Final report

1.1 Project details

Project title	PEMFCD
Project identification (program abbrev. and file)	12041
Name of the programme which has funded the project	Forskel
Project managing company/institution (name and address)	Department of Energy Technology, Aalborg University (ET-AAU)
Project partners	Dantherm Power A/S Hydrogen South Africa – Catalysis
CVR (central business register)	29102384
Date for submission	30.09.2015

1.2 Short description of project objective and results

English

The objective of this project was to further develop an existing computational model to simulate heat and mass transfer in proton exchange membrane fuel cells. This model was then employed to shed new physical insight and to make important suggestions that may substantially improve the performance and durability of air-cooled proton exchange membrane fuel cells. In addition, experiments have been conducted to verify these findings. In particular, a novel method to measure the fuel cell water balance was further developed and has led to a new patent application.

Dansk

Formålet med dette projekt var at videreudvikle en eksisterende beregningsmæssig model til at simulere varme- og masseudveksling i proton membran brændselsceller. Denne model blev derefter implementeret til at give ny fysisk indsigt til brug for at træffe nye beslutninger, der kan væsentligt forbedre ydeevnen og holdbarheden af luftkølede proton-udvekslings-membran brændselsceller. Desuden er forsøg blevet udført for at bekræfte disse resultater. Især blev en hidtil ukendt metode til at måle brændselscellen vandbalance videreudviklet og har ført til en ny patentansøgning.

1.3 Executive summary

This project was aimed at further advancing an existing computational fluid dynamics model that has been developed at ET-AAU over recent years. This model has several world-leading features and in particular is superior to commercially offered fuel cell models as offered by Fluent or Star CD. During this project the model was expanded in its capabilities and drastically improved in its numerical robustness which led to several publications in leading journals.

Numerous numerical studies conducted with our computational model and the findings have been and will be published in leading journals. These modelling publications will probably be among the leading articles for years to come.

Validation experiments were conducted with particular focus on the fuel cell water balance. We have developed a novel technique to measure the fuel cell water balance ad-hoc and in real time with great accuracy using hot wire anemometry. The original idea for this method stems from 2011 and a patent is currently being applied for. During this project we discovered a very elegant way how to treat the hot wire signal. This method is also being patented now.

Finally, we conducted water balance experiments on a commercial Ballard fuel cell stack using the hot wire methodology. These measured data are currently being analysed with our modified computational model to simulate air-cooled fuel cells with very good qualitative agreement. An invention disclosure has been submitted by the PI to AAU for a method of improving the performance of air-cooled fuel cell stacks as used by Dantherm Power A/S.

We are currently applying at EUDP for a follow-up project to improve the performance and durability of air-cooled proton exchange membrane fuel cells together with Dantherm Power A/S and Ballard Power Systems. The ET-AAU computational fuel cell model and our method to determine the fuel cell water balance with a hot wire anemometer will be a central part of this project, if granted.

1.4 Project objectives

In general, it was the objective of this project to further develop an existing computational fluid dynamics model to simulate heat and mass transfer in proton exchange membrane fuel cells which is based on the formerly commercial software package CFX-4. By further developing the existing model we wanted to shed new insight into heat and mass transfer in PEMFC. Previously, this model has helped to invent the "*Water Uptake Layer*", a potential break-through invention in the field of PEMFC because it may allow fuel cell operation on dry inlet gases and therefore can make humidifiers redundant which will significantly reduce the cost and complexity of fuel cell systems. The model development has also led to the invention of "*Dew Point Diagrams"* which can be used to optimize the operating conditions of PEMFC. It was also our goal to promote the use of this software and in the very least establish collaborations with various international partners so we can make use of our model and hopefully convince the fuel cell community of the advantages that CFX-4 clearly has over competing modelling efforts.

To give a rough overview, among the unique features of our model are:

- Leading multi-phase flow capabilities in the flow channels and the various porous media because of the use of the "multi-fluid approach".
- Leading implementation of the membrane water transport which makes our model capable of accurately predicting and understanding the fuel cell water balance.
- Capability of investigating both straight channel bipolar plates as well as the interdigitated channels. Our publications are the only ones that investigate the interdigitated flow field which is gaining increasing popularity in the fuel cell community as it allows for low stoichiometry operation. This was first shown in previous publications of our group.
- Capability of applying different pressures at anode and cathode as well as investigating co- or counter-flow. While the latter is not necessarily a given for commercial tools, the first part (different pressures) did require some advanced numerical manipulations. So far we have not seen in the literature other modelling results with different anode and cathode pressure.
- Capability of accounting for numerous "saturation jumps" between adjacent porous regions in case of multi-phase flow. Commercial tools usually do not account for the micro-porous layer whereas with our model it is easy.
- Applying non-isothermal boundary conditions by imposing a temperature gradient from anode inlet to anode outlet.

