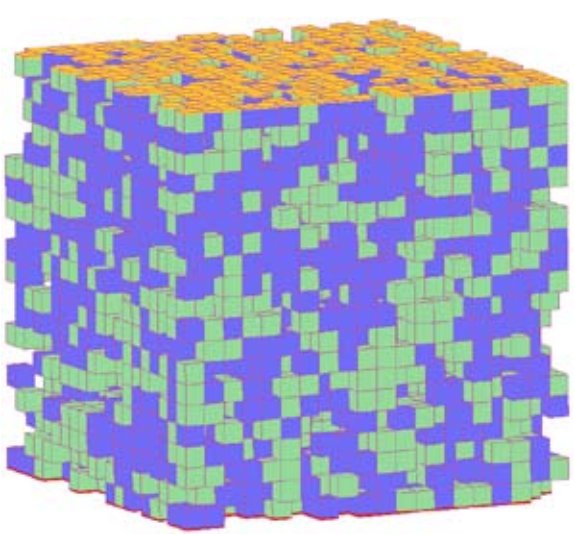
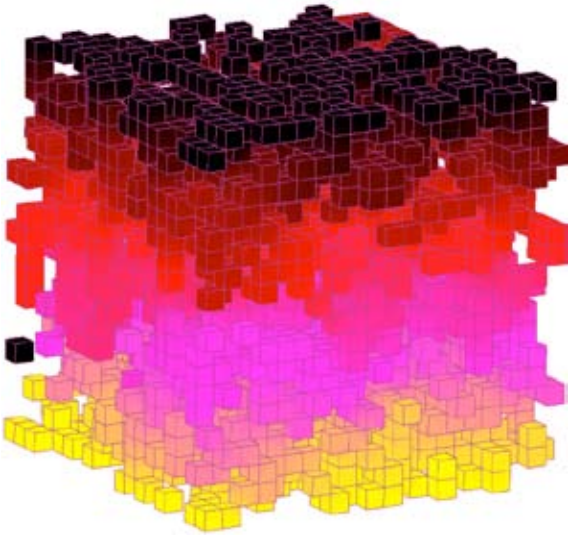
Zürcher Hochschule
für Angewandte Wissenschaften

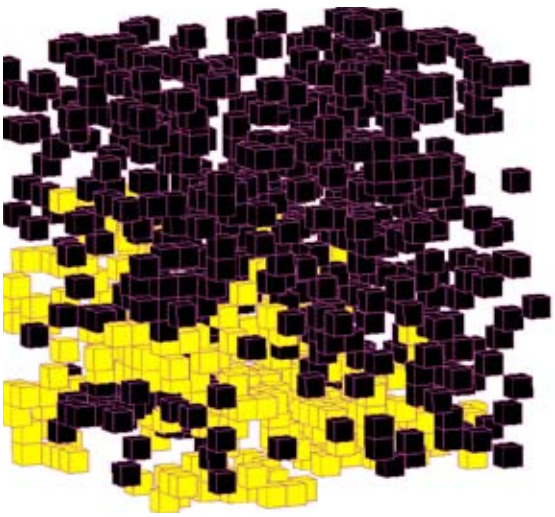
School of
Engineering

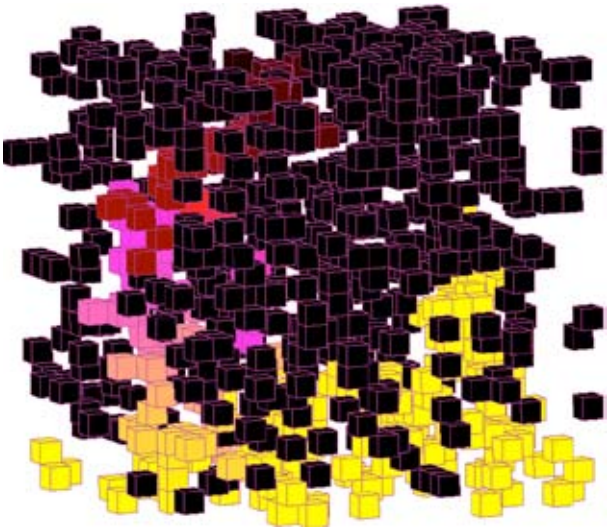
ICP Institute of
Computational Physics

Research Report 2008









Die Titelgrafiken zeigen einen Ausschnitt aus einer gemischt ionisch-elektronisch leitenden Elektrode einer Hochtemperatur-Brennstoffzelle. In der Elektrode finden Ladungstransport und Ladungstransfer (d.h. die Elektrochemie) statt. Die Bilder zeigen die ionisch-elektronischen Phasen (grüne und blaue Partikel) sowie die berechneten Verläufe elektrischer Potentiale für verschieden gut leitende Elektroden. So lassen sich in SESES Modellen reale Alterungsprozesse abbilden, die zu Leistungseinbussen führen.

The illustrations on the frontpage show sections of a mixed ionic/electronic conducting electrode of a high temperature fuel cell. Charge transport and electrochemical charge transfer occur in this electrode composed of ionic and electronic phases, see green and blue particles, respectively. The electrical potential distribution is calculated with our software SESES for electrodes of varying morphology and conductivity. This way one can study real aging processes that lead to performance reduction.

Contents

Chapter 1

Einleitung

Das Institute of Computational Physics hat im Jahr 2008 schulintern wie auch in der nationalen und internationalen Hochschulszene seinem Namen Ehre erwiesen. Es wurden verschiedene Forschungsprojekte im Bereich der numerischen Modellierung von Multiphysik-Systemen abgeschlossen und mindestens so viele neu lanciert. Wir durften in unserer Forschungstätigkeit viele spannende Herausforderungen zusammen mit unseren Industrie- und Hochschulpartnern meistern. An der Schnittstelle zwischen akademischer und angewandter Forschung sehen wir uns täglich neuen Herausforderungen gegenüber. Wie können wir mit unseren Modellen und Simulationen für unsere Forschungspartner einen Mehrwert schaffen? Die Antwort ist vielschichtig. Zum einen müssen wir das Vertrauen unseres Partners gewinnen und zeigen, dass wir mit unseren Berechnungen Erkenntnisse erzielen, welche allein durch experimentelle Untersuchungen nur schwierig zu erreichen sind. Andererseits müssen wir auch überzeugend darlegen, dass wir numerische Simulationen nicht nur unserem Handwerk zuliebe, quasi "l'art pour l'art", durchführen, sondern im Sinne der Projektziele optimal einsetzen. Eine Zusammenarbeit beginnt denn typischerweise auch mit einer umfangreichen Analyse des vorhandenen Problems und der Bedürfnisse des Partners. Oft ist es dann während der Zusammenarbeit zentral aufzuzeigen, wie unsere Simulationsresultate mit der Realität verknüpft sind. Dies erfolgt, indem wir z.B. mit Hilfe des Vergleichs zwischen Experiment und Simulation, Parameter bestimmen sowie ein System beschreiben oder mit Simulationen Wege zur Verbesserung der Systemeigenschaften aufzeigen. Auch wenn die Verfügbarkeit von schnellen Rechnern und benutzerfreundlicher Simulationssoftware weiter zunimmt, stellen wir fest, dass dies alleine z.B. einem Industrieingenieur nicht genügt um eigenhändig mit Multiphysiksimulationen Fortschritte zu erzielen. In der Regel ist einschlägige Erfahrung in der Beschreibung physikalischer Phänomene auf verschiedenen Längenskalen unabdingbar. Es gibt zu viele Beispiele, bei denen in der Industrie oder an anderen Hochschulen Simulationssoftware beschafft wird, welche dann aufgrund von Schwierigkeiten in der Einarbeitung kaum weiter genutzt wird. Es gibt also viele Anzeichen dafür, dass wir auch in Zukunft als Partner attraktiv bleiben. Die Opportunitätskosten für den Fall, dass man der Simulation als Entwicklungsmethode fern bleibt, steigen weiter an.

Um diesen Leistungsauftrag zu erfüllen, dürfen wir auf finanzielle Unterstützung von verschiedenen Förderagenturen und Forschungsstiftungen zählen. Letztlich sind für unsere Arbeit aber auch die Mitarbeiterinnen und Mitarbeiter zentral. Im Jahr 2008 durften wir mehrere neue Mitarbeiter am ICP begrüssen, welche unsere Kompetenzen verstärken. Mit Roger Häusermann und Evelyne Huber sind zwei ETH-Diplomanden zu uns gestossen, welche an unserem Institut eine Doktorarbeit absolvieren und von Professoren der ETH Zürich begleitet werden. Unser Umfeld mit internationalen Forschungspartnern und -Themen und der Status als wissenschaftliche Assistenten macht eine Dissertation an der ZHAW attraktiv. Mit Dr. Yasser Safa und Dr. Matthias Schmid sind zudem zwei Wissenschafter von der ETH Lausanne zu uns gestossen. Die Attraktivität einer Tätigkeit an unserer Schule bzw. unserem Institut wurde auch erhöht mit dem im Herbst 2008 lancierten Masterprogramm MSE (Master of Science in Engineering), das es den Master-Studenten ermöglicht, neben dem Unterrichtspensum in aktuellen Forschungsprojekten mitzuarbeiten. Dies ist denn auch ein Unterscheidungsmerkmal zu den Masterprogrammen an universitären Hochschulen. Die ersten Erfahrungen mit dem MSE Masterprogramm zeigen, dass

dies die Studenten wie auch die Dozenten gleichwohl fordert. Der Regelabschluss bleibt jedoch weiterhin der Bachelor und nur die bestqualifizierten Studenten werden im MSE Masterprogramm aufgenommen. Im Bachelor Unterricht waren Dozenten unseres Instituts in Modulen zur Physik, Mathematik, Signalverarbeitung sowie Thermodynamik tätig.
Unsere Sichtbarkeit als Institut in der Schweiz haben wir im Jahr 2008 auch mit verschiedenen Teilnahmen an Messen und Tagungen gepflegt, so zum Beispiel am Winterthurer Technologietag im Frühling sowie der Tagung der Electrosuisse zum Thema MEMS im Herbst. Am lokalen Anlass zum nationalen Tag der Technik und dem Thema Energieeffizienz referierten zwei ICP Dozenten, Thomas Hocker und Nils Reinke, zur Brennstoffzellen- bzw. Beleuchtungstechnologie. Anfang 2008 hat Jürgen Schumacher das ”5th Symposium on Fuel Cell Modelling and Experimental Validation” an der ZHAW organisiert. Dies ist ein Beweis für die internationale Anerkennung unserer Forschung auf dem Gebiet der Brennstoffzellenmodellierung und hat dem ICP weitere Impulse verliehen. Im Jahr 2008 gelang uns die Lancierung zweier europäischer Projekte ”AEVIOM” und ”Apollo” im Bereich der organischen Elektronik, eines davon finanziert durch das 7. Forschungsrahmenprogramm der EU.
Thematisch haben wir im vergangenen Jahr die Energieforschung deutlich verstärkt. So sind zwei grössere Photovoltaik-Forschungsprojekte angelaufen und auch das OLED EU-Projekt ist auf Energieeffizienz ausgerichtet. Auch ein Forschungsprojekt zum Thema Holzvergasung für die dezentrale Kraft-Wärmekopplung wurde am Ende des Jahres bewilligt. Somit leisten wir mit diesen Projekten einen Beitrag zu einem gesellschaftlich höchst relevanten Themengebiet.
Erwähnenswert ist auch der Aufbau des Mess- und Validierungslabors am ICP (kurz ”O-LAB”). Dank diesem Labor können wir künftig vermehrt eigene Messungen zur Validierung von Simulationsresultaten ausführen oder sogar einen Beitrag in der Entwicklung von Messtechnik leisten. Letztlich ist dieses Labor auch bestens geeignet um Studentenarbeiten auf Stufe Bachelor und Master im Bereich Mechatronik, Elektrotechnik und Informatik auszuführen.
Dass unsere Forschung anwendungsorientiert ist, zeigt nicht zuletzt auch der bisherige Erfolg der Spin-off Firma Fluxim AG, welche im vergangenen Jahr mit der Anstellung von Mitarbeitern und der Einmietung von Büroplätzen am ICP erste Schritte in die Unabhängigkeit unternommen hat. Mit der Kommerzialisierung der Software SETFOS macht diese Firma einen Teil der Forschungsresultate des ICPs einer internationalen Gruppe von Anwendern zugänglich. Die Anerkennung dieser Spin-off Firma auf nationaler und internationaler Ebene wurde bezeugt durch die Einladung zum Transferkolleg 2008 ”Industrial Photonics” der SATW (Schweizerische Akademie der Technischen Wissenschaften) und KTI (Kommission für Technologie und Innovation) sowie durch die Teilnahme am EU Projekt AEVIOM unter Leitung von Philips Research in Eindhoven. Die Zusammenarbeit unseres Instituts mit Spin-off Firmen hat sich auch mit Numerical Modelling GmbH erneut bewährt, welche im vergangenen Jahr gleich zwei neue KTI Projekte mit dem ICP lancierte. Numerical Modelling GmbH ist weiterhin ein strategisch wichtiger Partner.
Bei einem Blick ins kommende Jahr müssen wir davon ausgehen, dass sich die Finanzkrise auch in der Realwirtschaft auswirkt. Ob sich das auch in unserer Forschungstätigkeit bemerkbar macht, ist jedoch unklar. Es besteht sogar die Aussicht auf vermehrte Industrieforschungsprojekte, da Firmen in schwieriger wirtschaftlicher Situation gut beraten sind, vorhandenes Know-how und Personalresourcen von Hochschulen einzubinden. Der Beschluss des Bundesrates anfang des neuen Jahres zur Erhöhung des Budgets 2009 der KTI ist diesbezüglich ein deutliches Signal.
An dieser Stelle möchte ich im Namen des ICP Teams der School of Engineering der ZHAW für die Unterstützung und insbesondere unseren Förderagenturen für die erfolgreiche Zusammenarbeit danken. Ich freue mich, die genannten Herausforderungen gemeinsam im ICP Team anzupacken und möchte mich bei jedem einzelnen ICP Mitglied für den persönlichen Einsatz im vergangenen Jahr bedanken.

