows in Micro-Channels for Bio-Analytical Chip Applications

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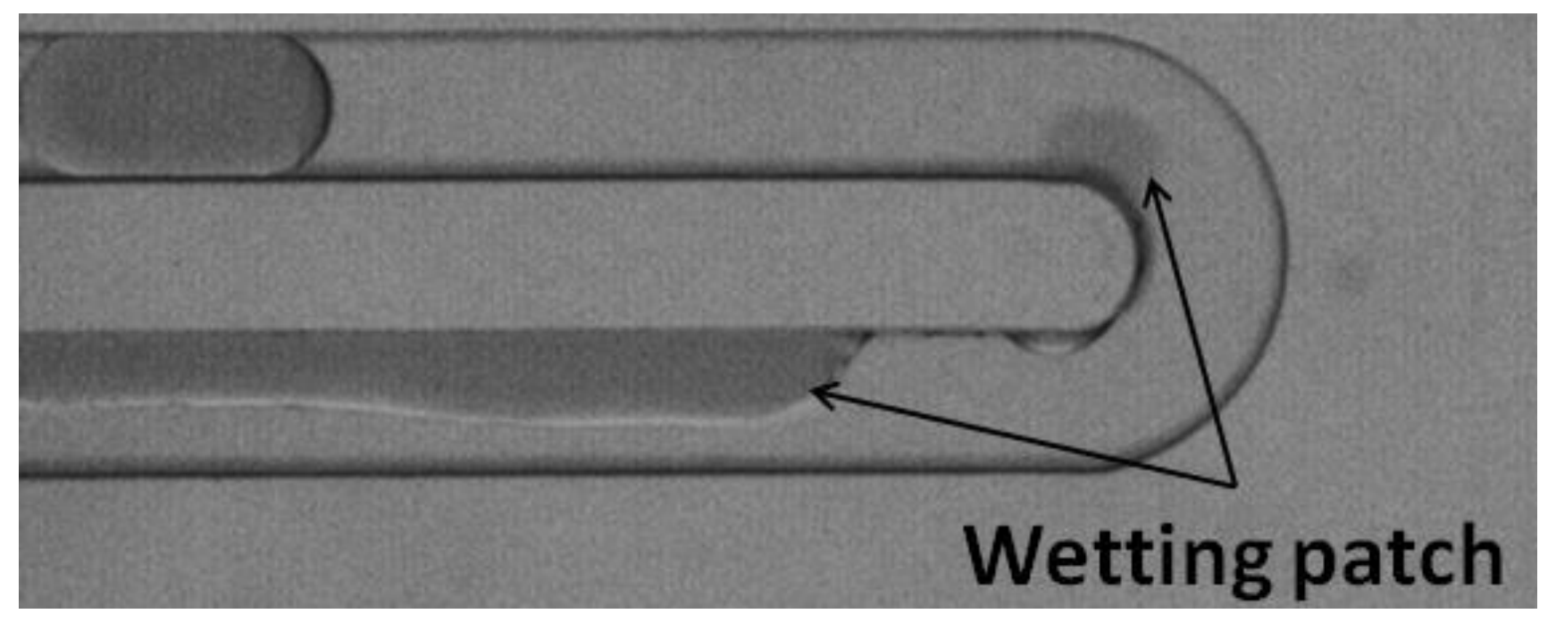
Background – Segmented Flows for Practical Applications

Segmented microflows (nanoliter-picoliter droplet scale) are a relatively novel advancement in bio-analytical assays. In addition to reduced sample sizes and high throughput, properly designed and treated chips can generate flows with no contact between the testing fluid and channel walls, preventing cross-contamination between droplets. However, we need a working understanding of the physics involved in order to predictably and optimally generate these flows.

For low-capillary number flows, an additional complication is the multi-scale nature of the flow. The film of carrier fluid separating the droplet from the walls may be orders of magnitude smaller than the width of the channel. Not only are these films difficult to visualise experimentally, but even modelling such different length scales numerically is not straightforward. Unfortunately, information from this region is vital to understanding things such as the pressure drop and droplet slip velocity, and to predict the stability of the thin film, which prevents the droplets from wetting the walls and interrupting the flow (see image).