Project Risks

It was stated in the project application that there were certain risks associated with it. The original motivation for this project was to advance a computational model of a proton exchange membrane fuel cell based on the so-called multi-fluid approach as offered by the formerly commercial software package CFX-4. It was our goal to demonstrate that our computational model is superior to commercial modelling tools such as the Fluent fuel cell module (ANSYS Inc.) or the model "*es pemfc*" offered by CD Adapco.

In a SWOT analysis it was pointed out that the fact that we deliberately use a software package that has been phased out and has not being distributed poses both opportunities and weaknesses because CFX-4 is often incorrectly considered to be not up to date. However, especially the multi-phase model and our implemented membrane water transport model into CFX-4 is unique and world leading. The fact that we have used CFX-4 did pose a problem for convincing other research groups to also use our model. This will be further elaborated upon at the end of this report.

It was also stated in the project description that the nature of the project is 80% research and 20% development. Despite the sometimes unpredictable nature of research we were able to comply very close to the original plan. A few minor adjustments had to be done while the project evolved, and these changes were made after consulting with PSO. They will be described in the summary of the work packages below.

Project Evolvement

Most of the milestones agreed upon were fulfilled and in particular the number of scientific publications plus the patent are very positive outcomes of this project. On the other hand, we also encountered difficulties that let to project delay and a need to change milestones due to changes at our passive project partner, HySA Catalysis (see below).

Project delays due to hiring of new staff

The fact that we had to hire a new post-doc for this project actually posed some delay. While the official project start was in July 2013, the internal hiring procedure at AAU is quite complex and has caused delays. Moreover, our original first-choice candidate declined the offer in the last minute due to the delays in the university administration, and therefore the post-doc effectively started on the project in June 2014. However, Dr. Saher Al Shakhshir has proven a very strong addition to our research team and has immediately generated a very good output.

Modification of work packages due to problems at our project partner, HySA

A passive project partner was Hydrogen South Africa – Catalysis (HySA Catalysis) located at the University of Cape Town, South Africa. Hydrogen South Africa is a government initiative to promote fuel cell technology and especially promote the use of Platinum catalyst. HySA constitutes of three different institutes: HySA – Catalysis (U. Cape Town), HySA – Systems (U. Western Cape, Cape Town), HySA – Infrastructure (Northwest U., Rustenburg). South Africa is by very far the largest producer of platinum with around 75 % of the world mining share. Around 45 % of this platinum is used by the automotive industry and many car companies have manufacturing lines in South Africa. The growing spread of battery electric vehicles, the fact that modern cars use ever less platinum and the fact that a very large fraction of the platinum in old vehicles can be recycled all give reasons for concern regarding this key economic pillar for South Africa. Because fuel cells will require platinum, the government of South Africa has identified this area as a key technology and is thus attempting to become a leading player in the world wide fuel cell market by launching HySA in 2008.

This project was an attempt from our side to establish a strategic partnership with HySA Catalysis, which is co-hosted by the University of Cape Town and *Mintek*. HySA Catalysis has world-leading experimental facilities and is capable of producing custom-made membrane-electrode assemblies (MEA's) which are central to fuel cells. It was our long-term plan to obtain MEA's according to our specifications from HySA and conduct experiments using custom-made fuel cell bipolar plates and channel geometries in our lab in order to advance fuel cell technology. In return, we wanted to make that group aware of our fuel cell modelling competences. By visiting there and demonstrating our CFD simulations we wanted to gain this potential key player in the field as a customer for our model. While from our side the collaboration was actively pursued during this project, there have been severe problems on the side of HySA in general with two of the three directors quitting during the first half of 2015 (one of them was Dr. Olaf Conrad from HySA Catalysis, our project partner). It is not surprising that in light of this turmoil at HySA the collaboration with our university was given a lower priority on their side. We are hoping to revive our relationship in the future, but for now it appears that we have reached a dead-end.

