Flexible Simulation of Fuel Cells with OpenFOAM

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Scientific work accomplished and results obtained

Results were attained within the following sub-projects:

- Electrochemical models
- Volume of fluid (VOF) models
- Electrochemical hydrogen purification

Electrochemical models

Heat and mass transfer are the dominant issues in polymer electrolyte fuel cell design. In the past year, the focus of Mr. S. Zhang (PhD student) has been on high temperature polymer electrolyte fuel cells (HT-PEFCs), which operate in the range 140-180°C, meaning that the reactants and products are in a vapor state, with the emphasis going forward on low temperature polymer electrolyte fuel cells (LT-PEFCs). Computational fluid dynamics (CFD) [A1, A2] is addressing transport and electrochemical phenomena at the continuum scale. The open source platform OpenFOAM [A3, A4] has been employed to perform large-scale calculations for single cells and stacks of cells using the JARA-HPC facilities.

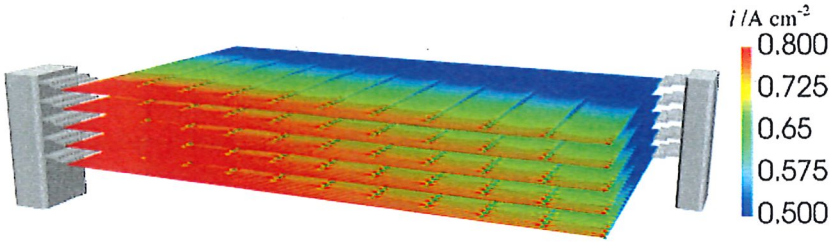

Figure 1. Current density distribution in a 5-cell HT-PEFC stack.

During the past year, Mr. Zhang performed detailed simulations of a 5-cell PEFC stack, with each cell having a nominal area of 200cm². The stack geometry was tessellated with a body-fitted mesh, produced with the commercial package ICEM-CFD, the flow-field calculations being performed with OpenFOAM. [P1, P2]. The mesh size was 170×10^6 compute cells, and the performance calculations were parallelized on 900 cores. Typical run times were of the order of 36-48 hours. The flux of fuel, air (and component species), cooling oil and charge were all considered along with the electric potential. Figure 1 shows the current density in the stack for a mean current density of 0.6 A/cm². Validation of the numerical results was achieved through comparison with experiments and with a simplified CFD stack model based on the distributed resistance analogy (DRA) [A5, A6]. Agreement was excellent; however, the fine-scale calculation displayed a resolution/fidelity that neither experiments nor DRA calculations can capture. This is important, as local extrema in current density, captured for the first time with the Juelich model, can affect the lifecycle performance and durability of a stack.

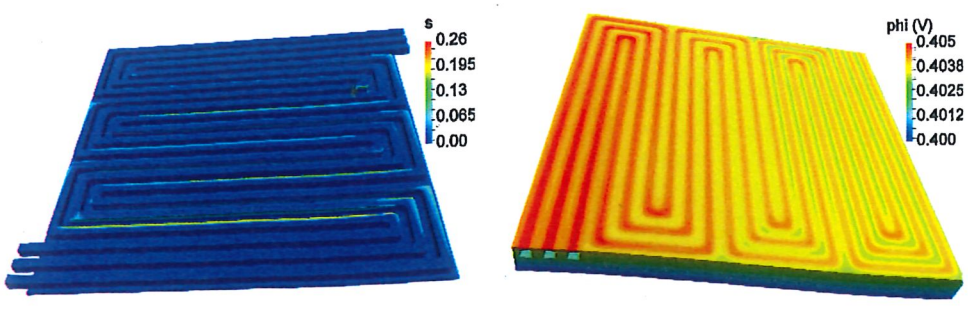

Figure 2. (a) Saturation and (b) potential distribution in an LT-PEFC.

Figure 2 shows some preliminary calculations for an LT-PEFC, which is a two-phase flow problem. The geometry follows that of the International Energy Agency Technology Collaboration Program on Advanced Fuel Cells, https://www.ieafuelcell.com/, benchmark PEFC, for round robin physical and numerical experiments. Figure 2(a) shows liquid water saturation, while Figure 2(b) exhibits the electric potential obtained from the solution of a detailed Poisson system of equations.

Substantial time and energy was successfully spent on making the basic fuel cell model more stable [P3]. The original motivation for the work was the realization that the basic algorithm did not provide stable solutions in the mass transfer limit at high current density. It was subsequently noted that there were also significant deficiencies at low current densities. Four specific remedies were proposed: (1) Relax the calculation for the local current density; (2) limit the minimum local ideal or Nernst potential; (3) linearize the mass transfer boundary condition in terms of the convection flux (coefficient) and transferred-substance state value as opposed to a Neumann condition (in a previous version of code); (4) apply a flux limiter to obviate negative values of mass fraction arising during the iterative procedure. Beale also developed 'simpleFuelCell', which is a simplified fuel cell model. This work was presented at the openFuelCell workshop held in Jülich in late October 2017. József Nagy has requested Beale put the case in the OpenFOAM tutorials, https://wiki.openfoam.com/ Tutorials. The basic idea is to modify the built-in incompressible solver, icoFoam, with an electrochemical reaction and mass transfer modules. The results of these calculations may then be compared to the analytical solution of Kulikovsky [A7]. At the workshop, Profs. Beale and Lehnert proposed a book of edited chapters entitled, "Electrochemical Cell Calculations with OpenFOAM", which now has 12 chapters under development by various authors worldwide.

