Karlsruher Institut für Technologie

Institut für Technische Chemie und Polymerchemie
Lehrstuhl für Chemische Technik
Prof. Dr. Olaf Deutschmann

Karlsruhe, 15.10.2015

Vergabe einer Abschlussarbeit Bachelor/Master

Title:
Physically based modeling of Solid Oxide Fuel Cells with Direct Internal Reforming (DIR-SOFC) in the counter-flow mode of operation

Description:

Fuel Cells (FC) are one of the leading members of the new brigade of clean and sustainable energy devices. It is essentially an open, continuously running battery that converts chemical energy of the supplied fuel (H_2, CO, etc.) directly into electrical energy with the help of an oxidizer (air). Since, there is no intermediate mechanical step, FCs are not restricted by the Carnot cycle and have no moving parts. Consequently, FCs are highly efficient, reaching efficiencies of 60-70%. Of the different kinds of FCs, SOFCs are the most efficient. The key feature of a SOFC is its solid ceramic oxide electrolyte which serves as an ion transport medium (oxide ions or protons) and as a membrane between the reducing cathode and oxidizing anode atmospheres. Ceramic electrolytes are key to enabling SOFCs to operate at temperatures up to 1000°C.

The one major drawback that has precluded the widespread commercialization of FCs in the power generation and transportation industry is its need for H_2 (and to a lesser extent CO) as fuel inputs. It is for this reason that the 'H_2 economy' model was conceptualized although never quite realized. A potential way to circumvent the problem is to use DIR-SOFCs. DIR-SOFCs can utilize CH_4, C_2H_6 and a few other higher hydrocarbons as fuel due to the ability of the anode to simultaneously dry/steam reform CH_4 into H_2 and CO and electrochemically oxidize H_2/CO to H_2O/CO_2 and produce electricity (Abbildung 1). The high operating temperatures of SOFCs are ideally suited to CH_4 reforming and water gas shift reactions. As a result, the understanding and development of DIR-SOFCs can play an important role in the clean energy sector. With that in mind, a physically based model of a DIR-SOFC has been developed in the group.

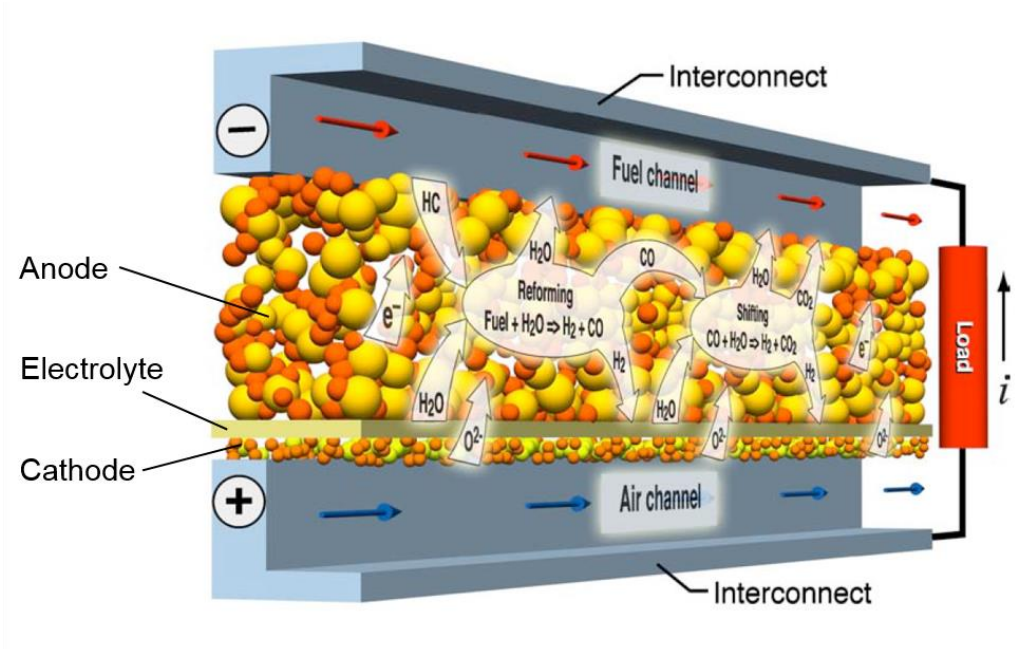

Abbildung 1: Schematic representation of a DIR-SOFC

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Physically based modeling of SOFCs is a key tool in better understanding the involved physics. The *a priori* model delves into greater depths and obtains keener insights than the traditional *a posteriori* equivalent circuits approach. It involves modeling the SOFC in the continuum scale using first-principle conservation equations of mass, momentum, energy and charge. Effective transport properties are used to model transport through the porous electrodes. Heterogeneous chemistry and electrochemistry are modeled using detailed elementary reactions. The formulated set of partial differential conservation equations are discretized spatially using the method of lines and the resultant ordinary differential equations (along with algebraic equations) are solved numerically using the robust differential-algebraic equation (DAE) solver, LIMEX. The complete code is written in Fortran 77 and is one of the modules that comprise the commercial software package, DETCHEM.

So far, the 2-D model has been only used to simulate the co-flow mode of operation i.e. the fuel and air streams flow in the same direction. The co-flow mode is currently solved using an upwind marching scheme for integration in the flow direction with inlet conditions for each element set to the outlet conditions of the previous element. To solve the SOFC in the counter-flow mode, the upwind scheme needs to be replaced with a scheme that integrates all axial volume elements simultaneously. The goal of this Masters project would be to implement such a scheme which enables the modeling of the SOFC in the counter-flow mode and then perform an analysis comparing the two operational modes for DIR-SOFCs.

Requirements:

Applicants require a basic understanding of fluid dynamics and heat and mass transfer, familiarity with numerical methods of solving differential equations like finite differencing and experience coding in a high-level programming language (Fortran would be best but C/C++/Java is also fine – It doesn't take long to learn Fortran if one knows C/C++/Java).

Starting date:

The starting date is flexible and can be decided on after an initial meeting.

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