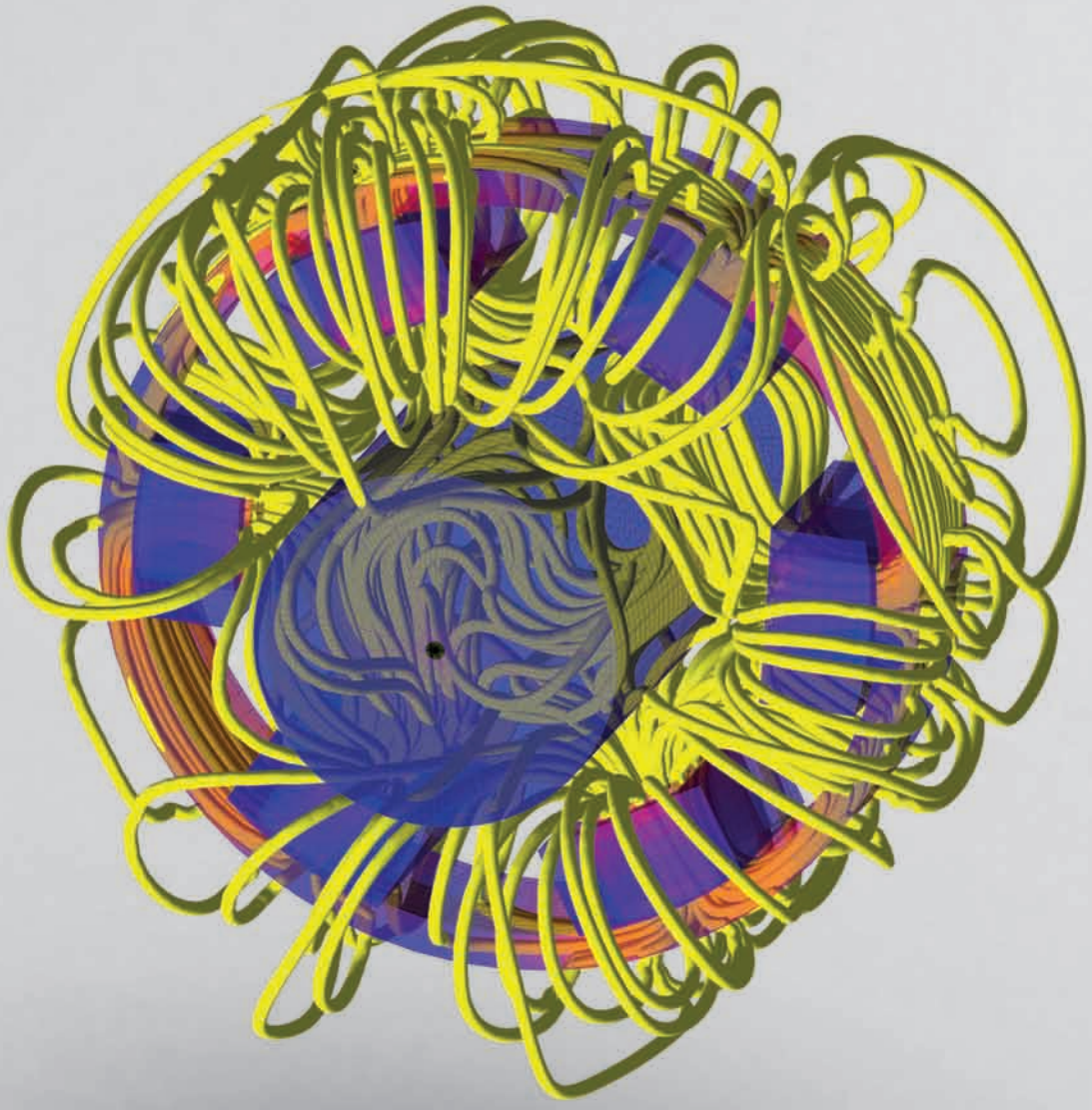
Zurich University
of Applied Sciences

School of Engineering

ICP Institute of Computational Physics

Research Report 2010



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Research & Development

Das Titelbild zeigt die magnetischen Feldlinien eines Asynchronmotors. Die simulierten Feldlinien wurden mit der am ICP entwickelten Multiphysik Software SESES erstellt.

The title graphic shows magnetic streamlines of an asynchronous motor. The simulation was performed with the multiphysics software SESES developed at ICP.

Contents

Einleitung

Am Institute of Computational Physics blicken wir auf ein ereignisreiches Jahr 2010 zurück. Wir bearbeiteten verschiedenste Forschungsprojekte im Bereich der numerischen Modellierung von Multiphysik-Systemen sowie Messtechnik und durften in unserer Forschungstätigkeit viele spannende Herausforderungen zusammen mit unseren Industrie- und Hochschulpartnern meistern. Thematisch haben wir uns verstärkt mit Forschungsfragen im Zusammenhang mit Energie auseinandergesetzt. So trägt unsere Forschung auf dem Gebiet der organischen Leuchtdioden als sparsame Beleuchtungstechnologie zur Energieeffizienz bei. Der Energieerzeugung dienen die organischen Solarzellen als auch die Farbstoff-Solarzellen, welche am ICP mit numerischen Modellen erforscht werden. Unsere Forschung an Brennstoffzellen und an Holzvergasersystemen widmet sich der effizienten Energieumwandlung. Schliesslich vermögen wir auch die Ressourceneffizienz zu steigern, indem wir photothermische Messmethoden für die zerstörungsfreie Schichtprüfung entwickeln. Denn die zuverlässige Messung von Schichtdicken ermöglicht Materialeinsparungen. Es ist zum einen eine gesellschaftspolitische Pflicht, dass wir uns mit Energie-relevanten Fragen auseinandersetzen. Zum anderen eröffnen sich in diesen Gebieten spannende und herausfordernde Forschungsthemen.

Im vergangenen Jahr mussten wir uns von unserem lieben Kollegen Hansueli Schwarzenbach verabschieden. Er verstarb im September nach schwerer Krankheit. Seine berufliche Laufbahn stand im Zeichen der Forschung. Er war ein Pionier der Forschung an Schweizer Fachhochschulen und verstand es hervorragend, die Brücke von der Theorie in die industrielle Praxis zu schlagen. Aus der von ihm initiierten Arbeitsgruppe für numerische Simulation von Sensoren und Aktoren hat er in unermüdlicher mehrjähriger Arbeit das Institute of Computational Physics aufgebaut und bis im Jahr 2007 geleitet. Seine Schaffenskraft führte auch zur ersten Spin-off Firma unserer Arbeitsgruppe, der Numerical Modelling GmbH. Er wird uns als Freund und grossartiger, lieber Mensch in bester Erinnerung bleiben.

In personeller Sicht kamen im vergangenen Jahr einige neue Mitarbeiter ans ICP. Simon Züfle und Remo Ritzmann arbeiten als wissenschaftliche Assistenten im Bereich organische Solarzellen bzw. angewandte Optik und Messtechnik. Dr. Matthias Bonmarin widmet sich der infrarot-basierten Messtechnik in unserem Optoelectronic Research Lab (O-LAB). Verschiedene ZHAW Bachelor und Master Studenten fanden den Weg ans ICP und arbeiteten bei unseren Forschungsprojekten mit. Insgesamt 3 IAESTE Praktikanten aus Hong Kong, Japan bzw. Finnland kamen für ein mehrmonatiges Praktikum zu uns. Zum Jahresende zählt das ICP fast zwei Dutzend Mitarbeiter und ist zu einem wichtigen Leistungsträger an der School of Engineering herangewachsen. In der Lehre sind wir inzwischen in nahezu allen Ingenieurstudiengängen tätig, nämlich in Mathematik, Physik aber auch im Unterricht zu Thermodynamik oder Signalverarbeitung. Ebenfalls bestreiten wir mehrere Unterrichtsmodule im nationalen Master of Science in Engineering.

Wir durften im vergangenen Jahr wieder verschiedenste Erfolge in der Forschung feiern. Zum Beispiel wurde die ICP Spin-off Firma Fluxim AG im Frühling 2010 in den KTI Start-up Coaching Prozess aufgenommen. Das im Rahmen eines KTI Projekts entwickelte photothermische Schichtprüfsystem wurde mit dem ITG Innovationspreis 2010 des Electrosuisse Verbands ausgezeichnet. Nils Reinke und Andor Bariska initiierten gegen Jahresende die Gründung der Firma Winterthur Instruments GmbH und werden die Kommerzialisierung des Schichtprüfsystems nun vorantreiben. Ein Technologietransfer am ICP wurde erneut auch mit den Firmen Numerical Modeling GmbH so-

wie Hexis AG gepflegt. Der vorliegende Bericht gibt einen Überblick über die im Jahr 2010 am ICP bearbeiteten Forschungsprojekte. Am Ende sind auch alle Studentenarbeiten sowie Publikationen und Konferenzbeiträge zusammengefasst.

Im Namen des ICP Teams möchte ich an dieser Stelle der School of Engineering der ZHAW sowie dem Kanton Zürich für die Unterstützung und insbesondere unseren Förderagenturen für die erfolgreiche Zusammenarbeit danken. Ich möchte mich bei jedem einzelnen ICP Mitglied für den persönlichen Einsatz im vergangenen Jahr bedanken und wünsche meinem Nachfolger Thomas Hocker viel Freude und Erfolg bei der neuen Aufgabe.

Nun wünsche ich Ihnen eine spannende Lektüre.

Beat Ruhstaller
Institutsleiter

Introduction

An eventful year at the Institute of Computational Physics has come to an end. We carried out numerous research projects in the field of numerical modeling of multiphysics systems and measurement techniques and enjoyed tackling many challenges in our R&D activities together with academic and industrial partners. We have been focusing ever more on energy related research topics. For instance, our research on organic light-emitting devices (OLEDs) eventually emerges into an energy-saving lighting technology. Organic solar cells and dye-sensitized solar cells, which we are investigating, are contributing to the generation of electrical power. Our research in fuel cells and wood gas processing systems is concerned with efficient conversion of energy. Finally, we are also addressing the efficient use of resources by developing novel photothermal measurement methods for coating analysis: an accurate determination of coating thickness can reduce material use. On the one hand it is a socio-political responsibility that we are addressing energy related research topics. On the other hand these topics open up many exciting and challenging research questions.

Last year in September our faithful colleague Hansueli Schwarzenbach passed away after a severe and long illness. His professional career was dedicated to research and he was a pioneer in research at Swiss Universities of Applied Sciences. He managed to efficiently bridge the gap between theory and industrial application. He had initiated a working team for numerical simulation of sensors and actuators and eagerly promoted it to the Institute of Computational Physics that he headed until 2007. His dedication and hard work has led to the first spin-off of our institute, Numerical Modeling GmbH. We will keep him in our memory as a great and faithful friend.

In terms of staffing, several new team members joined the ICP last year. Simon Züfle and Remo Ritzmann work as scientific assistants in the field of organic solar cells and applied optics and data acquisition, respectively. Dr. Matthias Bonmarin focuses on infrared based measurement techniques in the optoelectronic research lab (O-LAB) of the ICP. Several ZHAW bachelor and masters students have joined the ICP temporarily and contributed to research projects. A total of three IAESTE internship students from Hong Kong, Japan and Finland carried out an internship at our institute. Towards the end of the year, the ICP counted almost two dozen staff members and has become a crucial institute within School of Engineering. Regarding teaching we give lectures in almost all of the engineering curricula of our school, namely lectures in mathematics, physics but also in thermodynamics or signal processing. Moreover, we provide lectures in several national teaching modules of the Master of Science in Engineering.

In the past year, we celebrated several successes in research. For instance, the ICP spin-off company Fluxim AG entered the CTI startup coaching process. The photothermal coating analysis system developed within a CTI project has received the ITG innovation award 2010 from Electrosuisse. Nils Reinke and Andor Bariska have launched a start-up company towards the end of the year for commercializing this innovative measurement system. A technology transfer was again fostered with the companies Numerical Modeling GmbH and Hexis AG. The ICP research report gives an overview on the research projects at the ICP in 2010. The appendix informs about student projects, publications and conference contributions.

On behalf of the ICP team I would like to express our gratitute to the School of Engineering and the Canton of Zurich for supporting us and the research funding agencies for the successful collaboration. I would like to thank each ICP team member for her/his commitment in 2010 and wish my successor Thomas Hocker a lot of success with the new mandate.

Enjoy reading this report!

Beat Ruhstaller
Head of the institute

Chapter 1

Sensors, Actuators, and More

1.1 Analyse von thermisch induzierten Fertigungstoleranzen bei der Herstellung von Schwingquarzen

Contributors: T. Hocker

Partners: Patric Jacques, Micro Crystal AG, Grenchen
Funding: Direktfinanzierung
Duration: 2010–2011

Die Micro Crystal AG, Grenchen entwickelt und produziert piezoelektrische Schwingquarze, die als Taktgeber in Uhren und Mobiltelefonen verwendet werden, siehe figure 1. Als Teil der Swatch Group gehört sie mit 850 Mitarbeitern zu den in diesem Bereich weltweit führenden Firmen.

Fig. 1: Aufbau einer Quarzuhr.

Herzstück ist eine Stimmgabel aus Quarz, die in ihrer Eigenfrequenz (typischerweise mit 32’768 Hz) schwingt. Die Quarzstimmgabel wird über aufgedampfte Goldfolien, die als Elektroden fungieren, mit einer Wechselspannung angeregt. Für die Genauigkeit dieses elektrisch-mechanischen Resonators ist entscheidend, dass die Fertigungstoleranzen bei der Herstellung der Quarzgabel so klein wie möglich sind. Beim Aufdampfprozess der Goldfolien treten jedoch als Nebeneffekt unerwünschte Diffusionsprozesse auf, die zu ungleichmässigen Breiten der Quarzgabeln führen können. Dies ist schematisch in figure 2 dargestellt.

Fig. 2: Modellierung von Korn- und Korngrenzen Cr-Transport.

Chrom diffundiert durch Goldkörner und entlang von Korngrenzen und bildet an der Oberfläche der Goldschicht (bei hohen Temperaturen und in oxidierender Atmosphäre) Chromoxid. Zur Simulation des transienten Chromtransports in den aufgedampften Goldschichten und der Bildung von Chromoxid an der Goldoberfläche wurde ein 3D FE-Modell in unserer in-house Multi-Physik Software *Seses* entwickelt. Die darin enthaltenen Diffusionskoeffizienten wurden an Messdaten angepasst, siehe figure 3. Figure 4 zeigt typische Konzentrationsprofile für Chrom in Gold zu verschiedenen Zeiten.

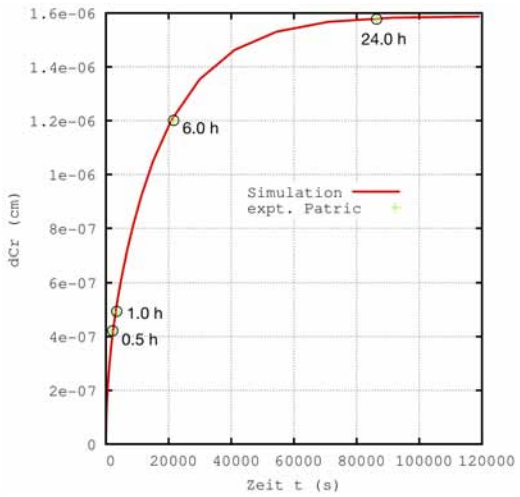


Fig. 3: Dargestellt ist die Schichtdicke an Chrom, dCr, die während eines Temperierprozesses in eine angrenzende Goldschicht diffundiert. Die Messdaten (Punkte) wurden im Modell durch Anpassen des Diffusionskoeffzienten gefittet.

