3-D thermo-electrochemical CFD modelling of solid oxide cell stacks with detailed electrochemistry

Context
Solid oxide fuel cells (SOFC) are direct energy conversion devices that allow the production of electricity with high efficiency while maintaining pollutant emissions at a low level. In reverse mode (solid oxide electrolyzer cell, SOEC), hydrogen can be produced. Their lifetime is currently not yet sufficient in both modes for large-scale commercialization. Therefore, the degradation phenomena that affect their performance need to be understood. They are related to the aggressive high temperature environment and they range from local alterations of the microstructure to cracking of the brittle ceramic layers that form the cells. The degradation depends on the spatial distribution of local conditions (gas composition, electrostatic potential, temperature, hence electrochemical potential) in the device in operation, the direct measurement of which in operation is very challenging. Therefore, detailed CFD models of solid oxide stacks that include a detailed electrochemical model are of interest to accurately predict the temperature profile in operation. This is also a prerequisite for understanding thermo-mechanical failures in the stack.

Objectives
The existing 3-D thermo-electrochemical model at GEM is a combination of a CFD Fluent model and a gPROMS finite-difference electrochemical model. The electrochemical model provides the sink/source term for the CFD calculations. In the current implementation, there is no feedback from the electrochemical model to the CFD model. The calculation of the sink/source terms assumes a gas-flow distribution close to one-dimensional. Therefore, slight inaccuracies remain in the predictions under ideal conditions and foremost, the approach is not amenable for simulating the effect of defects/dissymmetry. The objective of the project will be to improve the flexibility of the coupling between the CFD and FD software. The call from FLUENT to gPROMS using user defined functions (UDF) will be based on a grid that can be defined by the user, depending on the study (e.g. high local accuracy for defect modelling or low model runtime for design screening), and in an iterative manner. Both the CFD and electrochemical model, as well as the previous FLUENT-gPROMS interface in Matlab will be provided. Tools for automatic/systematic monitoring of the convergence will be also implemented. The model will be tested over a wide range of operating conditions, including internal steam-reforming and SOEC operation, but only in potentiostatic mode. The benefit of the developed model over the previous implementation will be quantified for a list of provided operating conditions and experimental data of the electrochemical performance and local temperature measurements.