The problems on the side of HySA did affect our project in the way that we were unable to obtain the custom-made membrane-electrode-assemblies that would allow us to further verify our previous modelling findings. As mentioned above, the original project plan was to obtain MEAs from HySA Catalysis and test them in a test rig in our fuel cell labs. We also wanted to use so-called interdigitated flow field plates and demonstrate fuel cell operation at low stoichiometric flow rates as had been demonstrated for the first time with our numerical model. However, in the second phase of this project it became more apparent that our research group at AAU may soon abandon the research activities in the field of low temperature PEMFC and put the focus in HT PEMFC. Therefore, we decided against purchasing expensive new equipment that may not be used after this project has been terminated. Especially in light of the fact that it is difficult for us to obtain custom made MEAs that we would need for model validation it was a reasonable choice to shift the attention on taking data on an existing Ballard fuel cell stack. This stack was modified in our laboratory by Dr. Al Shakhshir so that it operates on an open-ended anode. We then applied our newly developed method to obtain water balance data and compared it to our modelling predictions for an air-cooled fuel cell stack. This required modification of our existing fuel cell model and these simulations showed a different numerical behaviour as the previous ones on a water cooled fuel cell. These simulations are again world-leading in that they combine our non-isothermal multi-phase model of both anode and cathode side with our world-leading model for membrane water transport. The qualitative agreement between the measured water balance the calculated water balance is excellent and with our model we have shed very important physical insight which may lead to a patent.

The change in work packages away from using custom-made MEAs and a newly purchased test rig towards using an existing air-cooled fuel cell stack from Ballard as are utilized by Dantherm A/S was agreed upon with PSO in an e-mail exchange in January 2015.

Overview of work packages

- WP1: "*Implementation of the complete energy and entropy balances into the existing fuel cell model*".
  Final status: Completed
  A detailed energy analysis was conducted for an air-cooled fuel cell stack. This analysis will probably be published in a journal paper (T. Berning, et al.: *A thermodynamic and computational fluid dynamics analysis of air-cooled proton exchange membrane fuel cells – Part 1: Thermodynamic Analysis*, to be submitted to the Int. J. Hydrogen Energy, 2016). The implementation of heat transfer has been optimized and the numerical model has been made substantially more robust which allowed for a detailed analysis of heat transfer in the PEMFC and provided new understanding especially with respect to air-cooled fuel cells as are used by Dantherm A/S. This analysis will be published in a second journal paper (T. Berning, et al.: *A thermodynamic and computational fluid dynamics analysis of air-cooled proton exchange membrane fuel cells – Part 2: Computational Fluid Dynamics*, to be submitted to the Int. J. Hydrogen Energy, 2016). Hence, the outcome of this work package is two journal papers (to be submitted in 2016) and probably several future conference presentations. The late date of these publications is due to the fact that we are currently investigating whether a patent concerning air-cooled fuel cells is possible.

- WP2: "*Implementation of the electrical field equations and Butler-Vollmer equation into the existing model*".
  Final status: Partly completed
  The implementation of the electrical field equations will lead to the fact that our computational model would be able to predict the fuel cell performance curve which by some is considered the ultimate goal of a fuel cell model. On the other hand it is well known that even commercial fuel cell models are capable of predicting polarization curves, but they are usually not realistic. In the ET-AAU fuel cell model the implementation of the electrical field equation would add severe complexity and the convergence behaviour will be adversely affected. In the end the PI has spent more time as foreseen on conducting modelling simulations that can be immediately published as well as working out the theory behind our patented method of measuring the fuel cell water balance employing hot wire anemometry which has led to two journal papers and a potential patent new patent, see below.

- WP3: "*Debugging and improvement of convergence behaviour*".
  Final status: Completed
  Our numerical model in its current shape has proven to be very robust. This robustness also results out of numerical tricks that were devised by the PI. In particular, the PI developed and implemented the numerical treatment of the heat transfer between the various computational regions which greatly improved the numerical behaviour and eventually allowed for the numerical investigation of an air-cooled fuel cell as used by Dantherm Power A/S (WP1 and WP7). The fact that it is so numerically robust and capable of constantly producing world-leading modelling results is marvellous.