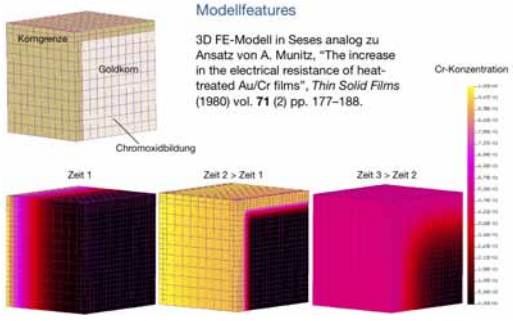


Fig. 4: 3D Seses FE-Modell für die Simulation des transienten Korn- und Korngrenzen Cr-Transports.

1.2 FE software for the industry

Contributors: G. Sartoris, H. Schwarzenbach, M. Roos

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

Goal of this project is to provide the industrial partner *NM Numerical modeling* with up-to-date software for the modeling of the Maxwell's equation in the low frequency regime where displacement currents may be neglected, i.e. the eddy current model. Of particular interest is the modeling of magnetic proximity sensors with common PC hardware and computational time limitations of a few hours. The new software has been implemented in the multi-physics numerical simulation tool SESES developed at ICP, its major strength being the possibility to solve and couple almost any governing equation of classical physics. Although SESES could already solve eddy current problems, their computation in 3D was far from being efficient and this project should provide up-to-date numerical algorithms. On the other side, since even optimized 3D eddy current computations can be still computationally expensive, from the industrial partner there was a need to know if reduced and less demanding models may be used to replace fully-fledged 3D computations.

From the software point of view, the first milestone was the introduction of edge finite elements within SESES. These elements are the natural framework when modeling eddy currents. Since they do not enforce the normal component of the vector field to be continuous and different from Lagrangian or nodal elements, they are well-suited to model sharp corners and sharp discontinuous material laws. The second milestone was the optimized solution of the system of linear equations. For 3D applications, the memory and computational requirements are too large for robust direct solvers to be used and one has to resort to iterative solvers. This is always the case when using edge elements, since here the eddy problem cannot be gauged, the assembled linear system is singular and direct solvers fail. However iterative solvers can solve singular systems, if the equations are assembled in a consistent manner. For iterative solvers, optimizing the solution consists in preconditioning the linear system, i.e. by solving a similar system much closer to the identity matrix so as to increase the convergence rate. In order to be effective, the associated similar system determined by the preconditioning matrix or simply the preconditioner, must be cheaply computed and a major drawback is that optimized and very effective preconditioners are problem dependent and need to be discovered for each application. Here the challange is to find robust preconditioners with convergence rates independent from the choice of the material parameters and the shape of the elements. For both nodal and edge elements of first and second order, we have implemented up-to-date preconditioners. For first order nodal elements, robust and fast is the ILU(0) preconditioner. The convergence rate is so good that the problems to be solved are generally bounded by the large memory requirements and not by the computational time. For second order nodal elements, the ILU(0) preconditioner can fail and the alternative is to use an auxiliary preconditioner based on the robust solution of first order nodal elements. Due to the singularity of the system matrix, the ILU(0) preconditioner fails also for edge elements. Here, the same auxiliary preconditioning technique can be used but the shape of the elements has a strong impact on its performance and we have not yet found an overall robust preconditioner.

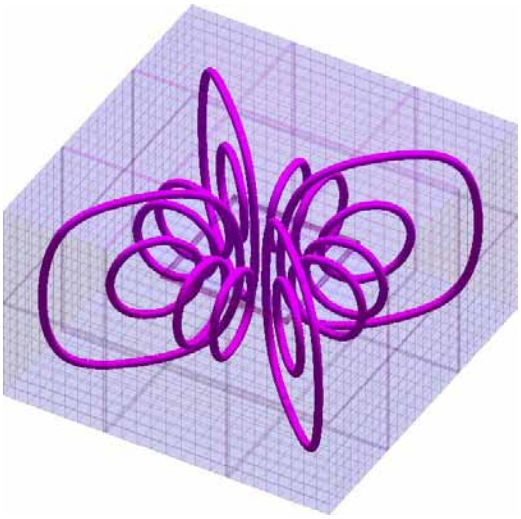


Fig. 1: Magnetic field streamlines of a rectangular coil.

1.3 Numerical modeling of laminates anisotropic plastic deep-drawing

Contributors: G. Sartoris

Partners: Alcan Technology and Management AG
Funding: Commission for Technology and Innovation (CTI)
Duration: 2008–2010

Modern laminates for the production of pharmaceutical blisters have a complex inner structure. Several layers of different plastic and alumina sheets are packed, stacked and glued together with the intent to provide the best environmental protection from external agents. 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 the industrial partner, which provides its customers with laminates for the production of pharmaceutical blisters and where the mechanical properties of the laminate must be guaranteed.

From the material point of view, the major concern is the correct description of the anisotropic elasto-plastic behavior at large strains, since actual models are not always able to correctly reproduce experimental data. More advanced and precise tools are required which was the first major goal of the project. The task is complex and includes both the writing and fitting of new material laws. From the numerical point of view, the anisotropic nature of the deformation process requires a full 3D nonlinear analysis at large strains. These computations are still quite expensive and the second goal of the project was to provide various optimizations at the software level to speed-up the numerical analysis within the multi-physics software tool Seses.

Solid-shell nonlinear elements have been implemented. These elements with a lot of internal degrees-of-freedom are little more sensitive to non-linearities than first order solid elements, they can be freely mixed with other elements and are for the global solution also as fast as first order elements, however, they are more expensive to assemble. A new interface to rigid-body contacts has also been implemented which can be used both for the algebraic and penalty method. The contact surface is interpolated either by first order or cubic polynomials. Frictionless contacts and the penalty method have been tested. The method is robust for all types of mechanical elements and can work with just a few elements. As an alternative to ill-conditioned penalty methods, there are algebraic methods. A method working directly with the globally assembled linear system and using the most recent residual forces has been developed. Not yet fully solved is the sticky problem and the writing of robust lock-out algorithms.

At project's end, we have accomplished all major goals and to our opinion a competitive and innovative framework for modeling the deep-drawing process of pharmaceutical blisters has been established. During the project development, it has been noticed that friction laws and contact modeling also play an important role. This aspect should further be considered together with other minor numerical optimization procedures.

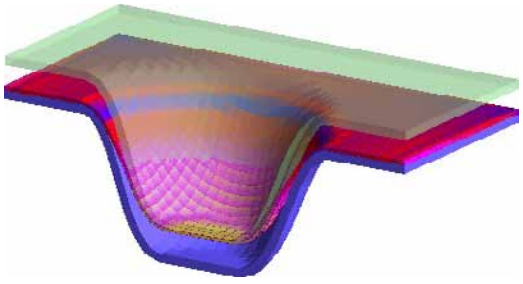


Fig. 1: Deep-drawing of a laminate to form a blister.

1.4 Populationsbilanzmodellierung von Mahlprodukten

Contributors: R. Axthelm

Partners: Novartis Pharma AG
Funding: intern
Duration: 2010

Mahl- oder Zerteilprozesse zur Herstellung feiner Feststoffpartikel spielen in vielen industriellen Anwendungen eine grosse Rolle. Dabei ist häufig das Ziel, den Prozess so zu steuern, dass die Partikel am Ende des Mahlprozesses eine bestimmte Grösse bzw. Grössenverteilung aufweisen. Die Frage, die sich zunächst stellt ist: Wie kann die Entwicklung der Grösenverteilungen analytisch beschrieben werden und wie hängt die gewonnene Darstellung von Einflussgrössen des Prozesses ab? Zu den Einflussgrössen gehören etwa Drücke und Geschwindigkeiten, die auf die Partikel wirken oder Materialeigenschaften wie Brüchigkeit der Partikel.
Der Vorgang des Partikelzerkleinerns wird durch ein Modell beschrieben, das zwei grundsätzliche Fragen beinhaltet, nämlich: Bricht ein Partikel? Und wenn ja, wie bricht es? Dieses Modell führt auf ein System von linearen, inhomogenen Differentialgleichungen, welche sich analytisch berechnen lassen.
Die Lösungen dienen als Ansatzfunktionen für Regressionen von Messdaten. Diese wiederum liefern eine Parametrisierung nach verschiedenen Einflussfaktoren. Figure 1 zeigt eine Überblicksdarstellung dieser Vorgehensweise.

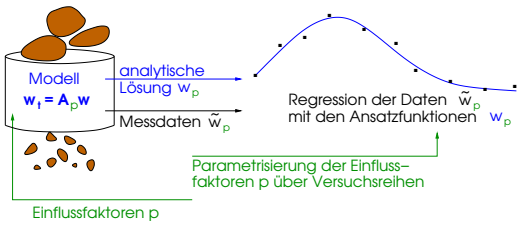


Fig. 1: Die Grössenverteilung w der Partikel hängt von den gegebenen Einflussfaktoren p ab.

Die Arbeitsschritte gliedern sich wie folgt: Der Anteil an Partikeln einer bestimmten Grössenklasse i wird in w_i zusammengefasst. Beim Bruchprozess bricht ein Anteil s_i (selectivity) von w_i in eine oder mehrere kleinere Klassen j. Die Verteilung auf kleinere Klassen wird in b_{ij} (breakage function) beschrieben. Für die Änderungsrate jeder Klasse i ergibt sich daraus

$$w_{i,t} = \quad s_i w_i + \sum_{j=i+1}^{n} b_{ij} s_j w_j$$

$w_{i,t}$ beschreibt die Zeitableitung von w_i. Weder die breakage function noch die selectivity sind a-priori bekannt. Zunächst werden diese beiden Ausdrücke zusammengefasst in eine Matrix $\mathbf{A}$ mit $A_{ii} = \quad s_i$, $A_{ij} = b_{ij} s_j$, $(i > j)$ und $A_{ij} = 0$, $(i < j)$. Damit stellt sich das Modell gleichermassen aber in neuer Form dar als das System gewöhnlicher Differentialgleichungen

$$\mathbf{w}_t = \mathbf{A}\,\mathbf{w}$$

mit $\mathbf{w} = (w_1 \qquad w_n)$. Die Lösungen dieses Systems ergeben sich durch die Rekursion: $a_{11} = 0$. Für $k = n \qquad 1$ berechne:

$$w_k(t) = \sum_{l=k}^{n} {}^{k}_{l} \mathrm{e}^{a_{ll}\, t}$$

$${}^{k}_{l} = \begin{cases} \sum_{j=k+1}^{n} \frac{a_{kj}\, \alpha_l^j}{a_{ll} - a_{kk}} \; {}^{k}_{i} & l > k \\ w_{k,0} \quad \sum_{i=k+1}^{n} {}^{k}_{i} & l = k > 1 \\ 100 & l = k = 1 \\ 0 & l < k \end{cases}$$

Die Unbekannten a_{kj} werden regressiv an die Daten ermittelt (siehe figure 2). Anschliessend können aus den a_{kj} die selectivity s_i und die breakage function b_{ij} berechnet werden.

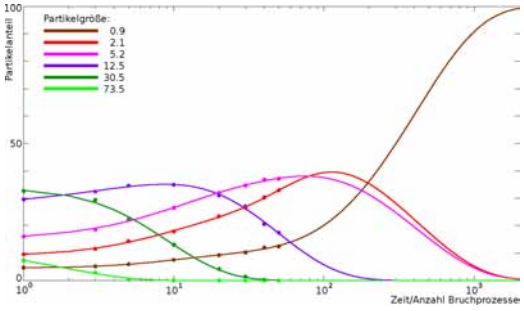


Fig. 2: Zeitliche Entwicklung der Partikelanteile je nach Grössenklasse. Dargestellt sind Messdaten ( ) und Lösungen ( ) der Differentialgleichungen.

Mit dieser Methode erhält man qualitativ gute Ergebnisse. Es lassen sich, wie in figure 2 zu sehen ist, ebenfalls die Ergebnisse des Mahlprozesses extrapolieren.

1.5 Thermal- ow analysis of pre-tempered chocolate in cooling tunnels

Contributors: T. Hocker, R. Axthelm

Partners: Manfred Suter, Max Felchlin AG, Schwyz
Funding: Swiss Food Research Network
Duration: 2010–2011

Max Felchlin AG, Schwyz, is well-known for the production of high-quality couverture, pastries and semi-finished confectionery products. Felchlin offers its customers comprehensive support and know-how for the manufacture and marketing of their end products. This support is based on both experience and understanding.

For an optimal product quality, the achieved state of crystallinity of the cocoa butter - a major ingredient of chocolate - plays a crucial role. This crystallinity state is manipulated during the so-called tempering process, where (stable) crystal seeds are generated. However, it also depends on the details of the subsequent cooling process, which so far has rather been neglected. Therefore, this project aims at developing methods to optimize the cooling process of pre-tempered chocolate in cooling tunnels. Figure 1 gives an overview about the planned combined experimental and modeling approach.

To describe the cooling process on different length scales, three different types of models need to be developed:

- a thermal-flow CFD model of the complete cooling channel
- a thermo-mechanical FE model of a single chocolate mould to simulate the crystallization of chocolate
- a thermal crystallization model to predict the heat release and consumption associated with different crystallization and melting processes

Based on the gained know-how, the following goals shall be reached:

- improving Felchlin's internal cooling process, i. e. to tailor it to specific products
- supporting industry customers in the further processing of chocolate products
- offer complete solutions to confectionary customers e. g. about the mold removing characteristics

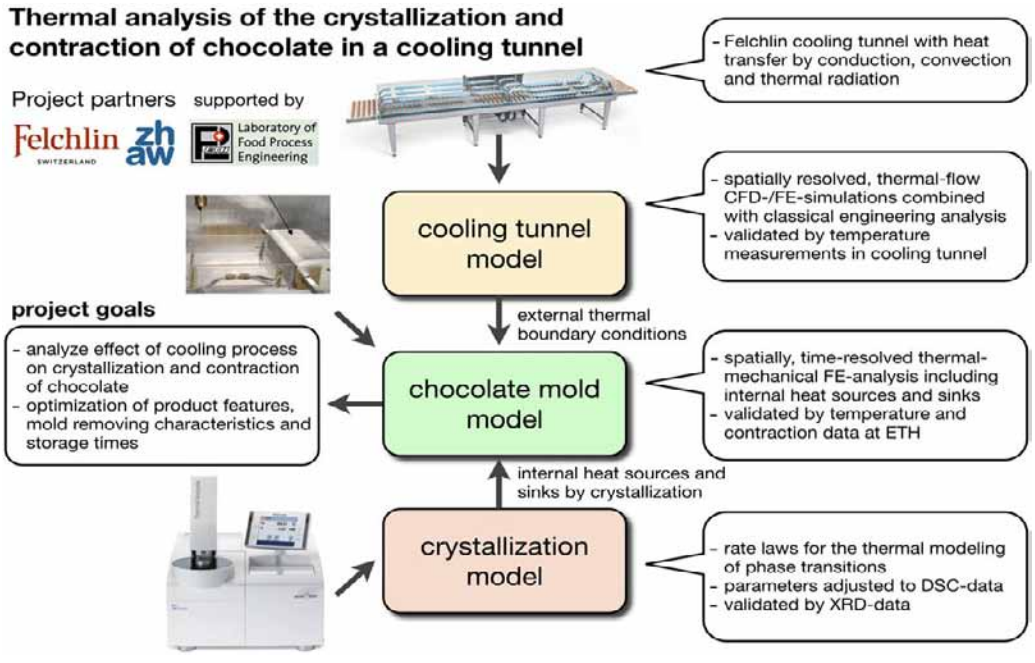


Fig. 1: Overview about the planned combined experimental and modeling approach.

