TU Clausthal

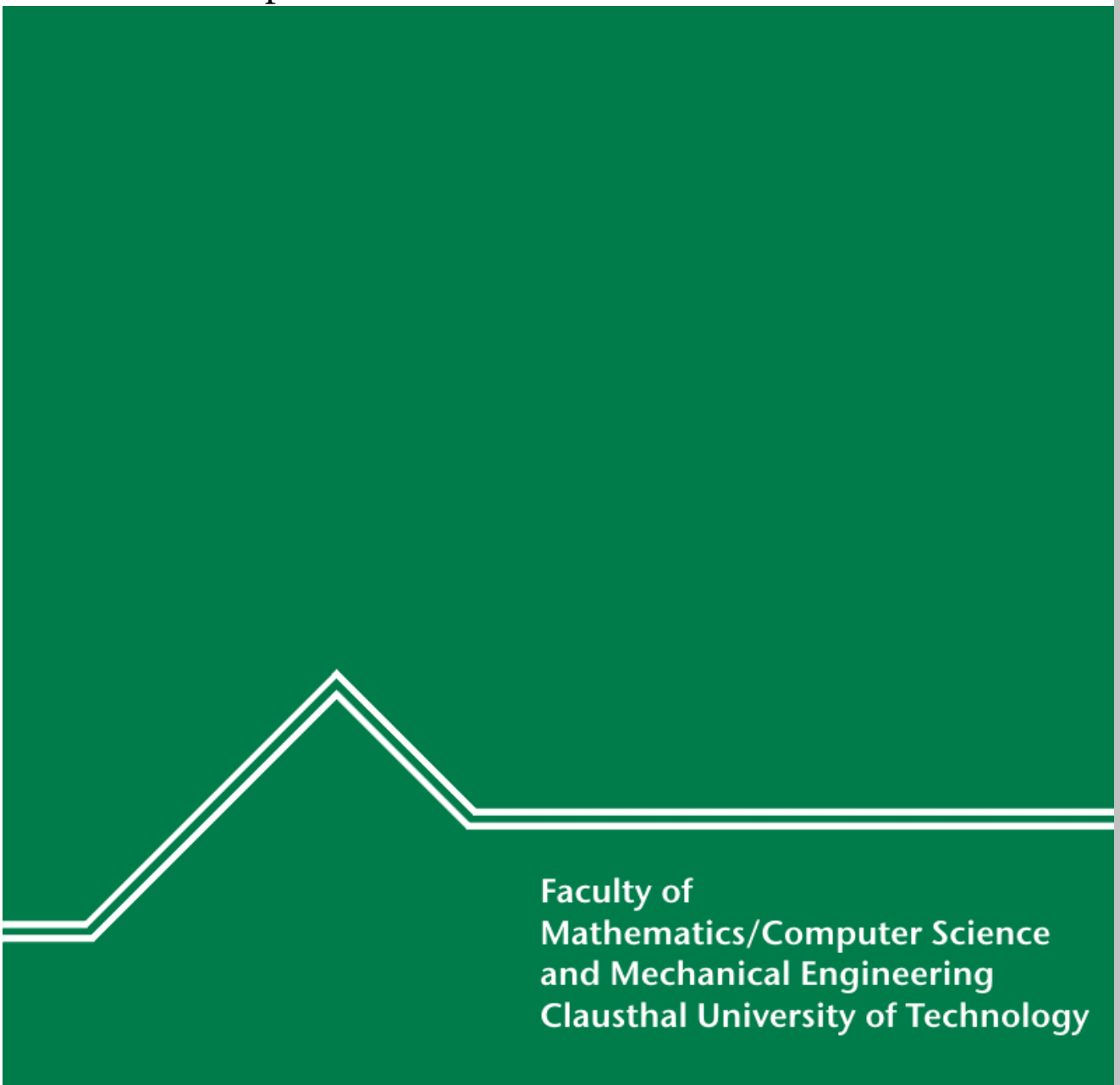
Clausthal University of Technology

Single-Fuel-Cell Simulation With CFX Under Consideration of Multi-Phase-Domains and Hydrogen-Oxygen-Interactions