Beat Ruhstaller
Institutsleiter

Chapter 2

Introduction

The Institute of Computational Physics has lived up to its name in 2008 with respect to its activities on national and international level. Several research projects in the field of numerical modeling of multiphysics systems were concluded and new ones launched. We enjoyed tackling many challenges in our R&D activities together with academic and industrial partners. At the boundary between academic and applied research we are facing many challenges on a daily basis. How can we generate value to our research partners with our numerical models and simulations? The answer is not straightforward. On the one hand we must earn the trust of our partners and demonstrate that our calculations indeed help gaining insights which could hardly be obtained by experimental means. On the other hand we must explain convincingly, that we do not perform numerical simulations just for the fun of it but rather because they are the most efficient way of achieving the objectives. Thus a collaboration typically starts with an analysis of the problems at hand and the needs of the partners. Generally it is crucial to demonstrate how the simulation results are connected to reality. This happens with the help of comparisons between experiment and simulation, parameter extraction or by formulating possible ways of improvement of the system properties. Although the availability of fast computers and user-friendly simulation software is further advancing, we can state that this alone won't allow an engineer to get up to speed with multiphysics simulations. In general, appropriate experience is indispensable. There exist too many examples of simulation software purchases in industry and at universities, in which the software is hardly used any longer after initial training difficulties. Thus there are numerous signs that we will remain attractive partners also in the future. The opportunity cost for the case in which simulation software is not taken advantage of is large.

In order to fulfill our mission we count on financial support of various research funding agencies. But after all, our staff members are crucial. In 2008 we welcomed new staff members which strengthen our competences. Roger Häusermann and Evelyne Huber are two ETH graduates that joined us for writing a Ph.D. thesis at our institute and in collaboration with professors of ETH Zurich. Our work environment with international research partners and topics and the status as scientific assistant makes a Ph.D. thesis at the ZHAW attractive. In addition, two scientists from ETH Lausanne joined us, Dr. Yasser Safa and Dr. Matthias Schmid. The attractivity of the working environment at our school and institute was increased also with the launch of the Master of Science in Engineering (MSE) program in Fall 2008. It allows the students to get practical training in research projects besides attending classes. This is a differentiation from the other academic master programs. The first experiences with the MSE show that it is demanding for both the students and involved lecturers. However, the bachelor degree will remain the standard degree at our school and only the best bachelor graduates are accepted as master students.

Lecturers of the ICP were teaching courses in Physics, Mathematics, Signal Processing and Thermodynamics this year. The visibility of our institute was maintained with the attendance of various conferences and symposia. For instance, the Winterthur technology day in Spring and the Electrosuisse MEMS meeting in fall. At the local event of the national day of technology with its focus on energy efficiency two ICP lecturers, Thomas Hocker and Nils Reinke, gave presentations in the field of fuel cell and lighting research. Moreover, Jürgen Schumacher organized the 5th Symposium on Fuel Cell Modelling and Experimental Validation (ModVal) at the beginning of 2008 in

Winterthur. This is one proof of the international recognition of our fuel cell research. The same year we succeeded in launching two European resarch projects (AEVIOM and Apollo) in the field of organic electronics, one of which financed by the seventh framework programme of the European Union.
In view of the research topics, we have strengthened our research activities in energy. Two larger research projects in photovoltaics as well as the OLED EU project are targeting energy efficiency. Moreover, a project in wood power was approved at the end of the year. Therefore we contribute in part to this societally highly relevant topic.
We are also proud to have set up a laboratory for measurement and validation in the past year. Thanks to this laboratory we will be able to carry out some of the measurements for validation of the simulation results on our own. We may even contribute to the development of suitable measurement techniques. This laboratory is also ideally suited for student thesis projects at bachelor and master level in the fields of mechatronics, electrical engineering and computational science.
The application-oriented nature of our research is proven by the success of the spin-off company Fluxim Inc., which has undertaken several steps towards an independent business by hiring a couple of staff members and renting office space at the ICP. With the commercialization of the software SETFOS, this company gives an international user community access to some of the research results of the ICP. The recognition of this spin-off company was proven by the invitation to the Transferkolleg "Industrial Photonics" by the SATW and the CTI in November 2008 as well as the participation in the EU project AEVIOM under leadership of Philips Research in Eindhoven.
The ICP collaboration with spin-off companies has proven valueable also in case of Numerical Modeling GmbH, which launched two CTI projects with the ICP. Numerical Modeling GmbH thus continues to be a strategic partner of the ICP.
Looking ahead into the coming year, we must assume that the financial crisis will also affect real economy. It is unclear, however, whether this is noticeable also in our research activities. There is even a chance for more research projects with industry, since companies are advised to consider engaging more know-how and human resources of the universities. The decision of the federal council to increase the budget for the commission for technology and innovation (CTI) for 2009 is a clear signal.
On behalf of the ICP team I would like to express our gratitute to the School of Engineering for supporting us and the research funding agencies for the successful collaboration. I am looking forward to tackle the above-mentioned challenges together with our team and would like to thank each ICP team member for her/his commitment in 2008.

Beat Ruhstaller
Head of the institute

Chapter 3

Sensors and Actuators

3.1 Finite element software for the industry

Contributors: Guido Sartoris, Hansueli Schwarzenbach, Markus Roos

Partners: ZHAW, Numerical Modelling GmbH
Funding: Commission for Technology and Innovation (CTI)
Duration: 2007 – 2009

The goal of this project is to provide the industrial partner *NM Numerical modeling* with up to date software for the modeling of Maxwell's equations in the low frequency regime where displacement currents may be neglected, i.e. the eddy current model. Of particular interest for SMEs is the modeling of magnetic proximity sensors with common PC hardware and computational time limitations of a few hours. At ICP we are developing our in-house software SESES, a general purpose multi-physics numerical simulation tool for the analysis of micro–macro, sensor–actuator devices by the finite element method in 2D and 3D domains. Its major strengh is the possibility to solve and couple together almost any governing equation of classical physics. In order to greatly improve the flexibility of the software, we have developed a functional input language allowing the user to define within the input generic material laws and coupling effects between the different physical fields. Although SESES may already be used to compute some eddy current problems, their computation in 3D is far from being optimal and efficient and one aim of this project is to improve this situation with up to date numerical algorithms. In particular, the multi-physics concept behind SESES allows to quickly couple together these new models with the available ones and for example to perform optimized computations by mixing up vector and scalar potential formulations which are coupled together along their common boundary. On the other side, since even optimized 3D eddy current computations are still computationally expensive, from the industrial partner there is a need to know if reduced and less demanding models may be used to replace fully fledged 3D computations. Such a comparison is shown in Fig. 1. The new numerical models will be used to validate such approximations and this part of the work will be done by the industrial partner.
From the software point of view which is the contribution from ZHAW to the project, the major work is the introduction of edge finite elements within SESES. These elements are the natural framework when working with the $\nabla \times \nabla$ operator since they do not enforce the normal component of the vector field to be continuous and differently from Lagrangian or nodal elements are well suited to model sharp corners and sharp discontinuous material laws. However, the eddy current problem cannot be gauged with edge elements and the linear system is singular. If the equations are assembled in a consistent manner, this is not a drawback for iterative solvers and here edge elements show in general a better convergence behavior than nodal elements. However, the good convergence is lost at middle-high frequencies or can be destroyed by using optimizations to reduce the number of unknowns, e.g. by using a mixed formulation with the magnetic potential together with boundary interface conditions, a cotree dof-reduction, a symmetrization or removal of the electric potential in the conductors. A two matrices approach may be useful to overcome the former difficulty at high frequencies, whereas the other optimizations must be combined with matrix preconditioning and are just used if they do not globally impair the computational expenditure. The greatest unknown is the convergence speed of the iterative solver and numerical investigations on the preconditioning's performance are required here. These numerical algorithms are pivotal for the overall success.

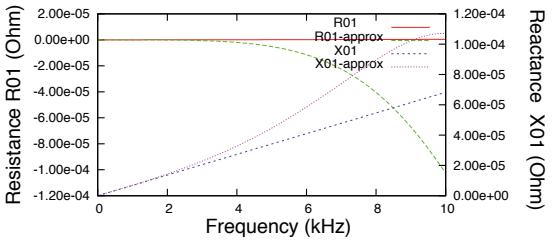


Fig. 1: Reactance matrix coefficients for a system of two coils computed by the eddy current model and a second order low frequency approximation.

3.2 Numerical modeling of laminates anisotropic plastic deep-drawing

Contributors: Guido Sartoris

Partners: Alcan Technology and Management AG
Funding: Commission for Technology and Innovation (CTI)
Duration: 2008 – 2009

Modern laminates for the production of pharmaceutical blister packages have a complex inner structure. Several layers of different plastic and alumina sheets of thickness between $5 - 100\mu m$ are packed, stacked and glued together with the intent to provide the best environmental protection from external agents. Each layer plays a different but important role, as for example, aluminum protects against light, oxygen and water vapor. When forming the blisters by deep-drawing, the overall functional role of the layers in the original laminate should be preserved and no holes, cracks or layer delamination are allowed to evolve during deformation. This is one of the major concern of Alcan, which provides its customers with laminates for the production of pharmaceutical packaging blisters and where the mechanical properties of the laminate must be guaranteed. Illustrations of blisters are shown in Fig. 1. One may try to get physical insight on the disruptive processes of the sandwiched layers by running complex, time-consuming experiments, but they do not necessarily yield ultimate and correct answers on the causes of failure. As well the material properties of the single layers have great influence on the overall results and there are large variations between production cycles which complicates the analysis further. Therefore a numerical approach to laminate deep-drawing is almost a necessity. Numerical modeling is expected to provide a better and more detailed insight of the deformation processes with respect to a solely experimental approach. At the present time, the numerical models used at Alcan are not able to correctly reproduce experimental data and more advanced and precise tools are required. This is the major goal of the project. The task is complex and includes both the writing and fitting of new material laws and optimizing the numerical software.
From the material point of view, the major concern is the correct description of the anisotropic elasto-plastic behavior at large strains, since at the present time, a theoretical definitive treatment is not available and several formulations have emerged.
Our intent is to use the more physically sounded multiplicative approach of plasticity instead of the additive one. The intent is to write generic anisotropic elasto-plastic laws for orthotropic materials at finite strains to be fitted with measurements performed at Alcan. This task is completely independent from the underlying numerical tools and for the in-house developed finite element tool SESES, can be performed completely in user space, i.e. without the need to compile any software code. This is also true for the curve fitting process based on simple experiments at constant strain values not requiring numerical simulations.
Because of the anisotropic nature of the deformation process, a 3D numerical non-linear analysis at large strains must be generally performed. These computations are still very expensive and the second goal of the project is to provide various optimizations at the coding level to speed-up the numerical analysis. Here generic non-linear volume elements are too expensive and non-linear shell elements supporting the same 3D material laws should be preferred. Forseen is also a mixing of both shell and volume elements by providing special interconnecting conditions. It is therefore possible to model the deep-drawing process on regions of small radii with the more precise volume elements and otherwise to use the less expensive shell elements.

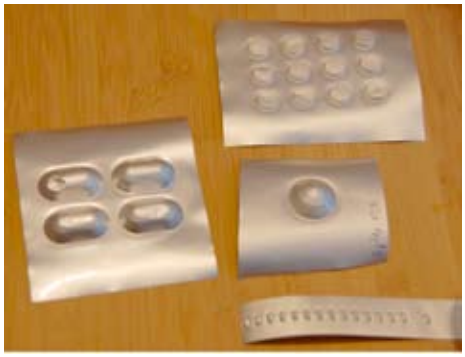


Fig. 1: Blisters formed by deep-drawing of a laminate.

3.3 Berührungsloses Signalanalyseverfahren für Schichtsystem

Contributors: Nils A. Reinke, Andreas Tiefenauer, Beat Ruhstaller, Andor Bariska (IDP)

Partners: Flo-IR und weitere 5 Industriepartner
Funding: Kommission für Technologie und Innovation (KTI)
Duration: 2007 – 2009

Wird nach einem optischen Energiepuls die IR-Abstrahlung von einer beschichteten Oberfläche zeitlich, örtlich und spektral gerastert gemessen, lassen sich Rückschlüsse auf die Schichtdicken oder auf thermophysikalische Stoffdaten ziehen.
Auf der Grundlage dieser Technik wird ein Auswertealgorithmus für die Messdatenanalyse sowie ein robuster Messprototyp entwickelt. Die folgenden beiden ZHAW Institute übernehmen dabei den Kernteil dieser Entwicklung in folgender Arbeitsteilung:

- IDP: Entwicklung eines Auswertealgorithmus: Aus Messdaten eines Mehrschichtensystems, sollen mittels eines physikalisch analytischen Modells Parameter wie Schichtdicke, und thermische Materialeigenschaften extrahiert werden können.
- ICP: FEM-Simulationen: Simulation von Anwendungssituationen; Entwicklung des Messprototypen: Es ist ein Messaufbau (Messhardware und Software) zu entwickeln, der den hohen Anforderungen an das System genügt (siehe unten).

In der Anfangsphase des Projekts wurden am ICP FEM-Analysen von Anwendungsfällen gemacht. Dazu wurde ein instationäres Schnittmodell der Schichtstruktur erstellt. Untersucht wurde beispielsweise der Einfluss von Semitranzparenz, Delamination oder auch Kontaktwiderständen. In der Hauptprojektphase wurde nach einer geeigneten Lösung der Datenerfassung gesucht. Die Herausforderung lag darin, ein System zusammenzustellen, welches die hohen Anforderungen an die Messdatenrate erfüllt ($>$ 10 kHz), eine hohe Empfindlichkeit im IR-Bereich besitzt, und über geeignete Möglichkeiten zur Ansteuerung über einen PC besitzt. Ferner sollten die Datenaufnahme der Kamera, sowie auch das Auslösen des Blitzes über eine Software koordiniert angesteuert werden können. Der Prototypenaufbau entspricht weitgehend dem in Fig. 1 abgebildeten Schema.

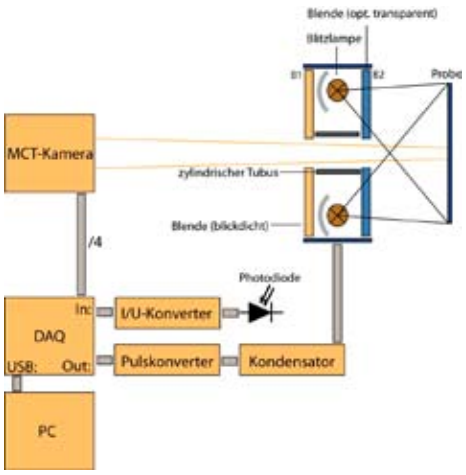


Fig. 1: Messaufbau am ICP bestehend aus Justierungseinheit mit Probe, der datenerfassenden Einheit (Kamera, U/IKonverter, Photodiode) und der datengerenierenden Einheit (Kamera, Blitz, Pulskonverter, Kondensator) sowie der Steuereinheit (Datanaqusisationsgerät (DAQ), Messsoftware).

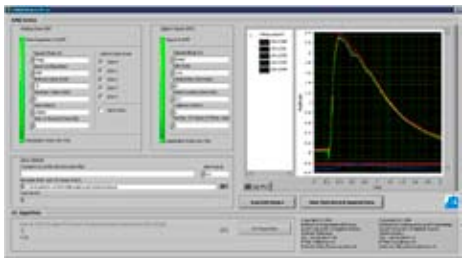


Fig. 2: LabView basierte Software zur Ansteuerung des Blitzes und Datenaufnahme inkl einfachem Datenmanagement.