Chapter 2

Electrochemical Cells and Energy Systems

2.1 A new model for detailed simulation of multiple transport and conversion processes in SOFC stack repeat units

Contributors: Y. Safa, T. Hocker

Partners: Hexis AG, HTceramix S.A., ETH-NIM, EPFL-LENI, EMPA
Funding: SwissElectric Research, Swiss Federal Office of Energy
Duration: 2008–2010

In 1994 Achenbach was among the first to publish a comprehesive 3D model for a planar repeat unit of a SOFC stack. A vast number of publications on SOFC models have appeared since then. Almost all publications discuss physical-chemical descriptions, model hierarchies (to capture phenomena on different length scales) and the resulting set of governing equations, but few deal with numerical issues. However, the robustness and speed of a SOFC model is critical for its usefulness as a design tool.

Progress in the study of local reactive transport phenomena in SOFC stacks has been achieved based on both advanced physical and numerical approaches. Specifically, the numerically unfavorable high aspect ratio of about 1’000 between a typical stack diameter and a typical cell thickness has been successfully treated using the ADI (Alternating Direction Implicit) numerical scheme. Unlike conventional methods, ADI allows one to predict local gradients of chemical species and electrical charges with low computing costs and unconditional numerical stability. This is especially important in the vicinity of a current collector rib and under extreme operation conditions, e. g. when the fuel gets depleted. Furthermore, the convection-dominant transport within the gas distribution channels has been accurately calculated without using a (unphysical) transverse numerical diffusion.

Concerning the gas flow in the channels along a porous electrode, another important feature of our model is the non-zero slip velocity at the electrode surface. In conventional approaches, this slip velocity is often estimated empirically. Alternatively, the hydrodynamic flow field is calculated from the Navier-Stokes equations which are simultaneously solved in the open flow channel and the porous electrode. Within the electrode, the velocity field is then penalized artificially by adding the Karman-Kozeny term. However, such a penalization suffers from inaccurate velocities in the vicinity of the electrode surface. In our approach, the compressible flow in both regions is treated in a unified manner in which the slip velocity is not known a priori, but follows from requiring continuous shear stresses at the electrode surface.

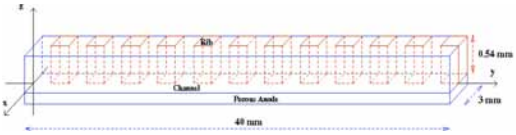


Fig. 1: Modeled repeat unit geometry including the anode, the open flow channel and the current collection ribs.

As an example, simulation results for the influence of the current-collection pattern (displayed in figure 1) on the hydrogen and ionic potential distributions within an SOFC repeat unit are shown in figure 2.

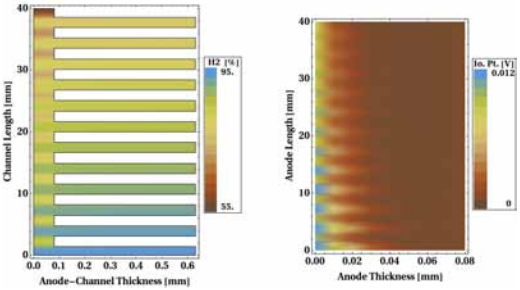


Fig. 2: Simulation results in a vertical cross-section of a SOFC repeat unit. Left: hydrogen distribution in channel and electrode, right: Ionic potential in electrode.

2.2 Time-dependent analysis of Hexis 5-cell stack (U,i)-data to predict degradation behavior on the stack level and for natural gas as fuel

Contributors: M. Linder, T. Hocker

Partners: Roland Denzler, Hexis AG, HTceramix S.A., ETH-NIM, EPFL-LENI, EMPA
Funding: AccelenT, Swiss Federal Office of Energy
Duration: 2009–2011

A simplified, *Mathematica*-based model to analyze the current-voltage characteristics of SOFC-stacks has been developed and is in regular use at Hexis. The model predicts the starting performance for a large number of current-voltage stack data without the need for any fitting parameters. It has been used to study the sensitivity of various input parameters such as changes in mass-flows, fuel composition, temperature, and humidity. The model is currently extended to the Hexis Galileo system to perform model-based analysis of field tests. Here, the goal is to explain unusual system behavior that, for example, could result from composition changes in the natural gas supply, and to assess long-term degradation from the field test results.

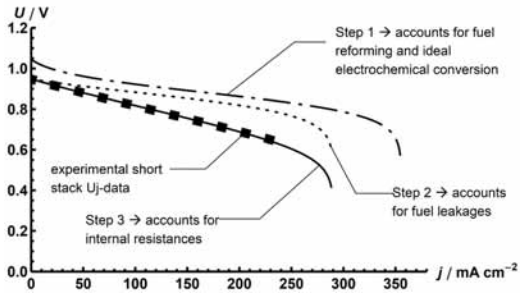


Fig. 1: Three-step procedure to adjust the model to Uj-data obtained from SOFC stacks measurements.

The model extracts the internal stack repeat unit resistance from an experimentally available current-voltage (Uj)-curve in a three-step procedure. This is shown in figure 1. As step one, an ”ideal“ Uj-curve is calculated under the assumption that the fuel reforming process and the subsequent electrochemical fuel conversion proceed under thermodynamic equilibrium conditions. Hence, for a given fuel composition at the reformer inlet and a given reformer temperature, the outlet composition is calculated using a thermodynamics software-package such as *Cantera*. To match the experimental open circuit voltage by the model, in step two, the corresponding leakage flux of hydrogen is removed and water is added to the anode gas mixture. Finally, in step three, we analyze the remaining differences between the experimental Uj-data and the simulated, dotted curve. These differences are caused by internal ohmic and polarization losses within the stack repeat unit.

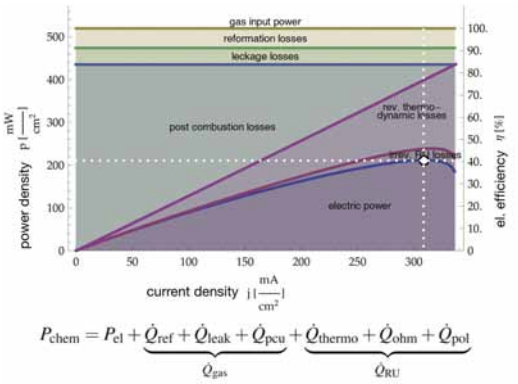


Fig. 2: Total energy balance for a Hexis SOFC stack at 920 °C that runs on CPO-reformed natural gas.

Besides analyzing Uj-data, the model also performs a full energy balance. Figure 2 shows how the various energy fluxes change with current density for a typical Hexis SOFC-stack. The maximum electrical efficiency (DC) at
320 mA cm^{-2} is around 40 % - relative to the heating value of the fuel input. This corresponds with a power-density of roughly 200 mW cm^{-2}. At this operation point, about 9 % is lost by the reforming of the natural gas, and 7 % by fuel leakages. An additional 7 % of the available fuel is burned in the post combustion unit (pcu) and another 7 % is lost by Joule’s heat related to internal repeat unit resistances. The largest loss comes from unavoidable reversible thermodynamic losses and is roughly 30 %. It also follows from the results that the maximum achievable electrical efficiency of a Hexis stack with electrolyte supported cell technology running on CPO-reformed natural gas is around 45 %.

2.3 Thermal management of a micro-fuel cell system

Contributors: C. Meier, T. Hocker

Partners: ETH-NIM, ETH-LTNT, EPFL-SAMLAB, CSEM, NTB
Funding: Swiss National Science Foundation Sinergia
Duration: 2010–2012

A simple but yet accurate model based on global mass and energy balances has been developed to predict the thermal characteristics of the ONEBAT micro-SOFC and similar systems that aim at powering portable devices. Our motivation was to assess the basic requirements on the thermal design of such a system that lead to a thermally self-sustaining operation. Figure 1 and table 1 give an overview of the main system components and specifications.

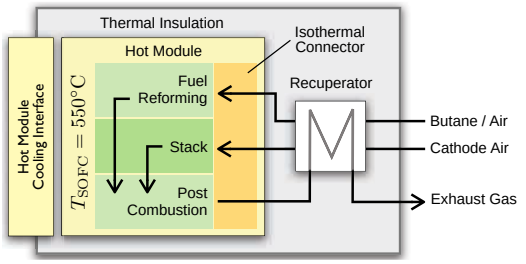


Fig. 1: Schematic overview of the MEMS based ONEBAT micro-SOFC with an isothermally (self-sustaining) operated hot module, a cooling interface, a recuperator and a thermal insulation.

The thermal characteristics of systems with an electrical power output between 2.5 and 20 W_{el} were obtained by dimensioning the hot modules and the surrounding insulations, calculate heat losses to the environment and solve the energy and the mass balance. The model thus links the energy balance to geometrical aspects of the system like the insulation volume.

Proposed micro-SOFC system specifications	
system electrical power, P_{el}	$2.5 \ldots 20\,W_{el}$
repetitive unit power, $P_{el,RU}$	$2.5\,W_{el}$
fuel	n-butane C_4H_{10}
air as oxidant	21% O_2 / 79% N_2
operating temperature, T_{SOFC}	550°C
reformer catalyst [15]	$Rh/Ce_{0.5}Zr_{0.5}O_2$
post combustion catalyst [2]	$Pt/Ce_{0.5}Zr_{0.5}O_2$
hot module substrate	Silicon or Foturan

Tab. 1: Main system specifications.

The air-to-fuel ratio λ is an appropriate parameter to control the operating temperature. However, a minimal λ of ≈ 2 is required by the electrochemical and post-combustion process (stoichiometric oxidation: $\lambda = 1$). At high electrical efficiencies and hence low heat release rates or in case of high insulation heat losses, a recuperator is required to achieve the desired operating temperature ($\rightarrow$*recuperator mode*). In contrast, at lower electrical efficiencies, disposing the released heat becomes an issue ($\rightarrow$*cooling mode*).

The basic thermal requirements for non-adiabatic systems are visualized in figure 2. In cooling mode (a), the required air-to-fuel ratio λ to not exceed an operating temperature of 550 °C is shown. In recuperator mode (b), the heat to be recuperated $\dot{Q}_{recu}$ and the dimensionless airflow preheating Θ_{recu} are shown that maintain the operating temperature.

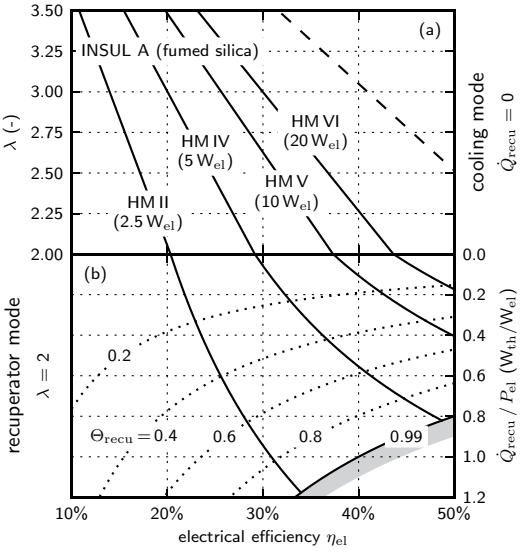


Fig. 2: Constant temperature operating plot for systems with 2.5 to 20 W_{el}. The increasing heat-loss-to-power ratio for systems with small electrical outputs shifts the characteristics to the left dashed line in (a): adiabatic operated system.

2.4 Modeling the reactive bonding process to connect silicon substrates

Contributors: C. Meier

Partners: ETH-NIM, ETH-LTNT, EPFL-SAMLAB, CSEM, NTB
Funding: Swiss National Science Foundation
Duration: 2010–2012

Reactive multilayer foils are used as local heat source in MEMS fabrication to melt a solder. After ignition on one end, an exothermic reaction front (Al+Ni $\rightarrow$ AlNi) propagates through the foil, see figure 1. The bilayer thickness influences the propagation velocity, the reaction duration and the specific heat of reaction. The thickness of the foil determines the total amount of heat released per bonding area. The whole solder layer above and below the multilayer foil has to melt to achieve mechanical strength and gas tightness.

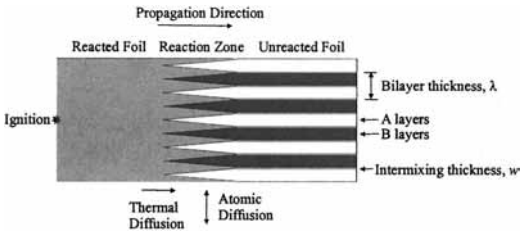


Fig. 1: Self-propagating reaction of a reactive multilayer foil (from Wang et al., 2004).

In an ideal (adiabatic) system, the required thermal energy is determined by the mass and the heat capacity of the multilayer foil and the solder, respectively, as well as the melting temperature and the heat of fusion of the solder, see e. g. Wang et al., "Joining of stainless-steel specimens with nano-structured Al/Ni foils", Journal of Appl. Physics (2004). In a real system, the heat diffusion away from the solder requires more heat to completely melt the solder.
To compute the temperature distribution within the bond and in its surrounds, a 1-dimensional model of the bonding system has been developed. The transient heat conduction equation is solved in our in-house FE-tool Seses. Only one half of the bonding is modeled, the adiabatic boundary at the reactive foil reflects symmetry, see figure 2. The heat is evenly released into the AlNi layer.
Figure 3 shows calculated maximum temperatures at different locations. A 2 μm thick silicon oxide layer on top of the substrate has been taken into account, which causes a steep
T-gradient between the solder and the wafer due to the low thermal conductivity of SiO2. Thanks to this thermal barrier, the temperature in the Si-wafer does not exceed the solder's melting temperature of 280 °C. As the assumed reaction duration goes toward small numbers, its influence on the temperature field around the reactive foil becomes small.

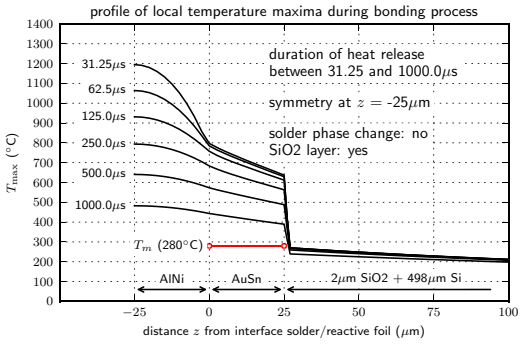


Fig. 3: Finite-element simulation results of maximum temperatures at different locations in the vicinity of the reactive foil, based on the transient heat conduction equation.

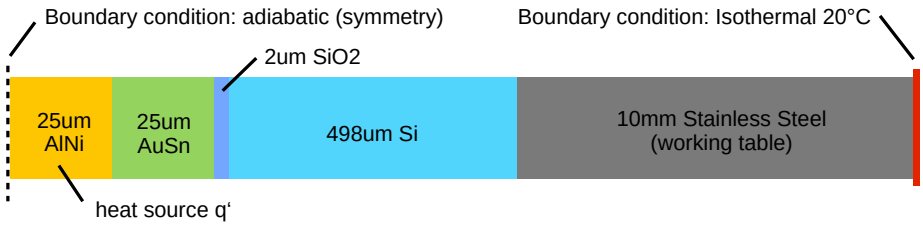


Fig. 2: Materials, layer thicknesses and boundary conditions of the 1D model.