- WP4: "*Parametric modelling studies, publications*".
  Final status: Completed (and more publications to come)
  The parametrical studies that have been conducted during this project have so far been published at several conferences and written up in conference proceedings. It should be noted that each of this paper constitutes a world-leading contribution to the field and demonstrates the unique capabilities of the ET-AAU fuel cell model. These parametrical studies include an investigation of the effect of the fuel cell channel geometry on the fuel cell performance and membrane hydration level, the effect of micro-channels in the micro-porous layer on the expected fuel cell performance and membrane hydration level, the detailed prediction of the fuel cell water balance, the effect of thermal material properties and the thermal contact resistance on the expected fuel cell performance and membrane water hydration level. A detailed list of publications and presentations is given below.

- WP5: "*Setting up the fuel cell test stations, test runs*".
  Final status: Completed
  We were fortunate to attract Dr. Saher Al Shakhshir to join our group as a post-doc, coming from the well-known fuel cell research group around Prof. X. Li at the University of Waterloo, Canada. Saher brought extensive experience in the handling of fuel cell test stations and excellent general lab skills into our group and the experimental progress has been very good in general.

- WP6: "*Making of membrane-electrode assemblies*".
  Final status: Cancelled and replaced
  The original plan was to use custom-made membrane-electrode-assemblies from Hydrogen South Africa - Catalysis to validate our fuel cell model. Due to the unforeseen problems at the side of HySA as described above and the fact that we would have to purchase expensive new equipment to conduct these tests it was decided to not use custom-made MEAs for model validation. Instead, we decided to conduct experiments on existing beginning-of-life and end-of-life Ballard fuel cell stacks, see WP 7.

- WP7: "*Water balance experiments*".
  Final status: Completed, but analysis still ongoing

We used an existing Ballard fuel cell stack and modified it so that it would yields data that can be comparable with our modelling predictions (steady-state operation). A beginning of life and an end-of-life stack were tested and the water balance was measured for different anode side stoichiometric flow ratios. A modelling study was conducted under comparable conditions. These tests and simulations were conducted towards the end of the project, and we still need to analyse the data in detail. A first quick glance revealed that the qualitative agreement between the experiments and the model is very good, but a detailed analysis will be time consuming. This will be University research work conducted until the end of this year.

- WP8: "*Model validation with polarization curves*".
  Final status: Cancelled and replaced
  While it was the original goal to validate the computational model against experimentally obtained polarization curves, it emerged that during course of the project the PI had to spend more time than anticipated on the analysis of the ex-situ data obtained with the hot wire sensor on a dry hydrogen stream and humidified hydrogen stream. The theory behind our patented method to directly determine the fuel cell water balance turned out to be very complex, and it took a substantial amount of the PI's time to interpret the data obtained by the post-doc and writing the publications. This is documented in the first two publications listed below which will probably comprise of the patent application resulting out of this project. Altogether, the original project description was too ambitious, also in light of the wealth of data that the experiments and modelling studies have produced which still need to be published. However, model validation was conducted with respect to the predicted water balance, see WP7, and these data still need to be thoroughly analysed and interpreted.

To summarize: Most of the originally planned work packages have been completed with very good success. Due to some delays in the hiring procedure, the experimental work was partly delayed and the project was extended. However, in such a case it usually hold true that it is better to hire the ideal candidate despite some delay than to hire a slightly lesser suitable candidate immediately. The work package of obtaining custom-made MEAs from HySA Catalysis and conducting validation experiments ("water uptake layer") was eventually cancelled due to unforeseen problems on the side of our project partner. This work package, however, was well replaced by modifying and using existing Ballard fuel cell stacks (beginning of life and end of life) to conduct diagnosis experiments with our exclusive method to directly measure the fuel cell water balance using hot wire anemometry. The numbers of publications has been very high and more publications will come where credit will be given to this project. We are in the process of filing one additional patent (actually a combination of two), and the simulations conducted to match the experiments on the air-cooled Ballard stacks have provided very important new insight that might lead to yet another patent. It is quite certain that our computational model has identified the main problem with operating air-cooled fuel cells, and it might be possible to substantially improve their performance.

1.5 Project results and dissemination of results

Despite the strategic set-backs especially with respect to the situation at HySA Catalysis, the technical outcomes for this project were very good, leading to several world-leading publications of our modelling results along with a new patent idea/application concerning our hot-wire technology.

It would be prohibitively long to list in detail all the technical outcomes of this project. Moreover, the details have been given in the publications that resulted out of this project, and they are listed as appendix.

