Zurich University
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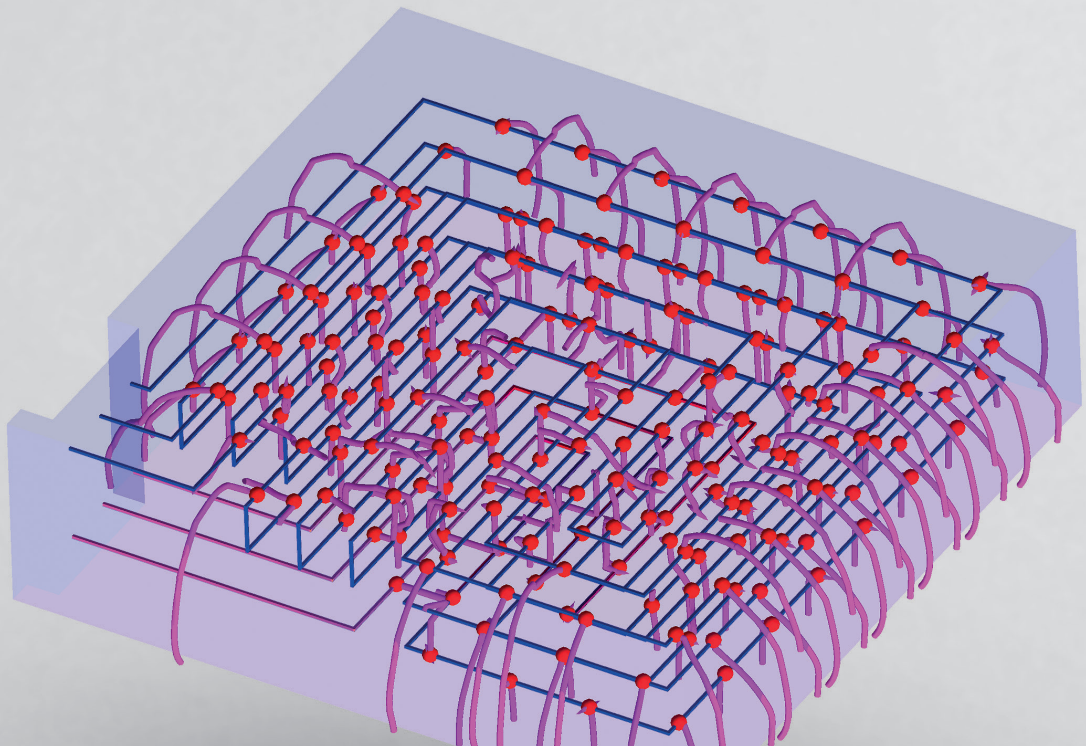
School of Engineering

ICP Institute of
Computational Physics

Research Report 2017



Zurich Universities of
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Research & Development

Short-term thermal flow in the soil of a $30\mathrm{m}^3$ earth collector reservoir during the summer months in order to reuse the stored heat during the heating season.

Kurzzeitige Wärmeausbreitungen im Erdreich eines $30\mathrm{m}^3$ grossen Erdkollektor-Speichers, der in den Sommermonaten solare Wärme im Erdreich einlagert, um sie während der Heizperiode zur Gebäudeerwärmung zu nutzen.

Contents

Vorwort

Digitalisierung, Virtual Reality, Industrie 4.0 und Cloud Computing

Wie geht man um mit den aktuellen Buzzwords? Teils bewegen diese Megatrends viel, da Fördergremien und Industriepartner diese Themen aufnehmen und die Innovation in die entsprechende Richtung vorantreiben. Aus manchen Quellen kommen zu den abgenutzten Schlagworten jedoch nur mittelmässige Beiträge. Letzteres möchten wir vermeiden, und wir tun dies, indem wir unserer Mission treu bleiben: Am ICP möchten wir mit anspruchsvollen Computersimulationen die Physik abbilden. Wir wählen Projekte aus, bei denen die Simulationen einen Mehrwert schaffen.
Wenn wir uns in der industrienahen Forschung engagieren und innovative Lehrkonzepte umsetzen, braucht es ein paar Jahre Zeit, um gute Resultate zu erarbeiten. Man kann also nicht sofort auf die neuesten Leitwörter reagieren. Wir haben früh konkrete Projekte angestossen und ein ansehnlicher Teil der im ICP-Report präsentierten Forschungsergebnisse haben einen entsprechenden Bezug zu den Schlagworten. Oft steuern wir damit ein wichtiges Puzzleteil bei in einer Disziplin, die viele Firmen überfordern, die aber mit zunehmendem Automatisierungsgrad zweifellos immer wichtiger wird.
Das süsse Beispiel zuerst: Industrie 4.0 in der Schokoladeproduktion (Seite 34). Ein Prüfstand zur Analyse der Erstarrung von Schokolade erlaubt die Validierung und Kalibrierung der numerischen Modelle, die zur Optimierung der Produktionsanlagen eingesetzt werden.
Ein weiteres Beispiel ist kickAR (Seite 32): Augmented Reality Tischfussball, bei dem der analoge Spielgenuss 100% erhalten bleibt. Mit Video-Tracking wird jeder Ballwechsel verfolgt und Spielern wie Zuschauern zusätzliche Informationen anzeigt. Als Lehrprojekt und Demoobjekt für die Bewerbung unserer technischen Studiengänge wird unverkrampfte Technikbegeisterung und Innovationskraft vermittelt. Wer es nicht glaubt, merkt es spätestes beim Selbstversuch.
Die hier erwähnten Projekte und viele weitere Beiträge aus dem Forschungsbericht zeigen auf, wie wir uns von den neuen Schlagworten inspirieren lassen und die dadurch entstehenden neuen Ideen und Technologien nutzen. Innovation ist aber untrennbar mit den Menschen verbunden, die sich kreativ und mit Sachverstand einbringen. Die Resultate entstehen in fruchtbarer Zusammenarbeit institutsintern wie auch mit den Projektpartnern. Deshalb ein herzliches Dankeschön an das ganze ICP-Team und Gratulation zu den erfolgreich akquirierten Projekten und den hervorragenden und vielseitigen Forschungsresultaten.

Andreas Witzig, Institutsleiter ICP, April 2018.

1 Multiphysics Modeling

Multiphysics modeling is a powerful tool for exploring a wide range of phenomena, coupling flow, structure, electro-magnetic, thermodynamic, chemical and/or acoustic effects. The past decades have been a period of rapid progress in this area. In fact, a Google search of this neologism returns more than 600'000 results. The possible range of applications has been widely expanded and numerical methods have become increasingly sophisticated and adapted to exploit available computational resources. Today, detailed physical-chemical models combined with robust numerical solution methods are almost a necessity for the design and optimization of multifunctional technical devices and processes.

At ICP, we perform applied research in the field of multiphysics modeling and develop finite element, as well as finite volume simulation software.

Our extensive experience in numerical analysis, modeling and simulation covers nearly all types of micro-macro devices and a wide range of governing equations of classical physics. We also develop single-purpose numerical tools specifically tailored to the needs of our partners, or use commercial software if better suited.

Among our specialities in this context is the application, extension and development of coupled models within our FE-inhouse code SESES, the CFD open-source software openFoam and/or commercial products such as COMSOL Multiphysics.


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1.1 Simulation of heating elements for industrial heat guns

In order to design optimized industrial air heating elements, a simulation model based on OpenFoam® was developed and relevant phenomena, such as heat transfer, temperature dependent fluid- and solid-parameters as well as multi-region characteristics were implemented. The goal of proposing a completely new design option according to customer demands was achieved.

Contributors: M. Boldrini, G. Boiger, T. Hocker
Partners: Leister AG
Funding: KTI/Leister AG
Duration: 2017–2018

Further development of the heating component was based on the findings of the earlier Fusilli geometry, see Fig. 1, which had been developed prior to 2017. Generally, the Fusilli showed strong advantages over the original product, especially in terms of a more homogenous heat flux.

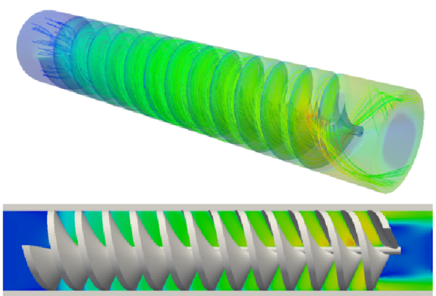

Fig. 1: Fusilli Geometry with velocity field.

However, the main shortcoming of the Fusilli was a relatively high pressure loss compared to the original design. The increased pressure loss resulted from the somewhat tight channels and high number of windings. Another problem with the geometry was that electrically contacting the component on the cold entry side was not possible. Based on these findings, a new type of geometry was developed which was able to overcome all the shortcomings of the Fusilli. Due to the pending patent application of the novel design only the results can be shared without detailing the geometry itself. Compared to the original product and the Fusilli, the new type of geometry showed a strong improvement on the pressure loss, as seen in Fig. 2. This improvement was achieved without a significant increase in local maximum heat fluxes. Additionally, the new geometry features a very homogeneous heat flux distribution.

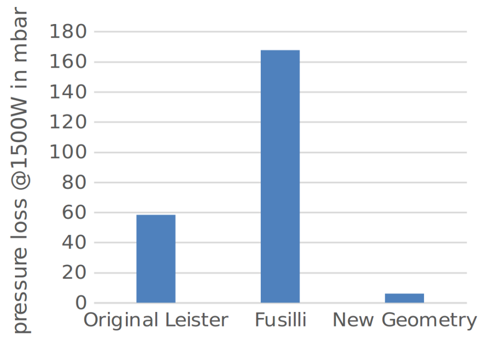

Fig. 2: Simulated pressure loss of different types of Geometries at a power input of 1500 W and corresponding air flow rates.

Another improvement compared to the original product and the Fusilli was achieved in terms of the maximum relative temperature difference within the geometry, see Fig. 3.

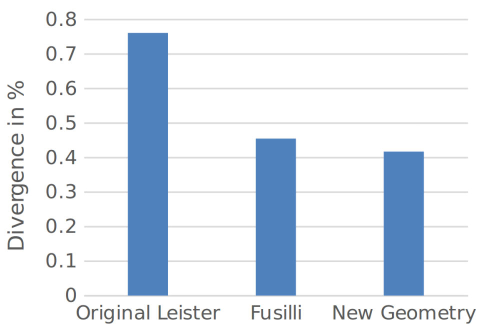

Fig. 3: Maximum relative temperature distribution over the geometries.

The latter advantage leads to a reduction of thermal stresses, which will lead to a longer lifetime of the component.

1.2 Simulation of agitation stress during pharmaceutical development

Agitation stress tests are a common way to test if a pharmaceutical drug can sustain the conditions during transport. In a vehicle such as a truck, the fluid is subject to vibrations and certain fluid structures are excited. The goal is to determine which flow structure are most harmful to the drug.