2.5 Development of a thermo-mechanical model to predict the buckling behavior of fuel cell membranes

Contributors: Y. Safa, T. Hocker

Partners: ETH-NIM, ETH-LTNT, EPFL-SAMLAB, CSEM, NTB
Funding: Swiss National Science Foundation Sinergia
Duration: 2010–2012

The presented model development is concerned with mechanical integrity issues. Hence it involves the analysis of different thermo-mechanical failure modes and the development of strategies to avoid them. At different stages during manufacturing and operation, both compressive and tensile stresses are exerted onto the fuel cell membranes. The membranes are thin ceramic layers with thicknesses of around 1 μm. Thus they represent the mechanically weakest component within the system. Compressive stresses can cause buckling and subsequent fracture. Tensile stresses can initiate cracks, which might as well cause fracture. Hence both types of stresses can severely damage or completely break the membranes. It is therefore mandatory to identify save "design spaces" as guidelines for the manufacturing and operation of the fuel cell membranes.
As main task, a complete buckling model has been implemented into the Mathematica software package. This model is based on the Railey-Ritz method as described by Yamamoto et al., "Nonlinear thermomechanical design of microfabricated thin plate devices in the post-buckling regime", *J. Micromech Microeng*, vol. **20**, pp. 035027 (2010). This approach uses trial functions for the buckling shapes that satisfy certain symmetry conditions. The membrane dimensions, its stress state caused by the manufacturing, its material properties and an applied thermal load are used to calculate the stress and displacement fields under compression. Note that the behavior of the membrane under compression is highly nonlinear since buckling is the result of a instability transition that is accompanied by a sudden energy release. Therefore standard mechanical theories such as Hooke's theory for linear-elastic materials are not applicable. In practice, several different buckling modes with different shapes can be observed.
Figure 1 (top left) shows schematically the allowed design space for a fuel cell membrane in dependence of the applied thermal load and the residual stresses imposed by the manufacturing.

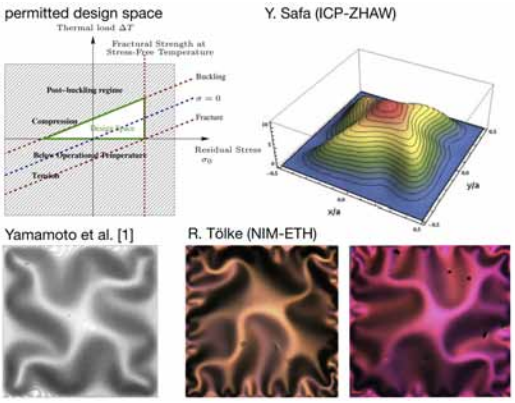


Fig. 1: top left: Schematic representation of the design space to ensure mechanical integrity, top right: simulation results of a buckled membrane under compression, bottom: experimental results for buckled membranes with similar shapes.

The design space is bound by too much compression (which causes buckling) and too much tension (which causes fracture). The diagram on the top right shows simulation results obtained by Y. Safa of a buckled membrane under compression. Note that the membrane is clamped at its boundaries. Note also that the warping exhibits four characteristic ridges. This is similar to the experimentally obtained buckling shapes shown on the bottom.

2.6 Development and application of an electrode micromodel to optimize performance and to predict degradation phenomena in mixed conductors Ni-YSZ anodes

Contributors: T. Hocker

Partners: Hexis AG, HTceramix S.A., ETH-NIM, EPFL-LENI, EMPA
Funding: SwissElectric Research, Swiss Federal Office of Energy
Duration: 2008–2010

The developed electrode model mimics the real 3D microstructure of mixed ion-/electron-conducting anodes and cathodes. It is especially suited for investigating the impact of microstructural details on electrode performance and aging. For example, it allows one to assess the effect of microstruture changes such Ni coarsening and electrode poisoning on the ohmic and polarization resistances of the electrode. The electrode model is part of a larger 3D local repeat unit model, which represents the full cell, contact layers as well as non-homogeneous current collectors (i. e. interconnects) on both sides. Hence the impact of electrode degradation on the local repeat unit performance can be predicted as well. To realistically mimic the electrodes solid-phase networks, up to eight different particle sizes can be specified for each phase. This allows one to adjust synthetic microstructures to real ones by matching their experimentally-obtained continuous particle size distributions (PSDs). Furthermore, the limiting effect of sinter necks on the solid-phase ion and electron transport is taken into account via additional contact resistances between neighboring particles. When compared with literature data, the electrode model possesses all main characteristics reported for real electrodes, see S. Sunde, "Simulations of Composite Electrodes in Fuel Cells", *Journal of Electroceramics*, **5**, pp. 153-182, 2000.
Figure 1 shows typical SEM pictures - on the left for a new Ni-8YSZ anode and on the right for the same anode after eight redox cycles. The electrode samples were provided by Boris Iwanschitz from Hexis, the image analysis was performed by Lorenz Holzer from EMPA. One can see that the redox cycles significantly increased the size of the Ni-particles, but left the 8YSZ-particles unchanged. Note also that the redox cycles caused a significant increase of pores. To adjust the synthetic microstructures used in the model to the ones shown in figure 1, continuous particle size distributions (PSDs) have been extracted from the SEM image data.

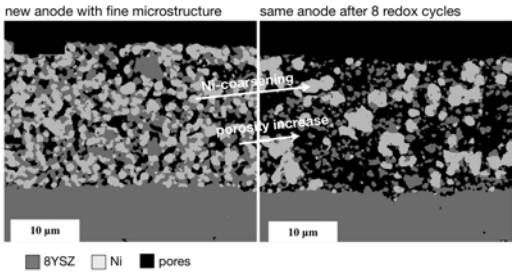


Fig. 1: SEM pictures for a new Ni-8YSZ anode (left) and the same anode after eight redox cycles (right).

This is shown in figure 2, where three anodes with initially fine, medium-fine, and coarse microstructures are compared to each other. The red bars represent experimental results for the new anodes as obtained from EIS-measurements. The corresponding simulation results based on artificial microstructures are shown as gray bars. They were obtained for 20 μm thick anodes with synthetic microstructures exhibiting PSDs similar to the experimental ones. It was observed that the model well describes the change of the polarization resistance with mircrostructure. The deviations from the experimental data lie within 20 %. The experimental and simulation results for the aged anodes after eight redox cycles are shown as well.

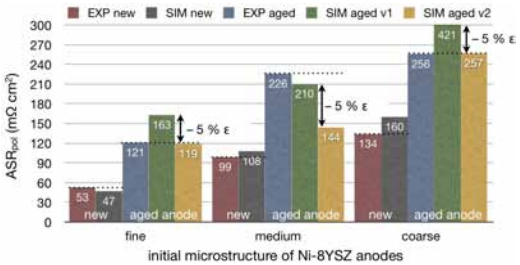


Fig. 2: Polarization resistances for new and aged Ni-8YSZ anodes (after eight redox cycles).

2.7 Holzvergasermodelle für dezentrale Kraft-Wärmekoppelung

Contributors: C. Meier, T. Hocker, R. Axthelm

Partners: Woodpower AG, Wila.
Funding: Gebert Rüf Stiftung
Duration: 2010–2012

Ziel des Projekts ist die Entwicklung von praxistauglichen Computermodellen, die die Umwandlung von Holz in Holzgas in Gleichstromholzvergasern abbilden. Die Modelle sollen die wichtigsten Prozessgrössen zueinander in Beziehung setzen und so helfen, Fragen zum (i) Reaktordesign, zum (ii) anfahren und (iii) kontinuierlichen Betrieb des Holzvergasers sowie zur (iv) Auswirkung von unvermeidlichen Schwankungen in den Brennstoffeigenschaften im Voraus zu klären.

Aufgrund der grossen Anzahl an Einflussgrössen und der Komplexität der im Vergaser ablaufenden physikalisch-chemischen Prozesse erfolgt die Validierung der Modelle über Messdaten, die hauptsächlich mithilfe eines eigens entwickelten Experimentalvergasers gewonnen werden.

Der für die Modellvalidierung benötigte Experimentalvergaser mit einer thermischen Leistung von rund 10 kW konnte 2009 gefertigt und 2010 in Betrieb genommen werden, siehe figure 1.

Fig. 1: ZHAW Experimentalvergaser im Aufbau und im Betrieb auf dem Dach des Maschinenlaboratoriums.

Figure 2 gibt einen Überblick der im Projekt verfolgten Modellansätze zur Beschreibung der Umsetzung von Holz zu Holzgas in Festbettreaktoren.

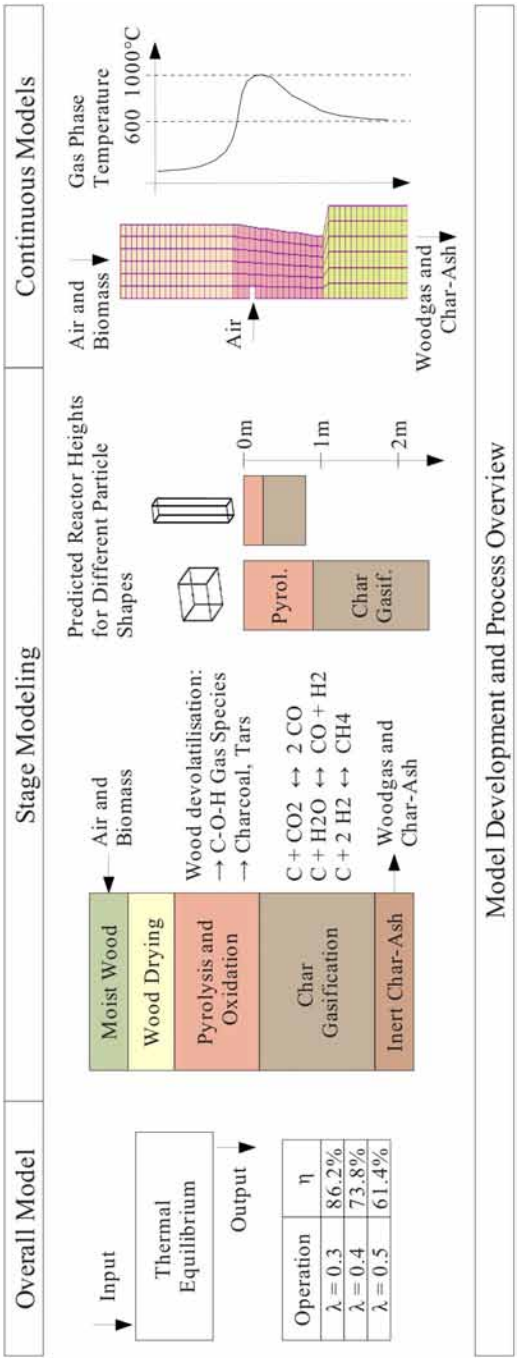


Fig. 2: Überblick Modellansätze zur Beschreibung der Holzvergasung.

Chapter 3

Organic Electronics and Photovoltaics

3.1 Efficient areal organic solar cells via printing

Contributors: M. T. Neukom, R. Ritzmann, T. Lanz, N. A. Reinke, B. Ruhstaller

Partners: TU/e Eindhoven University of Technology (NL), University Jaume I (E), CSEM, BASF
Funding: Swiss Federal Office of Energy
Duration: 2008–2011

This international research project with academic and industrial partners aims at creating more efficient and stable organic solar cells. The ICP is simulation partner and develops a comprehensive electro-optical model to numerically characterize organic solar cells.
An accurate determination of the charge carrier mobilities is essential to model and improve organic solar cells. A frequently used method to determine charge carrier mobilities is the CELIV technique (charge extraction by linearly increasing voltage). In this technique a voltage ramp is applied to the device in order to extract free charge carriers inside the bulk.
We simulate the photo-CELIV experiment with a fully-coupled electro-optical model and measure CELIV currents for several voltage slopes *a* and transient photo-currents of an organic bulk heterojunction solar cell. By fitting our numerical model to multiple curves we show that important material parameters like the charge mobilities, charge generation and recombination efficiency can be determined using numerical parameter extraction.
Figure 1 shows measured CELIV photocurrents with different voltage slopes and the corresponding simulations. For all voltage slopes the same set of simulation parameters is used. The transient currents can in general be reproduced with a numerical drift-diffusion model that simply assumes constant charge mobilities.

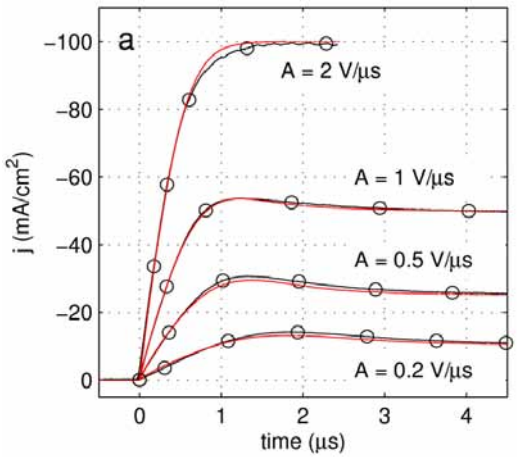


Fig. 1: Measurement (black) and simulation (red) of transient CELIV currents for different voltage slopes.

Measured and simulated IV-curves of a spin-coated cell are plotted in figure 2 as a function of illumination intensities. The measured current-voltage curves can be reproduced successfully by the simulations With the introduction of a light source with calibrated illumination intensity we obtain an additional scaling variable to investigate.

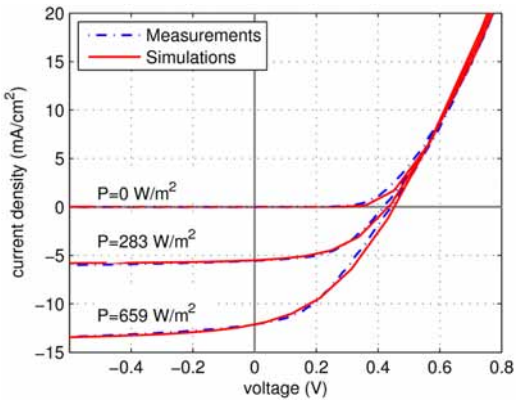


Fig. 2: Measured (blue) and simulated (red) current-voltage curves for spin-coated cells measured at different illumination intensities.

In the coming (last) project year, a series of bulk heterojunction blends dissolved in different solvents will be used for solar cell fabrication. The cell performance will be evaluated by model-based data analysis. The correlation of the cell performance with the blend morphology will be studied. Moreover, further experiments with time-dependent characterisation techniques (e.g. CELIV, impedance spectroscopy) will be carried out.