Among the publications that result directly out of this project are:

- T. Berning, S. Al Shakhshir: Applying hot wire anemometry to directly measure the water balance in a proton exchange membrane fuel cell - Part 1. Theory, *Int. J. Hydrogen Energy*, 2015.

- T. Berning, S. Al Shakhshir: Applying hot wire anemometry to directly measure the water balance in a proton exchange membrane fuel cell for a pre-humidified hydrogen stream, submitted, **status: under review**, *Int. J. Hydrogen Energy*, 2015.
- S. Al Shakhshir, N. Hussein, T. Berning: Employing Hot Wire Anemometry to Directly Measure the Water Balance in a Proton Exchange Membrane Fuel Cell, *Proceedings of the 11th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics*, South Africa, 2015.
- T. Berning: A Study of Thermal Effects in a Proton Exchange Membrane Fuel Cell with a Two-Fluid Model, *Proceedings of the 11th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics*, South Africa, 2015.
- T. Berning: The effect of Micro-Channels in the MPL on the Predicted Membrane Water Content in a PEMFC – A Modelling Study, *Proceedings of the 10th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics*, Florida, USA, 2014.
- T. Berning, S. K. Kær: A Theory on the Role of the Catalyst Layer Morphology on Water Transport in Proton Exchange Membrane Fuel Cells, **Conference Presentation**, 24th Annual Conference of the Catalysis Society of South Africa (CATSA 2013), Port Edward, South Africa, 2013.

Future publications resulting out of the PEMCFD (PSO) and EXC-CELL projects (EUDP):

- T. Berning, S. Al Shakhshir: *Applying hot wire anemometry to directly measure the water balance in a proton exchange membrane fuel cell - Part 2: Experimental*, to be submitted to *Int. J. Hydrogen Energy*, 2015.
- T. Berning, et al.: *A thermodynamic and computational fluid dynamics analysis of air-cooled proton exchange membrane fuel cells – Part 1: Thermodynamic Analysis*, to be submitted to the Int. J. Hydrogen Energy, 2016.
- T. Berning et al.: *A thermodynamic and computational fluid dynamics analysis of air-cooled proton exchange membrane fuel cells – Part 2: Computational Fluid Dynamics*, to be submitted to the Int. J. Hydrogen Energy, 2016.
- T. Berning: *A numerical fluid dynamics analysis of thermal effects in a proton exchange membrane fuel cell*, to be submitted to the Int. J. Hydrogen Energy, 2017.
- T. Berning: *A multi-phase flow study of heat and mass transfer in a proton exchange membrane fuel cell employing the interdigitated flow field – The effect of the channel width and the placement of micro-channels in the MPL*, to be submitted to the Int. J. Hydrogen Energy, 2017.

Several additional conference presentations and publications are planned for this and next year to market our patented technology to directly measure the fuel cell water balance by employing hot wire anemometry and to advertise our computational model.

Turnover and exports

One of the leading producers of hot wire anemometers is Dantec Dynamics A/S. Because our invented method of applying a hot wire to directly determine the fuel cell water balance is quite simple compared to previous methods, it is possible that fuel cell research groups around the world will try and adopt this method which will likely lead to an increased business for Dantec Dynamics.

The fact that with help of our computational model we have apparently identified the main problems of air-cooled PEMFC, such as are used by Dantherm Power A/S, can lead to substantial improvement in the performance and durability of such fuel cell stacks. The PI submitted an invention disclosure to AAU in July 2015, and if the proposed method of increasing the cell performance works, it can lead to another patent (see below) in addition to a drastic increase in exports and turnover by Dantherm Power because of a substantial price-drop of their units.

1.6 Utilization of project results

The newly developed method of applying hot wire anemometry for the direct determination for the fuel cell water balance will be further explored and developed at AAU. We are in the process of applying for two patents:

1. T. Berning: *A Method of Operating a Fuel Cell*, IPC No.: H01M8/04 (2006.01), H01M8/10 (2006.01). Patent No.: WO2013167134. Nov 14, 2013. This patent originally stems from Dec 2011 and resulted indirectly out of the PSO project "High Performance MEAs" (2008-1-10076). An application for a US patent has been made.

2. T. Berning, S. Al Shakhshir: *A Method of Directly Determining the Water Balance in Fuel Cells*, filed on Feb 13, 2015 under the number PA 2015 70084. This patent application results out of the current project. It is an extension of the first patent and covers the treatment of the hot wire voltage signal.

