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Simulation of Fuel Cell Powered Drive Trains

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Abstract

DLR is working on fuel cells and their application, whereby the interest in the mobile application of fuel cells is constantly increasing. The design of fuel cell systems is a multi-disciplinary task. It requires knowledge in electrochemistry, thermo- and fluid dynamics, electrical science and control. In the design of fuel cells systems for the energy supply of car engines, additional aspects have to be considered. Tools to optimise fuel cell systems should, therefore, be capable to link knowledge from several disciplines.

Consequently, DLR is currently developing a suitable design tool for fuel cell systems with respect to various applications. The presentation explains our approach of a physical model of a fuel cell and its implementation by Modelica. Some exemplary results highlight the application of the model.

Introduction

Recently German Aerospace Center (DLR) has initiated a new business division transport. The aim is to focus, strengthen and extend a number of already existing research activities within this sector. Among them are the research on transport systems e.g. analysis of the structure of transport systems, whereby DLR uses models developed for the analysis of air traffic. Other fields are the application of adaptronics and telematic in vehicle technology or use of advanced light weight materials for vehicle construction. It is well known that the transport sector contributes increasingly to the CO₂ – emissions. Therefore hybrid and fuel cell vehicles are discussed in order to reduce these emissions. A number of car manufacturers are currently developing fuel cell powered vehicle. DLR has performed research in fuel cells for space and stationary application for a number of years. A part of these capacities has been put into the transport division. There exist different types of

fuel cells. DLR is working on the high temperature Solid Oxide Fuel Cell (SOFC) and on the low temperature Polymer Electrolyte Fuel Cell (PEFC). The operating temperatures are around 800 C and around 80 C. Generally the PEFC is considered as the most promising type of fuel cell for power trains. Actually hydrogen is used as a fuel for the PEFC. The following paper deals with the PEFC.



Fig.1: Membrane Fuel Cell Test Facility PEMA at DLR Institute of Technical Thermodynamics

The design of fuel cell systems is a multi-disciplinary task. The fuel cell itself is an electrochemical energy converter. The detailed modeling of an fuel cell requires knowledge e.g. in electrochemistry, heat and mass transfer, multiphase thermodynamics, fluid dynamics. A fuel cell system consists of several sub systems:

- fuel cell
- air supply system
- fuel supply system = hydrogen supply system
- cooling system (heat and water management)
- control system

The air supply system has to deliver the oxidant usually oxygen to the fuel cell. It consists of blowers, fans valves and pipes. The fuel supply system could be a tank where the hydrogen is

stored and some pressure reducing and control valves reducing the pressure respectively metering the hydrogen to the fuel cell. Actually there exists no satisfying solution for the storage of hydrogen. Pressure tanks are bulky and heavy, which yield to limited ranges. The production of liquified hydrogen requires a significant amount of energy, furthermore the highly insulated storage tanks are very costly. An alternative is the on-board production of hydrogen by a reformers splitting a hydrogen rich hydrocarbon like methanol. Such reformer are chemical reactors which are followed by apparatus to purify the reformer gas in order To achieve sufficiently high reformer efficiencies often internal heat recovery is a must. To date the reformer is still a crucial sub system with respect to the dynamic operation of the fuel cell system. Having said this it is understandable why tools from chemical engineering like Aspen Speedup or other are used for the design and development of fuel cell systems. Having in mind that the current R&D in fuel cells yields to a steadily increasing knowledge base and also that the fuel cell system should be analysed with respect to the application in part load and transient operation, which especially the case for fuel cell powered drive trains, DLR has chosen MODELICA as a simulation tool for fuel cell systems.

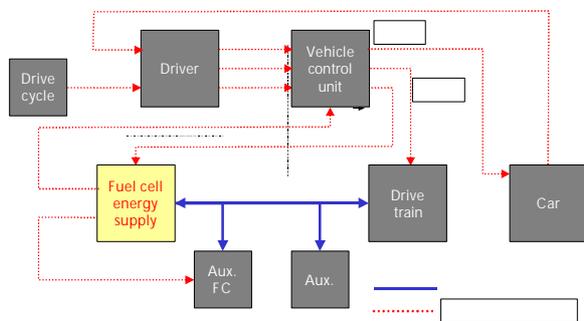


Fig. 2: Basic structure of the highest level of the fuel cell system model.