3.2 Numerical simulation and design of extremely thin absorber solar cells

Contributors: M. Loeser, B. Ruhstaller

Partners: EMPA Thun, ICP, FLUXIM
Funding: Swiss Federal Office of Energy
Duration: 2011–2012

This project is a joint research effort among the Laboratory for Mechanics of Materials and Nanostructures of the EMPA Thun and the Institute of Computational Physics of the Zurich University of Applied Sciences, to investigate and improve - both numerically and experimentally - the optical characteristics of nano-structured, extremely-thin absorber solar cells.
In recent years extremely thin absorber (ETA) solar cells have received considerable attention, and despite their yet low efficiencies, ranging about 2.5 %, they are considered as promising novel devices for converting sunlight into electric energy. The use of extremely thin absorber layers has numerous advantages. The probability that two optically generated carriers recombine before they reach the contact electrodes and are thus lost for energy conversion strongly decreases with the width of the absorber layer. In traditional photovoltaic (PV) applications this issue was dealt with by employing very expensive absorber materials with excellent electronic characteristics (i.e. long diffusion lengths). The high price prevents these solar cells from large-scale market penetration. In contrast, ETA solar cells do not only require a strongly decreased amount of absorber materials but also allow for the use of absorbers with significantly poorer electronic properties that come at a strongly reduced price. Together with rather inexpensive processing procedures ETA solar cells are very promising from both an academic and an economic perspective.
However, the efficiency of ETA solar cells is not only determined by their electrical, but also by their optical characteristics. The ability to efficiently trap and convert incident sunlight is a key feature that decides about economic success. In many cases the percentage of the incident light that is converted into free charges depends exponentially on the absorber thickness. In order to combine the advantages inherent to thin absorbers with the necessity of high optical absorption efforts must be made to enlarge the optical path in such way that the solar cell can absorb a significant fraction of the incident sunlight. To gain deeper understanding of the underlying complex optical processes and to obtain optimal device designs numerical simulations of the complete three-dimensional (3-D) problem are indispensible, as ill-chosen micro-structures can even decrease the device performance.

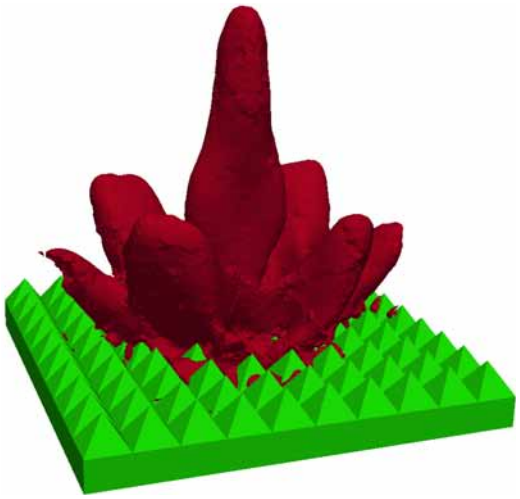


Fig. 1: Simulated three-dimensional full-wave emission beam of an LED featuring a micro-structured surface.

Yet, due to the combination of large devices and small micro-structures the accurate multi-dimensional simulation of such structures is most challenging. At the ICP we developed a 3-D simulation software that solves Maxwell's equations at greatly reduced computational cost thanks to a novel numerical method, the *Ultra-Weak Variational Formulation*. This software allows to obtain full-wave solutions for geometries that so far could not be numerically analyzed due to their large size.
A strong asset of this research project is the combination of both experimental and numerical methods. Whereas the EMPA Thun has profound knowledge in the field of device design, fabrication, and experimental characterization the Institute of Computational Physics provides profound expertise for numerical device simulation.

3.3 AEVIOM-Advanced Experimentally Validated Integrated OLED Model

Contributors: B. Perucco, E. Knapp, B. Ruhstaller

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

Funding: EU FP7

Duration: 2008–2011

The overall goal of the project AEVIOM is the development of a mathematical model for organic light-emitting devices (OLEDs) that is experimentally validated. This is what AEVIOM - Advanced Experimentally Validated Integrated OLED Model - stands for. In the long run an accurate numerical model is crucial for the improvement and optimization of OLEDs.

Simulations range from three dimensional Monte-Carlo simulations to our one dimensional continuum model which however integrates the disorder physics observed in the Monte-Carlo calculations. Thus, the Extended Gaussian Disorder model (EGDM) accounts for the disorder in organic semiconductors by a field, density and temperature dependent mobility model.

In the course of the third and last year of the EU-funded project the numerical solver, developed by the ZHAW in the previous two project years, has been extended for impedance modeling. With this approach we complete the set of simulations to be compared with measurements, i. e. we can now simulate steady-state current-voltage curves, dark-injection transients and impedance spectroscopy. Further, methods to extract model parameters from measurements were implemented.

Within the framework of the AEVIOM project, the interest was primarily on electrical parameter extraction from measured current-voltage curves to characterize the materials of an OLED stack. The algorithm to extract these parameters (mainly EGDM parameters) is based on a nonlinear least-square method which minimizes the error between the simulated and measured current-voltage curve. We observed that the method only needs a few iterations to solve the nonlinear least-square problem, typically around 10 iterations and further, we noticed a large convergence radius. The method was developed in collaboration between the ZHAW and FLUXiM and is available in the commercial semiconducting thin film optics simulator SETFOS. The method not only provides the model parameters which reproduce the measured current-voltage curve best, but also calculates other important key figures like the correlation between the extracted parameters, the landscape of the error function or the confidence region of the parameters. As an example, Figure 1 illustrates the error landscape as a function of the number and width of the density of states (DOS) for the electrons, N_0 and . The device analyzed is a single layer made of a polymer film which is embedded between the electrodes where the charges are injected. The mobility of the charges is parameterized according to EGDM.

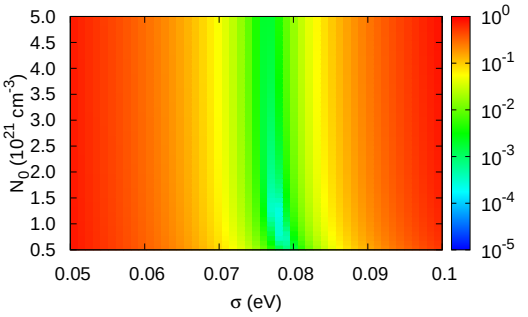


Fig. 1: The error landscape as a function of the number and the width of the DOS, N_0 and σ. The minimum is at $N_0 = 1 \cdot 10^{21}\ cm^{-3}$ and $\sigma = 0.078\ eV$

In order to reduce the correlation of the extracted parameters and thus provide a unique set of extracted parameters, we extended the method so that multiple measured current-voltage curves can be fitted simultaneously. Typically in the AEVIOM project, the current-voltage curves were measured for different layer thicknesses and for different temperatures of the device. We also introduced the possibility to specify parameters which must fit a single current-voltage curve and in parallel, we can optimize a parameter set which must fit multiple current-voltage curves. Moreover, SETFOS can be used to fit every physical quantity that can be simulated. This makes SETFOS a very flexible and useful tool in the application of parameter extraction.

3.4 Cost efficient thin film photovoltaics for future electricity generation

Contributors: T. Lanz, B. Ruhstaller

Partners: EPFL, EMPA, PSI, Oerlikon Solar, Greatcell, Solaronix, Flisom
Funding: SwissElectric Research
Duration: 2007–2010

In thin film silicon solar cells light scattering at rough layer interfaces is employed to increase the absorption. The roughness can be controlled by varying the deposition conditions of the transparent electrodes and the absorber materials. To perform an optical simulation of the light absorption in these devices it is necessary to take into account the scattering of the light at the rough interfaces as well as interference effects that may arise in thin layers. Our recently developed angular finite element method (aFEM) is capable of taking both effects into account. It is not as computationally expensive as full-wave methods and can treat - in contrast to ray-tracing approaches - light scattering in a direct, non-iterative procedure. Thin layers are treated coherently with wave optics (transfer-matrix formalism). In thick layers propagation of the intensity is employed. The light scattering at rough layer interfaces can be described in terms of angular distribution functions that also determine the fraction of scattered light. Figure 1 shows a block schematic of the individual steps in the computation.

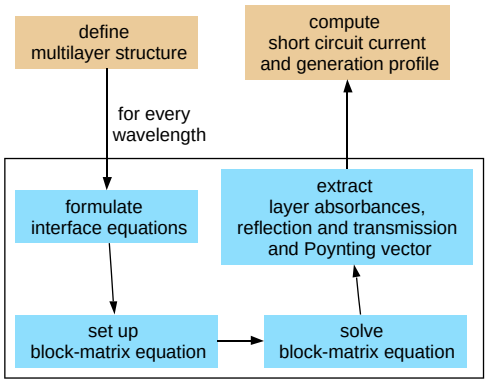


Fig. 1: Angular finite element method (aFEM) block schematic.

The necessary input parameters for the simulation are the layer thicknesses of all the individual layers, the refractive indices spectra of the materials and the scattering properties of the interfaces. In figures 2 and 3 the capabilities of aFEM are demonstrated for a micro-crystalline silicon solar cell developed at EPFL-IMT Neuchatel. The front and back contact are made of ZnO with a thickness of 4.8 um. The micro-crystalline absorber layer has a thickness of 1.1 μm. The ZnO front contact of this cell has been smoothed after deposition to limit the light scattering at this interface.

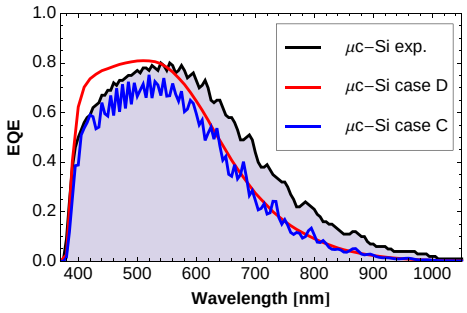


Fig. 2: aFEM calculations for the external quantum efficiency (EQE) of a micro-crystalline silicon (uc-Si) solar cell and measurement. Simulation cases C and D assume flat interfaces (no scattering). In case C the absorber layer is treated coherently, in case D incoherently (intensity only).

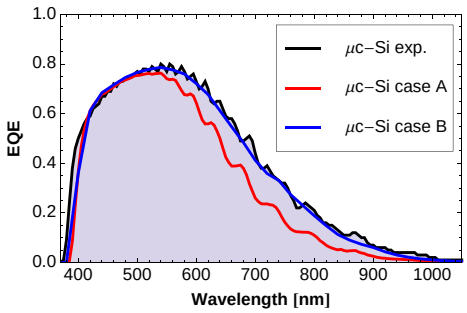


Fig. 3: aFEM EQE calculation of a uc-Si solar cell and measurement. Simulation case A assumes a coherent absorber layer and little scattering. Simulation case B assumes an incoherent absorber layer and a Lambertian scattering distribution.

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

Contributors: M. Schmid, A. Gentsch, J. O. Schumacher

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

From September 2008 to December 2010 the ICP carried out a research project for the modeling of dye-sensitized solar cells (DSCs). The objective of this project was to develop validated mathematical models for the DSC.

Steady-state parameter extraction

In the first period of the project we developed a validated model for the DSC. The model consists of an optical part, which simulates reflectance, transmittance and absorbance of the incoming light within the different layers of the DSC. The optical model is based on forward ray-tracing and thin-film optics. It allows to calculate the fraction of absorbed light in the active layer as well as the spatially resolved rate of generated excited dye states. The generation rate serves as an input for the electrical model, which simulates the injection of electrons into the TiO_2, the subsequent charge transport through the nanoporous layer and possible recombination with electrolyte species. In addition, the diffusive transport of redox species in the electrolyte is taken into account.

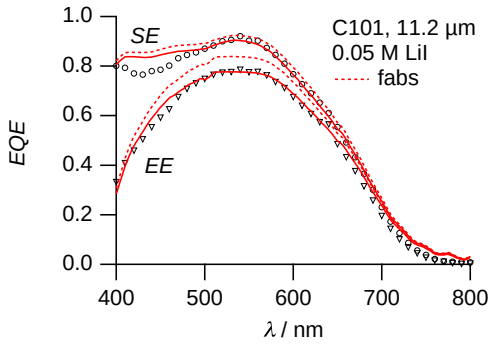


Fig. 1: Measured and simulated (bold red lines) EQEs for illumination from SE side (open circles) and EE side (open triangles) on a $11.2\ \mu$m thick test cell

The coupled optical and electrical DSC model is compared to steady-state measurement data in order to extract the essential parameters for the steady-state performance of the cell. Two important parameters characterizing the steady-state performance of the DSC are the electron injection efficiency, which describes how effectively the excited dye molecules insert electrons into the nanoporous TiO_2 layer, and the electron diffusion length, which characterizes the charge transport properties inside the semiconductor. By measuring the short-circuit current density and external quantum efficiency (EQE) for illumination from either the substrate electrode (SE) side or the electrolyte electrode (EE) side and comparing these measurement data to simulations, the influence of these two parameters can be disentangled. In this way injection efficiency and diffusion length of the DSC could be determined independently. This analysis (an example is shown in figure 1) was carried out for different types of DSCs (i.e. with different dyes, electrolytes with varying additives).

Transient simulations

Steady-state measurements are not sufficient to understand the detailed physical properties of the DSC. Two different DSCs may have the same photovoltaic parameters (IV-curve, power output, efficiency etc.), but behave differently, when the cells are perturbed by a small time-dependent signal around the steady-state.

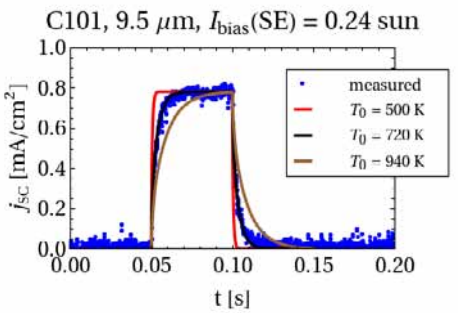


Fig. 2: Comparison of measured and simulated small perturbation current decay allows to extract trapping parameters.

Time-dependent measurement techniques such as electrochemical impedance spectroscopy and small amplitude photovoltage/photocurrent decay are crucial diagnostic tools. The developed simulation software allows to simulate

these measurement techniques. Then, by comparing experimental data to simulated data, the influence of the different model parameters on the response can be disentangled. Figure 2 shows exemplary a measured and simulated small perturbation photocurrent decay.

Quantitative loss analysis

A particularly instructive feature of the coupled optical and electrical DSC model is the quantification of optical and electric losses. As illustrated in figure 3, only a small fraction of the total incident solar spectrum is converted into electric power (10 - 11 % in high-efficiency DSCs). A large part of the solar flux is lost due to optical losses. Excited dye states might relax back to the ground state (injection loss). After injection, at least half of the photon energy is lost due to thermalization of the injected electron to the TiO_2 conduction band level, and due to the offset between the dye ground state and the redox energy level (potential loss). Also, the electrons may recombine with I_3^- in the electrolyte or with dye cations.

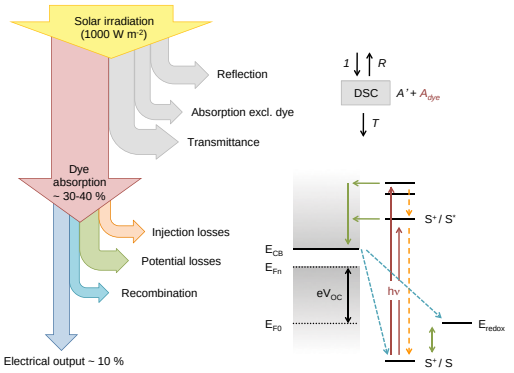


Fig. 3: Schematic of the various optical and electrical losses in a DSC.

