Hybrid DEM-VoF Multiphase Model for Microchannels of Electrochemical Devices

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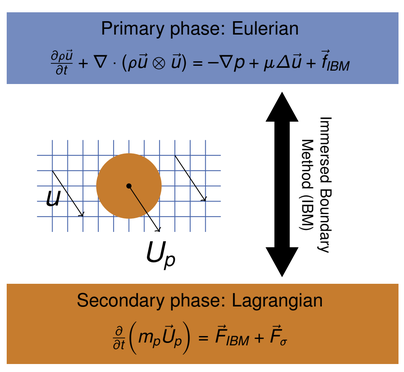
Discrete Element Method (DEM)

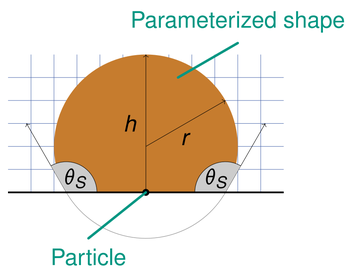
Concept

- Euler-Lagrange framework for finite-size particles [6]
- Rigid body assumption for small droplets



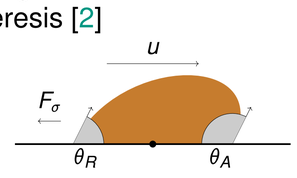
Droplet Shape

- Sphere cap with fixed static contact angle θ_S



Surface Tension

- Pinning force based on fixed hysteresis [2]



DEM Validation

Setup

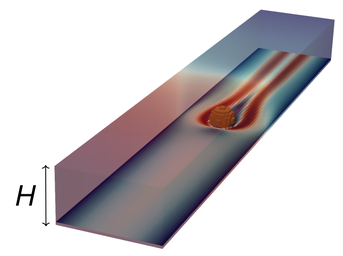
- Fully developed flow in rectangular channel of height H with a single droplet
- Variation of velocity and droplet size for one contact angle configuration

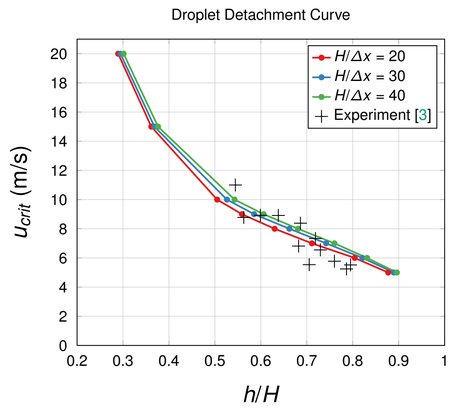
Results

- Droplet detachment curve
- Validation of
  - IBM forcing
  - Shape parametrization
  - Surface tension model

→ Accurate prediction of detachment curve with DEM

Note: The simulation assumes a 1.8 mm channel width vs. 1.6 mm in the experiment to match the determined hysteresis in [3].