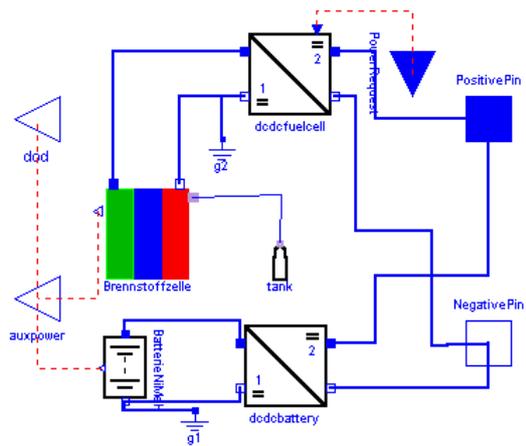


Fig.3: Model for the fuel cell energy supply system

As shown in Fig. 2 a *driver* compares the actual velocity of a *car* with the velocity of a certain *drive cycle*. The comparison results into an acceleration request to the *vehicle control unit*. The vehicle control unit contains strategies to fulfil the acceleration request with respect to the state of the energy supply system. This results into control signals for the mechanical brake and the *drive train*. Concerning the fuel cell activities, the main interest of DLR is the *fuel cell energy supply system* [Fig.3]. The modeling of the fuel cell system, mainly the fuel cell itself, is subject of this paper.

Some exemplary results are shown. Fig. 4 shows the results for the single fuel cell voltage (which is proportional to the thermal efficiency) in dependance of the current density for different air ratios. A higher air mass flow at the cathode of the

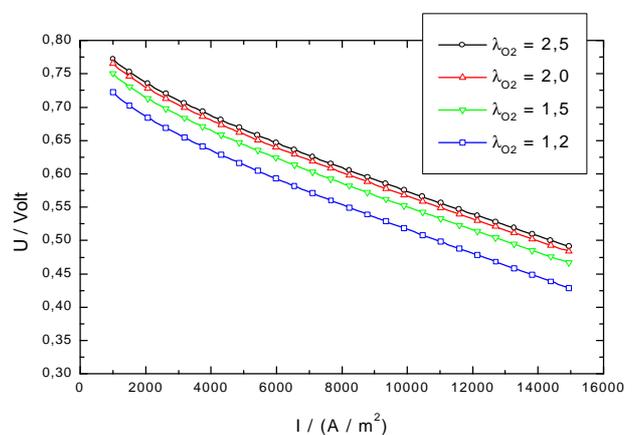


Fig. 4: Modelling effect of air ratio on single cell performance

fuel cells leads to a higher efficiency of the single fuel cell.

The necessity of simulating the complete system becomes obvious in Fig. 5: here, the efficiency of the complete system is calculated. In contrast to Fig.4, due to the parasitics of the compressor, the efficiency of the complete system is not best with the highest air mass flow.

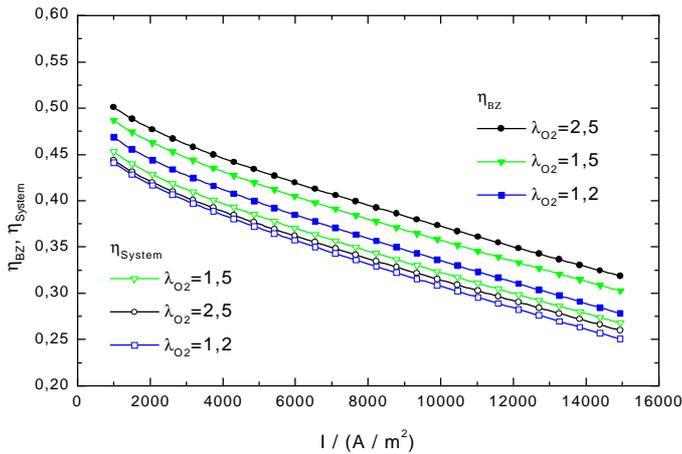


Fig. 5: Effect of air ratio on system performance and single cell efficiency.

