Karlsruhe Institute of Technology

Institute of Fluid Mechanics

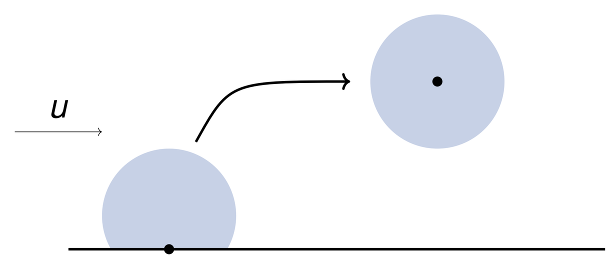
Discrete Element Method (DEM) for Gas-Liquid Flows with Wall Interaction in Microchannels

Ludwig Bossle | **Alexander Stroh**

Institute of Fluid Mechanics (ISTM), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract

In low-temperature fuel cells, liquid water condenses within the porous gas diffusion layer and is subsequently drawn into the gas microchannels. Efficient water removal is essential for optimal performance. Uneven distribution and blocked channels cause flow maldistribution and can damage the cell. The current range of multiphase models for large simulation domains is limited. Small domains are analyzed using the Volume of Fluid (VoF) method, while for larger domains usually two-fluid models are utilized that ignore wall interaction, despite surface tension dominating in microchannels. We propose analyzing droplet behavior in gas channels with a Discrete Element Method (DEM) based on an immersed boundary approach. This technique offers a significant speed-up over VoF while producing comparable results and being more robust. With this method droplet detachment in a single channel and in two parallel channels are analyzed.



Liquid Water in PEM Fuel Cells

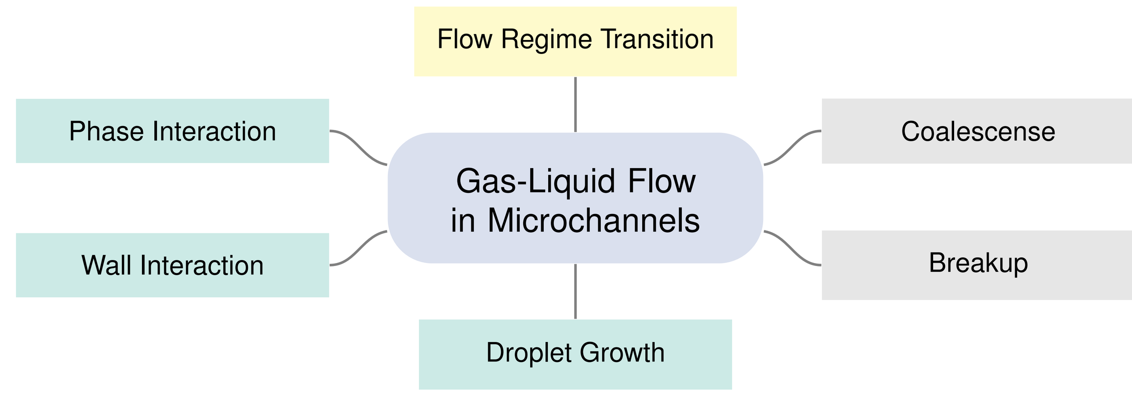
- Reaction: $2\,H_2 + O_2 \longrightarrow 2\,H_2O$
- Water condenses within the porous gas diffusion layer and is drawn into microchannels for removal

→ How is the gas distribution between channels?
→ Does blockage occur?

➡ **Robust simulation method suitable for larger domains while capturing necessary physics**

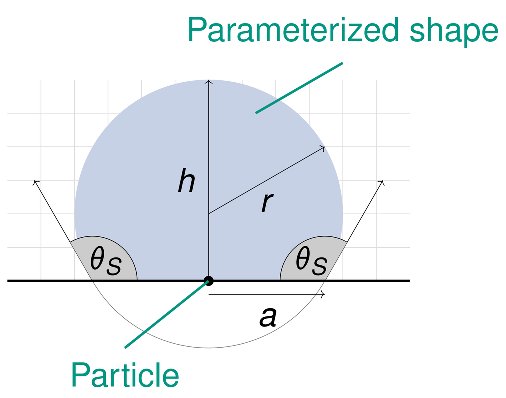
Dimensional analysis
- $Ca = \frac{\mu u}{\sigma} << 1$ → small viscous deformation
- $We = \frac{\rho u^2 D}{\sigma} << 1$ → small inertial deformation
- $Bo = \frac{\rho g D^2}{\sigma} << 1$ → small gravity-induced deformation