Problem Setup and Notation

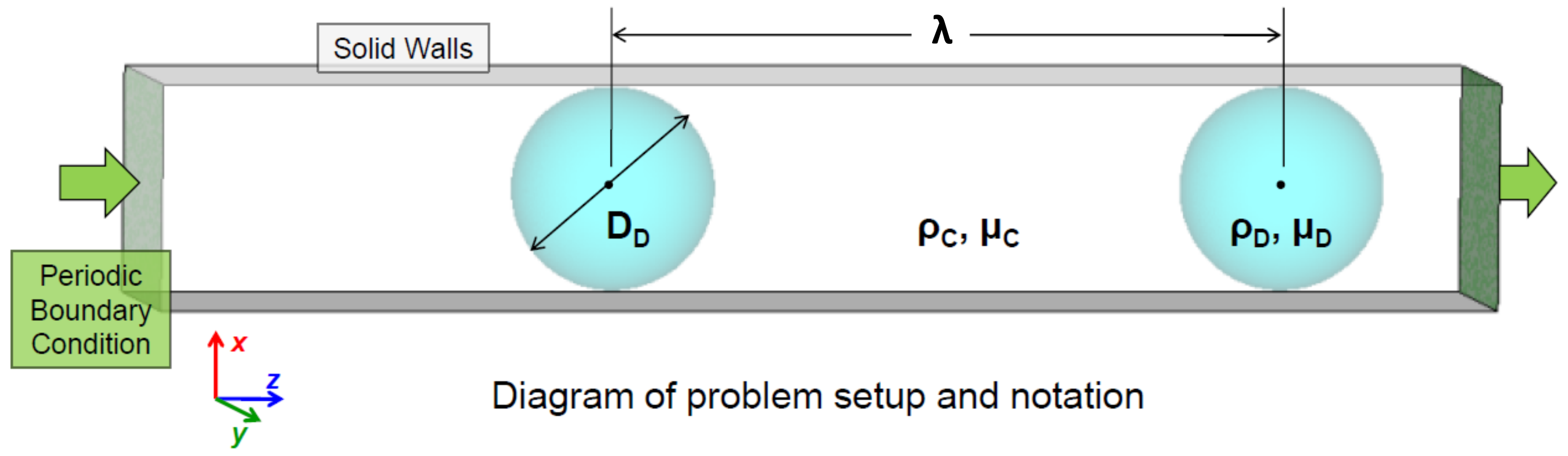
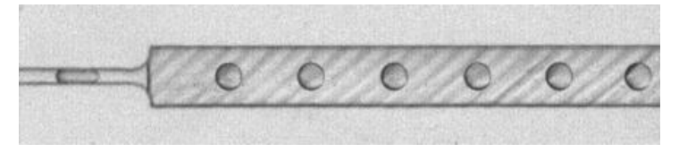
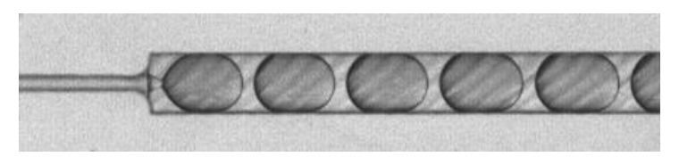


Diagram of problem setup and notation

- Periodic droplets/plugs of dispersed fluid (water) in an immiscible carrier fluid (fluorinated liquid + surfactant)
- Reynolds number, $Re_T = \frac{\rho_C \cdot (J_C + J_D) \cdot D_h}{\mu_C}$
- Capillary number, $Ca_T = \frac{\mu_C \cdot (J_C + J_D)}{\sigma}$
- Relative pressure drop, ${\varphi_T}^2 = \frac{|\overline{\nabla P}|_{2-phase}}{|\overline{\nabla P}|_{carrier\ fluid, J=J_C+J_D}}$
- Droplet effect parameter reflects localised pressure drop variation from constant pressure-drop profile, $\frac{\Delta P_{drop}}{Re_T} = \frac{\lambda}{Re_T} \cdot \left(|\overline{\nabla P}|_{2-phase} - |\overline{\nabla P}|_{carrier\ fluid, J} \right)$
- Capillary flows: $D_D < 1$, droplet shape dominated by surface tension except at very high Ca