Moreover, as described above, towards the end of the project the computational model was modified in order to simulate an air-cooled fuel cell such as are used by Dantherm Power A/S for UPS and telecom back-up. These simulations have led to additional insight and, if our idea to improve the fuel cell performance works, these simulations may lead to a new patent for ET-AAU in collaboration with Dantherm and Ballard Power Systems.

1.7 Project conclusion and perspective

Project Conclusion

Modelling work

The existing ET-AAU computational fuel cell model is based on the formerly commercial software package CFX-4 which is now owned by ANSYS Inc. It has been mentioned several times in this report that this model has numerous word-leading features because CFX-4 was originally developed around its multi-phase capabilities. CFX-4 has not been further developed since the year 2003 which is in part an advantage because the user can develop their own FORTRAN subroutines without the fear that with every software update the user-defined subroutines may not work anymore with the main code. However, ANSYS Inc. is successfully promoting the commercial Fluent fuel cell module which is being used by several fuel cell research groups around the globe. This model has severe weaknesses compared to CFX-4, and we tried to emphasize the strength of our model in the various publications that came out of the PEMCFD project. It appears certain right now that the publications resulting out of the PEMCFD model will be the leading ones in the field of fuel cell modelling and the PI believes that the Fluent model will not be able to generate similar results.

Experimental

The experiments in general have been a great success and we have learned that our previously patented method to determine the water balance in a PEMFC works better than we originally anticipated, a fact which has led to a second patent application. We are quite optimistic that we have developed the best and most elegant method of directly determining the fuel cell water balance by using hot wire anemometry, and we are hopeful that this method will be used in fuel cell research groups around the world in the future. Moreover, in our experiments we have also proven that the existing Ballard fuel cell stacks can in fact operate with an open-ended anode instead of dead-ended which requires periodic purging. While the effective stoichiometry in the latter case is typically between 1.05 and 1.1, wasting 5 – 10 % of hydrogen, we have so far managed to operate at a stoichiometry of 1.1 in the open-ended case. This means that we are wasting slightly more hydrogen, but it is also certain that the fuel cell durability in this case is much better. More work will hopefully be done in the future in the framework of an EUDP project with Dantherm and Ballard, see below.

Strategic

This project was also an attempt to form a strategic partnership between our research group at AAU and HySA-Catalysis in South Africa. While our group has world-leading modelling capabilities, HySA-Catalysis is also university based and has excellent experimental facilities especially with respect to the making of membrane-electrode assemblies. Moreover, it is part of the strategy of HySA to form collaborations with internationally renowned institutions because of a previous lack of expertise in South Africa in the field of fuel cell technology. While during the first half of this project this partnership was actively pursued from our side (in addition to the activities within this project one Danish PhD student spent his external research stay in the HySA Systems labs), we had to change some of the project work packages in part due to disruptions at HySA after the departure of Dr. Olaf Conrad, our main contact partner. Dr. Conrad had previously invited the PI to contribute to the three local workshops on fuel cell technology which were arranged by HySA Catalysis and held in Cape Town (2012-2014) and to co-supervise HySA Catalysis Master's and PhD students. While we are hoping to revive our partnership at a later point in time, for now it appears like we have reached a dead end.

Project perspective

Modelling work

In general, the outlook for our fuel cell model based on CFX-4 is uncertain. While it is the world-wide leading tool, the fact that is has been phased out more than 10 years ago makes it difficult to become wide-spread. On the other hand, the shortcomings of commercial tools such as the Fluent fuel cell module are becoming ever more obvious, and it is foreseeable that this module will become more and more a liability to Fluent (ANSYS Inc.). Our research group has by now numerous publications that show detailed and realistic results for the fuel cell water distribution, the membrane water content, the temperature and reactant distribution for very challenging operating conditions and geometries. Our multi-phase simulations of the so-called interdigitated flow field are still unmatched, and it is probable that the interdigitated flow field will gain popularity in the future. It is foreseeable that other fuel cell research groups would like to have the same modelling capabilities. We are hoping to obtain the research grant from EUDP in collaboration with Dantherm and Ballard that will allow us to further develop this fascinating modelling tool and generate more world-leading publications.