Tim Cramer of the Aachen High Performance Computing Group, together with Beale, set up the Jülich-Aachen OpenFOAM users group, which was initially a mailing list of 16 persons, and held a face-to-face meeting in Aachen on 27 April 2018, with a second meeting proposed for the autumn. Following discussions between Beale and Paul Gibbon (Juelich Supercomputing Center), Metin Cakircali, from the Institute for Advanced Simulation in the Juelich Supercomputing Center conducted some preliminary scalability performance measures on an openFuelCell test case provided by Shidong Zhang. Some bottlenecks were identified and the HT-PEFC cell and stack codes will be spun-off to a Danish PEFC manufacturer, SerEnergy A/S.

Detailed two-phase flow in porous media

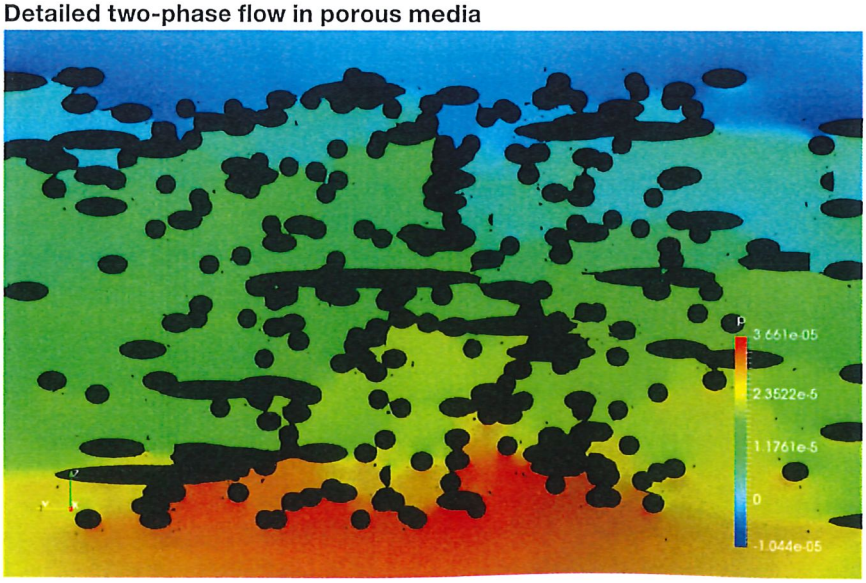

Figure 3. Pressure distribution in a porous structure.

Substantial effort was spent on meshing random cylindrical geometries using two open-source meshers, namely snappyHexMesh and cfMesh. In August 2018, Beale, together with Andersson and Mr. Zhang went to the University of Zagreb's School of Numerical Modelling of Coupled Problems in Applied Physics with OpenFOAM (NUMAP-FOAM). This is hosted by Hrvoje Jasak, one of the original developers of OpenFOAM [A8], with whom the IEK-3 are collaborating. At the same Messrs., Andersson, Zhang and Beale visited Franjo Juretić, Managing Director of Creative Fields Ltd. who produce cfMesh and work further on mesh refinement. Meshes produced by Engys (see https://engys.com/), developer of open source and enterprise versions of snappyHexMesh are being used to study single-phase transport in porous structures. This work is undertaken in collaboration with Martin Andersson (Lund University) and Pablo Garcia Salaberri (Universidad Carlos III de Madrid). This work will be used to consider both single- and two-phase flow in random porous structures in the coming months.

VOF models

Using OpenFoam (version 3.0.1), Andersson developed and solved a computational fluid dynamics (CFD) model for a single channel, which is of interest for the removal of liquid water inside a PEFC. The volume of fluid (VOF) approach (using the solver multiphaseInterFoam) was used to study the two-phase interface flow behavior, including the GDL/GC interface [P4-P8]. Note that our model is compared to synchrotron XTM measurements carried out at the Swiss Light Source at PSI (TOMCAT beamline). The model and the experiments share geometrical parameters. It was found in our last study that [P6]:

- The agreement between our model & the corresponding measurements is good considering droplet dynamics, for example the length from the liquid inlet to the first wall contact.
- We found that the two-phase flow inside the microchannel (illustrated in Figure 4) is connected to the liquid inlet size, gas flow velocity and contact angle, as well as the channel height. When the results from our recent work are compared to our previous effort [P5], it is clear that the influence of channel dimensions (width and height) is noteworthy.
- The model, as well as the experiments, present: detachment – flow in channel – wall attachment behavior when standard conditions apply. Exceptions include when the droplet is connected to the wall and GDL surface simultaneously: (1) from a decreased gas velocity; (2) from a decreased channel thickness; (3) from an increased liquid inlet area. Corner flow occurs at the wall on the side opposite to the GDL surface from: (1) a decreased gas velocity; (2) a decreased wall contact angle; or (3) an increased liquid inlet area.
- There is a strong dependence on the size of the droplet from the GDL surface liquid inlet area. A decreased liquid inlet area (with a constant liquid mass flow rate) yields noteworthy smaller droplets.
- The amount of droplets is increased from the higher gas velocity and consequently the droplets are smaller.
- The droplet moving behavior has a substantial impact on the channel height, with droplets attached to the wall (on the side opposite the GDL) and the GDL surface at the same time for the 150 µm case (thinnest channel), both for a constant mass flow rate (gas) and a constant velocity (gas).
- Smaller droplets can flow freely in the channel center for an increased period until the GC wall is attached.
- The hydrophilicity/hydrophobicity (e.g., the contact angle) has a strong impact on the droplet size (which may also be expressed as the time until detachment). A higher GDL contact angles yields a decreased droplet size. Note that a small (140° vs 153°) variance in the average contact angle has a significant influence on the droplet dynamics, determining if a (liquid) droplet remains connected to the GDL surface or if it detaches from the GDL surface, meaning that it later connects to the wall. It should be noted that the water droplet transport is somewhat stochastic.

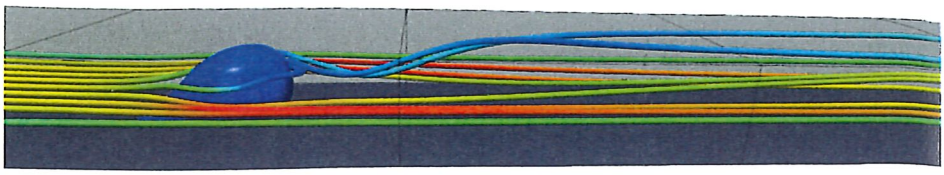

Figure 4. Gas flow around a droplet under detachment in a PEFC gas channel.

Electrochemical hydrogen purification

Within the European project, "MEMPHYS – membrane-based hydrogen purification system", the main objective is to develop an electrochemical membrane reactor for the separation of hydrogen from industrial gas mixtures. The CFD model developed by Reimer was applied to the laboratory test cell of an industrial project partner.

The behavior of the cell for two different gas mixtures, one with 80% hydrogen and one with 50% hydrogen, was compared. It is assumed that both gas mixtures are also humidified at 295 K. In previous discussions, it was mentioned that a cell voltage of 0.2 V should not be exceeded. Based on the polarization curve model, this translates into a current density of 0.32 A cm^{-2}. For both cases, the amount of 80% of the initial hydrogen should be removed from the gas mixture. This means that the same equivalent current density and same stoichiometry are used, which are the important parameters for electrochemical conversion devices. In other words, the same amount of pure hydrogen is produced with different inlet gas mixtures. This is of importance because the final application should work with a range of different gas compositions.

For 80% hydrogen, the modeling results showed that there was no mass transport limitation present under these conditions and the cell should work fine. The situation changed for the gas mixture containing 50% hydrogen. It can be seen that the hydrogen mass fraction reaches almost zero at the last outlet channel. This means that the limiting current is only reached within the applied model. In reality, the current density distribution would not be homogeneous, and therefore it is expected that the real limitation from mass transport may be present at higher currents (maybe factor 2 or 3). Nevertheless, it becomes clear that if the cell approaches its limiting current, the main problem will arise in the dark blue region of Figure 5.

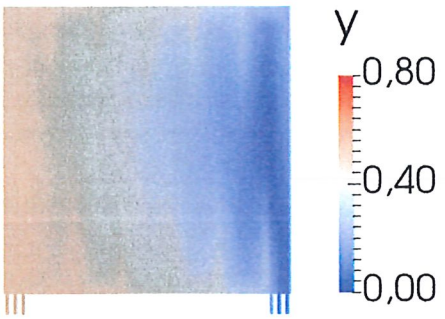

Figure 5. Hydrogen mass flow at the membrane for the 50% hydrogen gas mixture. The flow enters from the bottom left side.

Realization of this project

The simulations were run with OpenFOAM/3.0.1, as well as OpenFOAM/extend4.0. The communication via MPI is embedded, and only the application code must be developed. Several methods of domain decomposition are available with OpenFOAM.

Publications with project results

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Applied Energy. 2019;233-234:1094-1103.

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[P3] BEALE SB, REIMER U, FRONING D, JASAK H, ANDERSSON M, PHAROAH JG, LEHNERT W.
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