Basic Fuel Cell Model

A fuel cell is an electrochemical device that converts the chemical energy of a fuel to electrical energy without the Carnot cycle limitation of heat engines. The fuel and the oxidant are supplied continuously to the fuel cell. A fuel cell is composed of an anode, where the fuel is oxidized and a cathode, where the oxidant is reduced. The two electrodes are separated by the electrolyte, an ionic conductor. Solid polymer fuel cells (PEFC) use a solid polymer membrane as ionic conductor. The membrane is sandwiched between two porous electrodes. This makes the PEFC a robust fuel cell with simple design. With hydrogen as fuel and air as oxidant, a single PEFC reaches a voltage of about 0,7V. In order to provide higher voltages, single cells are connected in series to form a fuel cell stack. The performance of a PEFC is characterized by the polarization curve showing the relationship between cell voltage and current density. The cell voltage is proportional to the thermal efficiency. Voltage losses (overvoltages)

can be attributed to different mechanisms: at low current densities, the cell voltage is mainly reduced by the cathodic reaction. Mass transport limitations become dominant at high current densities. The voltage losses are increased by the resistance of the membrane. This resistance is not constant but dependent on the water content of the membrane. This demands an appropriate water management of the fuel cell. The aim of the numerical simulation is not only the calculation of the electrical power produced by the fuel cell, but also the computation of the water and heat balance.

Physical Model

Both electrodes of the fuel cell are separated into three different sections. The reactant gases flow in gas channels along the backside of the electrodes. A certain amount of the gases enters the porous electrode and diffuses to the catalyst layer adjacent to the membrane. At the catalyst-membrane-gas interface the electrochemical reaction takes place. The ions produced at the anode migrate through the membrane to the cathode.

The structure of the system always remains the same, the reason for using a modular modeling strategy is the ability to exchange submodels in an efficient way. This is necessary since the knowledge about the physical processes taking place in the fuel cell is in an early stage. As a result, different kinds of fuel cell models with a large variation in complexity are described in literature [e.g. 1-4]. The main aim of the modular modelling of the fuel cell is the development of an efficient engineering model by identifying the key mechanisms in the fuel cell.

Modelica Implementation

The basic structure of the fuel cell consists of the membrane-module that is connected to the anode on one side and to the cathode on the other side. Three models representing the reaction layer, the diffusion layer and the gas channel are connected in series to simulate the electrodes [Fig. 6]. In this paper we present the most basic fuel cell model.

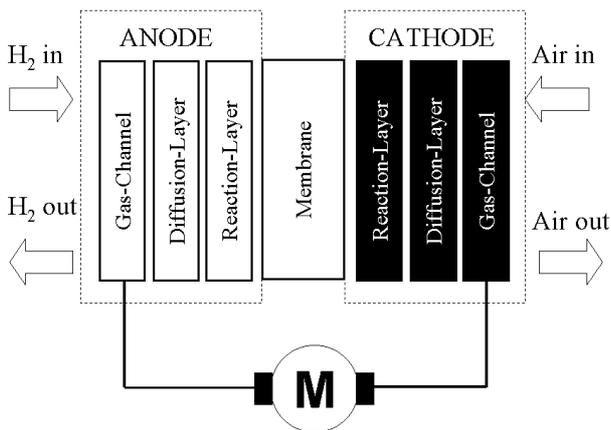


Fig.6: Schematic of the basic fuel cell model.

Connectors

In addition to the connectors used for heat transfer and electrical current, connectors for the different reactants are needed. Since the reactants are humidified before entering the fuel cell, connectors for multicomponent mass flow are used. For humidified hydrogen fed to the gas-channel of the anode the connector contains the molar flow \dot{m} , the total pressure p , the specific enthalpy h and the molar concentration $x[1]$ of hydrogen and $x[2]$ of water. The corresponding connector for humidified air at the cathode includes the \dot{m} , p , h and the molar concentration of nitrogen $x[1]$, oxygen $x[2]$ and water $x[3]$. Between the different layers of the fuel cell, the components must be treated separately, so there are also connectors for dry oxygen, dry hydrogen, dry nitrogen and water. All these connectors contain the variables \dot{m} , p , h but are defined as separate models to prevent connections between different species.

Physical properties of reactants

A library *properties* contains packages with the state equations of the different substances. Hydrogen, oxygen and nitrogen are treated as ideal gases. A partial model *idealgaslaw* with the functional relation between temperature, pressure and density serves as parent class for these gases. Water can occur both in liquid and gaseous state and plays an important role in heat and mass transfer. The package *water* contains functions with the saturation values of pressure, enthalpy and density. The algorithms used for the description of the relation between the state variables usually contain polynoms. The integration of these polynoms in acausal models proved to be difficult: although the isolated models worked, more complex system didn't converge. Instead of the models, functions are used to describe the relations between the state variables.