We show a sample calculation for a DSC cell in table 1 below. A large fraction (53 %) of the incident power is lost due to optical losses. Injection losses can constitute a significant loss channel (5.5 %). After injection, a major fraction of the photon energy is lost due to potential losses (20 %). Surprisingly, only a small fraction (0.7 %) is lost due to recombination. Another small fraction (1 %) is lost to electrical resistances in the electrodes. Finally, we find a power output of 75.9 Wm^{-2} (efficiency of 7.6 %) for the specific DSC considered her. In our opinion, the comprehensive loss analysis is an important tool for the optimization of the DSC.

Loss channel	Power ($W\ m^{-2}$)	Current ($mA\ cm^{-2}$)
Incident spectrum	872.0	51.5
Reflectance	85.2	5.2
Transmittance	317.3	22.4
Absorptance	126.7	9.3
Injection	54.9	2.3
Recombination	6.8	0.9
Potential	196.0	—
Series Resistance	9.6	—
Output	75.9	11.4

Tab. 1: Sample calculation for a DSC.

Graphical user interface

We implemented the developed DSC model into a simulation software called PECSIM (PECSIM=photoelectrochemical cell simulator)[1]. PECSIM is written in Mathematica and is equipped with a GUI. Currently, four simulation modes are available:

1. Steady-state analysis
2. Electrochemical impedance spectroscopy (EIS) simulation
3. Transient photovoltage and photocurrent decay simulation
4. Quantitative loss analysis

Outlook

The present project allowed the ICP to extend its experience of simulating optical devices to dye-sensitized solar cells and to broaden the know-how in the simulation of optical and electrochemical processes. The ICP currently evaluates the acquisition of several follow-up projects.

[1] http://www.pecsim.ch

3.6 In-line inspection of photovoltaic modules

Contributors: M. T. Neukom, T. Lanz, B. Ruhstaller, N. A. Reinke

Partners: Komax Solar, Altatec
Funding: Commission for Technology and Innovation
Duration: 2010–2011

This project is concerned with a new in-line inspection system for the quality control of photovoltaic modules during production. The photovoltaic modules shall be optically excited and electrically measured in order to determine key figures such as the maximum generated power under one sun condition. In this project, an innovative LED-based excitation is being developed that allows for a compact, high-intensity and homogeneous source of light suitable for solar cell characterization.
The industrial partner Komax Solar develops and sells in-line, high-throughput production and testing systems for industrial solar cell fabrication. Altatec is a microelectronics company with a strong competence in solutions for packaging of optoelectronic components. The Institute of Computational Physics provides its competence in the development of experimental characterization equipment and physical modeling. For characterizing the spectral photocurrent response of solar cells under test, a dedicated measurement system has been developed that servers as a benchmarking system. It makes use of a broadband light source, a monochromator and the lock-in technique for a low-noise measurement of the spectral photocurrent. A picture of the developed setup is shown in figure 1.
The project also deals with numerical modeling mainly of the optical part of the system and is still ongoing.

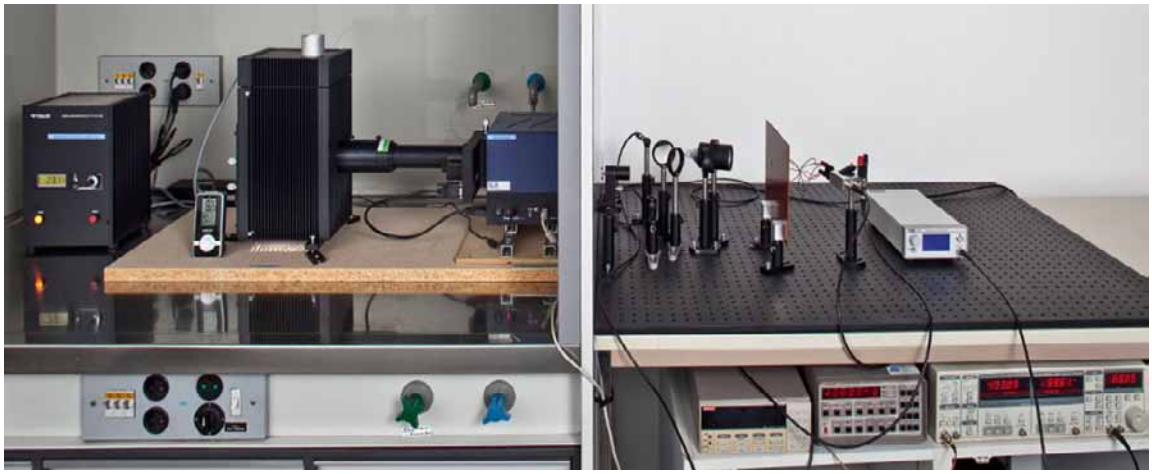


Fig. 1: Experimental setup for spectral photocurrent characterization of solar cells.

3.7 Optoelectronic research laboratory

Contributors: M. Bonmarin, K. A. Brossi, M. T. Neukom, N. A. Reinke, R. Ritzmann, S. Züfle

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) 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: Optical microscopy image of an organic photovoltaic cell.

The O-LAB is 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 optical spectroscopy
- Transient optoelectronic device characterization

Figure 1 shows a microscopical photography of electrode organic solar cell. An impedance analyzer used for the characterization of organic semiconducting devices is depicted in figure 2. Our experimental toolbox comprises fast oscilloscopes, signal generators, impedance analyzers, IR-sources, detectors and cameras, optical flashers and spectrometers covering the spectral range from 0.35 and 14 μm. A measuring setup for time resolved fluorescence and phosphorescence spectra is currently under construction.

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: Impedance analysing instruments for organic semiconducting device characterization.

Chapter 4

Student Projects

4.1 Optimisation of new generation silicon solar cells by means of 2D simulations

Students: Andreas Tiefenauer

Category: MSE Master Thesis
Mentoring: J. John (IMEC), B. Ruhstaller
Hand In: April 2010

This project has been conducted in the framework of a master thesis and internship at the Belgian interuniversity microelectronic center (IMEC) in Leuven. Solar cells are large area semiconductor devices. Other than for most semiconductor industry of microelectronic devices, the market driver for multi crystalline silicon solar cells is its cost structure. Since the silicon price makes about 30 % of the costs dealing with low quality silicon and with thinner and thinner wavers is imperative in the multi cristalline silicon solar cell industry. However the thinning of wafers brings new difficulties and asks for further optimisation in various domains of solar cell research.
Nevertheless, it emerges that reducing the cell thickness is not as straightforward as it seems. For technological and operational reasons it yields into structurally more complex solar cell concepts than the conventional thicker standard type cells. Thereby this increase of complexity naturally leads to more extensive Design of Experiments (DoE) which hardly could be done solely by experimental screening of parameters. At this point the need of simulations is essential. By virtually identifying insensitive parameters one can finally decrease the size of the experimental DoE matrix in the lab.
Since already existing 1D simulation tools such as PC1D are not sufficient anymore for more complex structures, it was the purpose of this work to develop a 2D model that is dedicated to simulate the opto-electrical behaviour of next generation solar cells. A first version of a 2D FE-model has been created and validated. By calculating IV characteristics under various parameter setups we have successfully shown that the 2D model is able to correctly reproduce trends and optimums for various cell parameters. The model showed in general good agreement with experimental data and some occurring discrepancies could be explained by the lack of certain - at that time - not yet implemented features.
The model has then been widely extended with many further features. To mention a few: A resistive circuit model has been added in order to take ohmic losses into account. In order to calculate the effect of textured front side an additional sub model had to be coupled to the 2D model. And a spectral characterisation mode has been added in order to also calculate IQE, EQE and spectral response. The final model contains thus a big variety of features and therefore allows extensive virtual characterisation of solar cells. The model is believed to have a great potential for availability in reasearch and developement and is further used and extended in the solar cell group of IMEC.

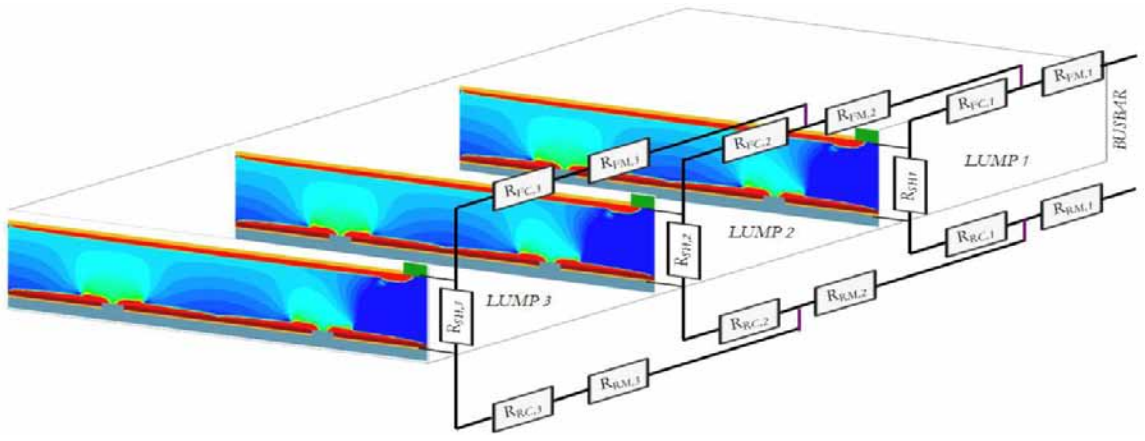


Fig. 1: Scheme of the 2D FE model coupled with a circuit model accounting for resistive losses.

4.2 SETFOS sweep data visualization

Students: André Götz

Category: Projektarbeit, Studiengang Systeminformatik UI
Mentoring: B. Ruhstaller
Hand In: Dezember 2010

Die ZHAW Spin-off Firma Fluxim AG (www.fluxim.com) entwickelt und vertreibt wissenschaftlich-technische Software (SETFOS) für organische Bauelemente wie Leuchtdioden und Solarzellen. Eine Anwendung der Software betrifft die systematische Variation von Eingabeparametern für die Simulation. Die Simulationen können so umfangreich sein, dass die Visualisierung der Rechenresultate in SETFOS und der Vergleich mit Messresultaten erschwert ist. In dieser Projektarbeit wurde eine eigene Java Applikation zur Visualisierung der vorliegenden Rechenresultate entwickelt. Die Applikation basiert auf Java-Bibliotheken und -Klassen, welche von der Hauptanwendung (SETFOS) stammen. Dies sind Bibliotheken und Klassen für wissenschaftliche Graphen, die interaktiv angepasst werden können. Die Applikation dient somit als Datenbrowser und eine beliebte Anwendung besteht darin, dass Anwender ihre Messdaten mit den simulierten Daten direkt vergleichen.

Diese Projektarbeit beinhaltete das Design und die Programmierung einer eigenständigen Java Applikation zur Visualisierung der durch den SETFOS-Kernel berechneten Simulationsresultate. Basierend auf einem Prototyp in Matlab wurde eine Oberfläche entworfen, welche es dem Benutzer ermöglicht, intuitiv Simulationsdaten mit mehreren Parametern mit Messdaten zu vergleichen. Der Benutzer kann dabei Datenspalten per Drag and Drop den Achsen der Graphen zuweisen, wo sie in zwei Dimensionen dargestellt werden. Eingangsparameter, wie zum Beispiel Schichtdicken oder die angelegte Spannung, können durch Schieberegler fixiert werden. Als weiteres Werkzeug wurde eine Kurvenschar-Funktion eingebaut, so dass durch Variation der Eingangsparameter mehrere Kurven in einen Graph geplottet werden können. Die Hauptfunktionalitäten, die gegenüber der Standard-SETFOS-GUI einen Mehrwert darstellen, konnten in dieser Arbeit alle erfolgreich umgesetzt werden.

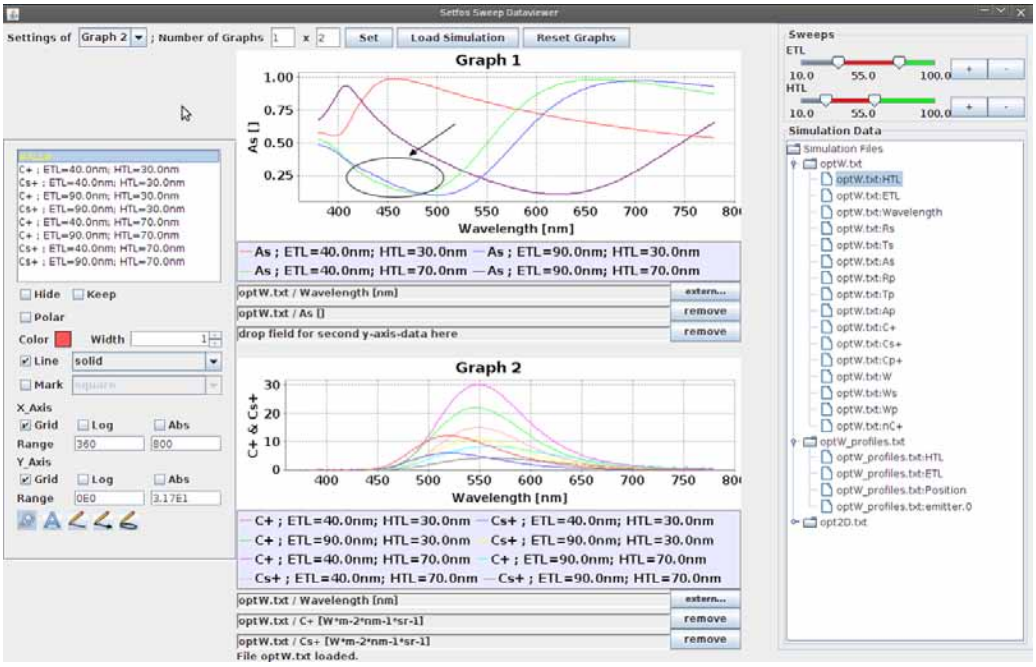


Fig. 1: Zeigt einen Screenshot des erzielten Software Prototyps.

4.3 Mass- and heat-transfer with two-phase ow, project "earth tube": cooling a school building in Tamil Nadu, India

Students: Remo Ritzmann

Category: Spare time project, MSE Lecture "Heat and Mass Transfer with Two-Phase Flow"
Mentoring: T. Hocker
Hand In: 2010–2011

Cooling buildings in hot summertime near the equator is an energy intense task. Two summer months with up to 40 °C are seen alongside three rainy season months around 30 °C. Additionaly there is a temperature gradient of approx. 10 °C between daily minimum and maximum. Air conditioning with an underground heat exchanger offers a low priced solution. This project shows how much cooling effect this brings.

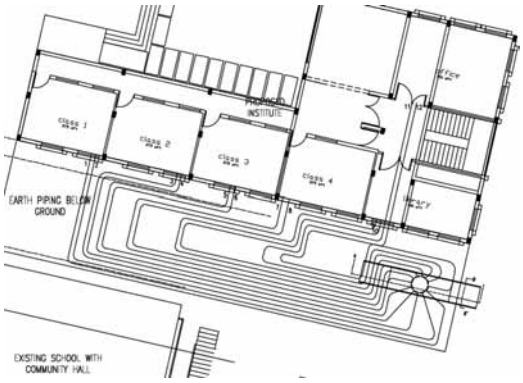


Fig. 1: Earth tube system with 20 tubes in India.

First of all a 1D transient heat coduction problem has been solved to calculate heat waves in the earth. The warm-up of soil around the earth tube was calculated by solving the global energy balance. Then a 2D stationary mass and energy balance lead to an understanding of the cooling process inside the earth tube.