V. Wesling, P. Giese, T. Kandelhardt

Technical Report Series

Fac3-10-01



Impressum

Publisher: Fakultät für Mathematik/Informatik und Maschinenbau,
Technische Universität Clausthal
Am Regenbogen 15, 38678 Clausthal-Zellerfeld, Germany
Editor-in-chief: Alfons Esderts
Technical editor: Martina Wächter
Contact: martina.waechter@tu-clausthal.de
URL: http://www.fakultaet3.tu-clausthal.de/forschung/technical-reports/
ISSN: 1869-8018

The Faculty of Mathematics/Computer Science and Mechanical Engineering Review Board

Single-Fuel-Cell Simulation With CFX Under Consideration of Multi-Phase-Domains and Hydrogen-Oxygen-Interactions

Prof. Dr.-Ing. V. Wesling
Dr.-Ing. P. Giese
Dipl.-Ing. T. Kandelhardt

TU Clausthal - Institute of Welding and Machining
Agricolastraße 2
38678 Clausthal-Zellerfeld
05323 / 722503

Abstract

A theoretical model for the simulation of complex systems, like the characteristics of chemical reactions in fuel cells, is important to enhance the effectiveness of PEM-FCs. With an appropriate approach it is possible to calculate the interactions between anode and cathode and to predict the flow performance of each gas. With respect to the velocity distribution in each flow-channel it is important to simulate all reaction products realistically. A Fortran program module was written and integrated into the commercial software Ansys CFX, which calculates the interactions of a 4-multiphase model in all channels, gas diffusion layers, and MEAs. Now, it is possible to obtain detailed information on the flow distribution in the flow channels. Simulation results show a nearly realistic distribution in the MEA. The volume fractions of the different gases in the channels correspond to reality, while, at the same time, the total system is in good electrochemical balance.

1 Problem description

The functionality of PEM-fuel-cells is based on an electrochemical process, where hydrogen and oxygen react in a controlled way. Both gases flow through a channel, while simultaneously interacting with a region called the gas-diffusion-layer (GDL). The membrane separating the two regions is only permeable by Hydrogen protons. Hydrogen dissociates at a platinum covered anode catalyst and while the protons permeate the membrane directly the electrons move through conductors to the oxygen side. There oxygen is ionized on the cathode catalyst. After this ionization, the protons react with the oxygen ions to form pure water. The electrons lead to a continuous current that can be gripped at the electrodes. Detailed information is described in [5].
The physical environment of both flow channels continuously changes depending on the mass flux through the gas-diffusion-layer. The volume fraction in the flow channels is directly dependent on the mass transportation through the GDL and membrane [1]. According to the flow channel, the mass flow either increases (on the cathode side) or decreases (on the anode side). To get correct results, it is not sufficient to simulate a flow channel alone, without changing the mass flux along the streamline. Therefore, a Fortran program was written and integrated into the commercial Software Ansys CFX. This program calculates the velocity and mass distribution realistically, with simultaneous consideration of the mass flux in the gas diffusion layer, for both the hydrogen and for the oxygen side. All other components of a fuel cell, like the gas-diffusion-layers, the catalysts, and the membrane are merged into one black box (see Fig. 1).