- Plug flows: $D_D > 1$, droplet (plug) approaches channel walls, high dependence on Ca



Project goals:

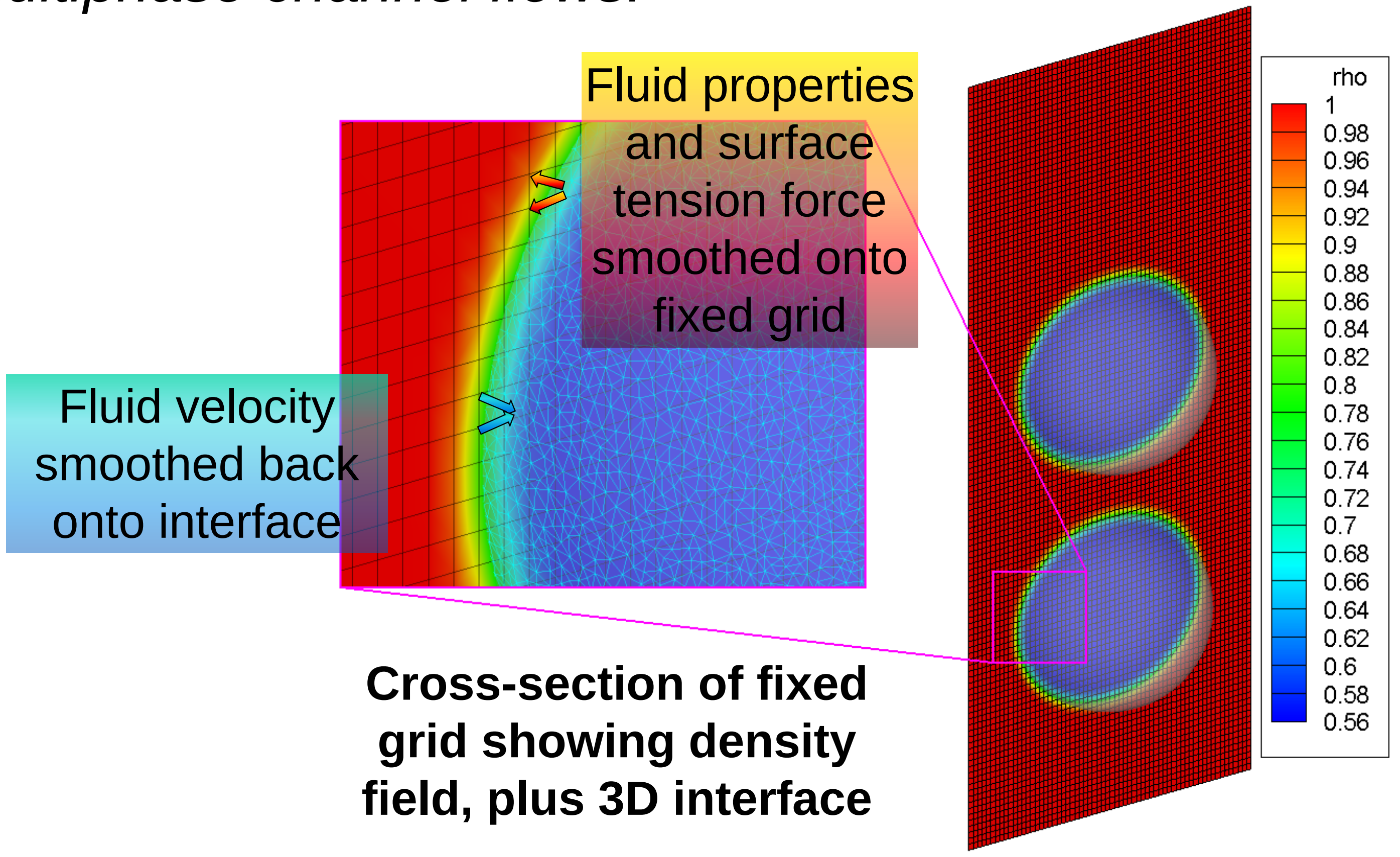
- *Investigate a wide range of flows, including those difficult or impossible to achieve in the laboratory*
- *Map the dependence/sensitivity of relevant parameters to different characteristic values*
- *Use simulation results to physically explain trends observed (both numerically and experimentally)*