Contributors: D. Brunner, G. Boiger
Partners: F. Hoffmann-La Roche Ltdl
Funding: F. Hoffmann-La Roche Ltdl
Duration: 2017–2018

Agitation stress tests are essential during the development procedure of a pharmaceutical drug. These tests are supposed to represent the conditions during transport in different vehicles such as trucks, ships or aircraft. In all vehicles, there will be characteristic vibrations with different intensities at different frequencies. In this study, we compare two different shaker types, which are commonly used within the EU for stress tests on pharmaceutical fluids, representing the conditions in the vehicles:

- Vibration table (vertical excitation);
- Horizontal shaker (excitation normal to gravity).

Both shaker types yield different flow patterns. The vibration table shows a standing wave, where the acceleration is normal to the surfaces. These waves are called *Faraday Waves* [1] and only appear above a certain threshold of the excitation amplitude. At lower frequencies (<30 Hz), three different modes were experimentally as well as computationally (CFD simulation) observed. The structures of these modes are shown in Fig. 1.

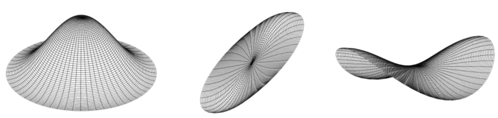

Fig. 1: Shape of surface wave mode 1 (left), 2 (middle) and 3 (right). [1]

On the horizontal shaker three different frequencies (70 rpm, 140 rpm, 200 rpm) were tested at a constant amplitude of 1cm of the deflection. All frequencies show a flapping motion with increasing intensity as the frequency increases. The flow structures at the end positions (left and right) are shown in Fig. 2 for 140 rpm. There is a good agreement between simulations and experiment.

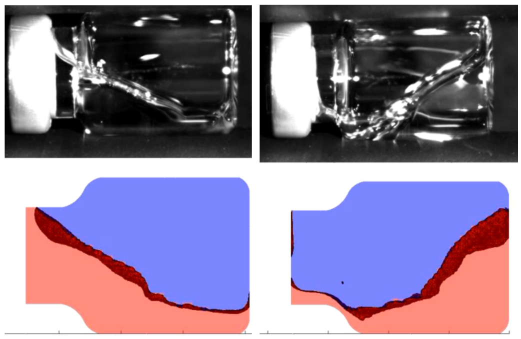

Fig. 2: Comparison of horizontal shaker at 140 rpm, amplitude 1cm, ETOH, state at max deflection (left and right).

The shear stresses of the two shakers have been compared. It has been found that the stresses increase with frequency at the horizontal shaker. In case of the vibration table, the shear stresses of mode 2 (flapping motion) are the most harmful. The stresses are approximately five times higher than for the other modes.

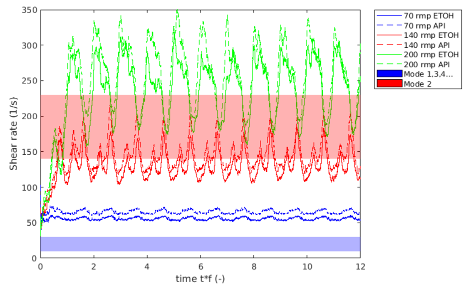

Fig. 3: Comparison of experimental data and derived models of tube sensor.

Literature:

[1] W. R. Batsom, Faraday Waves in Small Cylinders and the Side Wall Non-Ideality, University of Florida, 2013.

1.3 Modeling of electrostatic powder spray coating

Electrostatic powder spray coating is a widely used method to improve surface properties, by adding a protective layer onto the functional surface of a bulk material. A solver has previously been developed to predict the aerodynamics, electrostatics and particle dynamics effects within powder coating applications. Furthermore, an experimental procedure is being developed to validate the model and investigate several crucial factors affecting the final quality of the coating.

Contributors: B. Siyahhan, M. Boldrini, B. Rutz, N. Reinke, G. Boiger
Partners: Wagner International AG
Funding: Wagner International AG
Duration: 2014–2019

The experimental validation to be used for the flow solver developed previously [1], is for a flat plate configuration. The coating pistol is assembled on a mobile platform, which is free to traverse a rail to adjust its distance from a fixture supporting the substrate. The holder designed specifically for the plate provides angle adjustment with increments of 22.5° through the incorporated spokes (see Fig. 1).

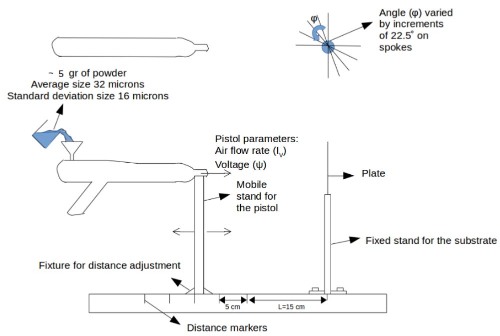

Fig. 1: The experimental set up with the variables, voltage, air flow rate, distance and angle.

It is desired to investigate the effect of voltage and air-flow rate of the pistol in addition to the distance to the substrate as well as the angle between the normal to the plate and the pistol. In order to achieve a comparison between the experimental results and the simulations, two parameters have to be tuned on the flow solver, namely the surface charge per unit area of the particles and the factor governing the effect of turbulence on the local flow velocity. The effect of varying the first parameter can be seen in Fig. 2. Here it can be observed that with high surface charge values, the electrostatic force will be more dominant than flow- and gravitational-effects and the particles will follow almost a straight line, projecting the nozzle shape onto the plate.

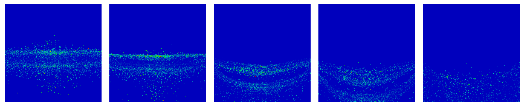

Fig. 2: Simulations with surface charge decreasing from left (1e-5 C/m^2) to right (1e-7 C/m^2).

An additional impact factor on particle movement was included in order to account for the random component of local flow velocity due to the turbulence field. It must be mentioned that the flow field has been obtained from a RANS model, which solves for the turbulence kinetic energy and the dissipation rate. From the turbulence kinetic energy with the assumption of isotropic turbulence, one can obtain

$$k=\frac{1}{2}\left(\overline{u'^2}+\overline{v'^2}+\overline{w'^2}\right)\overset{isotropic}{\Rightarrow}k=\frac{3}{2}\left(\overline{u'^2}\right)\Rightarrow|u'|=\sqrt{\frac{2}{3}k}$$
$$\vec{U}_{local}=\vec{U}_{av}+\gamma_k|u'|\vec{r}$$

Here the local velocity is a combination of the average velocity, Uav, the magnitude of the fluctuating component of the velocity u', a random unit vector r, and the turbulence kinetic energy factor γ_k. The charge per unit surface area of Shape of surface wave mode 1 (left), 2 (middle) and 3 (right) the particles and the kinetic energy factor will be determined based on the benchmark case where the plate distance is at 25 cm, angle 0°, the voltage varies from 15-100 kV and the air flow rate is 3 m^3/h.

Literature:

[1] G. Boiger, Euler-Lagrangian Model of Particle Motion and Deposition Effects in Electro-Static Fields based on OpenFoam, *Int. J. Multiphys.*, Vol. 10 (2), 2016.

1.4 Implementation of a batch production management using the example of Kistler Instruments Corp.

Kistler Instruments Corp. is a global leader in dynamic measurement technology for measuring pressure, force, torque and acceleration. Kistler makes a big effort moving towards digitalization and value chain transformation within the context of Industry 4.0. This journey starts with automation of processes and supply chain optimization. Therefore the possibility of coversion of the whole production to batch management in order to allow traceability has been evaluated.

Contributors:	H. Sotnikova, N. Reinke, K. Unzicker
Partners:	Kistler Instruments Corp.
Funding:	MSE
Duration:	2017–2018

Nowadays it is difficult to imagine any competitive enterprise aiming for growth and sustainable success without making an effort to introduce relevant data analysis. Production processes, in which the key data is continuously stored, analyzed and shared within the enterprise, help managers to make business and product decisions. Therefore, the process of moving towards the big data culture has been started in the Kistler Instruments Corp. Kistler has a know-how technology, focus on the further development and organization-wide commitment to quality. With this goal, the complete conversion of production into batch management, which offers the possibility of traceability over the entire supply chain has been checked. It allows prediction of damaged goods production in order to minimize recall costs, enables the batch allocation of recorded process data, as well as the analysis of quality problems and forms the basis for the introduction of MES with traceability.

The current production structure and technical possibilities for conversion have been analyzed based on three representative production groups: force sensors, RMS sensors and electronic devices. Technical and economic criteria have been used in order to evaluate the feasibility of the three different variants of the batch management. The extra time requirement has been calculated with the developed VBA tool, which can be used for further analysis with verified assumptions in the pilot project.

The results show that most of the extra time for the introduction of the batch production management is required for the set-up and inventory corrections. The source of high time consumption in warehouse shall be studied and reduced. In order to reduce the challenge of finding quality people at a reasonable cost, warehouse has become more efficient, automatized and standardized in order to reduce the human factor and back postings, scope of other errors. The most suitable variant for the realization in pilot project was considered Variant 3 with reasonably selected batch-production items, which requires 2 man-years extra. The introduction of 100% batch production management to allow full traceability up to the raw materials was found to be not economically feasible

Fig. 1: Kistler Force Sensor 9021A.

Literature:

[1] M. Barker, J. Rawtani, Practical Batch Process Management, 2005.

[2] G. F. Kaminske, Handbuch QM-Methoden, 2012.

[3] C. L. Smith, Control of Batch Procceses, 2014.

1.5 Crystal polymorphism, a micro-macro approach

Solidification phenomena observed in nature and industries involve different crystal forms that affect the thermo-physical properties of the materials. The quality of the product is not influenced only by the statement of macro-scale observation. Several static and kinetic effects are micro-scale players making departure from local thermodynamic equilibrium and change the properties of the bulk material. A new coupling model describing the interaction between macro and micro effects is formulated providing a consistent physical insight on undercooling phenomena that could be caused by grain curvature, attachment kinetics to the solid surface and solute trapping at the interface of melt and micro-grains

Contributors: Y. Safa, T. Hocker
Partners: IFNH ETHZ, and several industrial partners
Funding: Innosuisse
Duration: 2016–2018

In molding processes, an interaction between thermodynamic and kinetic effects takes several aspects. For instance, a high cooling rate of some materials from its melt phase promotes the growth of unstable crystal forms with limited latent heat release. On the contrary, a low cooling rate promotes the growth of stable crystal forms accompanied by a large release of latent heat. Furthermore, interconversion between different crystal polymorphs can be modeled as reaction equations with kinetic parameters (e.g. reaction constants) depending on the transition temperatures between phases in melt-crystals mixture. Another aspect from aforementioned interaction is expressed by the undercooling of the liquid phase below the melting point. This undercooling presents a departure from local thermodynamic equilibrium and could be observed under the conditions of high cooling rate; it is mostly attributed to the kinetic condition of the crystal growth. For instance, a strong attachment kinetic to the solid surface and a limited diffusion of the solute rejected from solid to melt (solute trapping on the interface) promotes kinetic undercooling. This in turn affects (decreases) the energy barrier of crystal nucleation and then increases the nucleation rate in the undercooled melt.