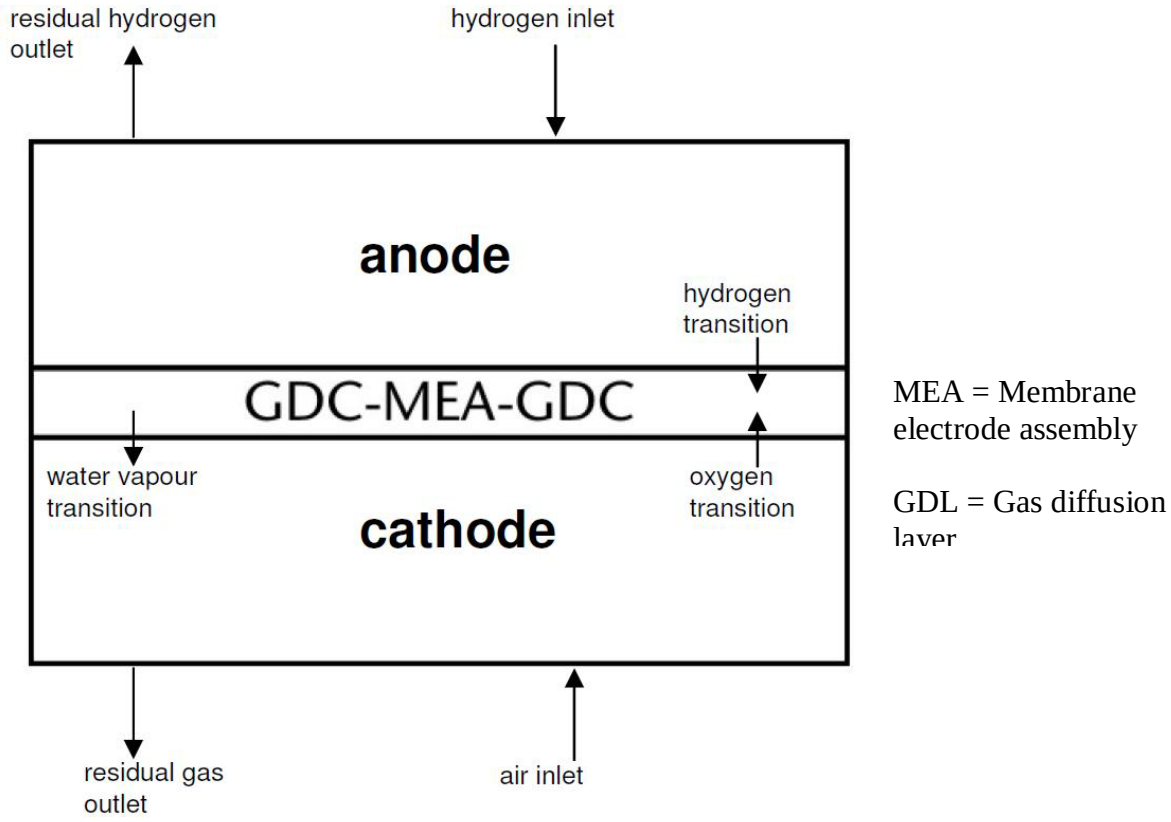


Figure 1: The model of the fuel-cell module

The use of one black box instead of five separated volumes in CFX, as it is shown in [7], has the advantage that the effort and duration of the iteration decreases. Because of this, the model couldn't regard every physical effect and so a small loss of accuracy is present. But for the design of fuel-cell flowfields the quantity of velocity and pressure distribution is more interesting than the exact values of speed and pressure. Especially the flux distribution of a flow field is important during the construction of a fuel cell. Consequently, the mass flux and streamlines have to be known in detail (see [2]). Information about water content, water saturation, or temperature is of second rank. With the information about the water content and water saturation (shown in [7]) it is possible to calculate the internal resistance of the cell and then the power dissipation. The temperature, occurring by forming pure water [5], is directly proportional to the gas distribution in both flow fields. The durability and efficiency of fuel cells depends on the temperature gradients. Of course a fuel cell should have small temperature gradients. And so the knowing of the gas distributions makes it possible to derive the temperature distribution.

2 Modelling and Simulation

All calculations have been done with the commercial software Ansys CFX, using a turbulent formulation, although the Reynolds numbers are extremely small. The latter implies that a laminar flow exists in the channels, but the turbulent formulation smoothes the flow distribution. Furthermore, all energetic losses are considered by the turbulent formulation. The anode gas is hydrogen (H2) at standard pressure (1013.25 hPa) and standard temperature (25 °C). The cathode is supplied with ambient air, which is represented as a nitrogen-oxygen-mixture. The mixture at the cathode-inlet is 80 % nitrogen and 20 % oxygen. All properties of both gases are also set at standard pressure and standard temperature. The reaction product pure water is set to steam at 100 °C.
The velocity distribution with respect to the mass losses is the result of the simulation. To get realistic results it is necessary to remove gas from the flow channel by means of negative mass sources. The environment and the operating condition of the fuel cell can be changed by varying the pressure or the temperature of the gases. To make all simulations comparable, the power density, which describes the operating condition, is set to a constant value of 200 mA/cm². Now it is possible to calculate the total mass losses. The hydrogen which was removed from the flow channel is set as the input mass flow into the gdl-mea-black-box. By knowing this input mass flow it is possible to calculate the necessary oxygen mass. Just as on the anode side, the calculated oxygen mass will be removed from the flow channel and set as an input mass flow into the gdl-mea-black-box. Because of this, the nitrogen volume fraction increases. The Black-box calculates also the mass of the formed pure water. As it is described above, this mass will be set as an input to the cathode channel. It is obvious that the total mass flow on the cathode side increases from the inlet to the outlet.