Research Code – Hybrid Front-Tracking/ Front-Capturing Method

Fortran research code initially developed by Dr. Gretar Tryggvason's research group

- ➢ Solves isothermal, incompressible Navier-Stokes equations on a regular 3-D Cartesian grid
  - Multigrid algorithm (fast propagation of solution)
  - Two-step predictor-corrector time integration
  - Code parallelized using MPI standard
- ➢ Liquid-liquid interface modelled as a mobile, adaptive triangular mesh with 2nd-order interpolation
  - Mesh used to calculate local fluid properties and surface tension; then interpolated onto fixed grid
  - Calculated velocity field used to advect the mesh
  - Peskin's smoothing used for grid-mesh interpolation to avoid discontinuituous coefficients

Project goal: *Evaluate, validate, and, where possible, improve the code as an efficient and robust solver for multiphase channel flows.*



Fluid properties and surface tension force smoothed onto fixed grid

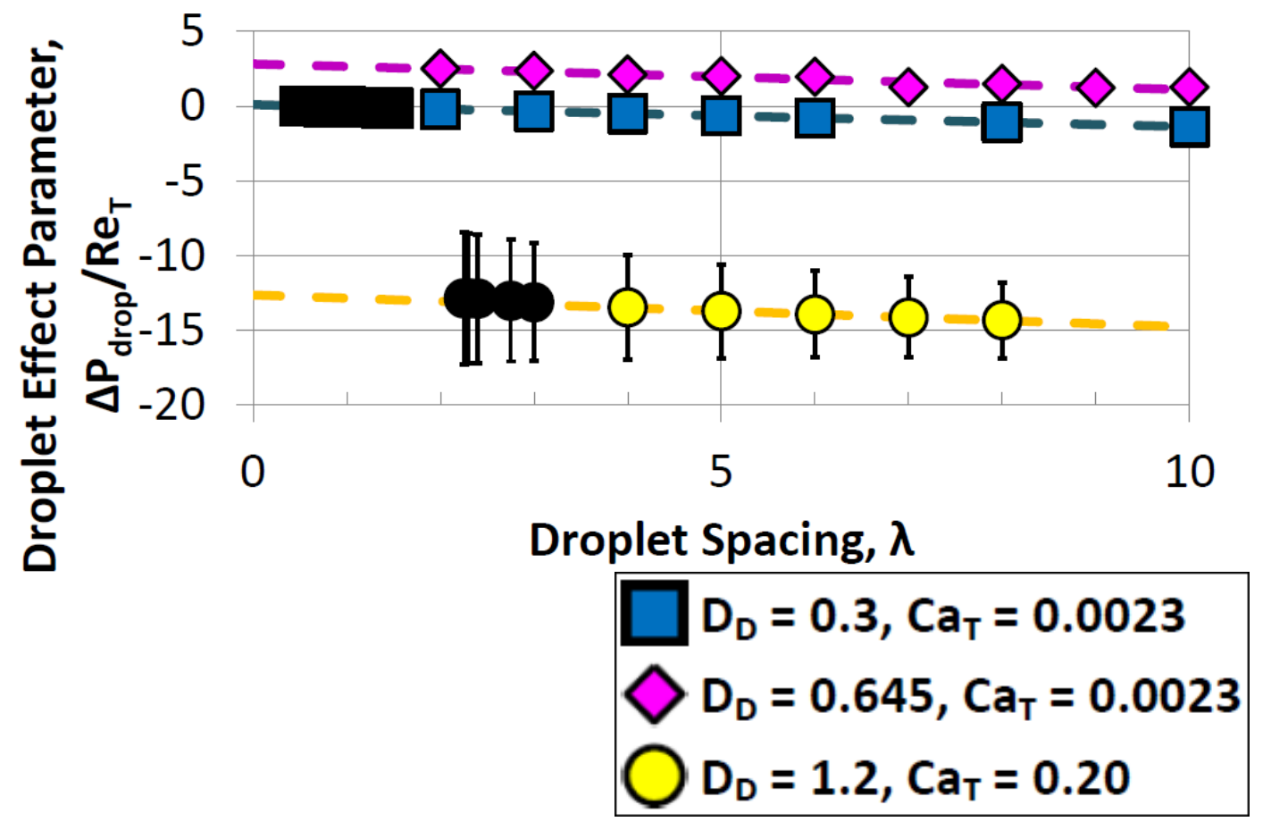
Fluid velocity smoothed back onto interface

