

Recent developments in the modeling of polymer electrochemical cells

Steven Beale, Shidong Zhang, Uwe Reimer, Werner Lehnert

TFEC-2020-33491

Submitted to the ASTFE 5th Thermal and Fluids Engineering Conference, New Orleans LA, 5-8 April 2020

Article Type: Presentation only

Keywords: Computational fluid mechanics, heat and mass transfer, fuel cells, electrolyzers

Abstract (3000 symbols or 250 word maximum)

Polymer electrolyte electrochemical cells (PECs) offer exciting possibilities as energy converters in the form of both fuel cells and electrolyzers. Computational fluid dynamics can be used to analyse the performance of virtual prototypes at the micro-scale, as well as the cell and stack levels. This presentation details a comprehensive program of development of open source tools to describe and predict PEC operation. The software employed is OpenFOAM, which mimicks the governing partial differential equations that describe the physics of PEC behaviour. Models range from detailed two-phase flow in porous transport layers based on digital reconstructions and the volume of fluid method, through single and multi-fluid cell models employing Eulerian-Eulerian solvers, to stack-level models whereby volume averaging or, also known as local homogenization are employed for both single-phase and two-phase formulations. The development of a multi-phase stack model represents an original and novel scheme not previously published.

The results of mathematical calculations are compared with analytical solutions for one-dimensional idealizations, previous three-dimensional (3-D) numerical work by other researchers, and detailed experimental data gathered in-house. Comparisons are made in terms of local current density and species mass/molar fractions, as well as current density vs. voltage, i.e., polarization characteristics. Different levels of model complexity are also considered, for instance comparisons of a 2-D electrochemical formulation based on a Kirchhoff-Ohm equation (ideal potential less losses/overpotentials) vs. a fully 3-D simulation of both ionic and protonic potential fields. The presentation concludes with an assessment of the needs/requirements of the next generation of PEC analysis tools.