Developing new Lattice Boltzmann CFD Methods for Phase-Change 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

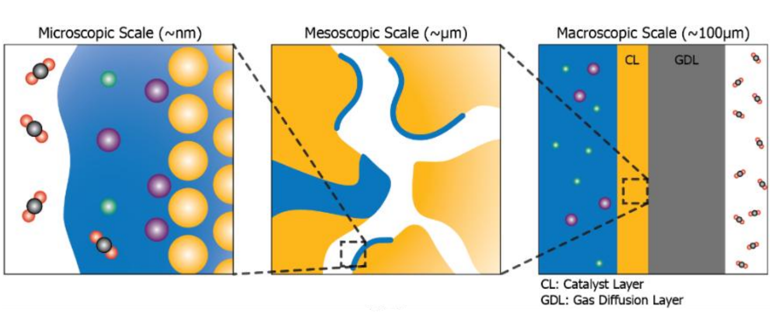
The **Lattice Boltzmann method (LBM)** is sometimes used for micrometer-scale CFD in electrochemical cells, due to its scalability and ease of implementing boundary conditions. LBM solves for the dynamics of large numbers of quasi-molecular particles, which can be shown to be equivalent to the behavior 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 enforces strict immiscibility between fluids, preventing straightforward modeling of phase-change relevant to dissolving gas bubbles in H_2 electrolysis, or **feed-gas dissolution in gas diffusion electrodes (GDEs) for CO_2 reduction.**

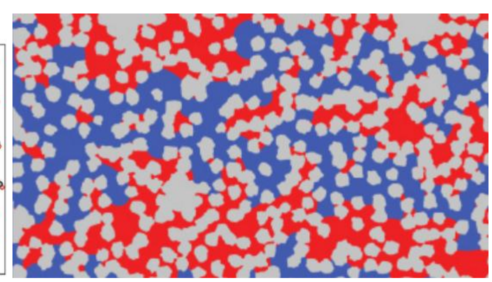
Indirect links between CG LBM other multiphase models suggest that it is possible to simulate phase-change in CG. In this project, **you will develop a novel phase-change framework for CG LBM**, validate it against analytical or experimental data, and characterize its range of applicability.

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 phase-change 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 phase-change 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 dissolution of CO2 (white) in the electrolyte (blue).***



*LBM simulation of the distribution of liquid (blue) in gas (red) in a porous solid (grey). In a GDE, **CO_2 gas dissolves in the liquid electrolyte**, affecting the electrolyte distribution. (10.1103/prh3-xhcb)*