The simulation showed the heat flow from the air into the soil. The temperatures are calculated from the given (turbulent) velocity-profile. With 20 m long pipes in a 30 °C ground the air temperature in the tube falls from 40 °C down to 32 °C. Since there is a climate with lots of humidity the simulation has shown that every hour 2 dl of Water is condensed per tube per hour. So in total 4 l h can be pumped out for watering the plants. Water condensation happens only near the tube walls.

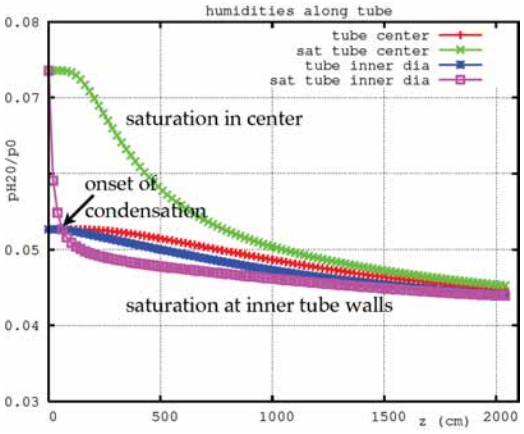


Fig. 2: Condensation conditions along earth tube.

The temperature T(x,t) in the ground at depth x and at time t has been simulated. The results showed that the air temperature can be reduced by 8 degrees. Another significant effect on human comfort will be that humidity is beeing reduced from 90 % to 60 %. Therefore one can perspire more easily in the airconditioned house with this low priced technique.

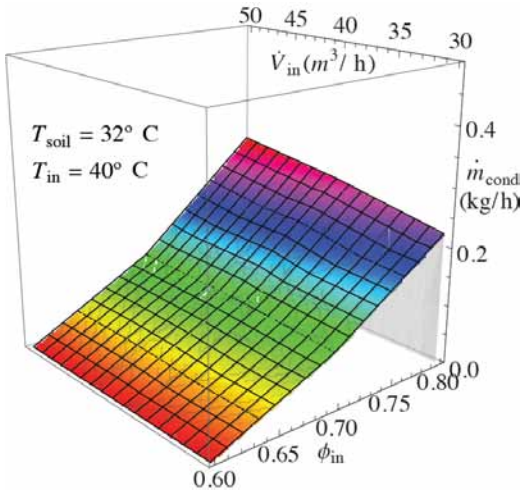


Fig. 3: Condensation & heat production rates at tube end in 3 m depth of sandy ground.

4.4 Complete List of Student Projects

1. Peter Bauer, Stephan Ernst, ”ICE-LED, Entwicklung eines LED-Screens für Werbung unter Eisflächen in Hockeyarenas“, *Projektarbeit Studiengang Elektrotechnik*, Betreuer: N. A. Reinke, R. Ritzmann, B. Ruhstaller, Firmenpartner: Martin Altorfer (Altira GmbH), Winterthur (2010).

2. S. Brunner, L. Imholz, ”Analyse von thermisch induzierten Fertigungstoleranzen bei der Herstellung von Schwingquarzen“, *Projektarbeit Studiengang Maschinentechnik*, Betreuer: T. Hocker, Firmenpartner: Micro Crystal AG (Swatch), Grenchen (2010).

3. L. Candrian, O. Hasler, ”Validierung einer Nernst-Sonde zur variablen Regelung der Erdgasreformierung im Hexis Brennstoffzellen-System“, *Projektarbeit Studiengang Maschinentechnik*, Betreuer: M. Linder, T. Hocker, Firmenpartner: Hexis AG, Winterthur (2010).

4. Chantal Eschbach, Ivo Günther, ”Charakterisierung von Solarzellen mit einem spektralen IU-Kennlinien-Messplatz“, *Projektarbeit Studiengang UI*, Betreuer: N. A. Reinke, M. T. Neukom (2010).

5. A. Götz, ”SETFOS sweep data visualization“, *Studiengang Systeminformatik UI*, Betreuer: B. Ruhstaller, Firmenpartner: Fluxim AG, Winterthur (2010).

6. Homajun Ahadyar, Pascal Schori, ”Temperatur-geregelter Gasstrom für die Untersuchung organischer Leuchtdioden und Solarzellen“, *Projektarbeit Studiengang* , Betreuer: N. A. Reinke, M. T. Neukom, S. Züfle (2010).

7. Fridolin Hösli, Stefan Kuch, Simon Lehmann, ”Algenreaktor“, *Projektarbeit Studiengang UI*, Betreuer: N. A. Reinke, K. A. Brossi (2010).

8. L. Kaufmann, R. Schmid, ”Optimierung eines Prüfstands für thermo-mechanische Belastungstests von keramischen Brennstoffzellen“, *Projektarbeit Studiengang Maschinentechnik*, Betreuer: T. Hocker, Firmenpartner: Hexis AG, Winterthur (2010).

9. Adrian Koller, Robin Jergen, ”ASURO Rasenmäher (ASMÄHRO), RPK - Rasenmähen Per Knopfdruck“, *Projektarbeit Studiengang MT*, Betreuer: A. Fassbind, R. Ritzmann (2010).

10. M. Linder, ”Modellbasierte Analyse der Spannungs- Strom-Kennlinie von SOFC Hochtemperatur Brennstoffzellen“, *MSE Masterarbeit*, Betreuer: T. Hocker, Firmenpartner: Hexis AG, Winterthur (2010).

11. Alexander Pohl, Marco Bär, ”1DES One Doctor Endoscopic Surgery, Foot operated laparoscopic telescope“, *Projektarbeit Studiengang Mechatronik*, Betreuer: T. Järmann, R. Ritzmann, Firmenpartner: Dr. J. Gnanaraj, India (2010).

12. Juan Romero, Fabio Lambreschi, ”Raytracing Applikation für die Simulation optoelektronischer Bauelemente“, *Projektarbeit Studiengang UI*, Betreuer: N. A. Reinke, M. T. Neukom, (2010).

13. R. Ringenberg, E. Schmidhauser, ”Entwicklung eines Injektors für die Brenngaszufuhr in Brennstoffzellensystemen“, *Projektarbeit Studiengang Maschinentechnik*, Betreuer: M. Linder, T. Hocker, Firmenpartner: Hexis AG, Winterthur (2010).

14. R. Ritzmann, ”Mass- and heat-transfer with two-phase flow, project "earth tube": cooling a school building in Tamil Nadu, India“, *Freizeitprojekt*, Betreuer: T. Hocker, Firmenpartner: Chance für Morgen, Winterthur (2010–2011).

15. Jonas Schumacher, Toni-Ante, ”LED-Blitz 2“, *Projektarbeit Studiengang UI*, Betreuer: N. A. Reinke (2010).

16. P. Specker, S. Wolff, ”Stationärer Betrieb eines Labor-Holzvergasers“, *Projektarbeit Studiengang Maschinentechnik*, Betreuer: C. Meier, T. Hocker (2010).

17. M. Steidinger, R. Christinger, ”Populationsbilanzen zur Modellierung des Bruchverhaltens von pharmazeutischen Wirkstoffen“, *Projektarbeit Studienrichtung Material- und Verfahrenstechnik*, Betreuer: R. Axthelm, T. Hocker, Firmenpartner: Novartis Pharma AG, Basel (2010).

18. A. Tiefenauer, ”Optimisation new generation silicon solar cells by means of 2D simulations“, *Master thesis and internship at the belgian interuniversity microelectronic center (IMEC)*, Betreuer: J. John, B. Ruhstaller, Leuven (2010).

19. D. Winter, V. Beer, ”Untersuchung des Rissbildungsmechanismus in Brennstoffzellen“, *Projektarbeit Studienrichtung Material- und Verfahrenstechnik*: Betreuer: D. Penner (IMPE), T. Hocker, Firmenpartner: Hexis AG, Winterthur (2010).

Appendix

A.1 Scientific Publications

1. J. Eller, J. O. Schumacher, G. Sartoris, B. Seyfang, and T. Colinart: *A 2+1D model of a proton exchange membrane fuel cell with glassy-carbon micro-structures*, Special Issue of Mathematical and Computer Modelling of Dynamical Systems (MCMDS) (accepted for publication, 2010).

2. L. Holzer, B. Iwanschitz, T. Hocker, B. Münch, M. Prestat, D. Wiedenmann, U. Vogt, P. Holtappels, J. Sfeir, A. Mai, and T. Graule: *Microstructural degradation in SOFC anodes: quanti - cation of nickel grain growth in dry and in humid atmospheres*, *Journal of Power Sources*, vol. **196**, pp. 1279–1294 (2011).

3. L. Holzer, B. Münch; B. Iwanschitz, M. Cantoni, and T. Hocker: *Quantitative relationships between composition, particle size, triple phase boundary length and surface area in Ni-cermet anodes for Solid Oxide Fuel Cells*, *Journal of Power Sources*, doi:10.1016/j.jpowsour.2010.08.006 (in press).

4. E. Knapp, R. Häusermann, H. U. Schwarzenbach, and B. Ruhstaller: *Numerical simulation of charge transport in disordered organic semiconductor devices*, J. Appl. Phys. 108, 054504 (2010).

5. E. Knapp and B. Ruhstaller: *Numerical Analysis of Steady-State and Transient Charge Transport in Organic Semiconductor Devices*, OQE, accepted for publication (2010).

6. J. Kuebler, U. Vogt, D. Haberstock, J. Sfeir, A. Mai, T. Hocker, M. Roos, and U. Harnisch: *Simulation and Validation of Thermo-mechanical Stresses in Planar SOFCs*, *Fuel Cells*, vol. **10**, pp. 1066–1073 (2010).

7. M.T. Neukom, N. A. Reinke, K. A. Brossi, and B. Ruhstaller: *Transient Photocurrent Response of Organic Bulk Heterojunction Solar Cells*, Proc. SPIE 7722 30 (2010).

8. B. Perucco, N. A. Reinke, F. Müller, D. Rezzonico, and B. Ruhstaller: *The in uence of the optical environment on the emission pro le and methods of its determination*, Proc. SPIE 7722 14 (2010).

9. B. Perucco, N. A. Reinke, D. Rezzonico, M. Moos, and B. Ruhstaller: *Analysis of the emission pro le in organic light-emitting devices*, Optics Express, Vol. 18, Issue S2, pp. A246-A260 (2010).

10. D. Rezzonico, B. Perucco, E. Knapp, R. Häusermann, N. A. Reinke, F. Müller, and B. Ruhstaller: *Numerical analysis of exciton dynamics in organic light-emitting devices and solar cells*, J. Photon. Energy 1, 011005 (2011).

11. B. Ruhstaller, E. Knapp, N. A. Reinke, M. Moos, B. Perucco, D. Rezzonico, and M. H. Lu: *Analysis of Exciton Distributions in OLEDs: The In uence of Optical Modes and Energetic Disorder*, SID Symposium Digest of Technical Papers, Volume 41, Issue 1, pp. 1894-1898 (May 2010).

12. S. Wenger, M. Schmid, G. Rothenberger, M. Grätzel, and J. O. Schumacher: *Understanding steady-state behavior in dye-sensitized solar cells using a validated coupled optical and electrical model*, Journal of Physical Chemistry C (in press).

A.2 News Articles

1. E. Heinzelmann: *Anti-Aging für Brennstoffzellen*, In Auftrag von Swisselectric Research (SWISS ENGINEERING STZ). Mai 2010

2. N. A. Reinke and A. Bariska: *Einfache Beschichtungskontrolle mit thermischer Schichtprüfung*, Bulletin 10s/2010 itg-Sonderausgabe / numéro spécial itg (2010).

3. N. A. Reinke and B. Ruhstaller: *Organische Elektronik*, Swiss Engineering STZ (Januar/Februar 2010). Organische Elektronik

4. N. A. Reinke: *Sicherheit dank Winterthurer Technik*, Winterthurer Stadtanzeiger, Ausgabe vom 21.12.2010 (21.12.2010).

5. N. A. Reinke: *Soirée Electrique*, blitz 04 Fachzeitschrift des AMIV an der ETH, 44. Jahrgang (17. November 2010).

6. N. A. Reinke: *Soirée Electrique*, Bulletin (2010).

7. N. A. Reinke: *Soirée Electrique*, Impact (2010).

8. N. A. Reinke: *Thermische Schichtprüfung*, Swiss Innovation Guide 2011 Handelszeitung Beilage im Handelsblatt (November 2010).

9. B. Ruhstaller and N. A. Reinke: *Organische Elektronik mit Perspektive*, Bulletin 9/2010 Jubiläumsausgabe/numéro du centenaire (2010).

A.3 Exhibitions

1. Control, Stuttgart, 2010.

2. Nationale Photovoltaik Tagung, Winterthur, February 2010.

3. Swiss Innovation Forum, Basel, 2010.

4. Symposium für virtuelle Produktentwicklung Schweiz, HSR, Rapperswil, April 2010.

5. Thurgauer Technologietag, Schönenberg, 19. März 2010.

6. Winterthurer Nacht der Technik, ZHAW, Winterthur, 2010.

A.4 Conferences and Workshops

1. K. A. Brossi and M. T. Neukom: *Fundamental Properties of Devices - Sensors, Transistors and Solar Cells*, Winterschool on Organic Electronics, Donnersbach (Austria), 6.–12.03.2010.

2. T. Hocker: *Model-based analyses of the Hexis SOFC system: from electrode degradation to overall system behavior*, invited talk, *IEA International Energy Agency Annex 25 Meeting*, Winterthur, April 2010.

3. T. Hocker, B. Iwanschitz, and L. Holzer: *Analysing microstructures to predict the performance and degradation of Ni-8YSZ anodes*, invited talk, *Workshop on Image Analysis in SOFC Degradation Research*, Brussels (Belgium), September 2010.

4. T. Hocker, B. Iwanschitz, and L. Holzer: *Assessing the effect of electrode microstructure on repeat unit performance and cell degradation*, *Modval7 - 7th Symposium on Fuel Cell Modelling and Experimental Validation*, Morges, March 2010.

5. T. Hocker, B. Iwanschitz, and L. Holzer: *Assessing the effect of SOFC electrode microstructure on its performance and degradation*, invited talk, *Symposium on Solid Oxide Cell Electrodes in 3D*, Risø, National Labs (Denmark), July 2010.

6. T. Hocker, B. Iwanschitz, and L. Holzer: *Using arti cial, computer generated electrode microstructures to predict the performance and degradation of SOFC anodes*, invited talk, *Transpore 2010 - International Symposium on Transport in Porous Materials*, PSI Villigen, August 2010.

7. L. Holzer et al.: *The microstructure of porous SOFC electrodes: new methodologies for reliable quanti cation and link with performance*, *9th European SOFC Forum*, Lucerne, June/July 2010.

8. B. Iwanschitz, A. Mai, T. Hocker, L. Holzer, and M. Schütze: *Degradation of Ni-Cermet Anodes in Solid Oxide Fuel Cells*, *9th European SOFC Forum*, Lucerne, June/July 2010.

9. E. Knapp: *Impedance Analysis*, International Simulation Workshop on Organic Electronics and Photovoltaics 2010, Winterthur, Switzerland, July (2010).

10. E. Knapp: *Impedance Analysis of Organic Light-Emitting Devices with Disorder*, SOLED Optics and Photonics Congress, Karlsruhe, 22/06/2010.

11. E. Knapp and B. Ruhstaller: *Numerical Analysis of Steady-State and Transient Charge Transport in Organic Semiconductor Devices*, NUSOD, Atlanta, USA, 07/09/2010.