Mit diesem Messaufbau wurden im ICP-eigenen Messlabor verschiedene Messreihen an den von Industriepartnern bereitgestellten Proben durchgeführt, welche der Entwicklung des Auswertealgorithmus am IDP dienen.

3.4 Velocimetry in railcars by a run-time measurement of thermal markers

Contributors: Nils A. Reinke, Andreas Tiefenauer, Beat Ruhstaller, Andor Bariska

Partners: Siemens TS
Funding: Commission for Technology and Innovation (CTI)
Duration: 2008 – 2009

State-of-the-art velocimetry using the Doppler method, dynamic image analysis and global positioning systems suffers from unreliabilities to a greater or lesser extent. This disaffection arises from a liability to interference towards environmental influences. Leaves, snowfall, rainfall and artificial lighting (light pollution) may lead to severe distortions in the measured velocity.
This feasibility project verifies a patent pending velocimetry technique which is based on a run-time measurement of thermal markers. The thermal-marker is applied from the railcar by optical excitation and subsequently photothermally detected by an infrared sensor. The velocity of the railcar can be determined by measuring the run-time from excitation to detection and the spatial distance between excitation and detection setup.

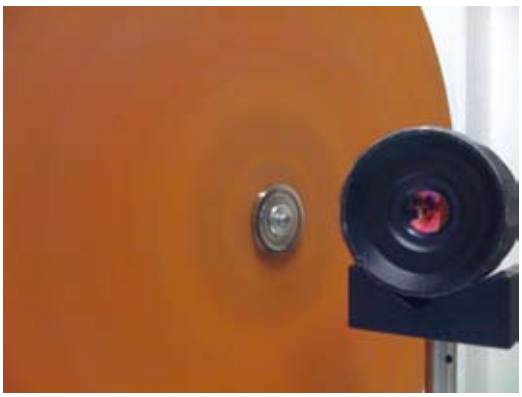


Fig. 1: Corroded steel disc spinning and a germanium zoom lens.

In recent years significant progress has been made in developing powerful, compact and inexpensive solid-state lasers. Nowadays, solid-state lasers replace traditional gas-lasers due to their higher reliability and low maintenance cost. At the same time, fast and inexpensive sensors for the mid-infrared regime become more and more available. Improvements in laser technique and MIR sensors enable to realize this innovative velocimetry technique.
This project subdivides into three sequential steps:

- Computational modeling for estimating the amount of light necessary to deposit the thermal marker with different optical excitation sources (Laser, LED, flashlamps). The optical deposition of the thermal marker leads to a transient temperature distribution inside the rail. In order to detect the deposited thermal marker by the infra-red sensor, the amplitude of this temperature distribution has to be sufficiently high.
- An experimental setup has to be developed from scratch. This experimental setup has to reflect conditions close to reality, e.g. the optical and thermal properties of the rail. Computational modeling will help to specify the individual components used in this experiment. The experimental setup will be controlled and data acquired by LabView.
- In a final step of the project test measurements will be performed and analyzed to verify results from computational simulations and to proof the concept of the pending patent.

A prototype experimental setup comprising a fixture for a spinning steel disc and an infra-red detector is shown in fig. 1. Results of this feasibility project will be further investigated in a field test, if the third step turns out to be successful.

3.5 Diagnostischer Atemanalysator mit elektronischer Mikronase

Contributors: Hansueli Schwarzenbach, Roman Gmür

Partners: Interstaatliche Hochschule für Technik Buchs, Hochschule Furtwangen, Universitätsklinik Innsbruck, Forschungszentrum Karlsruhe, SYSCA AG, GDS
Funding: Internationale Bodenseehochschule
Duration: 2007 – 2009

Das auf zwei Jahre angelegte Verbundprojekt namens DAMINA beinhaltet die Machbarkeit eines kostengünstigen, handlichen Atemgasanalysesystems für diagnostische Zwecke[1]. Es basiert auf einem Gassensormikrochip, der nach dem Prinzip der elektrischen Leitfähigkeitsmessung mit Metalloxid-Gassensoren die Atemgaszusammensetzung misst. Es unterscheidet sich von teuren, konventionellen, Grossgeräteanalysesystemen (Gaschromatographen, Massenspektrometer) durch seine Handlichkeit und ist in Arztpraxen zum kostengünstigen Einsatz ohne Spezialausbildung gedacht.

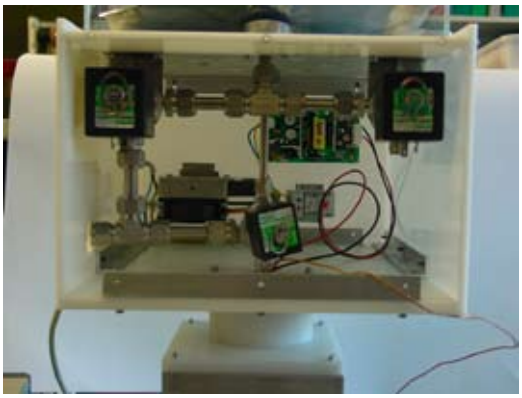


Fig. 1: Behälter Gasaufbereitung: A: Ventil, B: Vertikales Zuflussrohr Atemsack zum Messzylinder, C: Zuflussrohr Referenzgas zum Atemsack (Reinigung), D: Behälterheizung (vgl. Fig. 2)

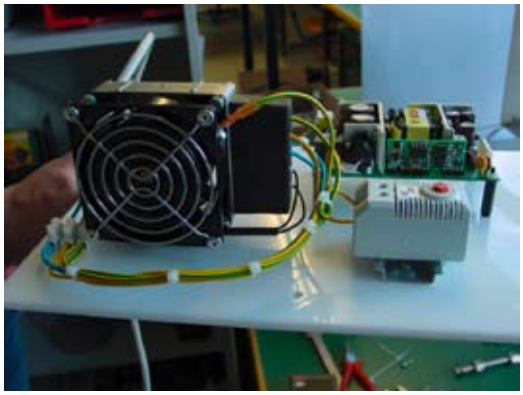


Fig. 2: Behälterheizung (an Rückwand am Behälter zur Gasaufbereitung montiert). A: Lüfter mit Heizung, B: Thermostat, C: Netzteil.

Das Projekt umfasste die Herstellung von Funktionsmustern zur Diagnose von Lungenkarzinomen. Bei Feldtests stellte sich heraus, dass die Nachweisgrenze des heutigen Systems für Formaldehyd bei 1 ppm in Atemgas liegt. Damit ist die Zielsetzung um einen Faktor 100 nicht erreicht. Zwar konnte der nachteilige Temperaturdrift der Sensorsignale durch ein verändertes Auswerteverfahren unterdrückt werden. Die Langzeitstabilität des Microchip ist heute dadurch wesentlich besser als vor 2 Jahren. Aus heutiger Sicht müssten alternative Messverfahren bezüglich der verlangten Nachweisgrenze für Formaldehyd und für andere Gaskomponenten evaluiert werden. Dies übersteigt die Möglichkeiten von SYSCA hinsichtlich einer Produkteentwicklung bei weitem. Auf der wissenschaftlichen Seite gibt es seit dem Hinschied von Kollege Goschnick am FZK im vergangenen Jahr keine weiteren Möglichkeiten für experimentelle Untersuchungen. Aus diesen Gründen wurde das Projekt vorzeitig gestoppt.

[1] ICP Research Report 2007

Chapter 4

Fuel Cells

4.1 Modeling PEM fuel cell performance with a focus on porous layer properties

Contributors: Yasser Safa, Jürgen O. Schumacher

Partners: Paul Scherrer Institute
Funding: Swiss Federal Office of Energy
Duration: 2007 – 2010

Proton exchange membrane (PEM) fuel cells are promising clean energy converting devices with high conversion efficiency, high power density and low to zero emissions.
Before reaching the full potential of this technology, some challenging tasks need to be overcome. In particular, the optimal control of the water flow in the fuel cell appears as a key issue in the design of fuel cell devices.
Under condensing conditions (the general case), liquid water will occupy part of the void in the porous structures of the fuel cell, and thus change the gas transport properties.
Actually, the water saturation inside the PEM fuel cell should be low enough in order to not block the porous Gas Diffusion Layer (GDL). In other words, the flow rate of water should be high enough to ensure the release of the produced water from the fuel cell. On the other hand, water in the cell is essential to maintain a high protonic conductivity of the proton exchange membrane. Consequently, for a successful water management in the PEM fuel cell, an accurate insight in the water distribution at different operating conditions is inevitably needed.

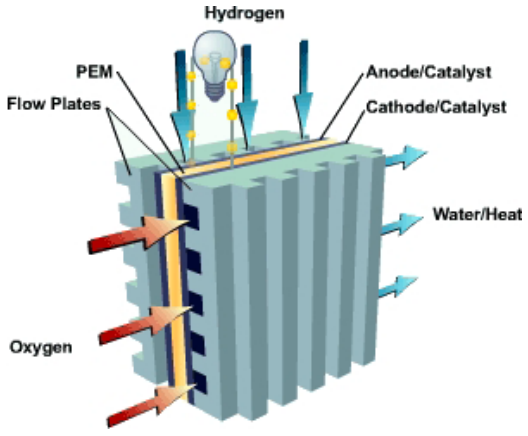


Fig. 1: Operation of a PEM fuel cell, the Gas Diffusion layer (GDL) is a thin material (fibers) located between the Flow Plate and the Catalyst Layer [1]

Fig. 2: The water distribution in a sample part of a Gas Diffusion Layer (GDL) presented in side view. The red color corresponds to the fibers and the blue color corresponds to the water. [2]

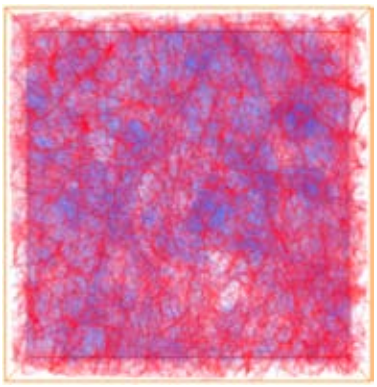


Fig. 3: The water distribution (blue color) in a sample part of a GDL presented in top view.

A combination of the measurement techniques that are applied at the Paul Scherrer Institute PSI and the numerical model that is being developed at the ICP is a practicable way to investigate the two-phase phenomena in a PEM fuel cell.
In this project, we are developing an advanced numerical two-phase flow model to describe the water transport in PEM fuel cells. Roughly speaking, we are applying the so called Multiphase Mixture (M^2) formalism to describe the water transport. This formulation allows to include the effects of vapor bubbles in the liquid

[1] www1.eere.energy.gov/hydrogenandfuelcells/animation/mod1.html
[2] Tomography performed at PSI, Switzerland

water flow as well as the effects of liquid droplets in the water vapor flow.
Compared to the traditional multi-phase flow model, different phases are considered as a single mixture fluid. The M^2 formalism is based on mixture variables for velocity, pressure and other values as viscosity, mobility and permeability.
Mathematically, we solve a time-dependent model that is composed of a convection-diffusion equation for the water saturation and of the Darcy-law with incompressibility condition for the fluid flow.
Due to a degeneracy of the equations, the transport coefficients are perturbed to obtain a non-degenerate problem with a smooth solution. The regularized solution should converge to the original as the perturbation parameter goes to zero with a specific convergence order.
To deal with space discretization, the finite element approximation is used for solving the regularized problem. It is combined with a stabilized mixed finite element method for solving simultaneously for velocity, pressure and water saturation.
Also, due to its convection-dominated feature, the stabilization tool SUPG (Streamline Upwind Petrov Galerkin) is applied when solving the saturation equation.
The time discretization of the global system is applied via an implicit scheme. Since the time scale of the total flow is longer than that of the water saturation evolution, we are choosing to introduce a multi-time step discretization in our approach.
In Figures (4-5) we present samples of numerical results on the liquid water distribution and the total pressure along the thickness direction of the GDL for an academic test case. The numerical simulations are achieved by developing a Mathematica code.

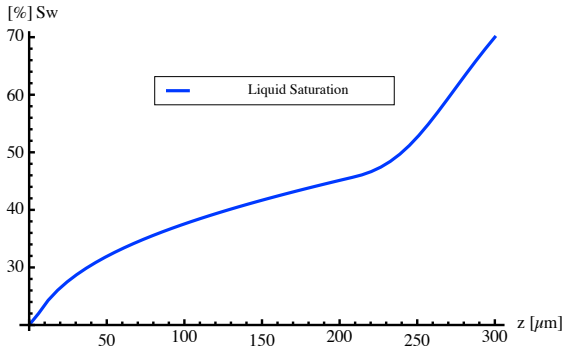


Fig. 4: Numerical results on the liquid water distribution in the thickness direction of the GDL.

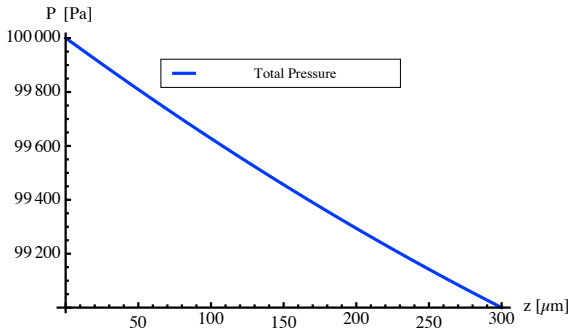


Fig. 5: Numerical results of the total pressure drop in the thickness direction of the GDL.

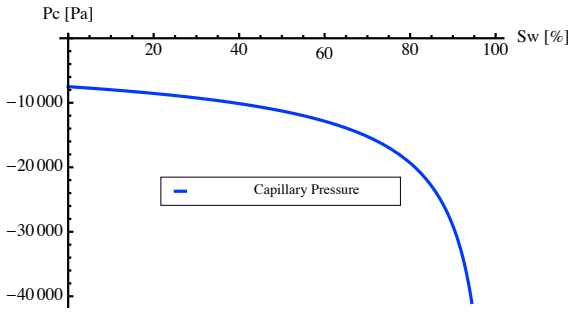


Fig. 6: The capillary pressure as a function of the liquid water saturation according to the Brooks-Corey model.

A change of the slope of the water saturation profile is observed in Figure 4 around the value of Sw = 50 %. The capillary effects (Figure 6) appear as a new contribution on the pressure driven flow phenomena. This has an impact on the distribution of the water saturation.

