Lattice Boltzmann Methods for Solute Dissolution and Transport 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).

Interested in **multiphase CFD**, **Lattice Boltzmann** techniques, **C/C++**, and modern **code development** (git, CI/CD) ? Send an email to e.kas@tudelft.nl: we will teach you the skills you need!

Background

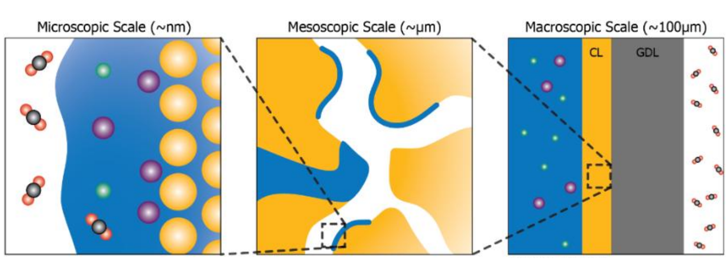
The **Lattice Boltzmann method (LBM)** is sometimes used for micrometer-scale CFD in electrochemical devices, due to its scalability and ease of implementing boundary conditions. LBM solves for the dynamics of large numbers of quasi-molecular particles, which can be shown to be equivalent to the behavior of a continuous fluid obeying Navier-Stokes. LBM can also similarly be used for solute **Advection-Diffusion**.

LBM allows unique control of particle fluxes along the links between lattice (mesh) nodes. By using **simple closure rules for fluxes** across these links, it is possible to **recover complex transport phenomena across sub-grid features**, such as **membranes or fluid-fluid interfaces**. Modeling gas diffusion electrodes requires resolving feed-gas dissolution into the electrolyte: by controlling gas flux across the interface, it should be possible to recover Henry's law naturally.

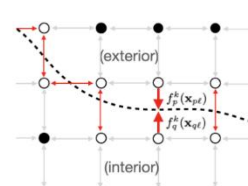
In this project, **you will develop LBM closure models for solute dissolution across a fluid-fluid interface**, validate it against analytical or experimental data, and characterize its range of applicability.

Goals

- **By the end of the literature review**, you will be able to:
  - Explain how LBM models macroscopic transport phenomena,
  - Evaluate shortcomings in how Henry's law is usually satisfied in LBM simulations,
  - Simulate simple fluid flow and advection-diffusion with your own LBM solver in C/C++,
  - Employ modern software development techniques (version control, continuous integration),
  - Recommend a course of action on how to implement your closure model.
- **Halfway through the thesis**, you will have:
  - Extended our group's in-house C++ code with a method to control flux across interfaces,
  - Examined how controlling LBM particle fluxes can confine solute species within a fluid phase,
  - Formulated simple flux closure rules that satisfy Henry's law across a flat interface.
- **By the end of the thesis**, you will have:
  - Explained your technique's underlying assumptions and tuning parameters,
  - Evaluated how LBM particle flux closure rules perform in satisfying Henry's law across curved moving boundaries,
  - 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 only allows for particle to move across lattice links (grey) between nodes (black and white). Thanks to this, **fluxes (in red) can be directly controlled across the interface** (dotted line) to recover macroscopically relevant phenomena.(10.1103/PhysRevE.107.024408)*