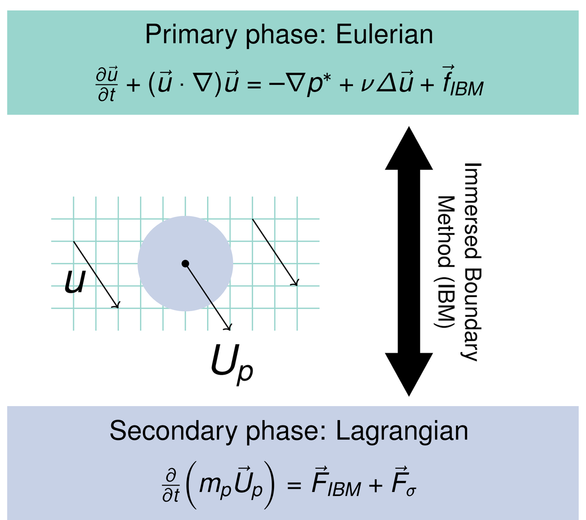
→ Surface tension is dominant
→ Assumption: Rigid-body model of droplet



Droplet Model

- Attached droplet modeled as a sphere cap with constant static contact angle θ_S
- Discrete element with point on wall
- Droplet growth via seeding points on surface





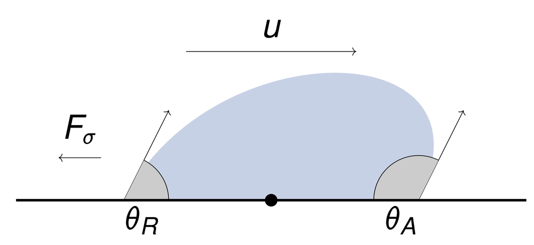
Wall Interaction

- Surface tension model

$$F_\sigma = a\pi\sigma(\cos(\theta_R) - \cos(\theta_A))$$

- Droplet detachment if

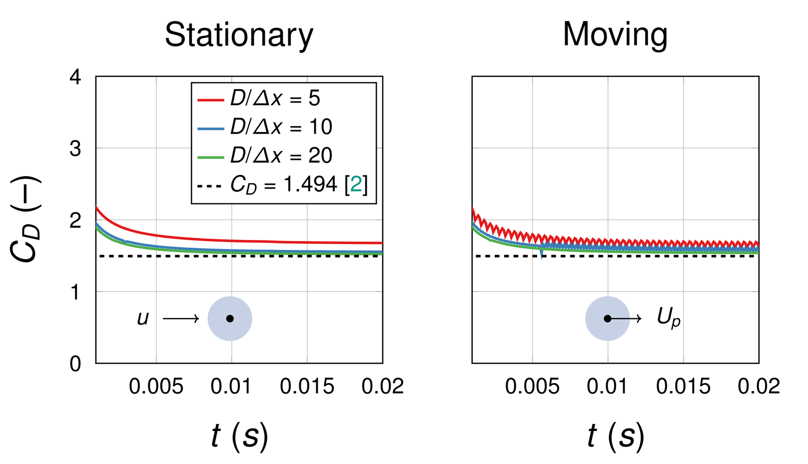
$$\vec{F}_{IBM}\cdot\vec{t} > F_\sigma$$



DEM Validation

- Flow around cylindrical particle for different mesh resolutions
- Moving and stationary cylinder at $Re_D = 40$