In the present work, we treat a phase change coupling energy transfer and mass transformation between different phases. This treatment involves advances in the formulation of numerical approach and physical model. From one side, the use of the developed numerical approach allows to predict the kinetic of crystal polymorphism of solid material undergoing thermal process like cold moulding, tempering and seeding, and further to derive relationships that can aid in process design. On the other side, the undercooling caused by grain curvature, attachment kinetics to the solid surface are analyzed at micro scale to be taken into account through a new coupling model describing the interaction between macro and micro effects. The developed approach in the present work contributes an applicable predictive tool to many industrial applications, as for example, polymer processing, cement manufacturing, food processing (chocolate) and pharmaceutical industries.

1.6 Model order reduction for underground energy storage

The goal of this study is the development of a fast and accurate dynamic model for underground thermal energy storage to be included into the *Polysun* design software.

Contributors: G. Sartoris
Partners: Vela Solaris AG
Funding: ICP
Duration: 2017

If a downhole heat exchanger inside a borehole is generally used as a source of heat combined with a geothermal heat pump, one can also think to use the same system for seasonal underground thermal energy storage, e.g. in summer to recycle the excess of heat collected by solar panels or the excess of electric energy by photovoltaic cells. From a modeling point of view, what is needed is a numerical model capable of yielding correct dynamic answers on the time scale of months with a time resolution of minutes. Such a model is readily available, however, it may require large computational resources not available in an embedded system, hence a model reduction with some loss of information is mandatory here.

Moment matching methods are classical reduction algorithms used for very large linear time-invariant (LTI) systems [1], i.e. well suited for FE discretized problems taken as referential systems. Now, by assuming the heat transport in our storage system is a linear process, the overall linear problem is not LTI due to the *on-off* behavior of the pump, making the velocity a function of time and so changing the *stiffness* or *time-response* of the linear system. However, for the velocity, we just have two possible on&off states, so we can perform two different model reductions and use them accordingly to the activity of their states; the problem is that the two projection spaces are different and switching dynamically between them does not a priori make sense. Hence at the end of each on&off state, we have to perform a lifting to the unreduced system followed by a projection into the next reduced one. This art of handling a piecewise time-dependency is connected to the *temporal localized model reduction* as of [2].

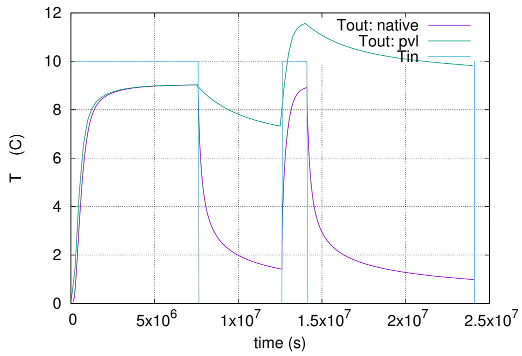

Fig. 1: Failure in computing $T_{\rm out}$ for the localized model order reduction using the *Padé Via Lanczos* approach for each single LTI-system compared to the native FE-model given some input temperature $T_{\rm in}$.

Although we successfully implemented model order reduction for each single LTI-system, we did not yet reach our goal of performing a model reduction for the whole non-LTI but linear thermal energy storage system, see Fig. 1. The reasons have been identified and new ideas already emerged how to solve this interesting problem. Here moment matching methods working in frequency-domain must be necessarily combined with reduction methods working in time-domain.

Literature:

[1] Z. Bai, Krylov subspace techniques for reduced-order modeling of large-scale dynamical systems, *Appl. Num. Math.*, 43, 9–44, 2002.
[2] S. Chaturantabut, Temporal localized nonlinear model reduction with a priori error estimate, *Appl. Num. Math.*, 119, 225–238, 2017.

1.7 Wärmepumpencontroller durch Simulationssoftware angesteuert

Drei magische Buchstaben verändern derzeit die Baubranche: BIM. Sie stehen für Building Information Modeling und bedeuten die umfassende Digitalisierung im Gebäudebereich. Während in einem ersten Schritt die Planungsabläufe neu strukturiert werden, versprechen die technologischen Neuerungen auch die Bewirtschaftung von Gebäuden zu revolutionieren. Diese Forschungsarbeit zeigt auf, wie direkt aus einer Simulationssoftware auf die zentrale Steuerungseinheit des Heizungssystems zugegriffen werden kann. Als wesentliche Erkenntnis wurde ausserdem aufgezeigt, wie mit einem kleinen Stück Software aus einem bestehenden Wärmepumpencontroller ein umfassender Datenlogger wird.

Contributors: R. Grosskopf, A. Witzig
Partners: ETHZ
Funding: Vela Solaris AG
Duration:

Für Neubauten oder Gebäudesanierungen sind die energetischen Anforderungen in den letzten Jahren stetig gestiegen. Komplexere Gebäudetechnik macht Planung und Inbetriebnahme anspruchsvoller, erlaubt aber langfristig eine effizientere Bewirtschaftung. Die Kommunikation zwischen allen Beteiligten an einem Bauprojekt wird neu konzipiert. Gewerkeübergreifend wird eine einheitliche Sprache entwickelt, die unter anderem auch die Simulation enger einbindet und die Programmierung der Gebäudetechnik standardisiert.

Diese Arbeit thematisiert die Umsetzung einer Schnittstelle zwischen der Simulationssoftware Polysun [1] und eines Wärmepumpencontrollers der Firma BS2, der in einem fortschrittlichen Gesamtkonzept eingesetzt wird [2]. Ziel ist es, den Controller direkt mit Hilfe der Software anzusteuern und dem Planer somit einen Zugriff auf die Einstellungen des Controllers zu schaffen. Dies ermöglicht nicht nur die Umsetzung der geplanten Einstellungen bei der Inbetriebnahme, sondern erlaubt eine stetige Aktualisierung, welche für weitere Analysen und Verbesserungen des Systems genutzt werden kann.

Aus den über 130 verfügbaren Parametern des Wärmepumpencontrollers wurden 28 Parameter ausgewählt, wie z. B. die Steilheit der Heizkurve oder minimale Stillstand/Laufzeiten. Die Parameter wurden in mehreren Simulationen in Polysun umgesetzt. Diese sollen schliesslich dem Wärmepumpencontroller übergeben werden. Hierfür konnten teilweise schon bestehende Steuerungen der Software verwendet werden, oder aber der Parameter musste in einer programmierbaren Steuerung umgesetzt werden.
Es wurde eine Übereinstimmung der Parameter aus der Simulationssoftware mit dem Wärmepumpensystem erreicht und eine Spezifikation der Schnittstelle für die programmierbare Steuerung in Polysun erstellt. Im Laufe der Arbeit hat sich zudem die Möglichkeit der Datensammlung des Systems mittels des eingebauten Loggers als höchst interessant erwiesen. In Bezug auf das kürzlich verabschiedete Energiegesetzt EnG und die damit verbundenen Auflagen bezüglich des Monitoring des Energieverbrauchs entstehen hier interessante Möglichkeiten.

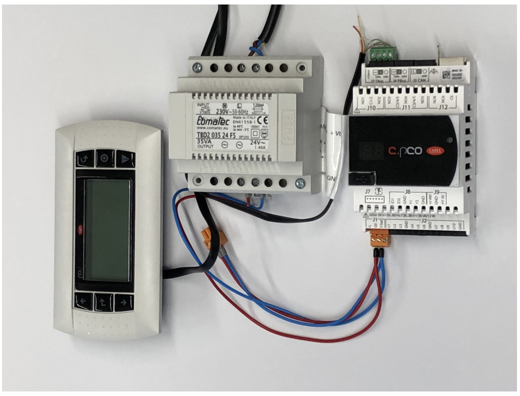

Fig. 1: Im Forschungsprojekt verwendeter Wärmepumpencontroller.

Literatur:
[1] http://www.polysunsoftware.com.
[2] P. Goffin: Evaluation of control strategies for lowEx residential buildings, PhD thesis ETH Zürich, 2014.

1.8 Analyzing the calibration of the Medyria velocity sensor based on an *openFOAM* thermo-fluidic CFD model

The *TrackCath* catheter developed by Medyria AG, Winterthur, has an integrated sensor to measure the flow-velocity and -direction in blood vessels. It has been observed that nominally equal catheters can exhibit significant deviations in their calibration curves. In order to better understand these deviations, a thermo-fluidic CFD model was developed in *OpenFOAM*. The goal was to perform a sensitivity analysis to determine the most influential parameters with respect to the sensor itself and the employed calibration procedure.

Students: L. Ruckstuhl
Category: Master of Science, Semesterprojekt
Mentoring: T. Hocker
Handed In: December 2017

The working principle of the sensor is the constant temperature anemometry (CTA). For a high measurement accuracy each sensor is calibrated separately. This is done by exposing the sensor to a water flow with given velocity and measuring the required electrical power to keep the sensor at a constant temperature. To mimic the calibration procedure in a CFD model, the mesh shown in Fig. 1 was set up. The sensing part of the catheter is represented by a heated surface of the shown cylinder. For accurately calculating the heat transferred over the sensor surface, a high-resolution mesh was employed in this region.

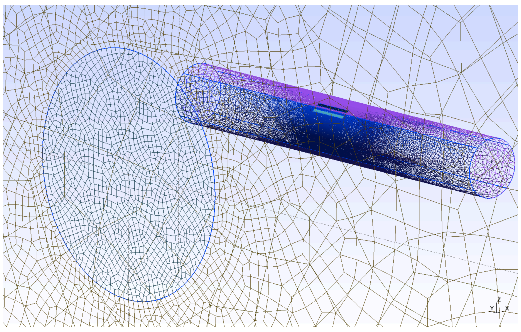

Fig. 1: Mesh used to model the thermal flow around a catheter equipped with the Medyria velocity sensor.

Preliminary simulations shown in Fig. 2 revealed that the calculated and measured thermal powers were of the same orders of magnitude, but major differences could be observed especially at low velocities. Further investigations indicated that the actual sensor temperature deviated from the surface temperature used as boundary condition in the CFD model. Both can be correlated with each other, but this correlation depends on the fluid flow velocity, as shown in Fig. 3. Using the latter led to a significant improvement of the model predictions. As next steps, the heat transfer characteristics predicted by the CFD model will be compared with literature data from [1]. Thereafter a sensitivity analysis of the geometry, improper positioning of the sensor in the crossflow and inaccuracies in the temperature measurements will be investigated.

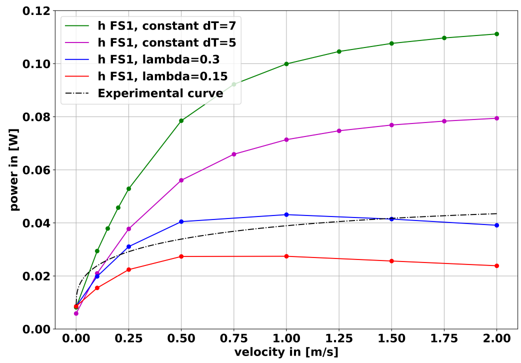

Fig. 2: Heating power versus flow velocity for a constant sensor temperature. Comparison between experimental data and simulation results for different parameter settings.