Cross-section of fixed grid showing density field, plus 3D interface

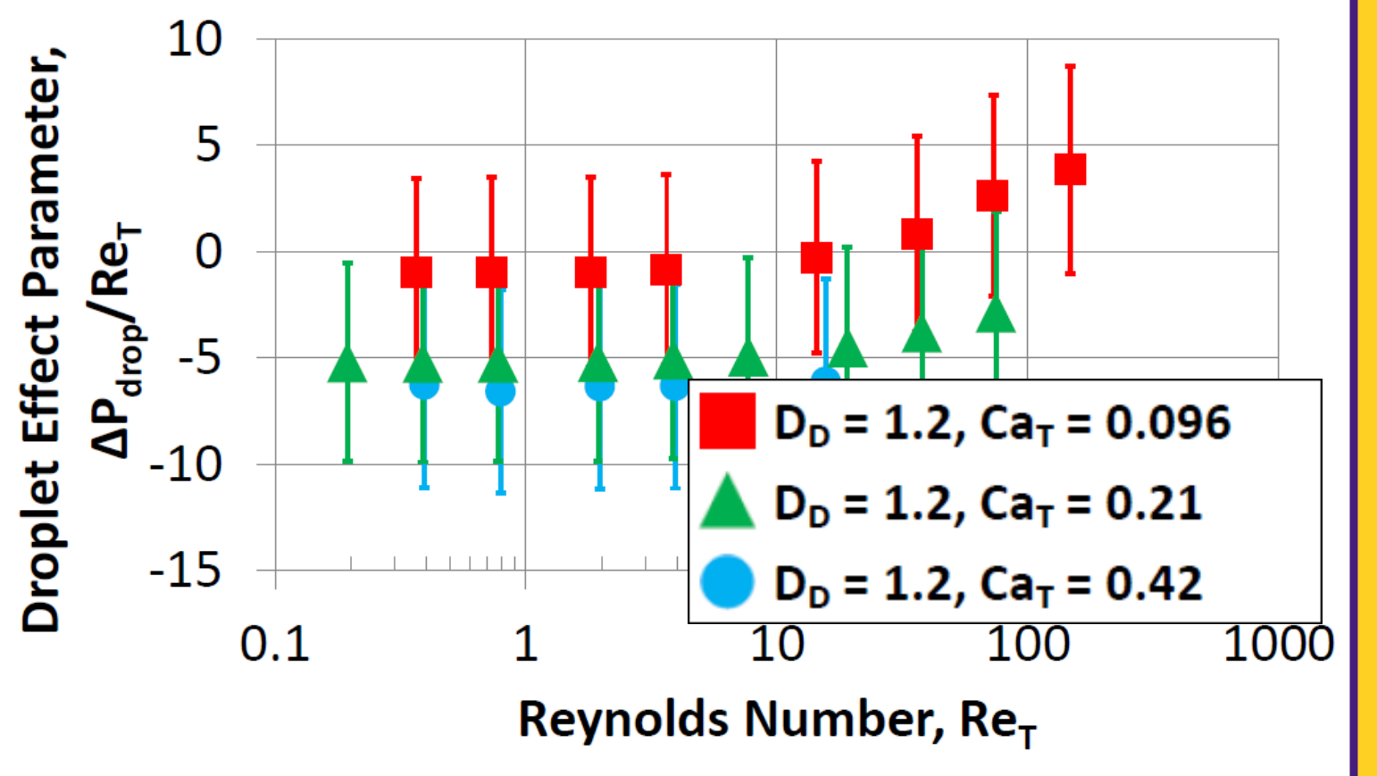
Results and Discussion

Parametric studies have revealed various trends.

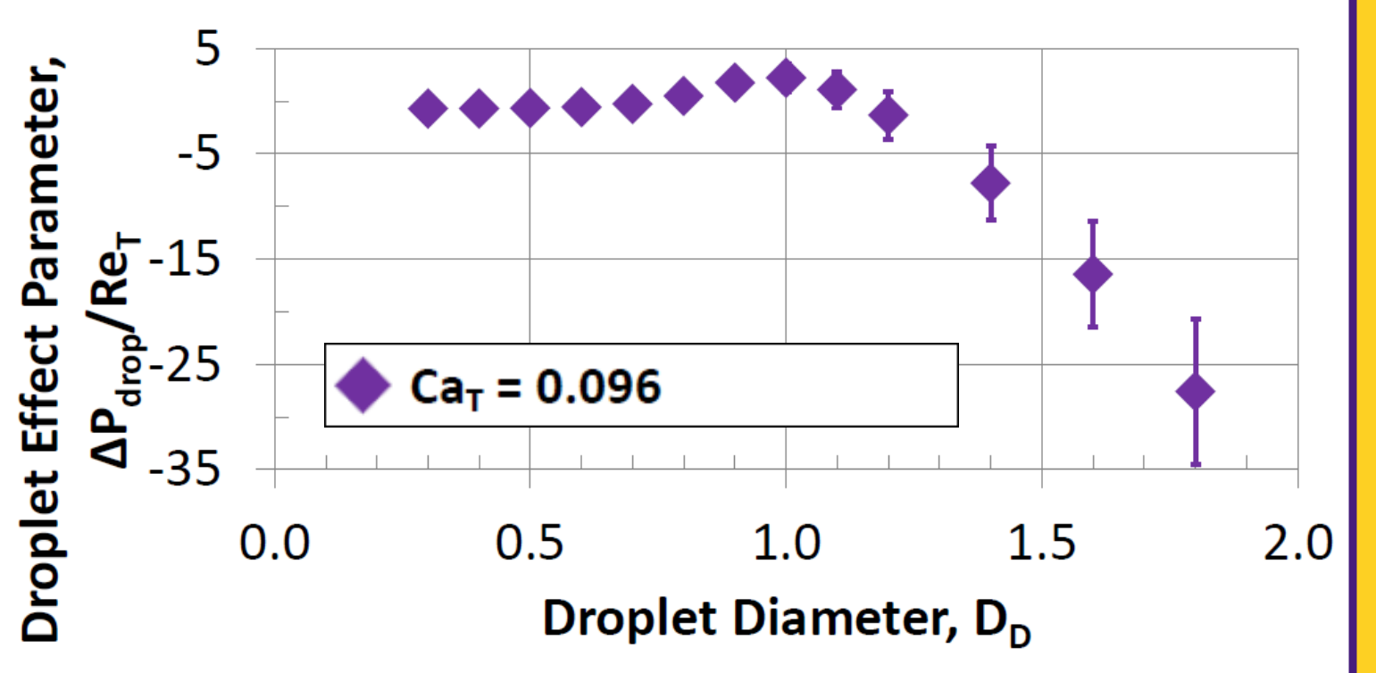
- Droplet effect parameter becomes linear with droplet spacing when droplets are sufficiently far apart. This allows the formulation of a relation to eliminate droplet spacing from consideration in other parametric studies.