12. T. Lanz and B. Ruhstaller, C. Battaglia, F.-J. Haug, and C. Ballif: *Light scattering model for optical simulation of thin lm silicon solar cells*, 25th European Photovoltaic Solar Energy Conference and Exhibition (EU-PV-SEC), Valencia, Spain, 2010.

13. T. Lanz and B. Ruhstaller: *Coherent and incoherent optical simulation of thin lm solar cells*, 12th Euregional Workshop on Novel Concepts for Future Thin-film Silicon Solar Cells, Delft, The Netherlands, 28.1.2010.

14. T. Lanz and B. Ruhstaller: *Light Scattering Simulation for Thin Film Silicon Solar Cells*, SOLED Optics and Photonics Congress, Karlsruhe, 22/6/2010.

15. M. Linder, T. Hocker, R. Denzler, A. Mai, and B. Iwanschitz: *Automated model-based analysis of i-V data for Hexis SOFC short stacks running on CPO-reformed natural gas*, *Modval7 - 7th Symposium on Fuel Cell Modelling and Experimental Validation*, Morges, March 2010.

16. M. Loeser and B. Ruhstaller: *Three-Dimensional Full-Wave Optical Simulation of LEDs*, SOLED Optics and Photonics Congress, Karlsruhe, 22/6/2010.

17. M.H. Lu, B. Perucco, D. Rezzonico, E. Knapp, N. A. Reinke, and B. Ruhstaller: *Exciton Distributions in OLEDs: In uence of Optical Modes and Energetic Disorder*, SID Symposium, Seattle, USA, 25/5/2010.

18. C. Meier and T. Hocker: *Modeling of Fixed-Bed Wood Gasi ers for Combined Heat and Power Applications*, *Modval7 - 7th Symposium on Fuel Cell Modelling and Experimental Validation*, Morges, March 2010.

19. M. T. Neukom and K. A. Brossi: *Fundamental properties of devices - sensors, transistors and solar cells*, Winterschool on organic electronics, Donnersbach Austria, 6–12 March (2010).

20. M. T. Neukom, N. A. Reinke, K. A. Brossi, and B. Ruhstaller: *Transient Photocurrent Response of Organic Bulk Heterojunction Solar Cells*, SPIE Photonics Europe, Brussels, 12/4/2010.

21. B. Perucco: *Analysis of Exciton Distributions in OLEDs*, International Simulation Workshop on Organic Electronics and Photovoltaics 2010, Winterthur, Switzerland, July (2010).

22. B. Perucco: *The in uence of the optical environment on the emission pro le and methods of its determination*, SPIE Photonics Europe, Brussels, Belgium, April (2010).

23. B. Perucco, N. A. Reinke, F. Müller, D. Rezzonico, and B. Ruhstaller: *The in uence of the optical environment and energetic disorder on the shape of emission zones in OLEDs and methods of their determination*, SOLED Optics and Photonics Congress, Karlsruhe, 22/6/2010.

24. B. Perucco, N. A. Reinke, F. Müller, D. Rezzonico, and B. Ruhstaller: *The in uence of the optical environment and energetic disorder on the shape of emission zones in OLEDs and methods of their determination*, SPIE Photonics Europe, Brussels, 12/4/2010.

25. D. Rezzonico, B. Perucco, E. Knapp, R. Häusermann, N. A. Reinke, F. Müller, and B. Ruhstaller: *Numerical analysis of exciton dynamics in organic light-emitting devices and solar cells*, SPIE Optics + Photonics, San Diego, USA, 2/8/2010.

26. D. Rezzonico, B. Perucco, F. Mueller, N. A. Reinke, E. Knapp, and B. Ruhstaller: *Design of Multilayer Organic Solar Cells and Light-emitting Devices*, LOPE-C, Frankfurt, 31/5/2010.

27. B. Ruhstaller: *Advanced simulation of OLEDs and organic solar cells*, Intl. Workshop on Organic Optoelectronic Devices: Simulation and Models of Operation, Castello, Spain, 5/10/2010.

28. B. Ruhstaller: *Simulation Software for Organic Electronics*, SLN/Opera Optoelectronics Meeting, Basel, 25/6/2010.

29. M. Schmid, A. Gentsch, S. Wenger, G. Rothenberger, and J. O. Schumacher: *Time-dependent coupled optical and electric modeling of dye-sensitized solar cells*, Hybrid and Organic Photovoltaics Conference HOPV 2010, Assisi, Italy, 23–27 May 2010.

30. M. Schmid, A. Gentsch, S. Wenger, G. Rothenberger, and J. O. Schumacher: *Time-dependent coupled optical and electric model for dye-sensitized solar cells*, International Simulation Workshop on Organic Electronics and Photovoltaics (ISW'10), Winterthur Switzerland, June 30–July 2 (2010).

31. J. O. Schumacher, and Y. Safa: *Modeling two-phase ow in the gas diffusion layer of a proton exchange membrane fuel cell*, 7th Symposium on fuel cell modeling and experimental validation, Morges, Switzerland, 23–24 March 2010.

32. S. Wenger, M. Schmid, G. Rothenberger, M. Grätzel, and J. O. Schumacher: *Understanding charge transport and recombination in dye-sensitized solar cells using an experimentally validated coupled optical and electrical model*, 2010 MRS Spring Meeting, San Francisco, USA, 5–9 April 2010.

A.5 Prizes and Awards

1. M. T. Neukom received the *Thales - Preis* for his Bachelor Thesis *Characterisation of optical pulsed solar cells*.
2. N. A. Reinke, Ausgewählter Aussteller auf dem Swiss Innovation Forum 2010
3. N. A. Reinke and A. Bariska, ITG Innovationspreis
4. N. A. Reinke and A. Bariska, Winterthur Instruments, Venture Kick Stage I ICP/IDP-SpinOff
5. B. Ruhstaller, Fluxim AG, CTI Startup Coaching Acceptance

A.6 Teaching

Bachelor of Science

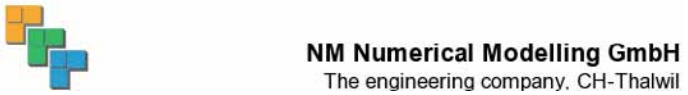
- "Mathematik für Ingenieure 1" (MAE 1) **- R. Axthelm**
- "Mathematik für Ingenieure 2" (MAE 2) **- R. Axthelm**
- "Mensch, Technik, Umwelt" für Maschinentechniker (MTU) **- T. Hocker, C. Meier**
- "Modellbildung und Simulation" für Material- und Verfahrenstechniker (MBS) **- T. Hocker, R. Axthelm**
- "Physik 1" für Elektrotechnik, Maschinentechnik und Systemtechnik (PHEMS1) **- M. Schmid, M. Loeser**
- "Physik 2" für Maschinentechnik (PHMT2) **- M. Schmid**
- "Physik 1" für Unternehmensinformatiker (PhUI 1) **- N. A. Reinke**
- "Physik 2" für Unternehmensinformatiker (PhUI 2) **- N. A. Reinke**
- "Reaktions- und Prozesstechnik" für Material- und Verfahrenstechniker (PRTMV) **- T. Hocker**
- "Signale und Systeme 1" (SiSy 1) **- J. O. Schumacher**
- "Signale und Systeme 2" (SiSy 2) **- J. O. Schumacher**

Master of Science

- "Applied Photonics" (Mirco and Nano Technolgoy) **- B. Ruhstaller**
- "Heat and Mass Transfer with Two-Phase Flow" (Engineering) **- T. Hocker**
- "Material Properties of Crystals / Tensors for Engineers" (Engineering) **- M. Roos**
- "Multiphysics Modelling and Simulation" (Engineering) **- J. O. Schumacher**

A.7 Spin-off Companies

Numerical Modelling GmbH



www.nmtec.ch

Numerical Modelling GmbH works in the field of Computer Aided Engineering (CAE) and offers services and simulation tools for small and medium enterprises. Our core competence is knowledge transfer: we bridge the gap between scientific know-how and its application in the industry. With our knowledge from physics, chemistry and the engineering sciences we are able to profoundly support your product development cycle. Numerical Modelling speaks your language and is able to conform to given constraints with respect to time and budget.
We often create so-called customer specific CAE tools in which the scientific knowledge required for your product is embedded. In this form, it is easily deployed within your R&D department and supports actual projects as well as improving the skills of your staff. Ask for our individual consulting service which covers all areas of scientific knowledge transfer without obligation.

FLUXiM AG

www.fluxim.com

FLUXiM is a provider of device simulation software to the display, lighting, photovoltaics and electronics industries worldwide. Our principal activity is the development and the marketing of the simulation software SETFOS which was designed to simulate light emission from thin film devices such as organic light-emitting diodes (OLEDs), thin film solar cells (organic and inorganic) and organic semiconducting multilayer systems.
Our company name FLUXiM is derived from flux simulation. Our software products are used worldwide in industrial and academic research labs for the study of device physics and product development. Check out our references and testimonials for more info. We develop swiss-made software in Switzerland and in addition also provide services such as consulting, training and software development, see services page for more details.

Winterthur Instuments

www.winterthurinstruments.ch

Winterthur Instruments GmbH develops measurement systems for fast non-contact and non-destructive testing of industrial coatings. These measurement systems can be used to determine coating thicknesses, material parameters (e.g. porosity) and contact quality (e.g. to detect delamination). The system is based on optical-thermal measurements and works with all types of coating and substrate materials. Our measurement systems provide the unique opportunity of non-contact and non-destructive testing of arbitrary coatings on substrates.

A.8 Team

The ICP team members as of December 2010 are listed below.

Name	Title	Function
Axthelm, Rebekka	Dr. rer. nat., Dipl. Math.	Research Associate
Bonmarin, Mathias	Dr. sc. nat., Dipl. Ing.	Research Associate
Brossi, Kai	B.Sc. in Systems Engineering	Research Assistant
Gentsch, Adrian	B.Sc. in Systems Engineering	Research Assistant
Hocker, Thomas	Prof. Dr. Chem. Eng.	Lecturer
Kaufmann, Lukas	B. Sc. in Systems Engineering	Research Assistant
Knapp, Evelyne	Dipl. Rech. Wiss. ETH	Research Assistant, PhD Student
Lanz, Thomas	M.Sc. Physics ETH	Research Assistant, PhD Student
Linder, Markus	M.Sc. in Engineering	Research Assistant, MSE Student
Loeser, Martin	Dr. ès. sc. ETH, Dipl. Ing. TUM	Research Associate
Meier, Christoph	Dipl. Ing. FH ZHAW	Research Assistant
Neukom, Martin	B.Sc. in Systems Engineering	Research Assistant
Perucco, Benjamin	M.Sc. in Engineering	Research Assistant, MSE Student
Reinke, Nils A.	Dr. rer. nat., Dipl.-Phys.	Lecturer
Ritzmann, Remo	M.Sc. in Engineering	Research Assistant, MSE Student
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. sc., M.Sc.	Research Associate
Sartoris, Guido	Dr., Dipl. Phys. ETH	Research Associate
Schmid, Matthias	Dr. ès. sc., Dipl. Phys. ETH	Research Associate
Schumacher, Jürgen	Dr. rer. nat., Dipl.-Phys.	Lecturer
Spiess, Esther		Administrative Assistant
Toniolo, Lilian		Administrative Assistant
Züfle, Simon	Dipl. Phys.	Research Assistant

The following visiting scientists were staying at the ICP for some time during 2010:

- Alfred Blaum, Dipl. Phys., Switzerland
- Moe Shibita, IAESTE Exchange Student, Japan
- Pekka Luomo, IAESTE Exchange Student, Turku University, Finnland
- Sung Man (Jack) Lai, IAESTE Exchange Student, The Hong Kong Polytechnic University, Hong Kong, China

A.9 Location

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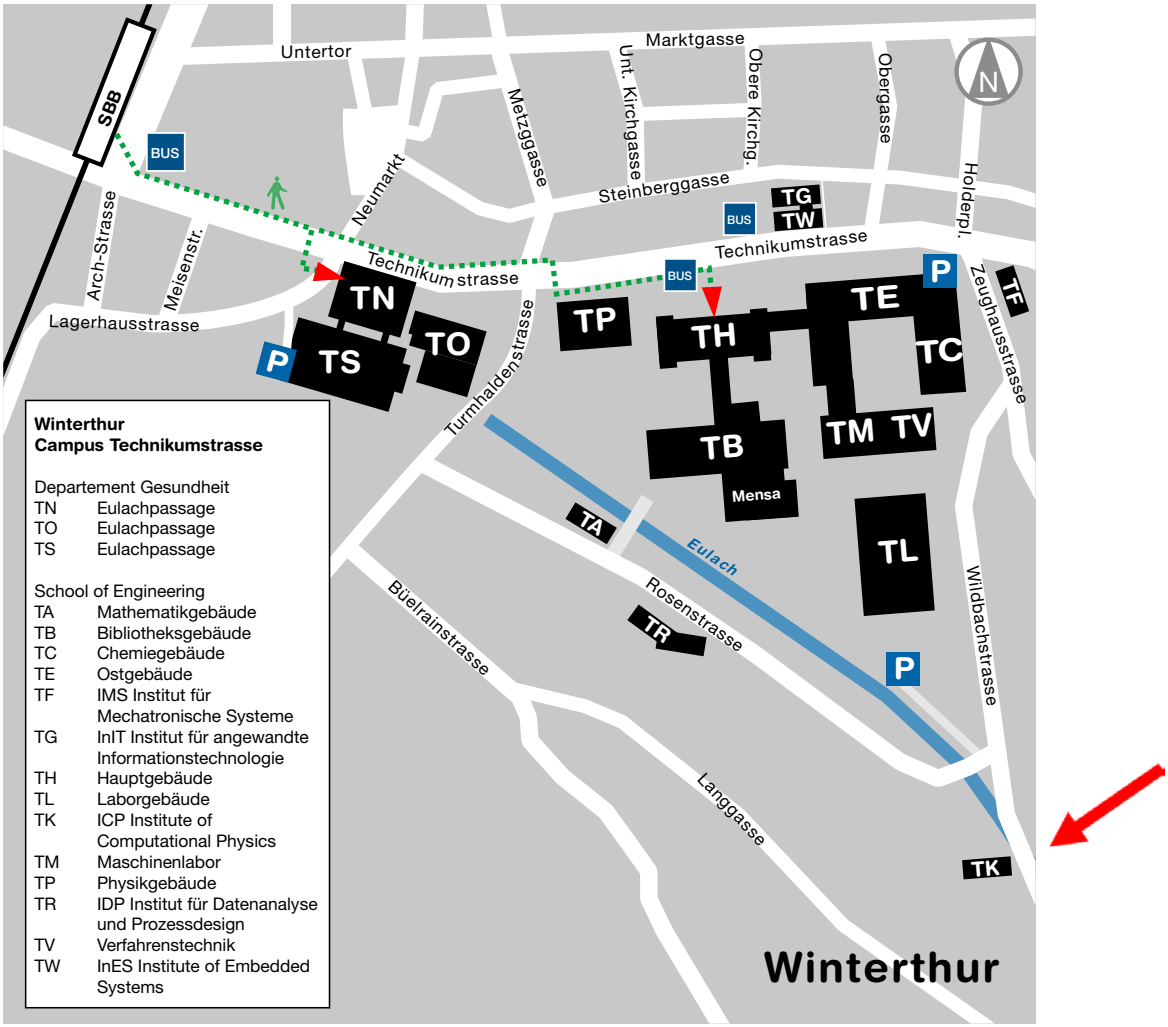

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