The further developed computational model might become a central part of a new EUDP project that the consortium of ET-AAU, Dantherm and Ballard have applied for to further improve the performance and durability of air-cooled fuel cells ("PEM Air"). One aspect of this project, if granted, will be to apply the ET-AAU fuel cell model to shed further insight into heat and mass transfer in air-cooled fuel cells. One example is that the general believe at Ballard and Dantherm is that the air has to be pre-humidified and the danger of membrane dry-out exists. Preliminary simulations with the ET-AAU fuel cell model, however, have suggested that in fact the membrane is ideally hydrated under almost all operating conditions even when the air that enters the fuel cell is completely dry so that no humidifier is required. The same simulations have also shown that no pre-heater is required under steady-state operation. Thus, the EUDP project, if granted, can lead to a substantial improvement in performance and durability of air-cooled fuel cells, and our model can play a central part.

Experimental

We will also further apply and refine our patented experimental method to directly measure the fuel cell water balance using hot wire anemometry. We are currently in discussions with Dantec A/S who have become interested in hydrogen technology – so far the constant temperature anemometers were meant to be used for air or water, but we have found that hydrogen and humidified hydrogen does give accurate and meaningful results. We are also in regular discussions with manufacturers of fuel cell test stations. The goal is to convince them to offer our patented hot wire technology as an integral part of their test stations so that they may license our patents. Our current plan is to possibly form a consortium with Dantec Dynamics A/S with a focus of developing hot wire sensors that are cheaper, simpler and more robust than current ones and dedicated to measuring the fuel cell water balance. From our side we are aiming to apply for a grant from the Danish Innovation Fund.

Additional notes

The PI was recently invited by Dr. George Tsotridis from the European Commission – Institute for Energy and Transport to attend a one-day workshop (June 2015). Dr. Tsotridis wanted to obtain an overview of the different fuel cell modelling efforts that are going on throughout Europe and he was especially interested in computational fluid dynamics (CFD) modelling as is done at ET-AAU. The outcome of this overview was sobering: only our group and the research group of ZSW, Ulm, Germany, were able to present advanced CFD models of a full fuel cell. The ZSW group, however, uses the Fluent commercial module whereas we have presented our own model development based on CFX-4. While the Fluent commercial tool does produce results, very great caution had to be applied in the analysis as several unphysical equations and sub-models are used. Therefore, we can claim to be Europe's leading group in fuel cell modelling using computational fluid dynamics.

The PI was also recently invited to serve as external consultant on a research project headed by the distinguished fuel cell researcher Prof. Frano Barbir and visited that group in September 2015. Dr. Barbir's research group at the University of Split, Croatia, is also using the commercial Fluent module. However, they have found that Fluent produces unrealistic results with respect to the fuel cell water balance. In addition, the membrane water content cannot be realistically predicted, and the Fluent manual discourages the use of the multiphase option.

More serious competition to our modelling efforts appears to be the wider spread of the free software Open FOAM which has been identified by some researchers as the tool of choice for developing future fuel cell models. However, so far there is still no proof that Open FOAM can actually handle the physical complexity whereas our group has repeatedly published world-leading results that are already obtained. Previous publications of fuel cell modelling results obtained with Open FOAM were not very convincing.

At a recent conference in July 2015 the PI talked to a researcher from the prestigious Paul Scherrer Institute (PSI) in Switzerland and he learned that PSI has until recently still used CFX-4 for the nuclear reactor modelling. In fact, they had purchased the CFX-4 source code from ANSYS. Hence, CFX-4 is still a very popular tool that is applied by some of the leading scientists world-wide. PSI has recently moved to the newer version of CFX (CFX-14), but they claim that the results obtained with CFX-4 were different, and better.

Summary

The ET-AAU computational fuel cell model is still unique and superior to all commercially available modelling tools. The development and application of this model has led to several break-through inventions in fuel cell technology and two (possibly three) patents for AAU in the field of fuel cell technology. The fact that it is based on the formerly commercial computational fluid dynamics package CFX-4, however, is still a problem for the wide-spread adaption of our tool. Currently, research groups in general prefer to use more "up-to-date" software packages such as Fluent, despite the fact that the computational results are not realistic and the models have severe shortcomings. A positive aspect is that the modelling results are unique in their quality and there is a growing desire in the fuel cell modelling community to do something similar, and this cannot be done with the commercial tools. The experimental work conducted during this project was both highly original and successful, and has led to a patent application. We are hopeful that this diagnosis tool will be wide-spread in fuel cell research in the coming years.

Annex

Pub_1.pdf
Pub_2.pdf
Pub_3.pdf
Pub_4.pdf
Pub_5.pdf