Liquid Water Transport in PEM Fuel Cell Gas Channel

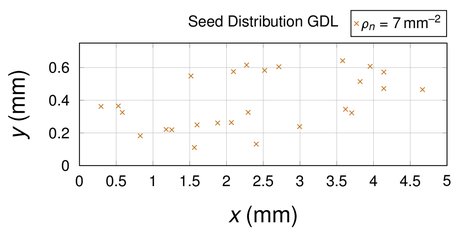
Setup

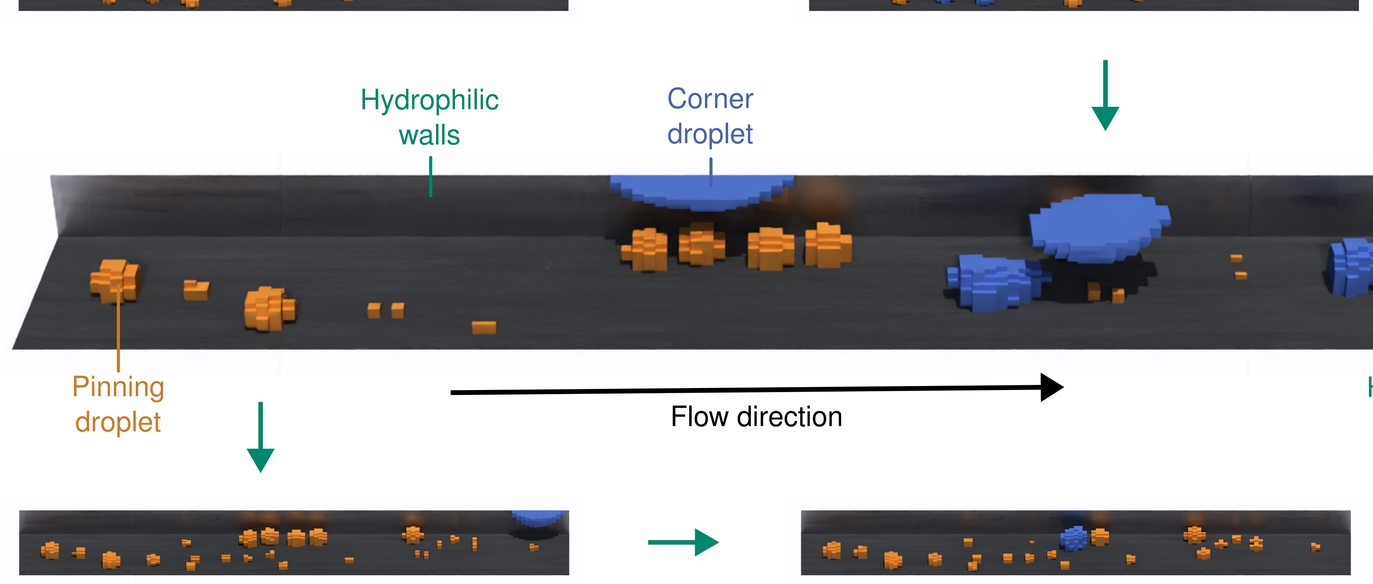
- Cathode channel section
- $j = 2\,\mathrm{A\,cm^{-2}}$
- $A_c = 0.1875\,\mathrm{mm^2}$
- No phase change
  → All reaction water is liquid
- Stoichiometry 1 for $A_{active} = 3\,\mathrm{cm^2}$
  → $u_b = 6.2\,\mathrm{m\,s^{-1}}$

GDL Boundary Condition

- Random distribution of seed points with density ρ_n [5]
- Constant mass flow rate per seed point (accelerated 100×)

$$\dot{m} = 5.4 \times 10^{-8}\,\mathrm{kg\,s^{-1}}$$





→ Oscillation between accumulation regime [1] and detachment events

$\theta_{S,wall} = 70°$
$\theta_{S,GDL} = 120°$
$\theta_{A,GDL} - \theta_{R,GDL} = 40°$

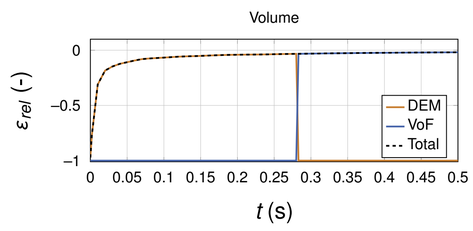
Transition from DEM to VoF

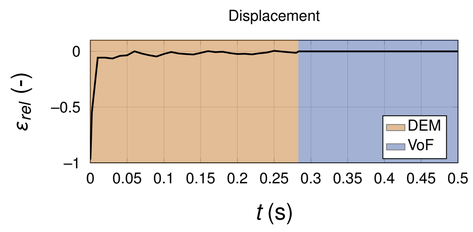
Single Droplet Injection

- Growth rate of $\dot{m} = 1 \times 10^{-7}\,\mathrm{kg\,s^{-1}}$
- Verification of added volume and displaced gas
- Transition to Volume of Fluid (VoF) method [4]:

$$IRQ = \frac{2}{(1/r)\Delta x}; \quad IRQ_{min} > IRQ_{crit} = 8$$

$t = 0.05\,\mathrm{s}$ $t = 0.25\,\mathrm{s}$ $t = 0.35\,\mathrm{s}$ $t = 0.5\,\mathrm{s}$





→ Volume and displacement captured in both models

Conclusion

- Coupled DEM-VoF framework demonstrates high numerical fidelity and computational stability
- Observation of different flow regimes (accumulation, droplet flow) → Short domain only generates small total liquid water amount

Outlook

- Generate flow regime map and validate with experimental data
- Consider DEM interaction with side walls
- Consider greater domain for analysis → Parallelization

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References

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