- Relative pressure drop decreases at higher capillary numbers, when plugs become elongated and films become thicker. Reynolds number is unimportant for $Re_T \leq 1{\sim}10$.

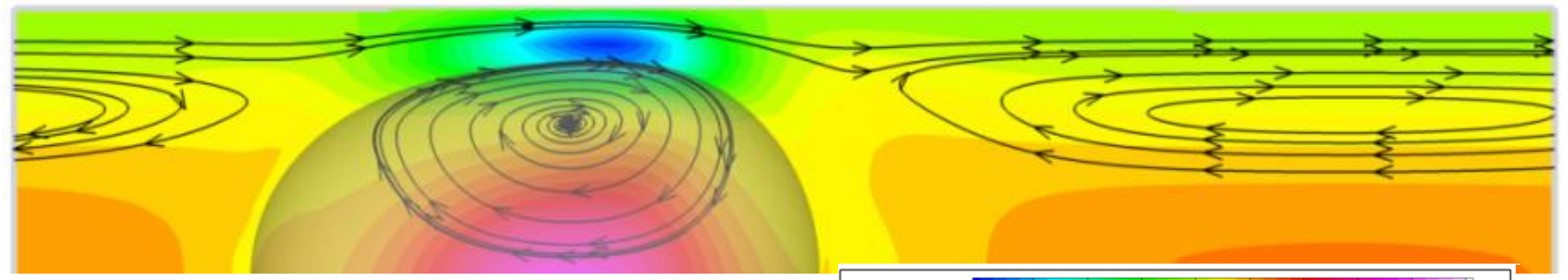


- Relative pressure drop reaches a maximum when droplet size approaches channel width, but decreases again as plugs become longer.

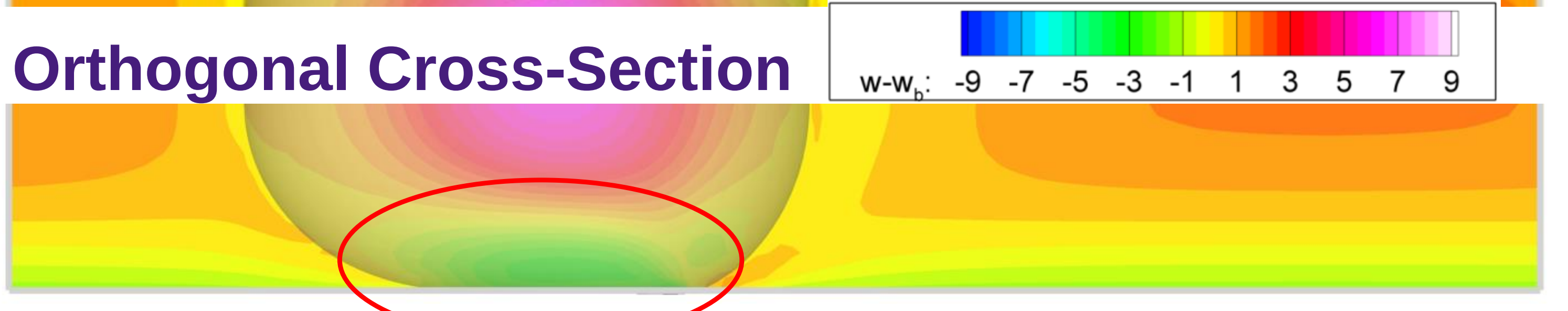


Further code modifications are needed to bridge the data gap with low-capillary number plug flows (thin films). A lubrication theory technique is being adapted to the current code in order to achieve this.

Diagonal Cross-Section



Orthogonal Cross-Section



Thin-film physics and wall wettability must be properly introduced

Acknowledgements

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IGERT on Multiscale Computational Fluid Dynamics - http://www.cct.lsu.edu/IGERT/