Finally, the introduction of the measurement results in the computational work is the future task devoted for an advanced technical exploitation of the code. The local water saturation in the Gas Diffusion Layers is determined experimentally at the Paul Scherrer Institute using x-ray micro-tomography. After phase separation of the image data, the water distribution inside the porous structure could be resolved on the scale of the pores. This enabled the measurement of the liquid saturation as function of the through-plane coordinate of the GDL and the capillary pressure. First experiments with complete cells are also performed. A comparison of the spatially distributed data of water saturation to the simulation results is an upcoming crucial task.

4.2 Simulation of polymer-electrolyte-membrane fuel cells and stacks

Contributors: Jürgen O. Schumacher, Jens Eller, Guido Sartoris

Partners: Paul Scherrer Institute
Funding: Gebert Ruef Stiftung
Duration: 2005 – 2008

We developed a computationally efficient model of a proton exchange membrane (PEM) fuel cell. In the framework of this "2+1D"-approach the anodic and cathodic fields are discretized in two dimensions with our finite element software SESES. The coupling between the anodic and cathodic side is established by a one-dimensional model representing the gas diffusion layer (GDL) and the membrane electrode assembly (MEA).
This approach is suitable for taking the high aspect ratio between the in-plane and the through-plane dimensions of fuel cells into account. The number of degrees-of-freedom (DOF) variables is significantly reduced in comparison to a full 3D model approach. Therefore, parameter variations for design studies of PEM fuel cell can be performed on standard PCs. Further, this modeling approach can also be applied to other fields, e.g. for the description of coupled electrochemical processes.
The gas flow channels and bipolar plates of the anode and cathode are discretized in two dimensions. Coupling between the anodic and cathodic side is established by a 1D model representing the membrane electrode assembly (MEA). Coupling between the 1D model of the MEA and the 2D models is achieved by using the values of the DOF variables of the 2D model as boundary conditions of the 1D model.
The 2+1D FEM model was applied to simulate a simplified micro polymer electrolyte fuel cell without gas diffusion layers (see Fig. 1). The gas flow-field of this fuel cell is made of microstructured glassy carbon plates. The electric current density distribution in the through-plane direction is shown in the figure. This current density is predicted by the 1D model, that is, in the direction perpendicular to the cell area. The plot corresponds to an average current density of $250\,mA/cm^2$. The current density is lowest near the gas inlet (top right), it increases to a maximum value in the cell center, and decreases towards the gas outlet (top left). The minimum value near the gas inlet is due to a low value of the membrane water content, i.e. the protonic conductivity in this region is lowest here. An increase of the membrane water content was found in the cell center.
The model approach is suitable to analyze different operation scenarios of proton exchange membrane fuel cells.

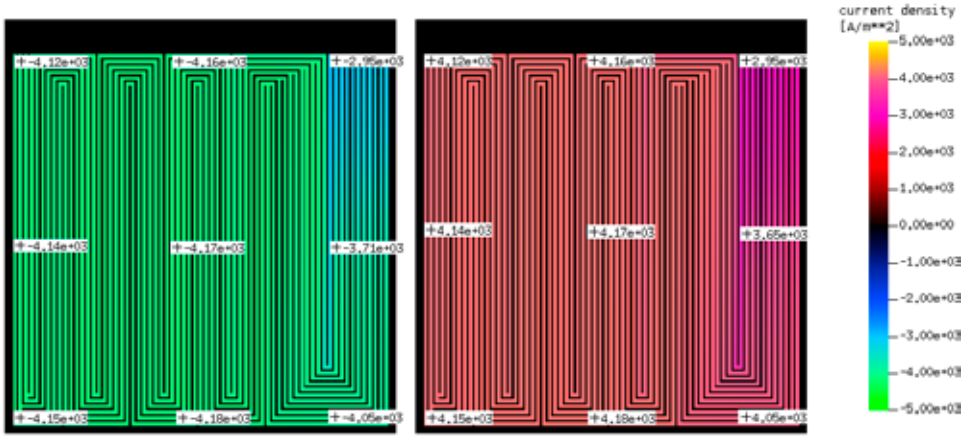


Fig. 1: Electric current density of a micro PEM fuel cell in the through-plane direction (left: anode, right: cathode).

4.3 Enhancing the lifetime of SOFC stacks for combined heat and power applications

Contributors: Thomas Hocker, Rolf Weiss (ITFE)

Partners: Hexis AG (Winterthur), EPFL Laboratoire d'Energetique Industrielle
Funding: Swiss Federal Office of Energy, SwissElectric Research
Duration: 2007 – 2010

Within 2008, our focus has been on modeling the thermo-mechanical and thermo-fluidic behavior of the overall system as well as on electrochemical micro-models for predicting the performance and the degradation behavior of single SOFCs.

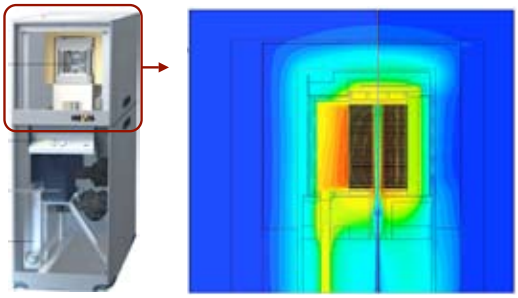


Fig. 1: Typical temperature-distribution within the Hexis SOFC-system as obtained from ANSYS-CFX thermal-flow modeling.

Together with our project partner ITFE, i. e. ZHAW's Institute of Thermo-Fluidic Engineering, a 3D thermal-flow model of the Hexis system has been implemented with the commercial CFD-software *ANYS-CFX*. The model consists of the stack, the heat exchanger, the reformer, and the thermal insulation, see Figure 1. Heat transfer by conduction, convection and thermal radiation (surface-to-surface and gas radiation with the post-combustion zones) have been considered. Chemical and electrochemical reactions are not explicitly modeled, but the corresponding heat-sources and -sinks (in case of methane steam reforming) have been taken into account. A typical simulation-run takes about 24 hours on a 12-CPU Linux cluster with 32 GB of RAM. Results show that the predicted stack temperatures are in good quantitative agreement with experimental results. The model development has been almost finished. A more realistic implementation of gas radiation (for CO2 and H2O molecules as well as soot particles) to accurately predict the heat transfer between the post-combustion zones and the stack remains to be included.

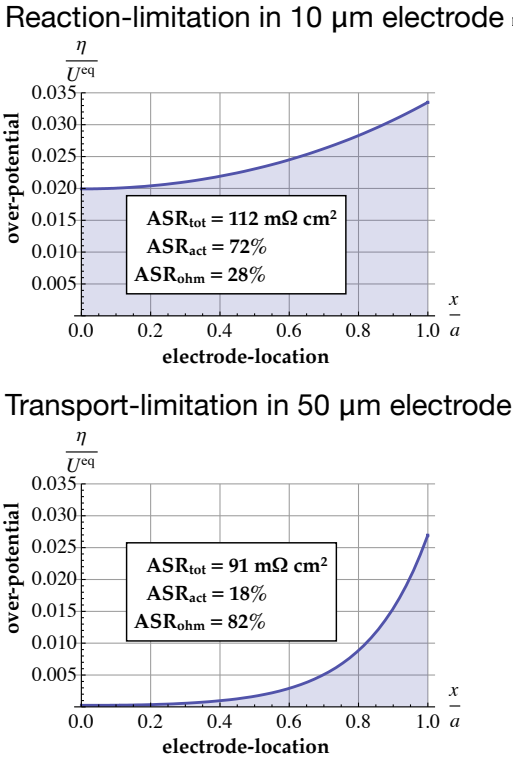


Fig. 2: Over-potentials predicted from the Costamagna electrode model for two limiting cases: electrode performance dominated by (a) reaction limitation, and (b) transport limitation.

The model by P. Costamagna et al.[3] for mixed ion-/electron conducting electrodes has been implemented into Mathematica, see Figure 2. Comparisons of the model predictions with experimental data have been made. They show good qualitative agreement and provide insight into the influence of particle coarsening on the electrode performance.

[3] P. Costamagna et al., *Electrochemical Acta*, vol.43, pp. 375–394, 1998.

4.4 Numerical simulation for the development of the Hexis SOFC-system

Contributors: Yasser Safa, Thomas Hocker

Partners: Hexis AG (Winterthur), Industrial Energy Systems Laboratory, EPFL (Lausanne)
Funding: Swiss Federal Office of Energy, SwissElectric Research
Duration: 2007 – 2010

The Solid Oxide Fuel Cell (SOFC) is a highly efficient producer of heat and power. As an electro-chemical device it consists of two porous electrodes, separated by a solid electrolyte. The oxygen molecule accepts an electron from the cathode and then an oxygen ion migrates through the electrolyte to the anode where it reacts with fuel. The electrons are then released and conducted through an external circuit to the cathode and thereby creating the electric current (Fig. 1-2).

The concept of SOFC heater “Galileo System”, established by our partner Hexis AG, is devoted to cover the essential power and heat requirement for a representative Central European single-family home.

A challenge task is to ensure a long lifetime service of Galileo with satisfactory performance. Therefore, an investigation of the long term degradation mechanism is highly needed.

Due to its novelty, little is known about the degradation behavior of the Hexis SOFC system and an experimental investigation may prove too expensive. In this respect, numerical simulation appears as an inexpensive tool to provide a computational prediction on the failure modes related to either electro-chemical or thermo-mechanical phenomena.

In this project we develop an advanced computational reactive flow modelling of the coupled transport phenomena in SOFC.

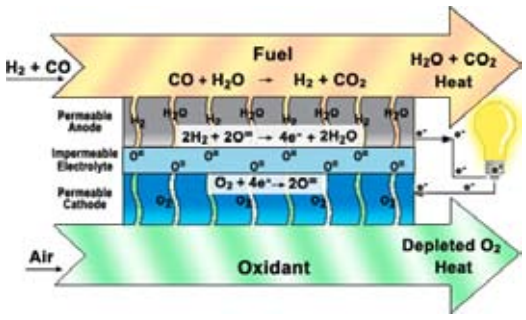


Fig. 1: Electro-chemical basic principle of SOFC [4]

[4] science.nasa.gov/headlines/y2003/18mar_fuelcell.htm

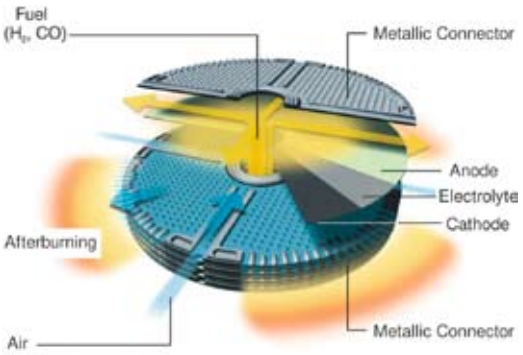


Fig. 2: SOFC Process (Courtesy HEXIS AG)

The physical model, that we study, is governed by a system of nonlinear partial differential equations describing the conservation law for mass, charges, energy and species. The fluid flow in the porous media is described by Darcy’s Law.

We apply the finite element approximation for the space discretization of the continuity equations. The convection dominant cases are stabilized by SUPG (Streamline Upwind Petrov Galerkin). To ensure the conservation properties in the results when solving for Darcy’s problem, we implement a stabilized mixed finite element method to solve simultaneously for velocity and pressure.

The mathematical system is linearized by means of a pseudo time step discretization via semi-implicit scheme. This stable iterative procedure is applied to a transient problem and it convergences unconditionally to the steady solution.

In order to overcome the geometrical complexities we start with a restriction in a representative sub-domain located in the so-called Cell Repeated Unit (Fig. 3).

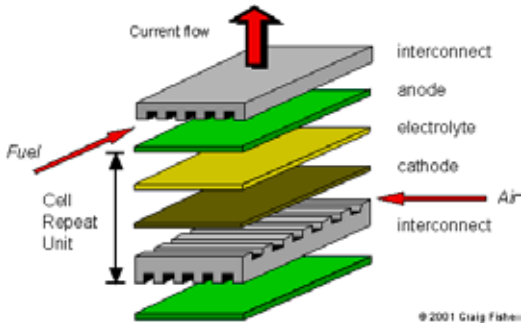


Fig. 3: A Cell Repeated Unit in a planar SOFC[5].

For an advanced insight in the coupled fields we solve, firstly, the system as one-dimensional (1D) problem through the thickness of the Cell Repeated Unit.
Nevertheless, in Figures (4-7) we present samples of numerical results on the gas-phase species distribution along the thickness direction in the anode for an academic test case. The numerical simulations are achieved by developing a Mathematica code.

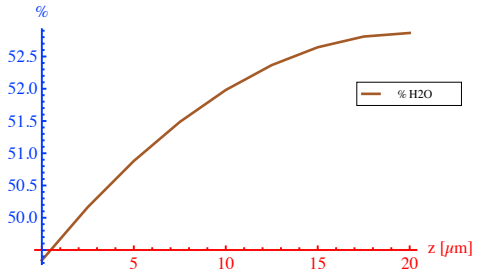


Fig. 4: Water vapor distribution along the thickness direction in the anode: the H_2O molecules are produced at the anode-electrolyte interface.

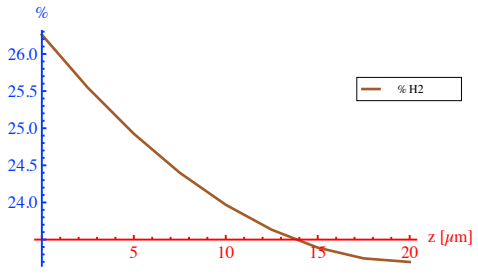


Fig. 5: Hydrogen distribution: the H_2 molecules are consumed by reaction with Oxygen ions.

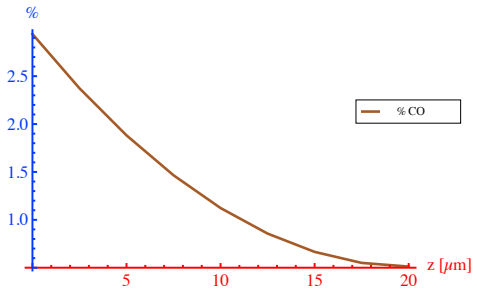


Fig. 6: Carbon Monoxide distribution: the CO molecules are consumed by Water Shift Reaction (WSR): $CO + H_2O \longrightarrow H_2 + CO_2$.

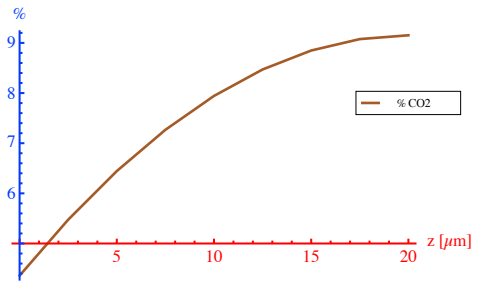


Fig. 7: Carbon Dioxide distribution: the CO_2 molecules are produced by water shift reaction.

