A flexible OpenFOAM-based framework for electrochemical systems

David Müller*   Sebastian Blessing   Wiebke Schrader   Alexander Stroh

Institute of Fluid Mechanics (ISTM)

Karlsruhe Institute of Technology (KIT)

In electrochemical systems such as proton exchange membrane water electrolysis (PEMWE) or fuel cells (PEMFC), relevant transport phenomena occur on multiple length scales: characteristic length may vary from nanometers in the catalyst layer (CL) to micrometers in the porous transport layers (PTL) and to millimeters in the bipolar plates (BP). These cells typically operate at high current densities, whereas the reaction rate, the heat release, the charge transport and the formation of bubbles or droplets are strongly coupled in an inherently unsteady and three-dimensional process [4].

With restrictions regarding the continuum hypothesis at the smallest scales and the available computational resources, a direct numerical simulation of a PEMWE or PEMFC is virtually impossible [4]. Depending on the scope of a study, appropriately detailed models for the electrochemistry and the multiphase flow are chosen a priori to their implementation to decrease the computational cost. As a result, the available solvers are specialized for either research or engineering purposes. Nevertheless, they still need customization to meet the requirements of the user. This process tends to be more challenging for each subsequent customization loop.

Based on the open-source software OpenFOAM [5], we propose a flexible, strongly object orientated framework designed to be easily extendable with respect to modelling physical behavior, solving transport equations and adapting numerical solution strategies. All transport equations to be solved are specified during runtime, including those for mass and momentum. Due to templating and the runtime-selection-mechanism available in OpenFOAM, the solver is highly customizable without the necessity of editing the source code. However, if an extension of the solver's functionality is needed, clear programming interfaces simplify the implementation of new runtime-selectable numerical methods. Additionally, they allow the inclusion of third-party software such as the Volume-of-Fluid library TwoPhaseFlow [1] or the chemistry and thermodynamics library Cantera [3].

During the conference, we present the key ideas behind the framework and how to efficiently take advantage of third-party code without reimplementing it. To demonstrate its functionality, the framework will be used to simulate a simple thermo-hydraulic flow and a PEMWE with different models for the multiphase flow – a mixture model to simulate a single channel/cell used typically for the development of PEMWE stacks and Volume-of-Fluid model [2] to study the mass transport within the PTL.

References

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*Email: david.mueller@kit.edu