Layers of the fuel cell model

Except for the reaction-layers, each of the seven layers of the model contains an ohmic resistor *elresistplusq* and an element *heatconduct* representing the thermal conduction in the layer. Due to the Joule heating the ohmic resistor represents a heat source that is connected to thermal conduction element [Fig.7].

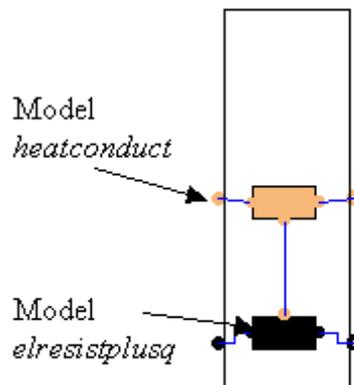


Fig. 7: Basic layer model.

Gas channels

The model for the gaschannel is *anodchannel* on the anode side and *cathchannel* on the cathode side. The model *cathchannel* is shown in Fig. 8. The connector for the inflowing humidified air is connected to the model *cathjunction* where the air is separated into its components. The separation of

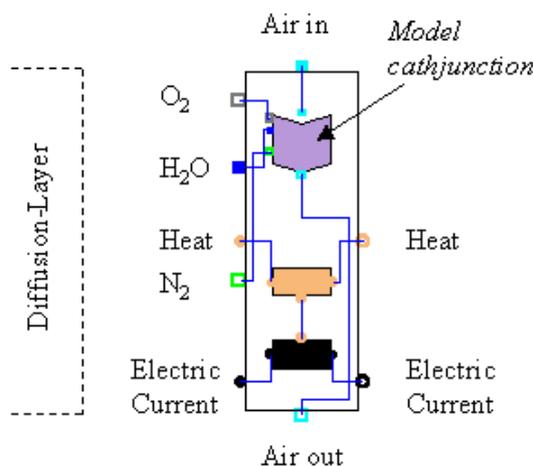


Fig. 8: Model *cathchannel* for the gas channel of the cathode

the air is necessary since the cathodic reaction consumes oxygen while water can flow in both directions at the interface between gas-channel and diffusion layer depending on the current density. Nitrogen is an inert component at the cathode. At the exit of gas-channel the different components are combined to leave the fuel cell in an wet air connector.

Diffusion layers

The reactants flow through the diffusion layer to or from the reaction zone of the electrode. An example for the range of complexity of physical models describing the processes in the fuel cell can be shown with the diffusion layer of the cathode. The most simple assumption is, that there is no loss in pressure of the oxygen. In this case, the model is reduced to the base model of a layer, the inlet connectors for the different gases are connected to the outlet connectors. The more complex model (Dusty-gas-model [5]) considers different kinds of transport mechanisms in the porous diffusion layer: the mass flow is regarded as combination of molecular diffusion, Knudsen diffusion and convective flow due to a pressure gradient. The Dusty-gas-model can be regarded as combination of different transport resistances [Fig.9].

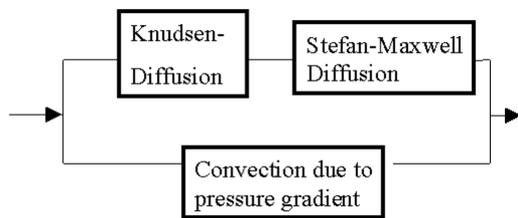


Fig. 9: Dusty-gas model for diffusion in porous media

In Modelica, for each of these three transport mechanism a partial model was created. These partial models were then completed by the transport-properties of the different gases. Finally, the models are connected according to the Dusty-gas-model. Calculations show, that the difference between the results of a fuel-cell model with the most simple model and the results of a fuel cell model with the Dusty-gas-model grow with the current-density. High current densities usually occur at low cell-voltages indicating low thermal efficiencies. For automotive applications, the current range where transport limitations become significant should be avoided since the efficiency of the fuel cell is not sufficient. For most