Clearly, it is inevitable to account for an interaction between the 1D computed fields and the two-dimensional (2D) in-plane flow in the gas channel. For this purpose, we are choosing to implement a 2+1D numerical model for solving the full problem with reduced computational cost. Finally, for a realistic simulation more mimicking the in-situ observations, we intend to adapt our inputs to new experimental values (Micro Structural Data).

[5]Craig Fisher: http://people.bath.ac.uk/cf233/sofc.html

4.5 Feasibility of a portable SOFC for Hilti's mobile machine tools

Contributors: Roman Gmür, Thomas Hocker

Partners: ETHZ Institute of Nonmetallic Inorganic Materials, Hilti Research Center
Funding: Hilti
Duration: 2007 – 2010

In contrast to conventional SOFCs, μ-SOFCs are characterized by membrane thicknesses of only a view micrometers and operation temperatures as low as $500\,^{\circ}\mathrm{C}$. Feasibility studies of such systems suggest electrical power outputs as low as $1\,\mathrm{W}$. μ-SOFCs could be employed in combination with or as replacement of batteries to power small to medium electronic devices, such as laptop computers, camcorders, or machine tools. Compared to energy storage devices such as Li-ion and NiMH batteries, higher energy densities (per volume or weight) are possible.
This project investigates the feasibility of a portable SOFC for Hilti's mobile machine tools. Having studied the current profiles of Hilti's mobile machine tools and specifications for mobile power sources, it is anticipated that a SOFC alone will not be sufficient for Hilti's high current peak applications. Therefore, the SOFC has to be coupled with an energy storage device such as a battery. The SOFC will charge the storage battery continuously, while the battery itself will deliver peak power during operation of the electrical tool. The SOFC can be designed as an external charger or as an internal unit.

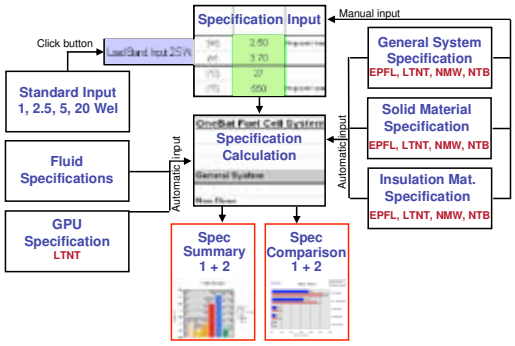


Fig. 1: Specification sheet for dimensioning the OneBat SOFC-system.

Figure 1 gives an overview of the newly developed specification sheet that has been developed for dimensioning the OneBat SOFC-system. It represents a accurate and self-contained description of all factors relevant for system design by a simple model based on global balances. This specification sheet has been checked against FE- as well as thermodynamic equilibrium calculations. It is a fast and flexible design tool to analyse dimensions, mass- and energy flows, as well as overall efficiencies and possible applications.

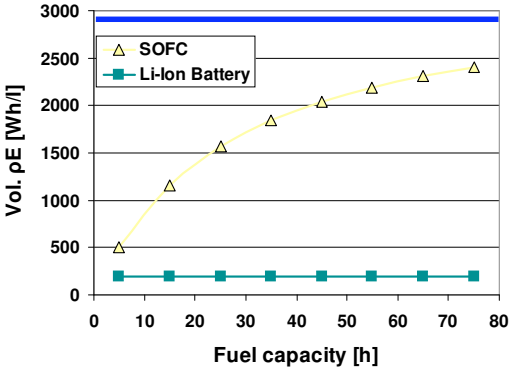


Fig. 2: Volumetric energy density of a SOFC as a function of its fuel capacity.

Figure 2 shows how the volumetric energy density of a SOFC increases with an increase in the fuel capacity. (The calculations were peformed for an SOFC with an electrical power of 2.5 W and an electrical efficiency of 40 %.) In the limit of a very high fuel capacity, the SOFC reaches the electrical capacity of butane which has been choosen as fuel. These results demonstrate the big volume advantage of an SOFC at higher fuel capacities in comparison with Li-Ion batteries.

Chapter 5

Organic Electronics and Photovoltaics

5.1 Advanced experimentally validated integrated OLED model

Contributors: Evelyne Huber, Beat Ruhstaller

Partners: Philips Research Aachen and Eindhoven, Technical University Dresden, FLUXiM, University of Cambridge, University of Groningen, Eindhoven University of Technology, Sim4tec

Funding: European Union FP7

Duration: 2008 – 2011

White Organic Light-Emitting Diodes (OLEDs) are highly efficient light sources that can potentially be used for general lighting. They can also be printed on flexible surfaces resulting in light-emitting flexible foils. Moreover, OLEDs have entered the small- and medium-size flat panel display market. The increasing complexity of OLEDs (layer composition and structures) demands an experimentally validated comprehensive OLED device model to design efficient and rational OLEDs. It has recently become clear that today's first generation models, based on conventional understanding of transport and photophysical processes, are insufficient for realistic OLED materials. The aim of the AEVIOM project[1] is to develop a numerical simulation tool for achieving breakthroughs in white OLED technology. Within the project, a second-generation OLED device model will be developed, within which the full three-dimensional character of the charge transport, recombination, and excitonic processes is taken into account. Thereby, the disordered nature of the organic materials is treated more properly than in today's first-generation OLED device models. The resulting integrated model will describe the complete interplay between OLED layer structure, charge carrier mobilities, excitonic processes and light-outcoupling. The task of the ZHAW within this project is the development of an effective 1-dimensional model that integrates the entire chain of physical processes that takes place in OLED operation. The main challenge is to incorporate novel physical models in the course of the project, which lead to strongly coupled partial differential equations, into an efficient solver. In this first year a solver has been implemented that solves the system of partial differential equations in a coupled manner and includes novel physical models like the Extended Gaussian Disorder Model (EGDM), the generalized Einstein diffusion and injection into Gaussian density of states. With the aid of the simulation we can calculate a) what is happening in the OLED (carrier profiles, see Fig. 1) as well as b) data that can be measured in an experiment (IV-curves, see Fig. 2).

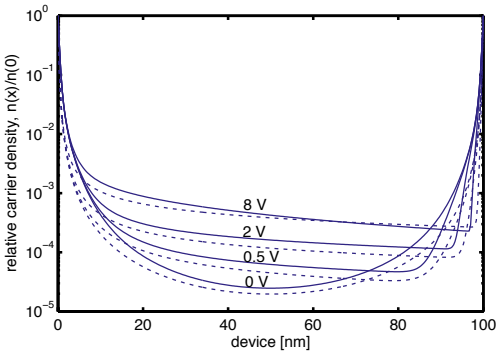


Fig. 1: Carrier concentration profile of a hole-only device. The dotted lines show the solution for constant mobility and diffusion while the solid lines represent the solution for the EGDM at different voltages.

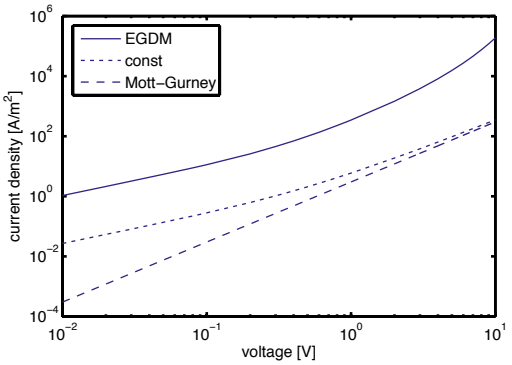


Fig. 2: IV-curve for constant mobility and diffusion and the EGDM. The Mott-Gurney law is plotted for constant mobility and neglecting diffusion.

[1] www.aeviom.eu

5.2 Efficient areal organic solar cells via printing

Contributors: Roger Häusermann, Nils A. Reinke, Beat Ruhstaller

Partners: CSEM Basel, Ciba Inc., TU Eindhoven (NL), Universitat Jaume I (E)
Funding: Swiss Federal Office of Energy
Duration: 2008 – 2011

This project with acronym Apollo aims to combine plastic electronics expertise in Europe for realizing organic solar cells for empowering printed electronics applications. Existing solar cell technologies cannot provide the attributes such as printability in ambient conditions, flexibility and low cost.
So far, the development of organic solar cells was to a large extent a semi-empirical trial-and-error process, in which organic semiconducting materials were selected on the basis of their known or partially known separate properties. It has recently become clear that this provides an insufficient sound basis for a further development. Therefore an interdisciplinary approach with new materials, device concepts, models and characterization methods is critical.
The focus of this project is on single cells and tandem cells with record efficiency that feature ease of production and proof-of-principle for the interdisciplinary research approach. The detailed understanding of device operation allows for steady improvements in efficiency.

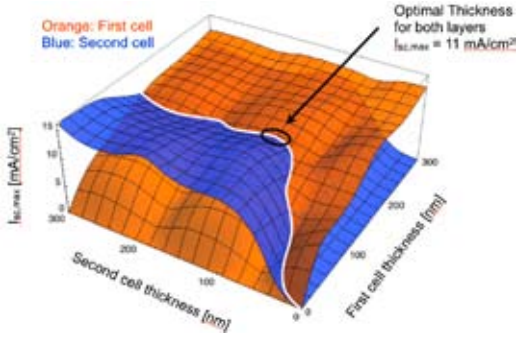


Fig. 1: Maximum achievable current in the two subcells of a tandem solar cell. The white line indicates current matching of the subcells, which is a precondition to reach high efficiencies.

A comprehensive device model for the study of operation mechanisms and the interpretation of measured data will be developed. It will cover the whole process chain from light absorption, exciton dissociation, charge carrier transport and collection by electrodes. The ICP has expertise in numerical modelling of optoelectronic processes in transient and steady state in OLEDs which is used to develop a simulation software for organic solar cells. The maximum achievable short circuit-current will be addressed with optical simulations that provide the spatial exciton generation rate density. It is intended to distinguish the detrimental effects of charge trapping, recombination and collection losses by the use of drift-diffusion simulations.

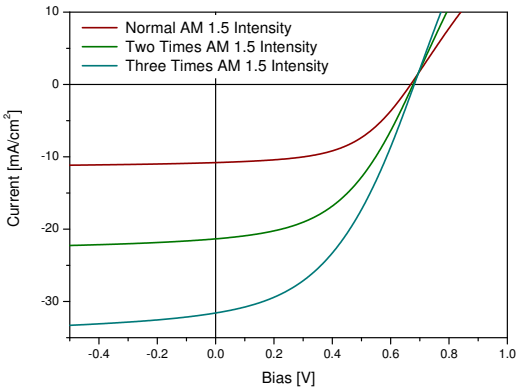


Fig. 2: Simulated current-voltage curves of an organic solar cell dependent on the illumination intensity.

In this early stage of the project an optical model has been developed to simulate multilayer organic solar cells. It is used to calculate the maximum achievable current in the solar cell. In Fig. 1 such a simulation is shown, where the generated current in a tandem solar cell is calculated for each subcell dependent on the thickness of these layers. This optical model has been coupled to a drift-diffusion solver to also simulate the electrical behavior of such a solar cell. First results can be found in Fig. 2 where calculated current-voltage curves are shown. These curves are simulated dependent on the illumination intensity which is varied from one sun intensity to three times the sun intensity. In ongoing work we investigate the exciton dissociation into free carriers and validate the results with experiments.

5.3 Cost efficient thin film photovoltaics for future electricity generation

Contributors: Roger Häusermann, Nils A. Reinke, Jürgen Schumacher, Beat Ruhstaller

Partners: EMPA, ETHZ, Univ. of Neuchatel, EPFL, PSI OC Oerlikon Solar, Solaronix, Flisom
Funding: SwissElectric Research
Duration: 2007 – 2010

The design of emerging thin film photovoltaic cells has several aspects in common: 1) The collection of ambient light in multilayers can be enhanced with the help of structured surfaces, 2) it shall be absorbed inside the thin film stack, 3) generate excited states that relax at nearby dissociation sites into electrons and holes, 4) which finally shall be transported to the electrodes with minimal loss.
In the course of the second ThinPV[2] project year the optical model has been finalized. For coherent optics an arbitrary layer setup can be simulated. Not only can the achieved short-circuit current I_{sc} be estimated, but also the absorption in each layer. This is shown in Figure 1. In the top part the optical field distribution is calculated inside a multilayer thin film solar cell stack. From this calculation the amount of absorbed photons can be calculated at every position inside the device, which can be seen in the lower part of Figure 1.
Subsequently, one can calculate the maximum achievable short-circuit current. By varying the layer thickness and materials one can optimize a given thin film solar cell. The extension of the multilayer optical model for mixed incoherent/coherent layer stacks is underway. This will provide the basis for designing several of the existing thin film photovoltaics technologies under investigation in this project.

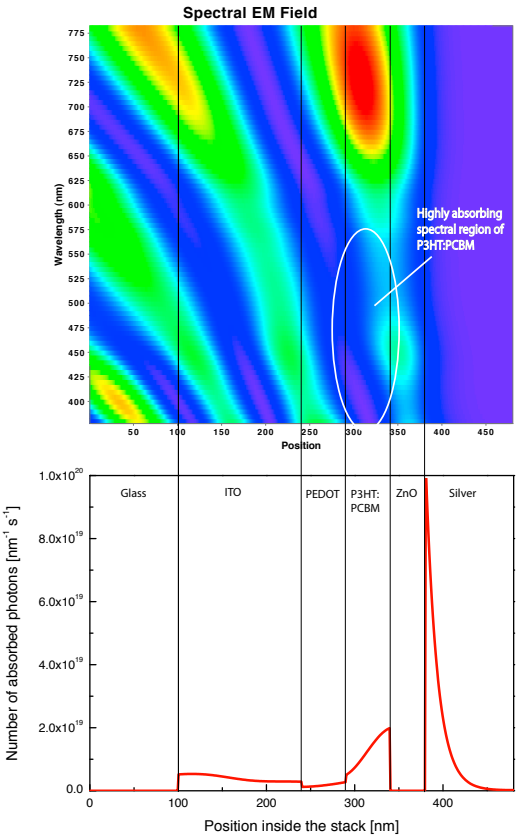


Fig. 1: Optical field distribution within a multilayer thin film cell (top) and profile of absorbed photons per second (bottom) under AM1.5 illumination.

[2] http://thinpv.empa.ch

5.4 Organic electroluminescent pictograms for push-button applications

Contributors: Nils A. Reinke, Roger Häusermann, Beat Ruhstaller

Partners: CSEM, Ciba, EAO
Funding: Commission for Technology and Innovation (CTI)
Duration: 2007 – 2009

The novelty of the envisioned product in this project is the possibility to produce very thin, custom-designed self-luminous pictograms for applications in push-buttons. They combine existing pushbuttons (EAO) with patterned emissive pictograms (CSEM) made from electroluminescent semiconductor materials (Ciba SC). The characterization and optimization of material properties, device and system architecture is supported by computational engineering and simulation software[3] development at ZHAW as illsutrated by prototypes in Fig. 1.

