Modeling and experimental validation of solid oxide fuel cell materials and systems

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In solid oxide fuel cell research, modeling activities take place at different levels, from the electrochemical reaction details at the electrode/solid electrolyte interfaces, to single cells, to stacks of cells and finally to entire systems, that include fuel preparation (reforming) and thermal management. For each level, one or more different simulation tools may be used. To stay in touch with reality, modeling and simulations are carried out on an existing SOFC cell and stack design of an industrial partner, aiming to improve the design and the materials requirements from the results indicated by the models. Fundamental input data to the models are obtained from in house experiments on the materials actually employed. Calibration and validation of the models is performed by electrical and thermal measurement of the same fuel cells and stacks mounted in house. The computational fluid dynamics (CFD) tool FLUENT is used for the detailed calculation of the distribution fields of temperature, current and gas species for large area unit cells (50 cm^2). The equation solver tool gPROMs is used for the same (using coarser meshing thereby reducing computing time) but especially for stack calculations (up to 50 cells). The data reconciliation tool BELSIM is used for the complete fuel cell system, defined as specific units (reactors,…) interconnected by streams (material or thermal). Examples of the different models and their results will be presented. Emphasis will be placed on the importance of the materials properties under different operating conditions of the fuel cell.