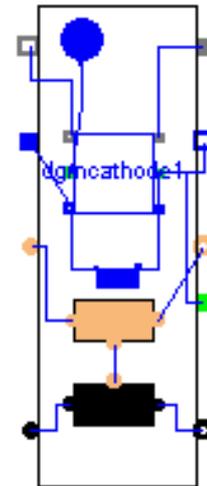


Fig. 10: Diffusion layer model with Dusty-gas model *dgm_cathode1*

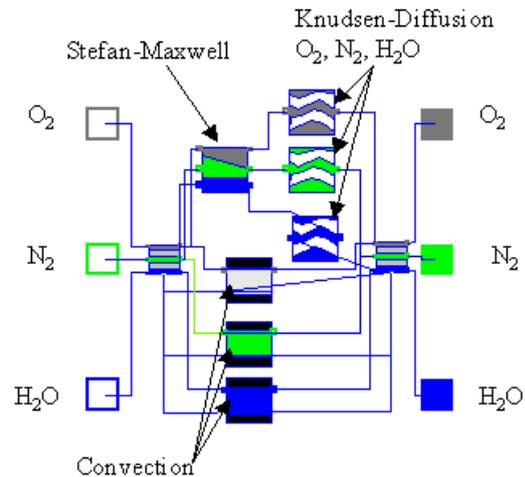


Fig.11: Dusty-gas model of the cathodic diffusion layer *dgm_cathode1*.

automotive applications, simulation models with simple transport models provide results that don't differ much from results calculated with more sophisticated models.

Reaction layers

The electrochemical reaction takes place in the interfaces between the membrane and the electrodes

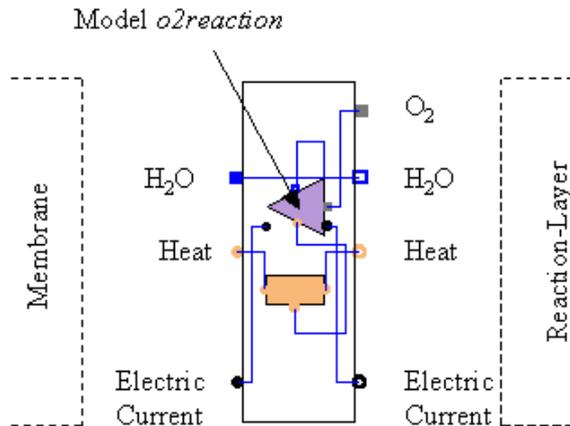


Fig. 12: Reaction layer of the cathode

The model *h2reaction* calculates the consumption of hydrogen and the heat produced by the splitting of the hydrogen molecules into ions. At the cathode, the model *o2reaction* determines the consumption of oxygen and the heat produced by the reaction. In contrast to the anode, significant voltage losses result from the reaction. These losses are dependant on current density, oxygen pressure and temperature.

Membrane model

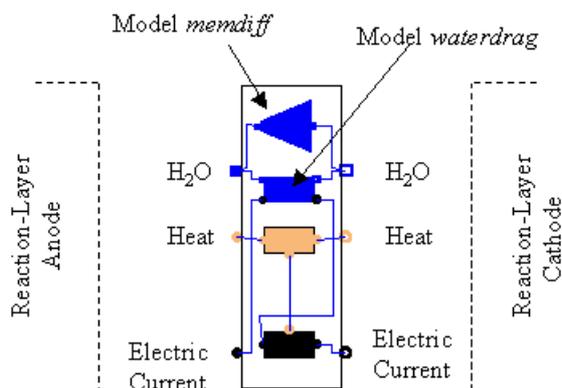


Fig. 13: Model of the polymer membrane

The ohmic resistance of the membrane is the most significant one in the fuel cell. The conductivity of the membrane depends on the wetness of the polymer. The model membrane contains the model

memresistor for calculating the ohmic resistance in dependance of a parameter defining the wetness of the membrane. Due to electroosmose water flows from the anode to the cathode. This drag is calculated in the model *waterdrag*. There is also diffusion of water through the membrane due to the concentration gradient of water between the both sides of the membrane. This flow is calculated with the model *memdiff*.

Conclusion

Modelica is applied to simulate transport systems using fuel cells. The modularity of Modelica supports the identification of the most efficient configuration of the basic components needed for a fuel cell system. The basic Modelica fuel cell model presented here is the starting point for the comparison of different physical models describing the processes in a fuel cell. The extension of the fuel cell library will continue with the aim of creating a efficient tool for the design of fuel-cell system.

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