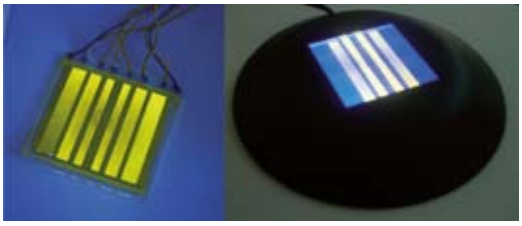


Fig. 1: Transparent PLED (left) and backlighted PLED prototype (right) developed in this project. The combination of blue backlight and yellowish emission from the PLED yields a white color emission.

The numerical simulation activities subdivide into electronic and optical device modeling as well as advanced analysis algorithms. The electronic device model contains charge drift-diffusion and exciton rate equations for modeling organic semiconductor devices including multiple excitons, several charge mobility and injection models and charge doping and trapping. The numerical algorithm delivers charge distribution profiles, transient electroluminescence, as well as current-voltage curves. The optical solver evaluates the angular emission characteristics as well as the substrate, thin-film and plasmon modes. The modes can be visualized and integrated to extract relative mode contributions and position-dependent lifetimes. Key performance figures such as luminous efficacy, CIE, CRI, etc. are calculated. Advanced analysis features allow to extract device parameters, for instance the shape of the emission zone, from experimental data. Our model fits experimental current-voltage curves of PLEDs considering a field dependent charge carrier mobility (cf. Fig. 2).

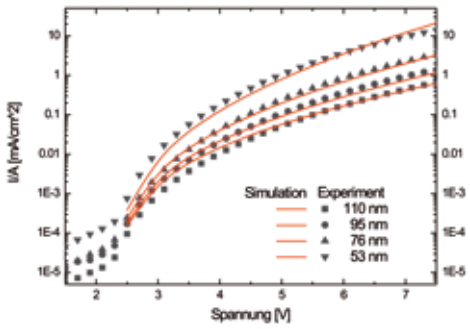


Fig. 2: Experimental and simulated current-voltage curves considering a field dependent mobility.

In large-area OLEDs non-uniformities in the luminance arise from potential drops across a low-conductive electrode. FEM-simulations allow to study such potential drops (cf. Fig. 3).

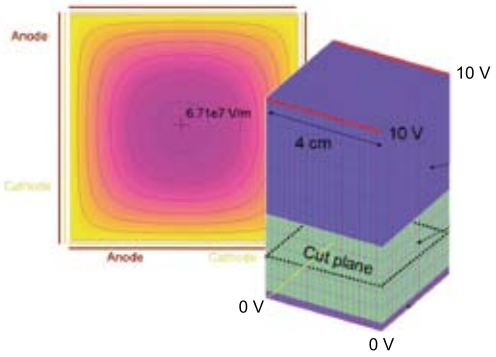


Fig. 3: SESES simulation of the potential drop.

[3] SETFOS Semiconducting Emissive Thin Film Optics Simulator, Fluxim AG, Switzerland, www.fluxim.com.

5.5 Modeling, simulation and loss analysis of dye-sensitized solar cells

Contributors: Matthias Schmid, Jürgen O. Schumacher

Partners: Laboratoire de Photonique et Interfaces (LPI), EPFL
Funding: Gebert Rüf Stiftung
Duration: 2008 – 2010

Dye-sensitized solar cells (DSCs) are an innovative technology for the production of electricity from solar energy. In contrast to conventional silicon semiconductor solar cells, light is absorbed in the DSC by dye molecules bounded to the surface of a highly porous structure of nanoparticles of transparent TiO_2. The production process of DSCs is based on relatively simple and inexpensive techniques, like e.g. screen printing. In addition no cost-intensive, exhaustible raw materials are needed. Therefore, the contribution of DSCs to an economic production of solar energy could be essential in the future.

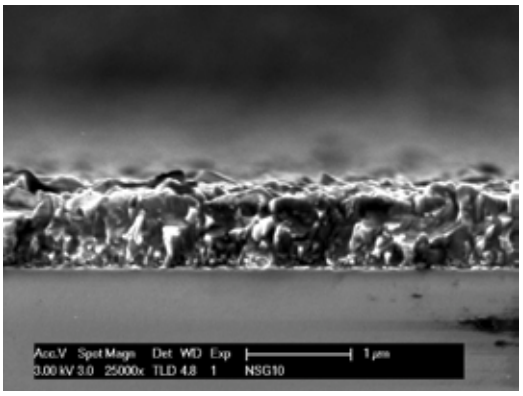


Fig. 1: SEM image of the F:SnO_2 glass used as front electrode in the DSC (image courtesy of EPFL). The SEM images are used to estimate the thickness and surface roughness of the F:SnO_2 layer.

In September 2008 we started a research project for the modeling of dye-sensitized solar cells. The project is carried out under the lead of the ICP in a close collaboration with the Laboratory of Photonics and Interfaces (LPI) at EPFL. The objective of this project is to develop validated mathematical models for the DSC. The models aim at describing the coupled optical, electrical and electrochemical processes taking place within the solar cell. This allows to analyze quantitatively the different loss channels of the energy conversion process. Research and development of DSCs could be accelerated to a large extent, if these new device models were implemented into accurate and efficient numerical algorithms.

Currently the ICP is developing an optical model of the DSC in order to simulate absorption, reflection loss and the spatially resolved sensitizer excited state generation rate. The optical model is validated by optical reflection and transmission measurements of the layers that constitute a DSC (F:SnO_2-glass, nanoporous semiconductor film, monolayer of dye, and electrolyte). The measurements are carried out by EPFL, see e.g. Fig. 1.

Simultaneously, a complete 1D through-plane model of the DSC is formulated, which uses the simulated generation rate profile from the optical model as an input. The through-plane model is based on a coupled nonlinear 1D system of partial differential equations (PDEs) to describe the electrochemical reactions and the transport processes. This 1D model is validated on laboratory DSCs by different measurements techniques such as photovoltage and photocurrent response and spectrally resolved quantum efficiency, see Fig. 2.

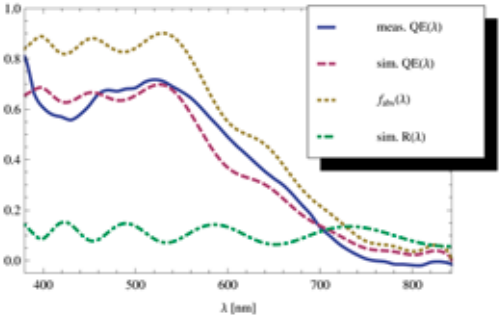


Fig. 2: Comparison of the simulated (solid line) and measured (dashed line) quantum efficiency $QE(\lambda)$ of the DSC as a function of wavelength of the incident light. The dotted line is the simulated fraction of absorbed light $f_{abs}(\lambda)$ and the dash-dotted line shows the simulated reflection loss $R(\lambda)$ of the front electrode.

5.6 Photovoltaics inspector

Contributors: Beat Ruhstaller, Nils A. Reinke

Partners: Fluxim AG
Funding: Transferkolleg "Industrial Photonics" funded by CTI and SATW
Duration: 2008 – 2009

The production of thin film solar cells demands high accuracy, quality and control on the process parameters in order to ensure highest possible power conversion efficiency, lifetime as well as yield. Quality-monitoring during and at the end of a production line is thus mandatory. Traditionally both optical and electrical methods are used to assess the quality, compare with Fig. 1. It is, however, not yet possible to automatically extract crucial material and device parameters with the help of an accurate numerical device model. Such a method would allow an early identification of process parameter deviation in production. In addition, a reliable numerical model is useful in the cell design phase in R&D. The software SETFOS is commercialized by Fluxim AG for organic semiconductor device simulation in R&D. So far, SETFOS does not yet provide physical models for charge transport and light scattering in **in**organic semiconductor devices. Both is relevant to inorganic solar cells that dominate the photovoltaics market today. The extended numerical device model shall combine a) an accurate description of the relevant physical processes, b) high computation speed and c) algorithms for parameter extraction.
In this feasibility study, the project idea is being evaluated and discussed with potential stakeholders and project partners. It includes a market study and analysis of industry needs and existing inspection methods.

Fig. 1: Illustration from Xenon Corp. of xenon flash lamps for photovoltaic module inspection.

5.7 Optoelectronic research laboratory

Contributors: Nils A. Reinke, Andreas Tiefenauer, Beat Ruhstaller

Partners: Various project partners
Funding: ICP, School of Engineering
Duration: ongoing

True-to-life modeling always is based on accurate input parameters from the real world. The purpose of the optoelectronic research laboratory (O-LAB) in this context is both providing such input parameters and experimentally validating simulation results. Combining advanced computational methods and state-of-the-art experimental methods allows us to develop innovations in measurement engineering.

Fig. 1: Photo-thermal characterization of an infrared-sensor.

The O-LAB is therefore a consequent expansion of our existing computational toolbox, facilitating the collaboration with experimentally-oriented partners and industry. Our current investigations comprise the following fields of interest:

- Ultra-fast photo-thermal heating and detection
- Thin film spectroscopy
- Transient optoelectronic device characterization

An exemplary setup developed at the OLAB is shown in Fig. 1. This setup allows to measure photo-thermal response times of infrared sensors down to 100 μs. An experimental setup measuring transient currents and electroluminescence from organic light emitting devices is depicted in Fig. 2. Our experimental toolbox comprises fast oscilloscopes, signal generators, IR-sources and detectors, flashers and spectrometers.
The O-LAB supports industrial needs in the characterization of sensors and actuators and several ICP projects related to thermal labeling, thin-film spectroscopy, organic light emitting devices and photovoltaics. In addition, our laboratory is ideally suited for educational purposes in teaching B.Sc. and M.Sc. students in mechatronics, electronics and informatics. The O-LAB gives young scientists and engineers the possibility of getting in contact with R&D and working on exciting issues in ongoing projects.

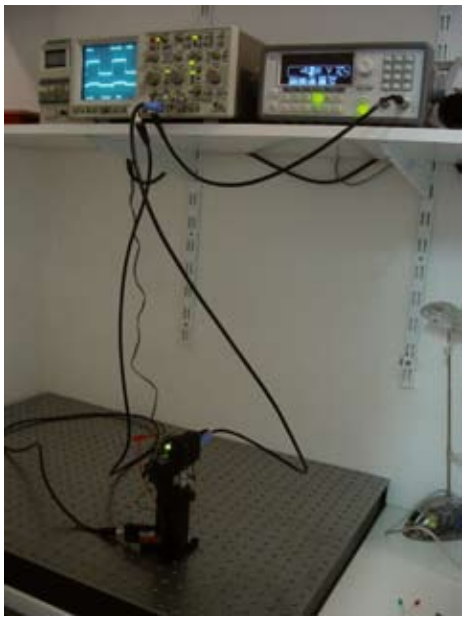


Fig. 2: Transient measurement of currents and electroluminescence in organic light emitting devices.

Chapter 6

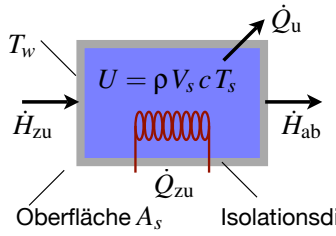
Student Projects

6.1 Wirtschaftlichkeit und Ökobilanz eines Blockheizkraftwerks mit regenerativen Energieträgern und 5 bis 20 kW elektrischer Leistung

Students: Martin Hauser, Marcel Ott

Category: Projektarbeit Maschinentechnik
Mentoring: Christoph Meier, Thomas Hocker
Period: Februar 2008 – Mai 2008

Ein Blockheizkraftwerk (BHKW) ist eine modular aufgebaute Anlage zur Erzeugung von elektrischem Strom und Wärme, die vorzugsweise am Ort des Wärmeverbrauchs betrieben wird. Sie setzt dazu das Prinzip der Kraft-Wärme-Kopplung ein. Der höhere Gesamtnutzungsgrad gegenüber der herkömmlichen Kombination von lokaler Heizung und zentralem Großkraftwerk (für die Stromproduktion) resultiert aus der Nutzung der Abwärme der Stromerzeugung direkt am Ort der Entstehung. Als Antrieb für den Stromerzeuger können Verbrennungsmotoren, aber auch Gasturbinen verwendet werden. Gasmotoren werden meist mit Erdgas betrieben. Jedoch auch ein Betrieb mit regenerativen Energieträgern wie z. B. Holzgas und Rapsöl ist denkbar.



$$\frac{dT_s}{dt} = \frac{\dot{Q}_{zu}(t) - A_s \alpha \left(\frac{T_s + \frac{\alpha}{\kappa/d} T_u}{(\frac{\alpha}{\kappa/d} + 1)} - T_u \right) + \dot{Q}_v(t)}{\rho V_s c}$$

Fig. 1: Einfaches Modell eines Systems aus Wärmeverbraucher, -quelle und -speicher.

Obwohl die BHKW-Technologie wegen der damit verbundenen CO_2-Reduktion (s. a. Kyoto-Protokoll) in vielen europäischen Ländern staatlich gefördert wird, blieb deren Verbreitung bisher unter den Erwartungen zurück. Deshalb ist das Ziel des Projektes, die BHKW-Technologie in Kombination mit regenerativen Energieträgern auf ihre Wirtschaftlichkeit und ihren ökologische Nutzen hin zu untersuchen. Für den wärmegeführten Betrieb wurde in Matlab/Simulink ein einfaches Modell aus Wärmeverbraucher, -quelle (BHKW) und -speicher implementiert, siehe Abbildung 1. Es konnte gezeigt werden, dass Mikro-BHKW-Anlagen unter der Voraussetzung eines minimalen Wärmebedarfs zu ähnlichen Kosten betrieben werden können wie konventionelle Pelletheizkessel, siehe Abbildung 2.

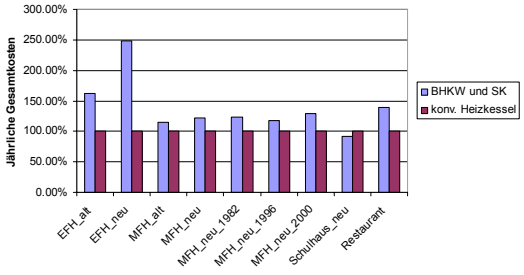


Fig. 2: Kosten BHKW mit Standardkessel für verschiedene Applikationen im Vergleich zu einem konventionellen Heizkessel.