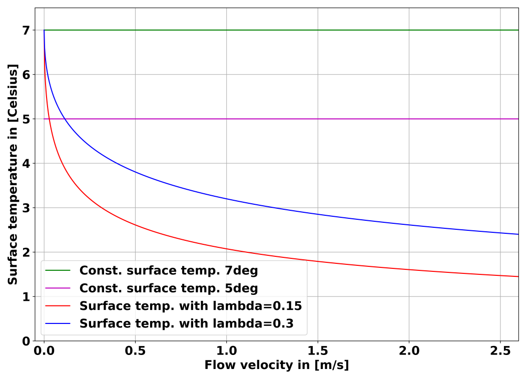

Fig. 3: Different options for correlating the sensor temperature in the model with the real sensor temperature.

Literature:

[1] S. Sanitjai, R. J. Goldstein, Heat transfer from a circular cylinder to mixtures of water and ethylene glycol, *Int. J. Heat. Mass. Tran.*, Vol. 47, 4785–4794, 2004.

2 Fuel Cells and Microstructures

Fuel cells are a prime example of electrochemical cells. They convert fuels such as hydrogen, natural gas or methanol into electrical energy and heat. Fuel cells can be used as a battery replacement in portable electronic devices, for combined production of heat and electricity in households and as electricity source in vehicles. Due to their flat design, fuel cells are easily scalable by connecting them in series to form stacks. Electrical efficiencies over 60 % are feasible which is much higher compared to other decentralized electricity generation technologies. Although the working principle among all fuel cells is the same – i. e. they all are galvanic cells –, they greatly differ in the choice of used materials and feasible operating temperatures.
The ICP supports the progress in fuel cell research by developing multiphysics computer models. In general, modeling helps to better understand the large number of chemical, thermal, electrical, mechanical and fluidic processes with the goal to detect weaknesses of the system and provide design improvements. Often these models rely on detailed information about the microstructures of the investigated materials. Hence the characterization of e. g. electrode and electrolyte microstructures in 2D and 3D is an integral part of our modeling efforts. Since this is a very time-consuming method we started a collaboration with the group of V. Schmidt, Universität Ulm, to use stochastics to generate virtual microstructures with identical properties to real microstructures. This allows one to test and optimize the performance of microstructured materials in a much more efficient way.
In addition to fuel cells, we also do research on novel hydrogen production techniques. For example, we model photo-electro-chemical cells (PECs) which use solar energy to split water and thus produce hydrogen fuel. Most research projects are conducted in collaboration with our strategic partners Hexis AG in Winterthur (SOFC), Paul Scherrer Institut in Villigen (PEFC), EPFL (hydrogen generation) in Lausanne and Universität Ulm (virtual microstructures).


David Bernhardsgrütter


Jürgen Schumacher


Matthias Schmid

2.1 Neuer Modellansatz zur Berechnung von UI-Kennlinien für Festoxidbrennstoffzellen unter Berücksichtigung verschiedener Verteilungen der Brenngasverweilzeit

Die vorliegende Arbeit befasst sich mit der Entwicklung und Anwendung von Modellen zur Simulation von Strom-Spannungskennlinien (UI-Kennlinien) von Festoxidbrennstoffzellen (SOFCs). Ergebnisse eines neuen Modells, das die Verteilung der anodenseitigen Brennstoffverweilzeiten in einer Stack Repeat Unit berücksichtigt, wurde mit früher entwickelten 0D- und 1D-Modellen verglichen. Das neue Modell transformiert den ortsabhängigen Brennstoffverbrauch über einer Zelle durch Verwendung von substanziellen Ableitungen in ein rein zeitabhängiges Problem. Mit diesem eleganten und sehr effizienten Ansatz lässt sich der Einfluss komplexer Brenngasverteilungen auf die Performance der Brennstoffzelle untersuchen und Letztere so optimieren.

Contributors: D. Meier, T. Hocker
Partners: C. Meier, Hexis AG, Winterthur, M. Linder
Funding: Swiss Federal Office of Energy
Duration: 2016–2018

Ausgangspunkt dieser Arbeit ist eine Lagrangesche Betrachtungsweise des Brennstoffverbrauchs in einer SOFC Stack Repeat Unit. Anstatt das Brennstoffzellenmodell für eine reale Geometrie der Strömungskanäle ortsabhängig zu implementieren, wurde hier ein Ansatz verfolgt, bei dem ein *Fluidpaket* mit einer gegebenen Brennstoffzusammensetzung am Eintritt auf seinem Weg durch die Repeat Unit verfolgt wird, siehe Abb. 1. Ist die Verweildauerverteilung des Brenngases aus Messungen oder CFD-Simulationen bekannt, lassen sich so Rückschlüsse auf die entsprechende Brennstoffzellenperformance ziehen.

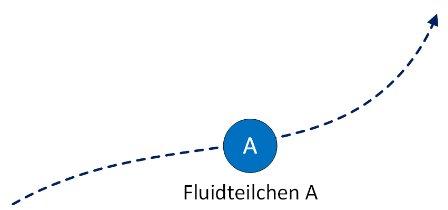

Abb. 1: Lagrangesche Betrachtungsweise des Brennstoffverbrauchs auf der Anodenseite einer SOFC Stack Repeat Unit.

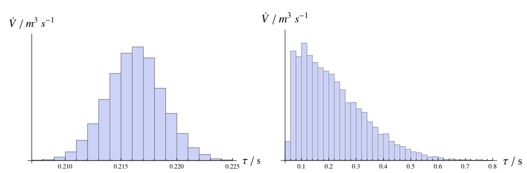

Abb. 2: Verschiedene Verteilungen der anodenseitigen Brenngasverweilzeiten. Links: sehr schmale Verweildauerverteilung nach Gauss, Rechts: breite Verweildauerverteilung gemäss dem CSTR-Modell.

Abb. 2 zeigt zwei theoretische Verteilungen anodenseitiger Brenngasverweilzeiten. Links ist eine sehr schmale Verweildauerverteilung, rechts eine breite, asymmetrische Verteilung dargestellt. Ähnliche Verteilungen lassen sich mit relativ wenig Aufwand für reale Kanalgeometrien aus CFD-Strömungssimulationen generieren.

Abb. 3 zeigt entsprechende Spannungs-Stromkennlinien für eine Brennstoffzelle der Hexis AG, die mit Wasserdampf-reformiertem Erdgas betrieben wurde. Erwartungsgemäss liefert die Repeat Unit mit der engeren Verteilung eine deutlich bessere Performance.

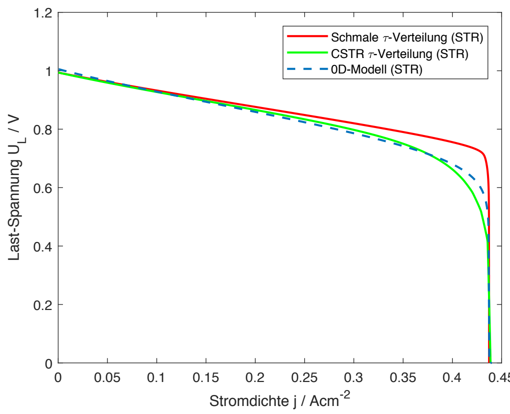

Abb. 3: Simulierte UI-Kennlinien für drei verschiedene Verteilungen von Brenngasverweilzeiten. Rot: schmale Verteilung, Grün: breite Verteilung gemäss CSTR-Modell, Gestrichelt: Verteilung gemäss 0D-Modell.

Literature:

[1] M. Linder et al., *Fuel Cells*, Vol. 11, 573–580, 2011.

[2] M. Linder et al., *J. Power Sources*, Vol. 288, 409–418, 2015.

2.2 Numerical modeling of SOFC electrodes

In this work, we are primarily interested in improving the performance of anode electrodes of high temperature solid-oxide-fuel-cells (SOFC) by means of numerical methods and by fitting electrochemical impedance spectroscopy data (EIS).

Contributors: G. Sartoris, L. Holzer
Partners: Hexis AG
Funding: SNSF
Duration: 2014–2017

Numerical models have been developed for modeling mixed ionic electronic conducting (MIEC) SOFC electrodes, computing impedance spectra and to solve the inverse modeling problem of parameter extraction from impedance data.

One important simplification is based by considering the role of the electrolyte (an ideal Ohmic conductor) as separator between anode and cathode. Since here we just solve for the electric potential, by additionally assuming its value on the electrolyte-MIEC charge transfer interface to be constant, mathematically we can split the modeling problem in three distinct anode, cathode and electrolyte submodels, with the impedance given by the sum of each single submodel's one. Since for the electrolyte the contribution is just resistive; we are left to study the MIEC and gas-channel domains both for the anode and cathode. Actually due to the geometry, the gas-channel is not limiting and we can assume constant concentrations there and so we are left to compute the electric potential, electron and ion concentrations in both MIEC-phases.

Although we have to solve locally for at most three scalar fields, the problem can be ill-conditioned with large gradients and sharp boundary layers showing up at the material interfaces. Therefore, the numerical effort for 3D simulations on imported tomographic topologies is daunting and simplified one- or two-field models are welcome. For each of these models, we have developed robust algorithms for fitting bulk material parameters.

In summary, we have tried to solve the inverse modeling problem of fitting bulk material parameters for SOFC MIEC-materials from impedance spectra. One advantage of this approach is that the analysis accompanying the inverse's evaluation may also help us to select the correct physical models. By comparing the results with published values, we can exclude the suitability of the one-field model and a two-field model approach is actually required. However, this latter is unable to model any contact's physics and a three-field model should be used for this purpose. Here computations show that the contact's model has a strong impact on fitting bulk parameters and therefore should be itself fitted; but at this point it looks like the (inverse) fitting problem is not anymore 100% solvable, i.e. some model parameters must be provided a priori. The fact that with various contact models, we have not been able to correctly reproduce the high frequency peak, gives us the impression that it is not possible to do it without a direct simulation of the contact metal layer, which has not yet been attempted. We also remind that all simulations were done for 2D domains and for 3D ones, an insurmountable ill-conditioning excludes a priori solving the inverse problem.

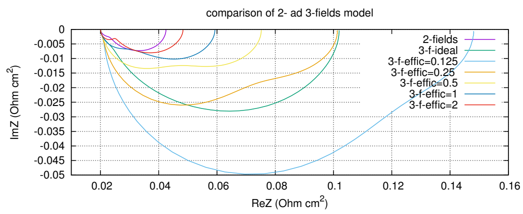

Fig. 1: Nyquist plots of impedance spectra for 2- and 3-field models, the latter for various contact's models.

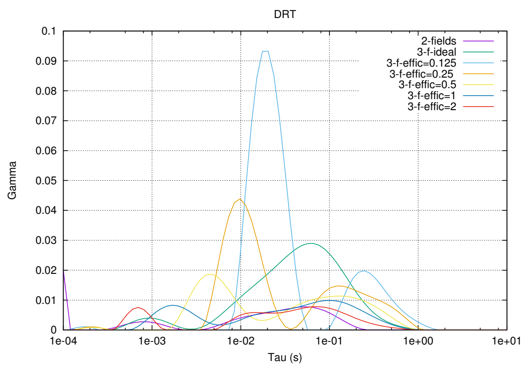

Fig. 2: Distribution of relaxation time for the impedance spectra to better spot single physical processes.