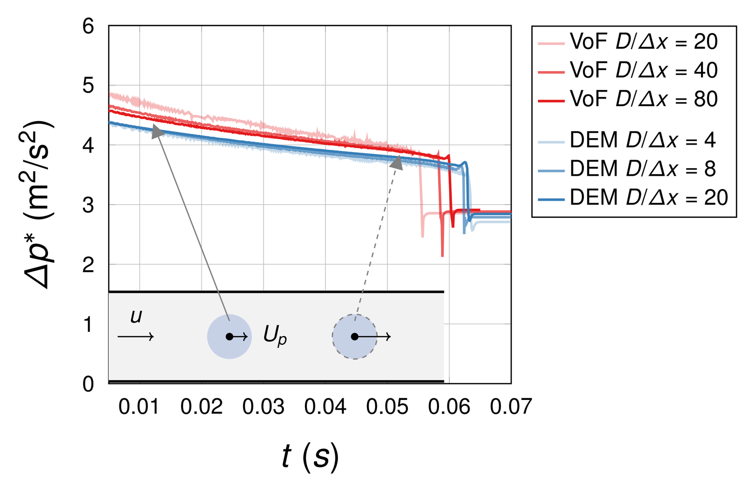
→ Convergence towards reference solution [2]



DEM vs. VoF

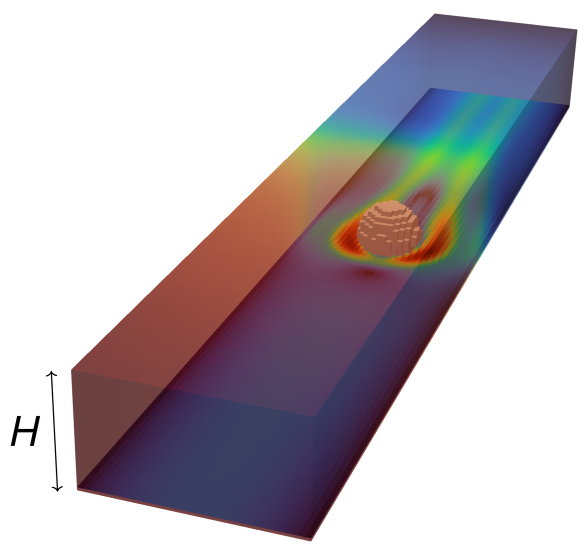
- Cylindrical particle accelerated through channel without wall contact until ejection ($Re_D = 40$)

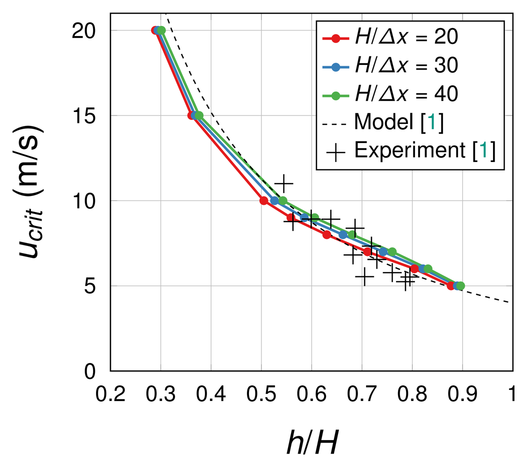
→ Comparable results between VoF (*interFlow*) and DEM
→ DEM remains stable for low mesh resolutions



Results: Single Channel

- Fully developed flow in rectangular channel of height H
- Analysis of droplet detachment velocity u_{crit} depending on droplet height h