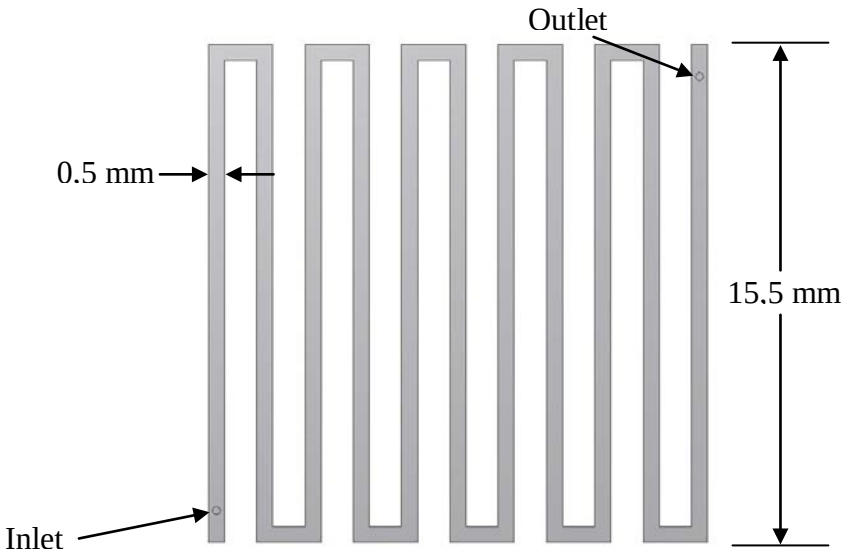


Figure 2: Model of the flow field

The structure of the PEM-FC-flow field is a simple short meander which covers a rectangle of 15.5 x 15.5 mm². The profile of the flow channel itself is also a square, with height and width set to 0.5 mm. The black-box of the GDL-MEA has a height of 0.3 mm and the same length and width as the flow field rectangle.

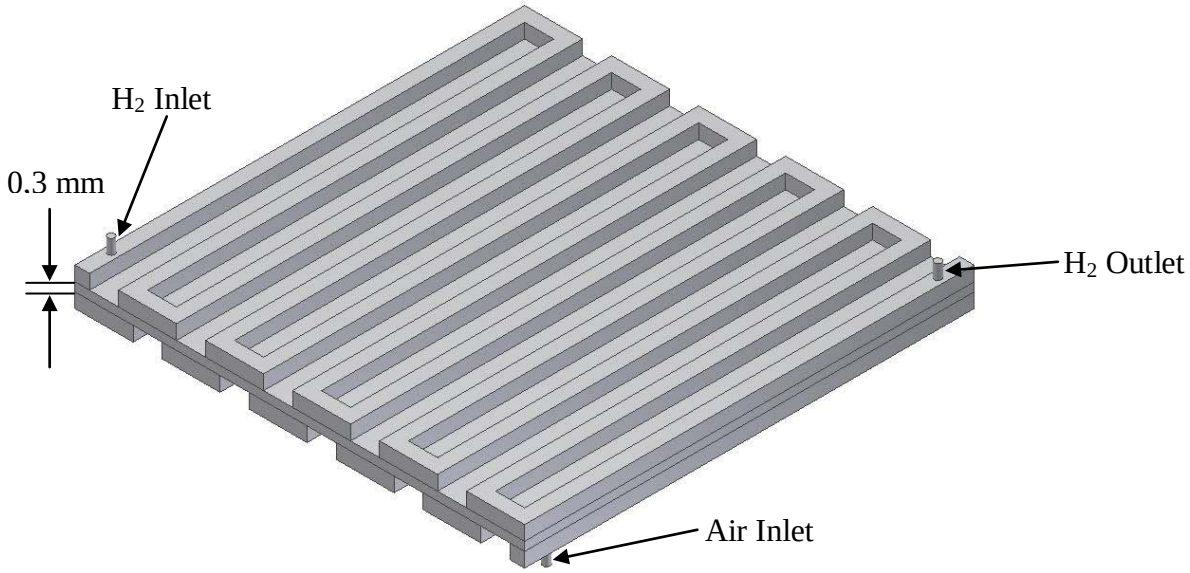


Figure 3: Model of the complete fuel-cell

All these volumes are meshed in CFX-Mesh with about 500,000 tetrahedron elements. Ansys CFX has the ability in spite of double faces and edges in the model to merge these faces and treat them as one. These merged faces are shown as contact faces in the program. It is now possible to set special properties at these contact faces.