2.3 Standalone open-source implementation of a steady-state two-phase PEFC model

In almost three decades of polymer electrolyte fuel cell (PEFC) modelling, a large number of numerical models have been developed in science and industry, but almost none have been made publicly available. In this project, we have developed the first open standalone implementation of a full-blown, two-phase, macro-homogeneous membrane electrode assembly (MEA) model for PEFCs. It implements the most dominant through-plane transport processes of charge, energy, gas species and water in a five-layer MEA.

Contributors: R. Vetter, J. Schumacher
Partners: Paul Scherrer Institute (PSI)
Funding: SNF, NRP 70
Duration: 2014–2018

As of 2017, there are two freely available open-source programs capable of simulating the state of the art in PEFC modeling at the cell scale: OpenFCST [1], a highly capable finite element package consisting of more than 120.000 lines of C++ code (not counting library dependencies) published under the MIT license, and FAST-FC [2], a finite volume tool built on top of OpenFOAM, consisting of about 12.000 lines of code (not counting the required OpenFOAM itself) published under the GNU GPL v3. Both of these codes are very heavyweight, in particular since they have library dependencies with many hundred thousand lines of code each. In addition to these usability limitations, the GNU GPL can pose an insurmountable legal barrier for commercial use of FAST-FC in industrial applications. In this project, we have developed the first open standalone implementation of a full-blown, steady-state, non-isothermal, two-phase, macro-homogeneous MEA model for low-temperature PEFCs [3]. It includes the most essential through-plane transport processes occurring in a five-layer MEA (Fig. 1): the transport of charges, thermal energy, gas species and the different phases of water. This results in eight coupled non-linear partial differential equations of second order, which are numerically solved together. The focus is on code simplicity, compactness, portability, transparency, accessibility and free availability. The model is implemented as a standalone MATLAB function and it utilizes MATLAB's default boundary value problem solver. With a total length of less than 400 lines of commented code and simulation runtimes in the order of a few seconds, our program offers great advantages over existing open-source solutions. Moreover, it will be released to the public under a license that is compatible with the BSD-3 license, permitting unrestricted use for commercial and non-commercial purposes.

An example output of the program is shown in Fig. 2 for a typical modern PEFC under operating conditions similar to those found in automotive applications.

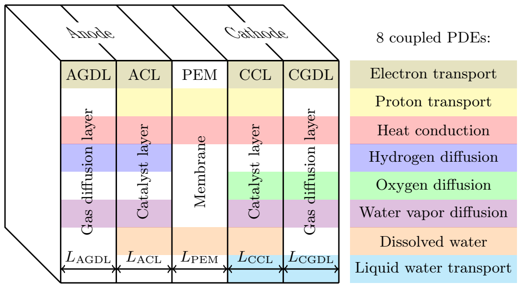

Fig. 1: Sketch of the geometry of the 5-layer MEA model (not to scale) and the simulated transport processes.

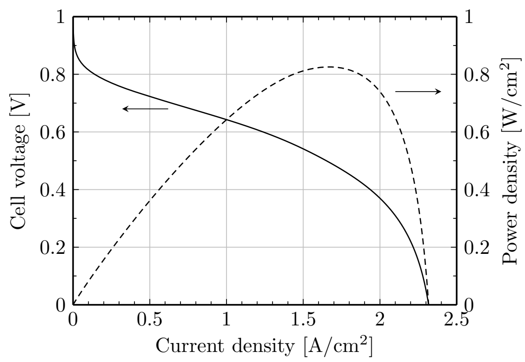

Fig. 2: Simulated polarization curve of a differential PEFC at 80°C, 2 bar and 90% relative gas humidity.

Literature:
[1] M. Secanell et al. *ECS Transactions*, 64, 655–680, 2014.
[2] D. B. Harvey, J. G. Pharoah, K. Karan, https://www.fastsimulations.com.
[3] R. Vetter, J. Schumacher, submitted to *Comput. Phys. Commun.*.

3 Organic Electronics

Organic semiconductors have received great attention since 1987 when organic light-emitting devices were invented by leading scientists at Kodak USA. After 30 years of R&D and commercialization efforts world-wide, we are now witnessing a wide range of OLED displays in consumer products ranging from mobile phones to 77-inch TVs. The particular advantages of OLEDs is their thin construction, large viewing angle, color gamut and high energy conversion efficiency. OLEDs consist of a sequence of thin organic semiconductor layers placed in-between two metallic electrodes. Organic semiconductors have equally gained attention as strong light absorber and charge transport materials in organic solar cells, with which flexible PV modules can be built. In recent years, organic semiconductors have also been key to the ground-breaking hybrid organic-inorganic perovskite solar cell technology, which is the hottest emerging photovoltaics technology and shows great potential for LED applications, too. Further into the invisible range of electromagnetic waves, terahertz photonics is a growing technological field for non-invasive diagnostics applications. The ICP carries out R&D in the field of OLED, OPV, perovskite PV and non-linear optical crystals for terahertz photonics technology by employing multi-physics computer models and devising novel measurement systems. In the laboratory of the ICP, we fabricate OLEDs and novel solar cells on a small scale for R&D purposes and are setting up a terahertz photonics measurement system. We focus on device and material characterization methods by a combination of advanced measurement and simulation technology. This chapter gives an overview on ongoing R&D projects carried out in this interdisciplinary research field of the ICP.


Balthasar Blülle

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Markus Regnat


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Tobias Bach

3.1 Verbesserte Lichtausbeute in organischen Leuchtdioden dank einer neu entwickelten Streuschicht

Im Rahmen des Forschungsprojektes FlexOLED wurden Materialien, Messgeräte und Simulationssoftware entwickelt, um die Energieeffizienz von organischen Leuchtdioden (OLEDs) zu verbessern.

Contributors: M. Regnat, T. Beierlein, B. Blülle, M. Diethelm, M. Jazbinsek, K. Lapagna, K. Pernstich, B. Ruhstaller
Partners: Avantama AG, PV-LAB (EPFL), ZPP (ZHAW), Fluxim AG
Funding: KTI
Duration: 2015–2018

Immer mehr Bildschirme, Handy-Displays und neuerdings auch Beleuchtungslösungen werden heute aus organischen Leuchtdioden (OLEDs) gefertigt. Dazu werden dünne Schichten verschiedenster Halbleitermaterialien so kombiniert, dass die beim Anlegen einer Spannung bewegten Ladungsträger rekombinieren und Licht erzeugen. Ein Teil dieser Strahlung wird jedoch wegen des unterschiedlichen Brechungsindexes zwischen den einzelnen Schichten totalreflektiert und bleibt innerhalb der OLED gefangen.

Im Rahmen des FlexOLED-Projektes wurden neue Materialen entwickelt, die helfen mehr des in einer OLED erzeugten Lichts an die Umgebung abzustrahlen. Dazu wurde eine zusätzliche Schicht entwickelt, welche zwischen dem Trägersubstrat und der eigentlichen OLED aufgebracht wird und das Licht streut. In dieser Streuschicht sind einerseits Nanopartikel eingebettet um den effektiven Brechungsindex zu erhöhen und andererseits sorgen ebenfalls eingebettete Mikropartikel für eine effektive Streuung des Lichtes auch bei grossen Winkeln, welches ansonsten totalreflektiert würde. Die neuartigen Streuschichten wurden von der Firma Avantama entwickelt und anschliessend im Labor der ZHAW getestet.

Die Entwicklung einer solchen Streuschicht wäre ohne geeignete Simulationssoftware kaum möglich gewesen. Mithilfe von Simulationen konnten nämlich die optimalen Materialparameter gefunden werden. Denn für ein optimales Ergebnis werden je nach Aufbau der OLED unterschiedliche Schichtdicken und Partikelkonzentrationen benötigt. Am ICP wurden in Zusammenarbeit mit der Firma Fluxim neue Softwarealgorithmen entwickelt, mit welchen diese optimalen Materialparameter gefunden werden konnten.

Durch die Herstellung von eigenen OLEDs mit den internen Streuschichten konnte deren Entwicklung wesentlich verbessert werden. Durch das Testen der Schichten unter realen Bedingungen wurden Schwachstellen erkannt und die Materialkombinationen konnten weiter optimiert werden. Wichtiger Bestandteil einer OLED ist insbesondere eine transparente Leiterschicht. Das dazu benötigte Material ist schwierig in guter Qualität abzuscheiden. Im Zuge dieses Projektes wurde an der EPFL auch ein neuartiger transparenter Leiter entwickelt der ohne das wertvolle Edelmetall Indium auskommt. Die restlichen Schichten der OLED wurden im hauseigenen Labor des ICP hergestellt.

Die internen Streuschichten beeinflussen die Winkel, unter denen das Licht der OLED abgestrahlt wird. Generell ist dieses Abstrahlverhalten ein wichtiges Kriterium und in dieser Arbeit wurde ein Messgerät entwickelt, um das winkelaufgelöste Abstrahlverhalten von OLEDs zu messen. Dazu wurde ein Prototyp an der ZHAW (ICP und ZPP) entwickelt, der von der Firma Fluxim zur Serienreife weiterentwickelt wurde (Abb. 1). Der Erfolg dieses Projektes lag mitunter darin, dass die gesamte Kette in der Entwicklung von den beteiligten Partnern abgedeckt wurde, also von der Materialentwicklung über die Optimierung der Materialparameter durch Simulation, bis zur Herstellung und Charakterisierung eigener Proben zum Verifizieren der erwarteten Spezifikationen.

Abb. 1: Vom Prototyp zum Produkt: Das im Projekt entwickelte Messgerät PHELOS zur Bestimmung des winkelaufgelösten Abstrahlverhaltens von OLEDs.

3.2 Understanding physical processes in Perovskite solar cells and OLECs

Perovskite is a promising material for solar cells. Devices show record efficiencies of more than 20 %, which is almost twice the conversion efficiency reached by organic solar cells. With the aid of numerical simulations and measurements the ICP aims at understanding these devices in more detail. Ionic transport is a key ingredient for a realistic simulation. The devices are in terms of simulation related to organic light-emitting electrochemical cells (OLECs).

Contributors: E. Knapp, M. Neukom, A. Schiller, B. Ruhstaller
Partners: EMPA, Fluxim AG
Funding: CTI
Duration: 2016–2019

The name of the Perolec project is composed of the two words ”perovskite” and ”OLEC” since the project aims at developing simulation and measurement tools for the emerging perovskite solar cells and organic light-emitting electrochemical cells. It is assumed that the two types of devices have ion transport in common, in addition to electron and hole transport. Ion transport is relatively slow in comparison with electron and hole transport. This behaviour requires an adaptation of the measurement system to record a time-dependent response from microseconds to minutes. To fully characterize the devices, measurements from high to low frequencies are necessary. The frequencies can be so low, that the experiments take from several hours up to some days. Intrigueing features such as negative capacitance or an inductive loop can be observed at low and mid frequency in impedance spectroscopy. An example of a measured inductive loop is shown in Fig. 1.