Für Einfamilienhäuser und andere kleine Bauten ist der Wärmebedarf allerdings zu gering. Die Möglichkeit von Wärmeverbundanlagen, wo mehrere EFH durch dasselbe BHKW beheizt werden, stellt hier sicherlich eine interessante Alternative dar. Voraussetzung für einen störungsfreien Betrieb der Anlage sind technisch ausgereifte Komponenten. Dieser Entwicklungsstand ist bei gasbetriebenen Blockheizkraftwerken erreicht worden, bei den kleinen Holzvergasern muss allerdings noch weiterer Entwicklungsaufwand betrieben werden. Ein weiterer ungeklärter Punkt ist die Auslegestrategie verschiedener Hersteller: entgegen unserer Auslegung werden keine, oder nur sehr kleine Pufferspeicher verwendet, was den Deckungsgrad und somit den Anteil gekoppelt erzeugter Energie deutlich verkleinert.

6.2 Modell-basierte Analyse der U–I–Kennlinie von SOFC Hochtemperatur-Brennstoffzellen

Students: Markus Linder

Category: Vertiefungsarbeit Masterstudium (MSE)
Partner: Hexis AG
Mentoring: Thomas Hocker
Period: Oktober 2008 – Februar 2009

Die Hexis AG, Winterthur, gehört zu den führenden Unternehmen in der Entwicklung stationärer Hochtemperatur Brennstoffzellensysteme. Hexis entwickelt Brennstoffzellen-Heizgeräte im kleinen Leistungsbereich, die für die dezentrale Wärme- und Stromversorgung in Einfamilienhäusern eingesetzt werden.
Um die Brennstoffzellen in ihren elektrochemischen sowie thermo-mechanischen Eigenschaften gezielt weiter zu entwickeln, müssen diese möglichst exakt charakterisiert werden. Dazu wird im Betrieb die elektrische Spannung in Abhängigkeit des elektrischen Stromflusses gemessen und als sogenannte Strom-Spannungskennlinie ((U,i)-Kennlinie) aufgezeichnet. Diese Kennlinie ist von zentraler Bedeutung, da damit die Leistungskurve dargestellt und Verluste typisiert werden können. Das Ziel dieser Vertiefungsarbeit war die Entwicklung eines Modells, mit dem die umfangreichen Messdaten von Zellen-Prüfständen effizient analysiert werden können. Dazu wurden die unterschiedlichen Effekte und Einflüsse auf den Gesamtverlust quantifiziert. Für den Betrieb der Brennstoffzelle wird Erdgas, das primär aus Methan ($\mathrm{CH_4}$) besteht, verwendet. Auf der Zelle selbst wird Wasserstoff ($\mathrm{H_2}$) umgesetzt. Dazu wird das Erdgas, in einem Reformer in Wasserstoff und Kohlenmonoxid CO umgewandelt. Über die Menge des verbrauchten Wasserstoffes an der Zelle, wird dann die ideale (U,i)-Kennlinie berechnet. Die (U,i)-Kennlinie aus den Messungen, unterscheidet sich von der berechneten (U,i)-Kennlinie. Diese gut erkennbare Differenz ergibt sich aufgrund der Verluste, die im realen System auftreten. Mit dem entwickelten Modell können, nebst dem Erzeugen der idealen (U,i)-Kennlinie, die Leckage- und Repeat Unit-Verluste (eine Repat Unit eines Zellenstapels besteht aus der Zelle und den Stromsammler-Platten) quantifiziert werden, vgl. mit Abbildung 1. Dazu wird die ideale (U,i)-Kennlinie in mehreren Schritten an die gemessene (U,i)-Kennlinie angepasst.
Das in *Mathematica* implementierte Modell erlaubt eine weitgehend automatisierte Auswertung der Messdaten. Einzig die Zusammensetzung des Erdgases nach der Reformierung und der Verbrauch an der Zelle müssen vorgängig ermittelt werden. Eine Zusammenfassung der Resultate und Inputdaten der Modellrechnung wird als Excel-Sheet ausgegeben. Für die Überprüfung auf mögliche Fehler wurden die Resultate des Modells mit denen einer alten Auswertung verglichen. Da diese Verifizierung erfolgreich war, darf das Modell für Auswertungen und Analysen eingesetzt werden. In weiteren Arbeiten ist geplant, die Benutzerfreundlichkeit des Modells weiter zu verbessern. Es soll künftig bei Hexis für die routinemässige Analyse von (U,i)-Kennlinien eingesetzt werden. Vorgesehen ist zudem eine Auswertung und statistische Aufbereitung einer grösseren Anzahl von (U,i)-Kennlinien.

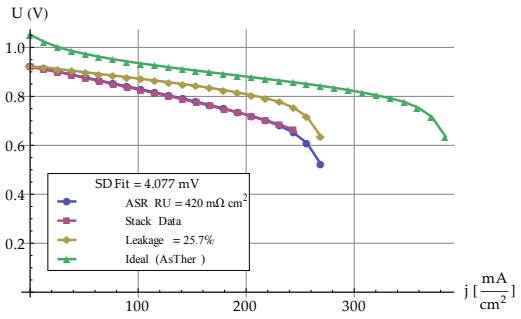


Fig. 1: Modellbasierte Analyse der Spannungs-Strom-Kennlinie einer Hochtemperatur-Brennstoffzelle.

6.3 Modell-basierte Optimierung der Holzvergaseranlage in Wila

Students: Roger Bächtiger, Fabian Kekeis

Category: Diplomarbeit Maschinentechnik
Partner: Woodpower AG, Wila, Globutech Services, Freiburg im Breisgau
Mentoring: Thomas Hocker
Period: August 2007 – Oktober 2007

Unter Holzvergasung versteht man den verfahrenstechnischen Prozess der Teilverbrennung unter Luftmangel um aus Holz das brennbare Holzgas zu gewinnen. Holzgas wird beispielsweise als Brennstoff für stationäre Gasmotoren eingesetzt, um über einen Generator elektrischen Strom zu produzieren. Die Woodpower AG und die Elektrizitätswerke des Kantons Zürich (EKZ) betreiben seit Anfang 2007 die erste kommerzielle Anlage für Holzvergasung in der Schweiz. In der Anlage werden nach der oben beschriebenen Methode ca. 450 kW Strom und zusätzlich ca. 1000 kW Wärme aus Altholz erzeugt. Projektziel war die modellbasierte Optimierung der Holzvergaseranlage in Wila über Massen- und Energiebilanzen sowie thermodynamische Gleichgewichtsmodelle. Die hierfür benötigten Grössen wie Temperaturen, Konzentrationen und Massenflüsse wurden aus Messungen vor Ort bestimmt. Aus den Modellen lassen sich wichtige Kenngrössen wie die Höhen der verschiedenen Reaktionszonen im Reaktor ermitteln, siehe Abbildung 1.

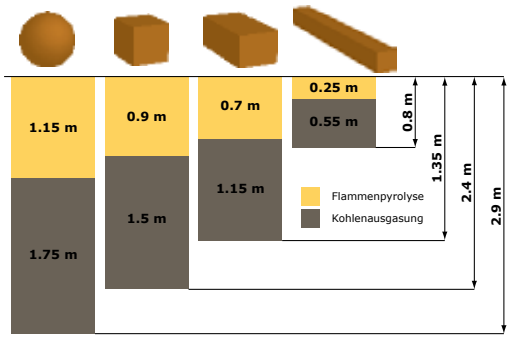


Fig. 1: Berechnete Höhen der Flammenpyrolyse- und Reduktionszonen in Abhängigkeit von der Form der verwendeten Holzschnitzel.

Hierfür muss man wissen, wie lange die Pyrolyse (d. h. der Ausgasungsprozess) einzelner Partikel dauert. Die in Abbildung 2 gezeigten Messungen von Pyrolysezeiten stimmen gut mit den von E. R. Huff[1] publizierten Werten überein.

Fig. 2: Messung der Pyrolyse- und Reduktionszeit an einzelnen Holzpartikeln.

Ausserdem wurde berechnet, wie sich der unerwünschte Austrag an Holzkohle mit dem Feuchtegehalt der verwendeten Holzschnitzel sowie den Wärmeverlusten über die Reaktorwand verändert, siehe Abbildung 3. Bei einem Wassergehalt von 15 % und einem Wärmeverlust von 20 kW ergibt sich ein Holzkohleaustrag von knapp 5 Gew.-%. Dieser Wert stimmt gut mit den Erfahrungswerten der Woodpower AG überein.

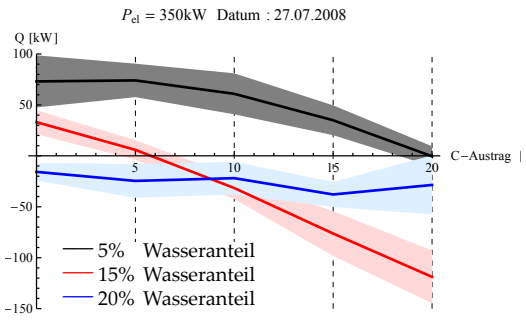


Fig. 3: Einfluss des Feuchtegehalts der Holzschnitzel und der Wärmeverluste über die Reaktorwand auf den Austrag an Holzkohle.

[1] E. R. Huff, "Effect of Size, Shape, Density, Moisture and Furnace Wall Temperature on Burning Times of Wood Pieces," in *Fundamentals of Thermochemical Biomass Conversion*, Ed. R. P. Overend, 1985.

6.4 Prüfstand für thermo-mechanische Belastungstests von Brennstoffzellen

Students: Matthias Kocher, Florian Baumberger

Category: Diplomarbeit Maschinentechnik
Partner: Hexis AG
Mentoring: Thomas Hocker
Period: August 2008 – Oktober 2008

Zur Erhöhung der Zuverlässigkeit und Langlebigkeit des Hexis Brennstoffzellensystems müssen die Materialeigenschaften der Brennstoffzellen weiter optimiert werden. Insbesondere müssen sie den thermomechanischen Beanspruchungen im Betrieb besser standhalten. Zur Überprüfung der Stabilität der Zellen wurde deshalb ein Prüfstand für thermomechanische Belastungstests entwickelt. Die Idee ist, die Zellen bereits vor Einbau ins System einem realistischen Belastungstest zu unterziehen.

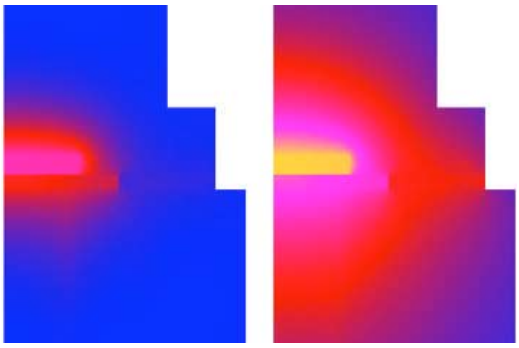


Fig. 1: Temperaturplot aus thermischem FE-Modell zur Analyse des Aufheizens des thermomechanischen Zellenprüfstands.

Im Prüfstand müssen sich deshalb ähnliche Temperaturverteilungen wie im Zellenstapel des realen Systems einstellen lassen. Hierfür wurde zunächst ein ”virtueller Prüfstand“ mit Hilfe der Finite Element Software SESES entwickelt, siehe Abbildung 1. Das Modell berücksichtigt neben der Wärmeleitung in den Feststoffen den Wärmetransport über thermische Strahlung in Kavitäten sowie die Wärmeabfuhr über die Oberflächen via Naturkonvektion.
Durch Vergleich einer grossen Anzahl verschiedener Designs wurde via FE-Analyse ein Konzept erarbeitet und anschliessend umgesetzt. Abbildung 2 zeigt den fertigen Prüfstand. Daran ist besonders, dass sich hohe Temperaturgradienten in den Zellen auch ohne eine erzwungene, externe Kühlung einstellen lassen.

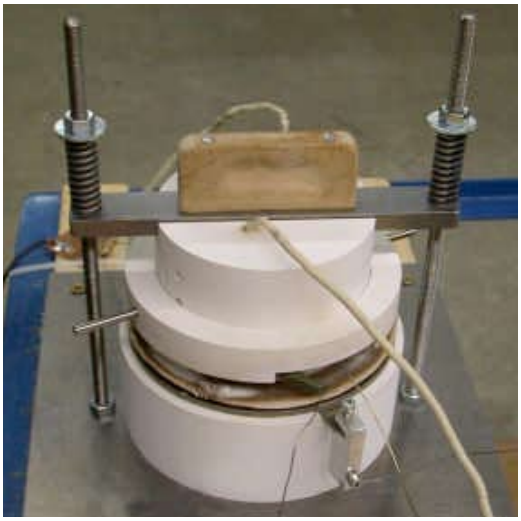


Fig. 2: Prüfstand für thermomechanische Belastungstests von Hochtemperatur-Brennstoffzellen.

Um die Temperaturverteilung innerhalb der Zelle in einer hohen Auflösung zu messen, wurden 20 Thermoelemente verbaut. Hierbei handelt es sich um eine Spezialanfertigung der Winterthurer Firma Sawi. Die Thermoelemente halten sehr hohen Temperaturen stand und lassen sich über Feingewinde sehr genau positionieren. Aus den gemessenen Temperaturverteilungen auf den Zellen wurden in einem nachfolgenden Schritt die induzierten mechanischen Spannungen via thermo-mechanischer FE-Analyse berechnet.

6.5 High Performance Grating Spectrometer

Students: Martin Neukom, Simon Hübscher

Category: Project Work in Mechatronics
Mentoring: Nils A. Reinke, Christoph Stamm
Period: Oktober 2008 – Januar 2009

In this work a grating spectrometer with a focal length of 30cm is constructed from scratch. The exploded assembly drawing in Fig. 1 shows the external and internal compartments of the device. The spectrometer offers both fixed entrance slits ranging from 20$\mu\mathrm{m}$ to 1mm and an adjustable entrance slit. An additional mount allows to connect optical fibers to the device. A holographic grating with 1200 $\mathrm{lines/mm}$ is used as a dispersive element. The concave curvature of the grating defines the focal length of the device making additional optical components needless. The curved grating thus allows a very compact design of the device and reduces optical aberrations and losses. The spectrum is detected with a highly sensitive CCD line sensor comprising 3000 pixels.