3 Results

The primary target of this fuel-cell simulation is to see the realistic mass ratio in each channel. With the newly developed module it is also possible to calculate large complex flows regardless of the vast size of the model.

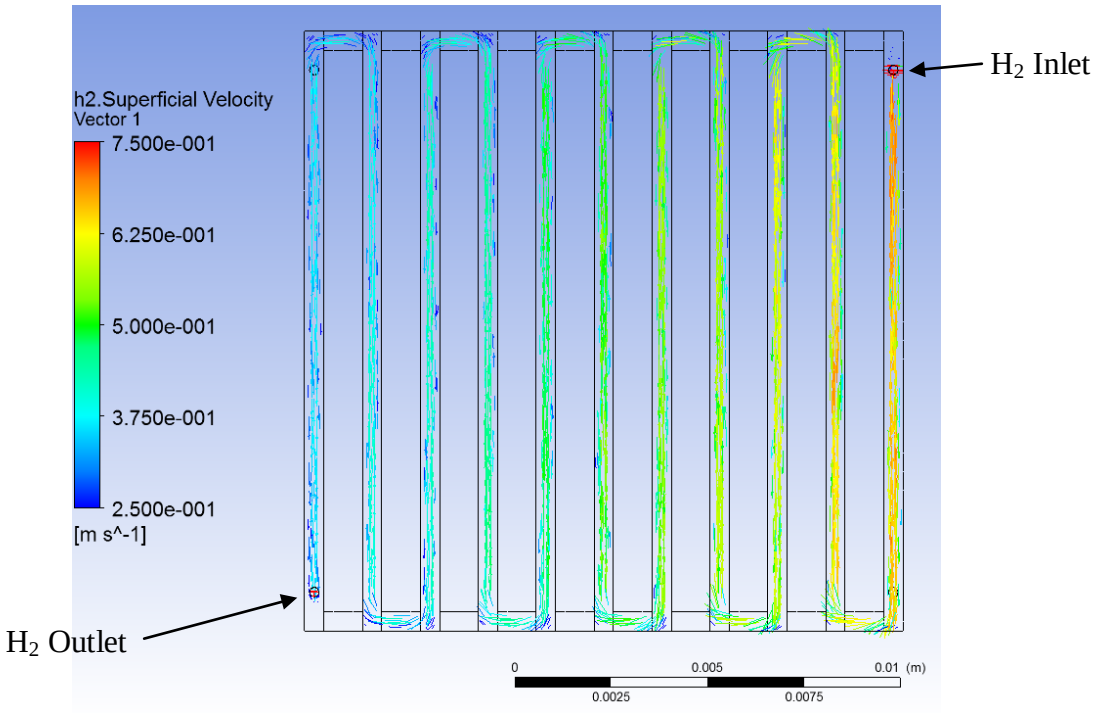


Figure 4: Velocity distribution of the Anode side

As shown in Fig. 4, the anode side of the fuel cell shows a decrease of the hydrogen from the inlet to the outlet. Because of this, the velocity of the hydrogen reduces stronger in comparison to a normal perfusion of a meander channel with no mass fluxes.

Mass flow	
Air Inlet	6,630 e-7 [kg s^{-1}]
Air Outlet	- 8,073 e-7 [kg s^{-1}]
Hydrogen Inlet	1,007 e-8 [kg s^{-1}]
Hydrogen Outlet	-5,054 e-9 [kg s^{-1}]
Volume fraction	
O2 (Air Outlet)	11,467 %
N2 (Air Outlet)	79,387 %
H2 (Air Outlet)	0 %
Water (Air Outlet)	9,285 %
O2 (Hydrogen Outlet)	11,467 %
N2 (Hydrogen Outlet)	79,387 %
H2 (Hydrogen Outlet)	0 %
Water (Hydrogen Outlet)	9,285 %

Table 1: Mass flow and Volume fraction of the Simulation

The simulation is in electrochemical balance which means that the mass of the converted hydrogen atoms has the correct size. The results show that the set inlet mass flow is a little bit too high (see Table 1) and to many unused gas coming out of the outlet. Because of the assumption that the reaction in the black-box is ideal, all hydrogen atoms which flow into the black-box react with oxygen.