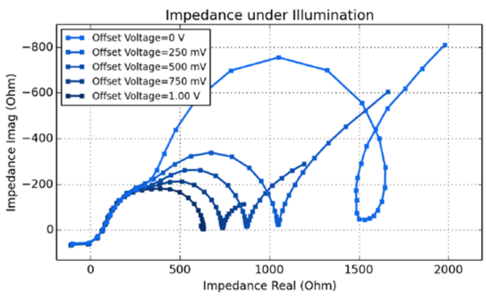

Fig. 1: Measurement of the impedenca spectra. At mid-frequency an inductive loop occurs.

For the simulation, a 1D model is used where a set of five partial differential equations is solved. Charge transport of ions differs from electrons and holes in terms of the low mobility of charge carriers and boundary conditions. The simulation can be performed in steady-state, time-dependent and as small signal analysis. The simulation helps to understand the physical processes taking place in the device. In Fig. 2 the inductive loop as displayed in Fig. 1 is reproduced by simulation. The inductive loop depends on the ion mobility.

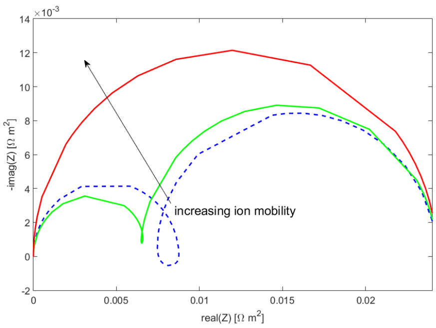

Fig. 2: Simulation of the impedance spectra in qualitative agreement with measurements shown in Fig. 1. A variation of the ion mobility shows an significant impact on the inductive loop.

The collaboration with the ICP spin-off Fluxim allows for the implementation of the new tools into the simulation software Setfos and the integrated measurement solution Paios. Both are commercially available and widely used by customers. The research partner EMPA fabricates OLECs and perovskite solar cells, which are then measured at ICP and Fluxim to test and validate the new tools. With the Perolec project, the ICP contributes to an emerging field in academic and industrial research.

3.3 High-power THz photonics based on molecular crystals

In this Korean-Swiss joint research project, we aim at developing next generation high-power THz sources delivering ultra-broadband, as well as narrowband tunable radiation based on organic molecular crystals. The ICP is developing theoretical and numerical models to support molecular crystal development at Ajou University (Prof. O-P. Kwon) and experimental high-power THz-wave generation demonstrations at PSI (SwissFEL Laser Group, Prof. C. P. Hauri).

Contributors: M. Jazbinsek, U. Puc
Partners: PSI-SwissFEL, Ajou University
Funding: SNSF, NRF
Duration: 2016–2018

THz photonics is a growing research field and future scientific and technological breakthroughs rely strongly on advanced THz sources. Highly nonlinear optical molecular crystals offer unique advantages for THz-wave generation compared to alternative methods. However, phonon-induced absorption of most organic crystals in the THz region leads to undesired modulation of the spectrum and limits the THz output efficiency. To overcome such drawbacks, phonon-mode engineering by modification of molecular structures has been suggested as one possible solution. [1] We propose an efficient alternative approach for generating intense broadband THz waves based on a tandem configuration that combines two complementary nonlinear organic crystals [2]. The ICP developed a theoretical model for the proposed tandem cell, which has been successfully confirmed in the THz experiment performed at KAIST, based on the crystal tandem cell produced at Ajou University. Such configuration compensates for the spectral gap of the generated THz waves and additionally enhances the optical-to-THz conversion efficiency. As a result, such tandem configuration provides a versatile platform to generate gapless broadband THz spectra with suppressed phonon absorption and contributes to advancing the development of intense broadband coherent THz sources.

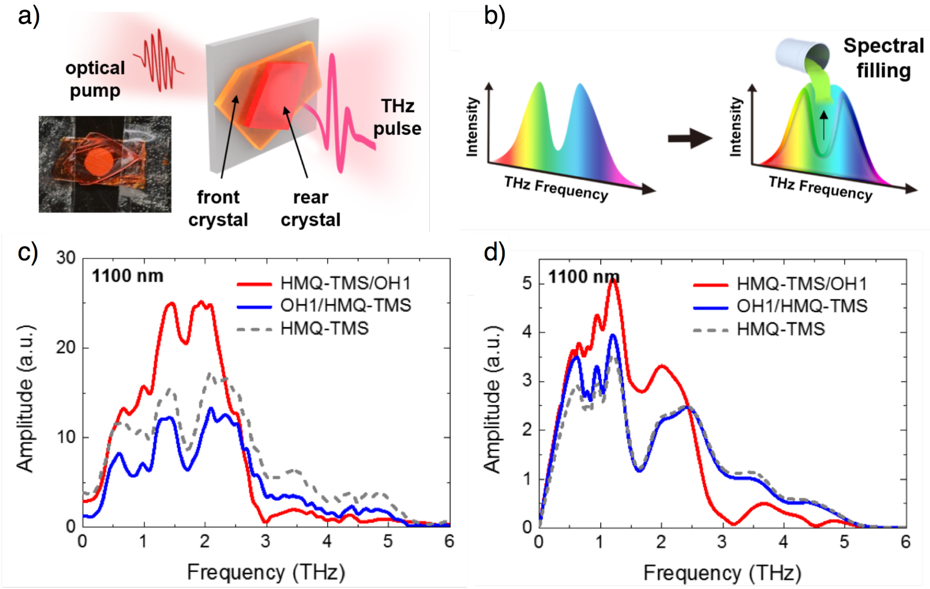

Fig. 1: (a) A schematic diagram of organic tandem THz generator based on two distinct crystals (HMQ-TMS and OH1 crystals) and photography of a tandem crystal. (b) Conceptual diagram of spectral filling by a tandem THz configuration. Distribution of the THz spectral amplitude generated in parallel tandem configurations at the pump wavelength of 1100 nm: (c) Experimental and (d) theoretical results for a single HMQ-TMS crystal and a tandem with OH1. For the tandem configuration with the rear OH1 crystal (solid red curve), the phonon mode gap at about 1.5 THz of a single HMQ-TMS crystal is reduced significantly.

Literature:

[1] S. H. Lee, B. J. Kang, B. W. Yoo, S. C. Lee, S. J. Lee, M. Jazbinsek, H. Yun, F. Rotermund, O. P. Kwon, *Adv. Funct. Mater.*, 27, 1605583, 2017.

[2] B. J. Kang, S. H. Lee, W. T. Kim, S. C. Lee, K. Lee, G. Benacchio, G. Montemezzani, M. Jazbinsek, O. P. Kwon, F. Rotermund, *Adv. Funct. Mater.*, 1707195, 2018.

3.4 Ultrabroadband Terahertz spectroscopy and imaging

The goal of this project is to develop a new compact instrument for terahertz non-destructive material testing and characterization. The new system will allow for THz spectroscopic measurements, THz imaging and THz thickness measurements with an ultrabroadband spectral range beyond 15 THz, which is presently not available on the market.

Contributors: U. Puc, M. Krajewski, T. Bach, M. Jazbinsek
Partners: Rainbow Photonics AG
Funding: CTI
Duration: 2017–2019

Organic electro-optic crystals are very promising and efficient THz-wave generation materials. They allow for both very high THz electric fields, exceeding several GV/m using optical rectification of femtosecond laser pulses, as well as the possibility for extremely broad bandwidth extending well beyond 10 THz. However, the usual laboratory THz systems based on these crystals exploit very bulky and expensive Ti:sapphire fs laser systems, which are not desired for industrial THz imaging and spectroscopy applications. We are therefore developing a compact THz time-domain spectroscopy and imaging system based on relatively low-cost and small-size femtosecond fiber lasers operating at telecommunication wavelengths.

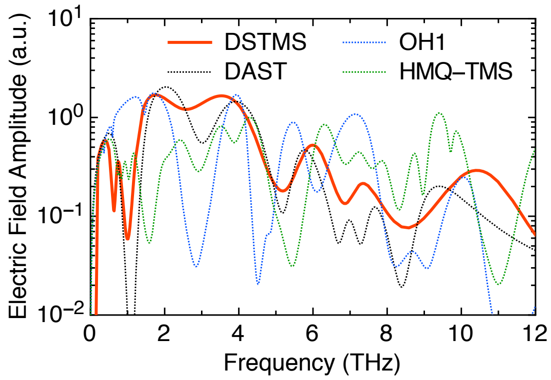

Fig. 1: Theoretical THz electric field amplitude using various state-of-the-art organic crystals using 1560 nm and 50 fs pump pulses and the generation and detection crystals of 0.5 mm thickness.

As the THz generation and detection material, we choose the organic crystal DSTMS (4-N,N-dimethylamino-4'-N'-methyl-stilbazolium 2,4,6-trimethylbenzenesulfonate), since it reaches the highest overall efficiency and the flattest spectrum among the presently known state-of-the-art organic crystals (Fig. 1).

We use a very compact commercial femtosecond laser from Menlo Systems with pulse length of 40 fs, 190 mW average power, 100 MHz repetition rate and 1.55 μm wavelength as pump beam. Fig. 2 shows the acquired THz time-domain electric field and the corresponding power spectrum obtained in dry air atmosphere. We achieve a very large frequency bandwidth extending beyond 15 THz, with a high dynamic range of up to 60 dB.

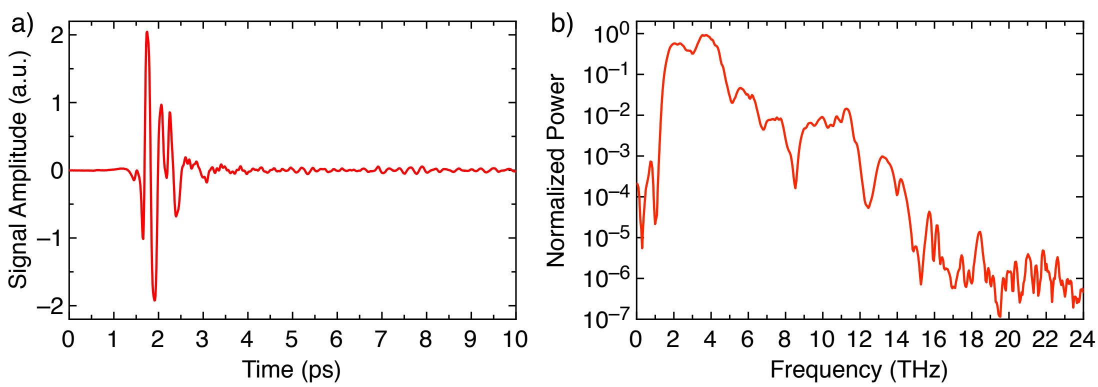

Fig. 2: THz time-domain signal (a) and the corresponding power spectrum (b) of the compact terahertz setup.