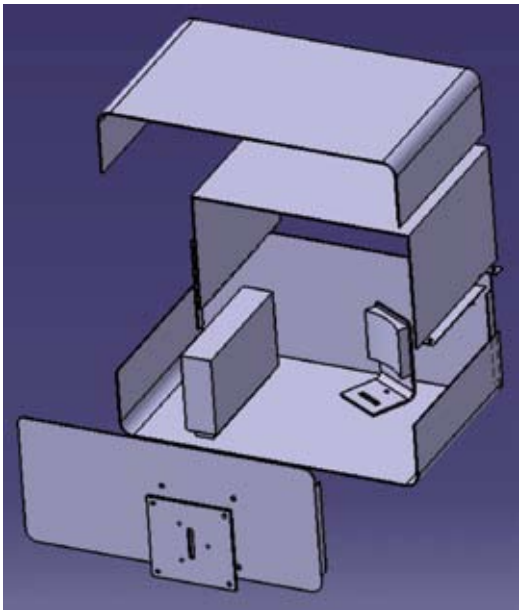


Fig. 1: Exploded assembly drawing of the spectrometer comprising the internal and external body, the mounted holographic grating and the CCD line sensor.

The inner shielding of the device encapsulates the CCD sensor from optical noise. The detectable spectrum ranges from $450\mathrm{nm}$ to $750\mathrm{nm}$ at a maximum spectral resolution of 0.1 nm depending on the width of the entrance slit. The sensor is both powered and controlled by an USB 2.0 interface. The developed LabView software allows calibrating both spectral positions and absolute intensities by a build-in polynomial fitting routine and reading calibration data from a file, respectively. A screenshot of the developed LabView software is displayed in Fig. 2. The software offers the basic functionality of background subtraction and setting the integration time. During long acquisition processes the user is informed about remaining recording time. Transient processes can be recorded at a speed of 300 scans per second which can be accelerated up to 3000 scans per second using an alternative line sensor.

Fig. 2: Spectrometer software developed in LabView.

This high performance spectrometer offers high resolution, high sensitivity and high speed making it competitive with upper-class commercial products. This spectrometer will thus be a valuable tool for prospective projects in the field of thin-film optical spectroscopy and bio-sensing applications.

Chapter 7

Appendix

7.1 Publications

- Light extraction and optical loss mechanisms in organic light-emitting diodes: influence of the emitter quantum efficiency: *S. Nowy, B. Krummacher, J. Frischeisen, N. A. Reinke, W. Brütting*, J. Appl. Phys. 104, 123109 (2008).
- Surface plasmon resonance sensor utilizing an integrated organic light emitting diode: *J. Frischeisen, C. Mayr, N. A. Reinke, S. Nowy, W. Brütting*, Opt. Express 16, 18426-18436 (2008).
- B. Ruhstaller, T. Flatz, D. Rezzonico, M. Moos, N. A. Reinke, E. Huber, R. Häusermann, B. Perucco: *Comprehensive simulation of light-emitting and light-harvesting organic devices*, Proceedings of the SPIE Conference, Vol. 7051, ISBN 9780819472717, San Diego, USA (2008).
- R. Häusermann, N. A. Reinke, E. Huber, B. Ruhstaller: *Towards Comprehensive Simulation of Organic Solar Cells*, Proc. EOS Annual Meeting (2008).
- N. A. Reinke, B. Perucco, M. Moos, W. Brütting, B. Ruhstaller: *Emission Zone Extraction and Analysis of Loss Channels in Organic Light-emitting Devices*, Proc. EOS Annual Meeting (2008).
- S. Nowy, N. A. Reinke, J. Frischeisen, and W. Brütting: *Light extraction and optical loss mechanisms in organic light-emitting diodes*, Proc. SPIE (2008).
- J. Frischeisen, N. Reinke, C. Ostermayr, J. Neumann, S. Nowy, W. Brütting: *Surface plasmon resonance sensor based on a planar polychromatic OLED light source*, Proc. SPIE (2008).
- K. Steinkamp, J.O. Schumacher, F. Goldsmith, M. Ohlberger, C. Ziegler: *A non-isothermal PEM fuel cell model including two water transport mechanisms in the membrane*, Special issue of the Journal of Fuel Cell Science and Technology, Volume 5, Issue 1, 011007 (2008).
- A. Bieberle-Hütter, D. Beckel, A. Infortuna, U. Muecke, J. Rupp, L. Gauckler, S. Rey-Mermet, P. Muralt, N. Hotz, M. Stutz, N. Bieri, D. Poulikakos, P. Müller, A. Bernard, R Gmür, T. Hocker: *A micro-solid oxide fuel cell system for battery replacement*, Journal of Power Sources, 177, 123ff (2008).
- H. Schwarzenbach: *Modellbildung in der Mikrosystemtechnik - Kreativität ist gefragt*, SWISS ENGINEERING STZ Nummer 7/8 (2008).
- H. Schwarzenbach: *Multiphysikalische Werkzeuge im Kleinstformat*, Technica 7 (2008).
- R. Alther, R. Weiss, E. Lang, T. Hocker: *Self-opening closure with air inlet channel for composite packaging or for container necks to be sealed with foil material*, International Patent Application PCT/CH2008/000339 (2008).

7.2 Conferences and Workshops

- E. Huber, R. Häusermann, N. A. Reinke, B. Ruhstaller, T. Flatz, M. Moos: *Mobility Models for OLED Device Simulation*, International Krutyn Summer School, Krutyn, Poland, May (2008).
- R. Häusermann, E. Huber, N. A. Reinke, B. Ruhstaller, T. Flatz, M. Moos: *Design Rules for Organic Photovoltaic Cells: Reflective Electrode Material*, Olla Summer School, Krutyn, Poland, May/June (2008).
- N. A. Reinke: *OLED Light Outcoupling*, 1st International User Workshop, Winterthur, Switzerland, July (2008).
- R. Häusermann: *Organic Photovoltaic Cell Simulation*, 1st International User Workshop, Winterthur, Switzerland, July (2008).

- B. Ruhstaller, T. Flatz, D. Rezzonico, M. Moos, N. A. Reinke, E. Huber, R. Häusermann, B. Perucco: *Comprehensive simulation of light-emitting and light-harvesting organic devices*, SPIE Optics & Photonics Conference, San Diego, USA, August 2008.
- B. Ruhstaller, T. Flatz, D. Rezzonico, M. Moos, N. A. Reinke, E. Huber, R. Häusermann, B. Perucco: *Comprehensive simulation of light-emitting and light-harvesting organic devices*, IBM Almaden Research Center, San Jose, USA, August 2008.
- R. Häusermann, N. A. Reinke, E. Huber, B. Ruhstaller: *Towards a Comprehensive Simulation of Organic Solar Cells* , EOS Annual Meeting, Paris, France, September/October (2008).
- N. A. Reinke, R. Häusermann, D. Rezzonico, B. Perucco, E. Huber, B. Ruhstaller: *Emission Zone Extraction and Analysis of Loss Channels in Organic Light-emitting Devices*, EOS Annual Meeting, Paris, France, September/October (2008).
- D. Rezzonico, B. Ruhstaller, T. Flatz, M. Moos, N. A. Reinke, E. Huber, R.Häusermann, B. Perucco: *Comprehensive simulation of light-emitting and light-harvesting organic devices*, Organic Semiconductor Conference, Frankfurt, Germany, October 2008.
- R. Häusermann, N. A. Reinke, E. Huber, B. Ruhstaller: *Opto-Electronic Simulation of Organic Solar Cells* , ThinPV Workshop: “A look inside solar cells”, Ascona, Switzerland, November (2008).
- R. Gmür, T. Hocker: *Thermal-Flow Modeling of the OneBat Micro-SOFC System*, 5th Fuel Cell Research Symposium on Modeling and Experimental Validation, ZHAW, Winterthur, 2008.
- T. Hocker, B. Iwanschitz, J. Sfeir, A. Mai, R. Denzler: *Model-Based Analysis of Degradation Phenomena and Performance Losses in Hexis SOFC-Stacks*, 5th Fuel Cell Research Symposium on Modeling and Experimental Validation, ZHAW, Winterthur, 2008.
- J. Eller, J.O. Schumacher, G. Sartoris, M. Roos: *Computationally Efficient Simulation of PEM Fuel Cells and Stacks*, 5th Fuel Cell Research Symposium on Modeling and Experimental Validation, ZHAW, Winterthur, 2008.
- A. Bieberle-Hütter, D. Beckel, A. Infortuna, U. Muecke, J. Rupp, L. Gauckler, S. Rey-Mermet, P. Muralt, N. Hotz, M. Stutz, N. Bieri, D. Poulikakos, P. Müller, A. Bernard, R Gmür, T. Hocker: *Micro-Solid Oxide Fuel Cells: From Thin Film Membranes to a Micro-Fuel Cell System*, 8th European Fuel Cell Forum, Lucerne, Switzerland, 2008.
- AJ. Sfeir, A. Mai, B. Iwanschitz, U. Weissen, R. Denzler, D. Haberstock, T. Hocker, M. Roos: *Status of SOFC Stack and Material Development at Hexis*, 8th European Fuel Cell Forum, Lucerne, Switzerland, 2008.
- H. Schwarzenbach: *Überblicksvortrag Numerische Modellierung*, electrosuisee Fachtagung der ITG Fachgruppe Hardeware-Technologie: Elektronik der Zukunft, Trilogie MEMS - NANO - ORGANIC, September 2008.
- Th. Hocker: *Mit Hochtemperatur-Brennstoffzellen effizient und dezentral Strom und Wärme gewinnen*, Nationaler Tag der Technik zum Thema Energieeffizienz, ZHAW, Winterthur, 5. November 2008.
- N. A. Reinke: *Effiziente Lichtquellen der Zukunft*, Nationaler Tag der Technik zum Thema Energieeffizienz, ZHAW, Winterthur, 5. November 2008.

7.3 Prizes and Awards

- Thomas Hocker received the title ”Professor ZFH” from the board of the Zurich University of Applied Sciences.
- Roger Häusermann received the Springer Presentation Award for Students for his talk ”Towards a Comprehensive Simulation of Organic Solar Cells” at the European Optical Society meeting in Paris at the end of September.
- Nils A. Reinke received the ”Augsburger Universitätspreis” for his Ph.D. thesis entitled ”Photophysical Processes and Light Extraction in Organic LEDs” at the University of Augsburg.

7.4 Teaching

- ”Physik 1 & 2” für Unternehmensinformatiker (PhUI 1 & 2) **- N. A. Reinke**
- ”Physik 2” für Unternehmensinformatiker (PhUI 2) **- B. Ruhstaller**
- ”Applied Photonics” (Master of Science in Engineering) **- B. Ruhstaller**
- ”Fluid-Thermodynamik“ für Maschinentechniker (FTh1) **- Th. Hocker**
- ”Mensch, Technik, Umwelt” für Maschinentechniker (MTU) **- Th. Hocker**
- ”Diskrete und Numerische Mathematik” für Mechatroniker (DNM2) **- H. Schwarzenbach**
- ”Signale und Systeme 1 & 2” (SiSy 1 & 2) **- J.O. Schumacher**
- ”Physik 1 & 2” für Wirtschaftsingenieure (PhWI 1& 2) **- M. Roos**
- ”Material Properties of Crystals / Tensors for Engineers” (Master of Science in Engineering) **- M. Roos**

7.5 ICP Team Members

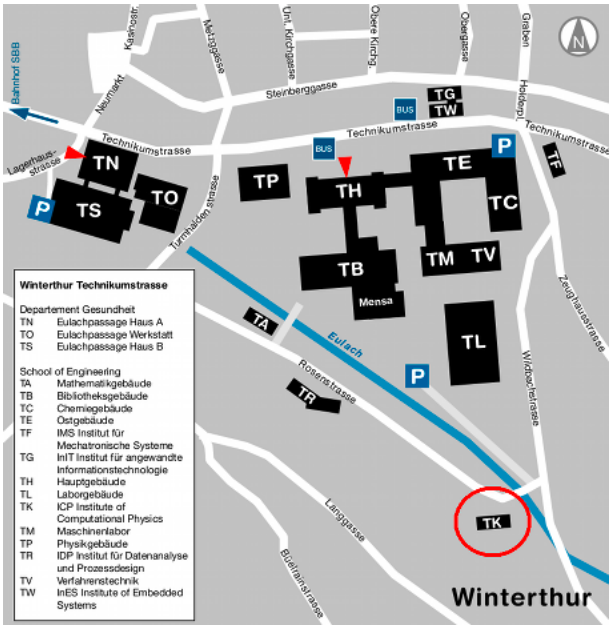
The ICP team members as of December 2008 are listed below.

Name	Title	Function
Eller, Jens	Dipl. Rech. Wiss. ETH	Research Assistant
Gmür, Roman	Dipl. Ing. FH	Research Associate
Häusermann, Roger	Dipl. Phys. ETH	Research Assistant, PhD student
Hocker, Thomas	Prof. Dr., Dipl. Verfahrensingenieur	Lecturer
Huber, Evelyne	Dipl. Rech. Wiss. ETH	Research Assistant, PhD student
Lindner, Markus	Dipl. Ing. FH	MSE Student
Perucco, Benjamin	Dipl. Ing. FH	Research Assistant, MSE Student
Reinke, Nils A.	Dr. rer. nat., Dipl.-Phys.	Lecturer
Roos, Markus	Prof. Dr., Dipl. Phys. ETH	Lecturer
Ruhstaller, Beat	Prof. Dr., Dipl. Phys. ETH, e-MBA	Lecturer, Head of the ICP
Safa, Yasser	Dr. ès sc., MSc.	Research Associate
Sartoris, Guido	Dr., Dipl. Phys. ETH	Research Associate
Schmid, Matthias	Dr. ès sc., Dipl. Phys. ETH	Research Associate
Schwarzenbach, Hansueli	Prof. Dr., Dipl. Math. ETH	Lecturer
Schumacher, Jürgen	Dr. rer. nat., Dipl.-Phys.	Lecturer
Tiefenauer, Andreas	Dipl. Ing. FH	Research Assistant, MSE Student
Toniolo, Lilian		Administrative Assistant

The following visiting scientists were staying at the ICP for some time during 2008:

- Jose Montero, Ph.D. candidate, Universita Jaume I, Castellon, Spain: February - March 2008
- Kemal Celebi, M.Sc., MIT, Boston, USA: June - September 2008

7.6 Location and Contact Info



Institute of Computational Physics
Zurich University of Applied Sciences
Wildbachstrasse 21 (TK)
8401 Winterthur
Switzerland

Prof. Dr. Beat Ruhstaller
Phone +41 58 934 78 36
Fax +41 58 934 77 97

www.icp.zhaw.ch
E-Mail: beat.ruhstaller@zhaw.ch

Administration:
Lilian Toniolo
Phone +41 58 934 73 06
E-Mail: lilian.toniolo@zhaw.ch

Zürcher Hochschule
für Angewandte Wissenschaften

School of Engineering

ICP Institute of
Computational Physics

Technikumstrasse 9
Postfach
CH-8401 Winterthur

Telefon +41 58 934 71 71
Fax +41 58 935 71 71
E-Mail: info.engineering@zhaw.ch
Web www.icp.zhaw.ch