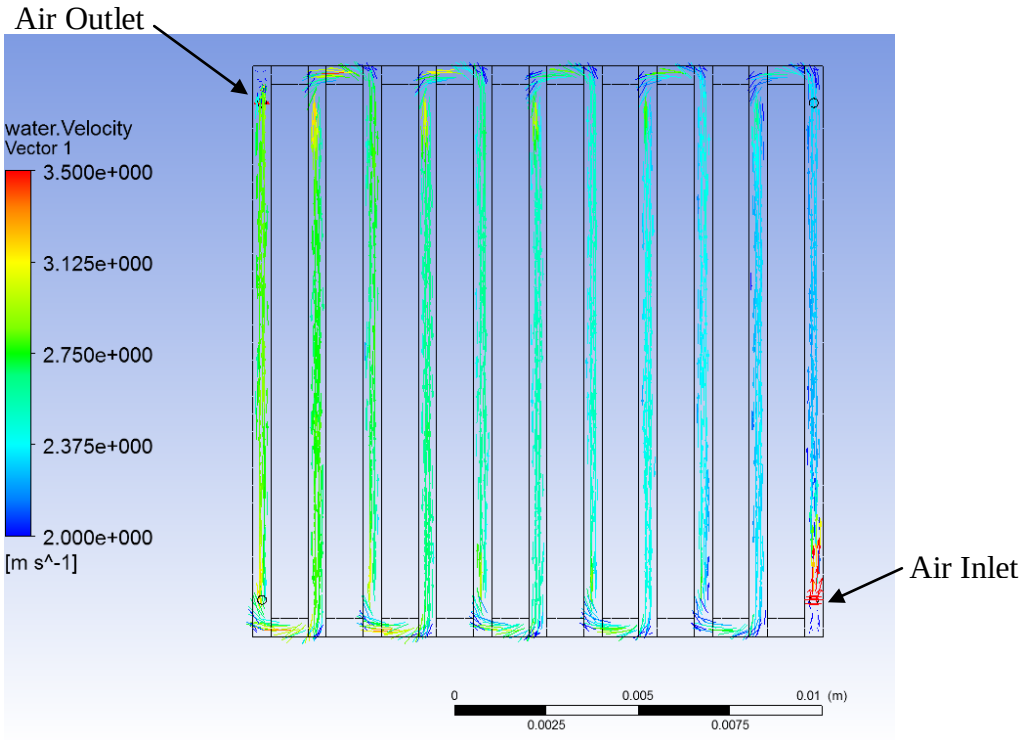
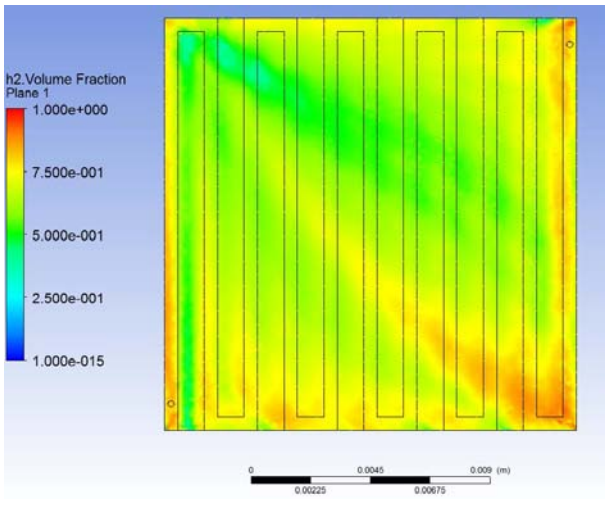


Figure 5: Velocity distribution of the cathode side

The cathode side shows an increase of the gas from the inlet to the outlet. This is the result of the produced water vapour. The volume fractions of the different gases vary stronger than expected from the increase of the gas alone. The nitrogen mass remains constant from the inlet to the outlet, but its volume fraction decreases. It would even increase, because of the oxygen flow into the black box, but this effect is more than compensated by the water vapour. The volume fraction of the oxygen decreases. The pure water, as the result of the hydrogen–oxygen-reaction, starts with a volume fraction of zero and increases towards the outlet.