3.5 Charge carrier dynamics in organic electronic devices

This project employs different layer architectures such as organic light-emitting diodes (OLED), solar cells, and monopolar devices in order to study charge carrier transport. For this purpose we investigate new and improved measurement techniques in experiment as well as by numerical simulation. We develop reliable parameter extraction methods that are supported by numerical simulations. SNF and DFG give joint funding for two PhD projects.

Contributors: S. Züfle, M.T. Neukom, B. Ruhstaller
Partners: Universität Augsburg
Funding: SNF, DFG
Duration: 2015–2018

Many material parameters in organic electronic devices are difficult to evaluate, especially in complex stack architectures involving many layers. This is why for parameter extraction usually single-layer and unipolar devices are investigated. However, in the complete device the parameters can be different, making the transfer of the results error-prone. This project focusses on the development of new approaches for reliable extraction of charge transport parameters. By combining new experimental methods with drift-diffusion modelling, we aim to achieve these goals.

A promising technique for the determination of the charge carrier mobility is the CELIV (charge extraction by linearly increasing voltage) technique performed on MIS-diodes (metal-insulator-semiconductor). This type of layer stack can be fabricated by adding an insulating layer on top of the material to investigate, thereby ensuring unipolar behavior. We have found that bilayer OLEDs comprising a polar electron transport layer (ETL) show a voltage regime where they behave like a MIS-diode in accumulation. Therefore, the MIS-CELIV technique can be employed to determine the hole mobility in the hole transport layer (HTL).

Temperature-dependent MIS-CELIV curves can be used to determine the thermal activation of the charge carrier mobility. By comparing simulation and experiment we could show that this activation energy can be deduced with a relatively small error. Furthermore, by adding temperature-dependent impedance measurements it is also possible to evaluate the injection barrier for holes from the electrode into the HTL. The simulation-based analysis shows that in the impedance experiment both this injection barrier and the mobility activation contribute to the analysed activation energy. Therefore, by combination of the two measurement techniques these parameters can be disentangled.

From the modelling we can give recommendations on how to perform the measurements in order to most accurately determine the mobility. Furthermore, we investigated how reliably the mobility thermal activation can be extracted. From an analysis of consistency between extracted and input activation energy we deduced a correction factor which can then be used for analysing experimental data.

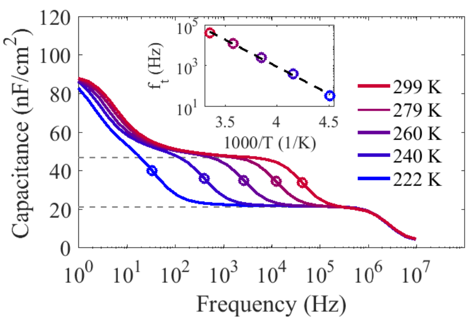

Fig. 1: Measured capacitance-frequency at varied temperature. An Arrhenius analysis of the transition frequency give the activation energy.

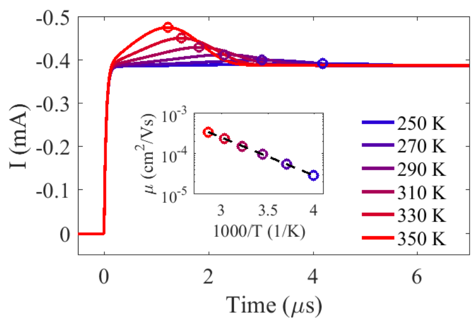

Fig. 2: MIS-CELIV simulation for varied temperatures. The transient peak position is related to the temperature-dependent hole mobility.

3.6 Large-area electrothermal simulation

In organic light-emitting diode (OLED) modules, the electrical conductivity often increases with temperature. The temperature, on the other hand, increases as electric current flows. This positive-feedback effect can be explored in the new thermal module of the simulation software Laoss by Fluxim AG, for which the ICP developed and tested numerical methods.

Contributors: C. Kirsch, S. Altazin, R. Hiestand, M. Regnat, T. Offermans, R. Ferrini, L. Penninck, B. Ruhstaller
Partners: CSEM SA, Fluxim AG
Funding: CTI
Duration: 2016–2018

In large-area thin-film semiconductor devices the electrical sheet resistance of the thin films may adversely affect the charge transport inside the device. Therefore, the applied voltage required to achieve a prescribed electric current increases with the device area. Because the light emission in OLED modules is proportional to the electric current, a lot of energy is required to achieve a high brightness in large-area OLED modules. Also the uniformity of the light emission is an issue in large-area devices. Additional structures such as metal grid lines are sometimes used as a remedy. Furthermore, a larger applied voltage also produces stronger electric fields inside the device, which leads to more heat generation by Joule heating. This in turn may lead to a thermal breakdown of the OLED module.

The new thermal module in the large-area semiconductor device simulation software Laoss by Fluxim AG allows the user to investigate these aspects. The temperature distribution in an OLED module can be simulated, for example, as shown in Fig. 1.

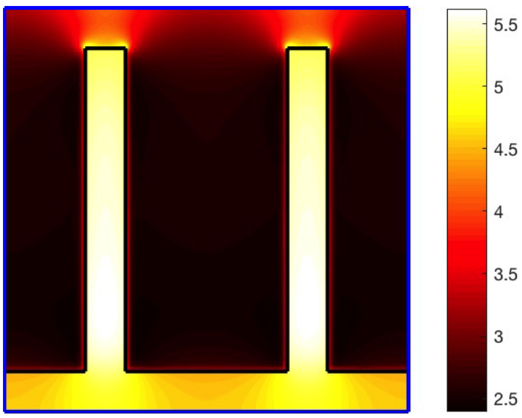

Fig. 1: Temperature distribution inside a $5\,\mathrm{cm} \times 5\,\mathrm{cm}$ OLED module with a busbar and two metal fingers. The values indicate the temperature above the ambient temperature of $300\,\mathrm{K}$.

Such simulations allow the user to identify hot spots inside the device and to explore the effect of various heat dissipation strategies.

For this purpose, the ICP added a thermal model together with an electrothermal coupling to the existing electrical semiconductor device model, which is based on the finite-element method and which employs a coupled 1D-2D modeling approach for computational efficiency [1]. The calculation of the temperature distribution requires an electrical→thermal coupling, in which heat generation occurs due to Joule heating; it arises from the electric fields in the lateral directions inside the (2D) top and bottom electrodes and from the heat generation inside the (1D) semiconductor stack.

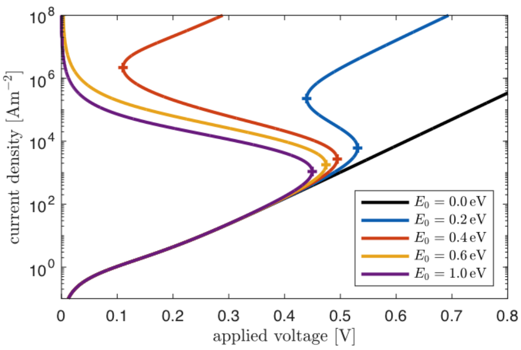

Fig. 2: S-shaped current-voltage characteristics of an OLED device (for different values of the activation energy E_0) due to the thermal→electrical coupling (positive feedback).

Another interesting phenomenon is observed when the thermal→electrical coupling is active. In this case the electrical conductivity in the semiconductor stack increases with the temperature, and because of the Joule heating due to electric current flow there is a positive feedback. This effect leads to an s-shaped current-voltage characteristics of the OLED device (cf. Fig. 2), along which the current density may increase even if the voltage decreases, if the temperature increases at the same time. This phenomenon has been simulated and also measured in OLED devices recently [2].

References:

[1] C. Kirsch et al., Int. J. Multiphys. 11, 2017
[2] M. Liero et al., Opt. Quant. Electron. 49, 2017

3.7 Limits of triplet harvesting in fluorescent organic light emitting diodes

The objectives of this research project are, first, to investigate the mechanism of triplet harvesting in state-of-the-art fluorescence based exciplex organic light emitting diodes (OLEDs) and, second, to investigate and quantify the efficiency limit and roll-off at high excitation as well as the degradation phenomena during prolonged operation of these OLEDs. An electro-optical drift-diffusion model is used to describe and predict the characteristics of the OLEDs.

Contributors: M. Regnat, K. Pernstich, B. Ruhstaller
Partners: Jang-Joo Kim group from Seoul National University, Korea
Funding: SNF
Duration: 2016 – 2018

Fluorescence based OLEDs have particular advantages compared to phosphorescence based OLEDs: lower cost of materials because no precious metals (Ir, Pt) have to be used, long device lifetime, a narrow emission spectra leading to saturated colors, and a better intellectual property landscape. One major drawback, however, is the low efficiency related to the low singlet exciton yield of 25 %. This low efficiency can be significantly increased when the OLED materials are capable of converting (non-radiative) triplet states to emissive singlet states.

In this project we use the abilities at the ICP for advanced OLED device characterization (Paios) and advanced OLED device simulation (Setfos) to investigate the highly-efficient TADF OLEDs with fluorescent emitters, provided by the team of Prof. Jang-Joo Kim from Seoul National University.

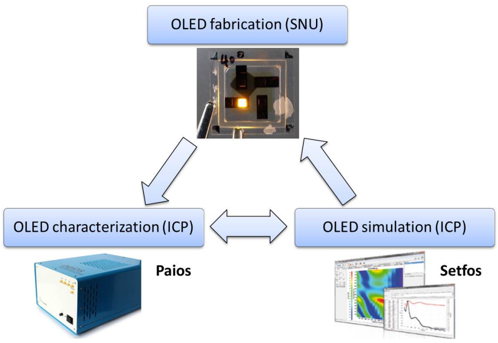

Fig. 1: Project approach for the investigation of high efficient state-of-the-art fluorescent exciplex OLEDs.

Due to the all-in-one measurement tool Paios and new in-house developed add-on measurement setups at ICP, we were able to characterize these OLEDs with several different methods, such as standard current density – voltage curve, impedance and capacitance – voltage measurements, as well as angle-dependent electroluminescence (EL) spectra and temperature-dependent transient EL measurements. Based on the OLED characterization results, an electro-optical drift-diffusion OLED model was established with the simulation software Setfos. Fig. 2 shows the good agreement of measurement and simulation for the example of the temperature-dependent transient EL decay behavior of the OLED after voltage turn-off.

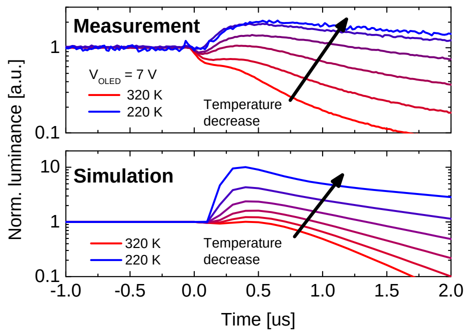

Fig. 2: Measured and simulated temperature-dependent transient EL decay behavior of the OLED after voltage turn-off (t = 0 us).

