Developing new Lattice Boltzmann CFD Methods for Electrolyte Wetting in Electrolyzers

- **Supervisors**: Ezra Käs (daily supervisor e.kas@tudelft.nl), Dr. R.M. Hartkamp (Process & Energy, ME)
- **Prerequisites**: ME Advanced Fluid Mechanics (or equivalent), some numerical modeling experience (ME Multiphysics transport in Energy Materials **or** CFD for Engineers **or** AE CFD2: Discretization Techniques **or** WI Numerical Analysis **or** relevant personal/educational project).

Are you interested in learning about **multiphase CFD**, **Lattice Boltzmann** techniques, and **code development** in **C/C++**? Send an email to e.kas@tudelft.nl: we will teach you the skills you need!

Background

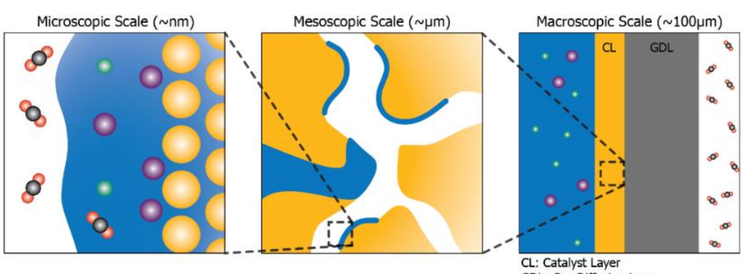
The **Lattice Boltzmann method (LBM)** is sometimes used for micrometer-scale CFD in electrochemical cells, due to its scalability and ease of implementing boundary conditions. LBM solves for the dynamics of large numbers of quasi-molecular particles, which can be shown to be equivalent to the behavior of a continuous fluid obeying Navier-Stokes. **Color-Gradient (CG)** is a multiphase LBM that conserves some of LBM's remarkable algorithmic simplicity.

CG LBM fluid-fluid surface tension is enforced differently than solid-fluid wetting, despite being physically related phenomena. A self-consistent model would enable more confident modeling of the effects of wetting on **liquid electrolyte filling in gas diffusion electrodes (GDEs) for CO_2 reduction.**

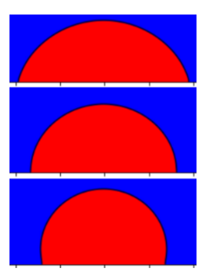
A previous MSc thesis suggests that it is possible to **assign surface tension between solids and liquids** in CG LBM, bringing all capillary phenomena under the same framework. In this project, you would **finish developing this novel wetting implementation**, validate it against analytical or experimental data, and characterize its range of applicability.

Goals

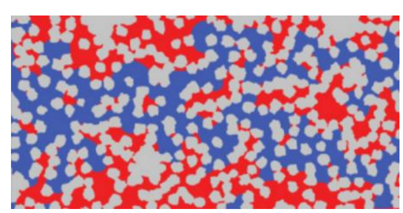
- **By the end of the literature review**, you will be able to:
  - Explain how LBM models single- and multiphase systems,
  - Discuss shortcomings of CG LBM in electrochemical device modeling,
  - Simulate simple multiphase systems with your own CG LBM solver in C/C++,
  - Recommend a course of action on how to implement a new wetting implementation in CG LBM.
- **Halfway through the thesis**, you will have:
  - Extended our group's in-house C++ code with a CG model,
  - Formulated a new wetting framework for CG LBM.
- **By the end of the thesis**, you will have:
  - Extended our group's in-house code with your novel CG extension,
  - Explained your technique's underlying assumptions, tuning parameters, and thermodynamical implications through careful analysis of the equations,
  - Validated your extension against analytical or experimental data in tests relevant to electrochemical device modeling,
  - Assessed your extension's range of applicability, through analysis of your validation results.



*Different physical scales in Gas-Diffusion Electrodes used in CO_2 reduction. This projects supports **mesoscopic-scale** modeling by developing tools to **model wetting of the electrolyte (blue) and gas (white) on the solid catalyst (yellow)***



*Droplet displaying different contact angles on a solid surface by adjusting **solid-liquid surface energies in CG-LBM.***



*LBM simulation of distribution of liquid (blue) in gas (red) in a porous solid (grey). In a GDE, **surface-tension varies with local conditions and solid-surface heterogeneities**, requiring a flexible and tunable modeling approach (10.1103/prh3-xhcb)*