The computed velocity distributions on the anode and cathode side are realistical. Because of the individual treatment of the different gases it is possible to make accurate predictions of the behaviour of the fuel cell. The streamlines are also very realistical and show the gas flow in the fuel cell's channels during operation. Under these circumstances it is possible to design new flow field structures which have a positive effect of the operation and performance of the fuel cell. Not only the single view of each flow channel is important, also the interaction of both gases is essential.



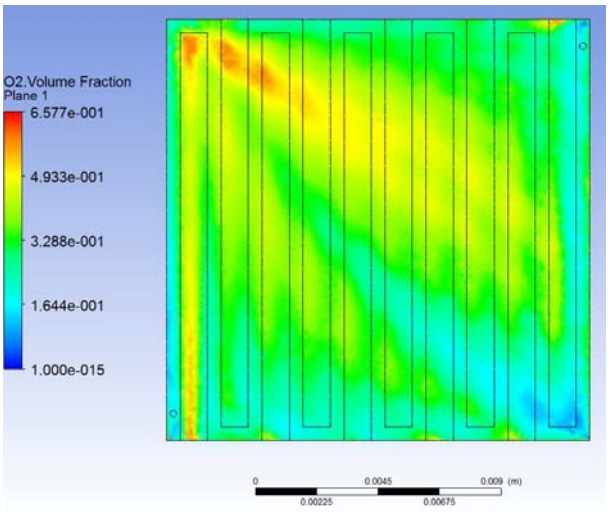


Figure 6 and 7: Volume fraction of H_2 and O_2 in the MEA-GDL-Black-Box

The interaction of hydrogen and oxygen are shown in the black-box. Unlike the flow channels, the black box has no inlet and outlet. Because of this, it is not possible to get a convergent result. Nevertheless, the mixture ratio of the gases is shown and calculated with sufficient accuracy. With the knowledge of the mixture ratio in the GDL-MEA the flow field structures can be modified more effectively in order to increase the performance of the fuel-cell.

4 Summary

Developing a numeric model, which shows realistic streamlines and velocity distributions, is an important step on the way to find new efficient flow fields. The simulation is more favourable and faster than building every constructed flow field and comparing the data from time consuming tests.
In this technical review, a procedure of a fuel-cell simulation in due consideration of the mass transport through the membrane was described. With a newly developed module for the simulation software Ansys CFX it is possible to compute the streamlines and velocity distribution realistically. Furthermore the interaction between the anode and the cathode can be examined in more detail. The 3-volume model of a fuel-cell, where the gas diffusion layers and the membrane are represented by only one volume, has also been developed to run larger, more complex models. First simulations were made with a 15.5 mm rectangle cell including a meander flow field. The volume fractions and velocity distributions of the anode- and cathode side are realistically shown. Also the mixture ratio in the membrane volume can be predicted reliably despite of no present inlet and outlet. From the visual representation of the streamlines of the flow channels it is possible to design new flow fields to increase the performance of the fuel-cell. Also the interaction between the anode and the cathode helps to adjust the flow field structures.

Literature

[1] V. Gurau, F. Barbir, H. Liu: An Analytical Solution of a Half-Cell Model for PEM Fuel Cells, Journal of The Electrochemical Society 147, 2000

[2] K. Tüber: Analyse des Betriebsverhaltens von Polymer-Elektrolyt-Membran Brennstoffzellen für portable System, Dissertation, Uni Duisburg-Essen, September 2004

[3] H.S. Chua, C. Yeh, F. Chenb: Effects of porosity change of gas diffuser on performance of proton exchange membrane fuel cell, Journal of Power Sources 123, 2003

[4] H.E. Siekmann, P.U. Thamsen: Strömungslehre: 2. aktualisierte Auflage, 2008

[5] F. Barbir: PEM fuel cells: theory and practice, 2005

[6] Ansys CFX-Solver Modeling Guide, Chapter User Fortran, Ansys, 2006

[7] Fluent 6.3 Fuel Cell Modules Manual, September 2006