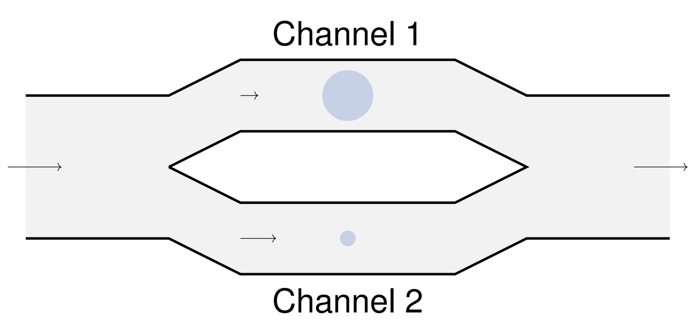


$H/\Delta x$	RMS to Model (m/s)
20	1.37
30	1.12
40	0.93

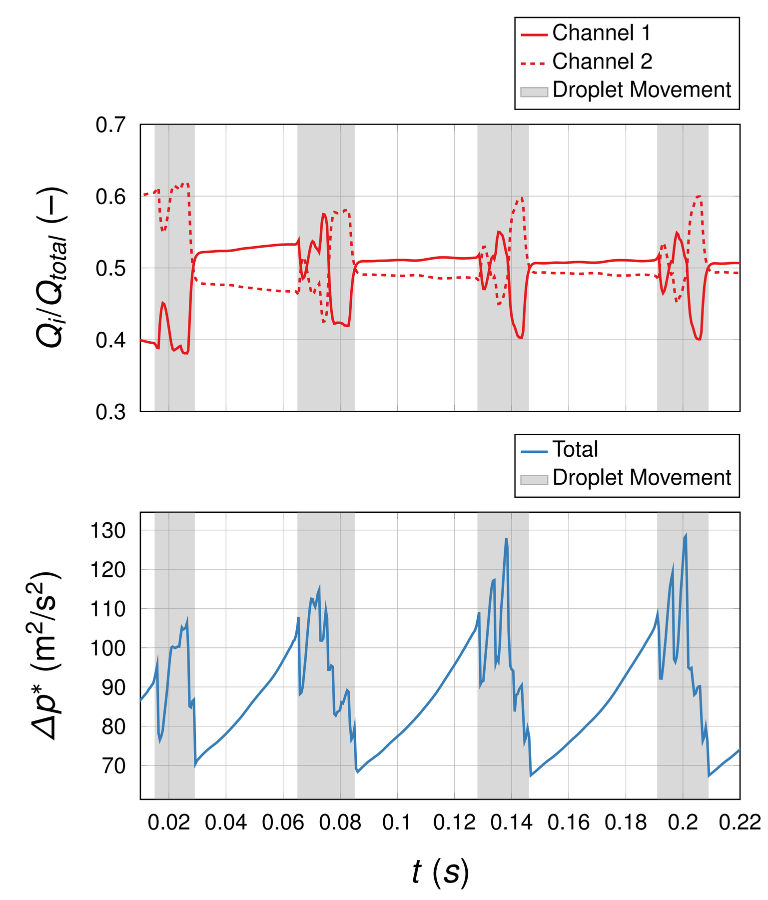
Note: The model and simulation assume a 1.8 mm channel width vs. 1.6 mm in the experiment.

Results: Two Channels

- Bifurcation with constant droplet growth rate
- Initialization with bigger droplet in channel 1
- $u_b = 5$ m/s

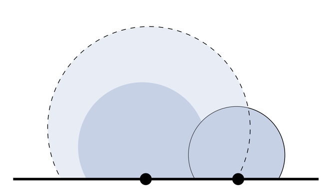


→ Initial maldistribution turns into symmetric steady osciallation between channels



Summary and Outlook

- DEM gives comparable results to VoF while enabeling a coarser resolution for this application
- DEM can be used to predict droplet detachment in microchannels
- DEM can be used to analyze interaction between multiple microchannels
- Add other flow types (e.g. film flow, slug) like [3]
- Add particle-particle interaction (e.g. coalescense)
- Implement parallelization of finite size particles



We gratefully acknowledge the funding of Schaeffler Technologies AG & Co. KG.

References

[1] S. C. Cho, Y. Wang, and K. S. Chen. "Droplet Dynamics in a Polymer Electrolyte Fuel Cell Gas Flow Channel: Forces, Deformation and Detachment. II: Comparisons of Analytical Solution with Numerical and Experimental Results". In: *Journal of Power Sources* 210 (July 2012), pp. 191–197.
[2] R. Gautier, D. Biau, and E. Lamballais. "A Reference Solution of the Flow over a Circular Cylinder at Re=40". In: *Computers & Fluids* 75 (Apr. 2013), pp. 103–111.
[3] D. Niblett, S. M. Holmes, and V. Niasar. "Discrete-Particle Model to Optimize Operational Conditions of Proton-Exchange Membrane Fuel-Cell Gas Channels". In: *ACS Applied Energy Materials* 4.10 (Oct. 25, 2021), pp. 10514–10533.