In Fig. 2 a slower EL decay for decreasing temperature after voltage turn-off (t = 0 us) is observed, which is a typical behavior for OLEDs with triplet harvesting mechanism. The deviation of the peak height in the simulation to the measurement in Fig. 2 indicates that the electro-optical model parameters have to be adjusted and/or new mechanisms added, which is under current investigation. At the end of the project a comprehensive model should be established to describe and predict the OLED efficiency limit and degradation phenomena of this state-of-the-art fluorescence based exciplex OLED, leading to the realization of improved TADF OLEDs.

3.8 Weiterentwicklung des PAIOS-Kryostaten zum marktfähigen Produkt

Im Rahmen einer Projekt- und anschliessenden Bachelorarbeit wurde ein Kryostat entwickelt, welcher als Erweiterung zum PAIOS-System von Fluxim verwendet werden kann, um temperaturabhängige Messungen an OLEDs und Solarzellen durchzuführen.

Contributors: A. Meier, R. Ropelato, M. Neukom, A. Gentsch, B. Ruhstaller, K. Pernstich
Partners: Fluxim AG
Funding: –
Duration: 2016–2018

Um die Proben von organischen Leuchtdioden (OLEDs) und Solarzellen bei unterschiedlichen Temperaturen testen zu können, wurde ein Kryostat als Erweiterung zum PAIOS-Messgerät entwickelt. Bereits während der Projektarbeit und Bachelorarbeit 2016-2017 wurde zusammen mit Dr. Kurt Pernstich und der Firma Fluxim AG ein Prototyp für eine solche Vorrichtung erstellt. Diese wird nun in weiteren Schritten bis hin zum marktfähigen Produkt weiterentwickelt.

In den meisten wissenschaftlichen Aufbauten werden Stickstoff-gekühlte Kryostaten verwendet. Damit erreicht man zwar sehr niedrige Temperaturen (<100 K), das Hantieren mit Stickstoff ist jedoch umständlich. In diesem Projekt werden Peltier-Elemente zur Kühlung verwendet. Diese werden elektrisch betrieben. Dadurch wird die Bedienung des Kryostaten für die Nutzer vereinfacht und die Kosten reduziert.

Die Wärme der Peltier-Elemente wird mit Hilfe eines aktiven Umwälzkühlers abtransportiert. Dieser kühlt die Flüssigkeit im Kühlsystem auf -20 °C. Somit kann die Probenplatte bei stabilen -50 °C gehalten werden. Für Anwendungen die einen weniger grossen Temperaturbereich benötigen, wurde auch eine Variante mit aktiver Luftkühlung entwickelt. Damit kann eine Temperatur der Probenplatte von -20 °C erreicht werden. Für beide Varianten gilt eine maximale Temperatur von +80 °C. Diese wird durch den Anwendungsbereich der Peltier-Elemente begrenzt.

In Abb. 1 wird der aktuelle Stand und ein beinahe marktfähiges Produkt gezeigt. Das Produkt wurde so konzipiert, dass für die Luft- resp. Wasser-gekühlte Lösung nur wenige Teile ausgetauscht werden müssen. Zudem muss für unterschiedliche Device-Layouts der Proben nur eine Platte für die Messstifte neu gestaltet werden. Des Weiteren kann der *Automated Measurement Table* direkt unter den Kryostaten montiert werden. Dadurch können Tests mit Photodetector, Spektrometer, etc. durchgeführt werden, wobei die Messgeräte automatisch gewechselt werden.

Die ersten Geräte sollen bis Ende Mai geliefert werden.

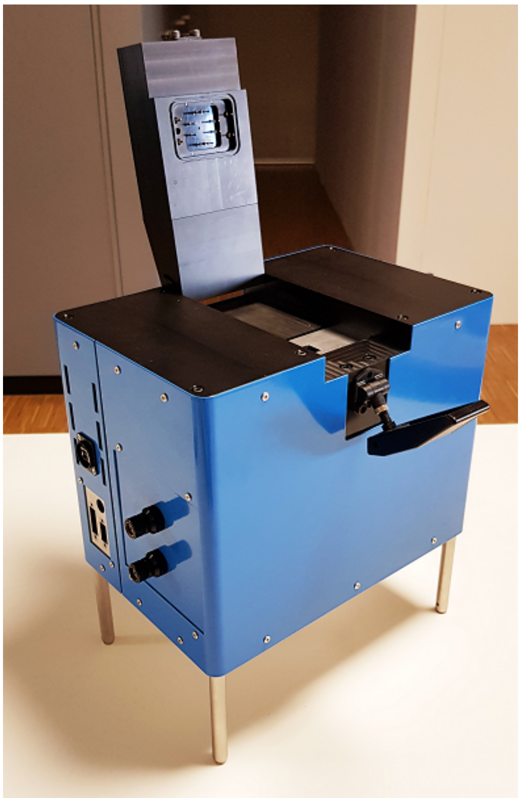

Abb. 1: Aktueller Stand des PAIOS-Kryostaten mit Wasserkühlung.

3.9 Electrochemical characterisation of NPB organic semiconductor films

The density of states is an important material property for devices from organic semiconductors. To measure it electrochemically, an add-on for the Paios measurement system was developed. This was then used to characterize NPB films with different measurement techniques.

Students: J. Dunst
Category: Master Thesis
Mentoring: K. Pernstich, B. Ruhstaller
Handed In: 23.2.2018

Devices from carbon based semiconducting materials like organic light emitting diodes (OLED) and solar cells are a promising technology, which has already been applied to commercial products. To get a deeper insight into the physical mechanisms via simulation, the parameters of the used materials need to be known. The aim of this work was to characterise thin organic films with electrochemical measurements such as cyclic voltammetry, electrochemical voltage spectroscopy and impedance spectroscopy. The main interest was in determining the density of states, the highest occupied and lowest unoccupied molecule orbital (HOMO and LUMO energies) as well as the trap density. The measurements were carried out on films of N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB), which is a widely used hole transport material in the OLED community.

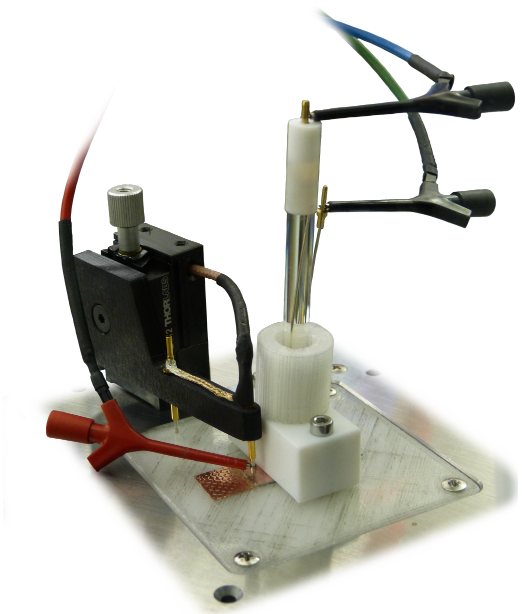

Fig. 1: Measurement setup used for characterization.

To implement these measurement techniques, an add-on for the measurement system Paios had to be developed. The development, the realisation as well as the testing of the electrical circuit and a sample holder for this add-on had been part of this thesis. With the final version, both transient and frequency dependent measurements up to 100 kHz can be realised.

The cyclic voltammetry measurements provided a HOMO of -5.33 eV and a LUMO of -2.17 eV which is in good agreement with literature values. In addition to this, a Gauss distribution of the density of states was fitted to the measurement curve of the HOMO, which had a maximum at 5.46 eV and a width of 0.06 eV. The impedance measurements resulted in a similar density of states distribution with a center at -5.41 eV which is close to the Gaussian fit, but it also shows some differences in shape and width see Fig. 2 below.

In summary, it has been shown that cyclic voltammetry as well as impedance spectroscopy yield valuable information about the density of states. Furthermore, various interesting questions for further investigations arose from this thesis.

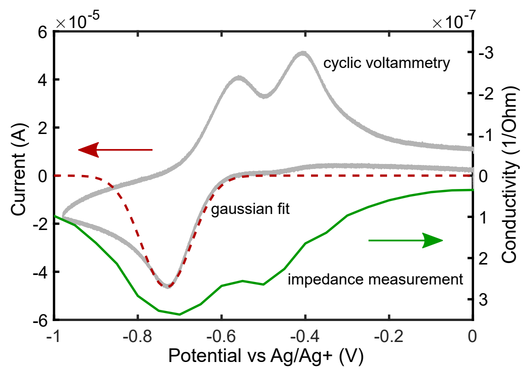

Fig. 2: Comparison of the density of states resulting from cyclic voltammetry and impedance measurements.

4 Sensor and Measuring Systems

Nowadays almost every object of everyday life carries a functional coating. The coating not only determines the appearance but also affects its properties such as its scratch or corrosion resistances. In order to ensure the quality of coatings, its thickness, homogeneity, material composition and adhesion properties have to fulfill certain standards. Previously, these coating properties often could only be determined in rather few individual samples. To minimize errors this often resulted in coatings being too thick, thus wasting material.

Lock-in thermography is a relatively new, non-destructive and non-contact testing method. In this case, a surface is thermally excited over a temporally changing heat flux. The resulting thermal radiation is recorded by infrared sensors and evaluated by means of computer algorithms. This allows one, for example, to detect invisible surface defects, whereby the depth range can be varied over the applied modulation frequency.

At ICP, lock-in thermography has been further developed for several years in the framework of numerous R&D projects. For example, in cooperation with the industrial partners J. Wagner, Oerlikon Metco and AkzoNobel the CoatMaster was developed to measure coating thicknesses. In addition, ICP uses lock-in thermography to detect skin diseases.


Daniel Fehr


Göksel Gülay


Samuel Hauri


Nils Reinke


Claude Ritschard


Benjamin Schmid


Urs Vögeli

4.1 Heat exchanger for gasifying Eucalyptus in Portugal

Due to massive import in the 20th century, non-native Eucalyptus has become the predominant wood species in Portugal. In order to slowly get rid of the population, a team of ICP researchers is supporting the Aberta Nova foundation near Melides to develop a prototype wood gasification reactor. The novel gasification system can basically turn wood chips into thermal energy, combustible gas and highly needed electricity. This year's focus was on devising a suitable gas-water-air heat exchanger to utilize 20 kW of excess thermal energy.

Contributors: G. Boiger, D. Neeser, A. Fassbind, P. Caels
Partners: Aberta Nova Foundation
Funding: Aberta Nova Foundation
Duration: 2017–2018

Wood gasification is a potential core technology in the context of sustainable, de-centralized heat- and electricity supply for homeowners as well as small and medium businesses. For years the ICP has conducted research in this field. Aside from extensive model-based analysis of the process, we have helped our research partner, the Aberta Nova foundation, to construct a prototype 20 kW gasifier at their site in Melides, Portugal. While the aggregate runs quite smoothly on Pine, Eucalyptus still causes problems concerning long-term stationary operation. While having made significant progress in running the system on Eucalyptus, in the spring of 2017 our team of ICP researchers still encountered problems with the high amount of excess thermal energy, released by the gasification reaction.

Fig. 1: Heat exchanger featuring 52 exchange tubes (left) and D. Neeser welding in the workshop at the Aberta Nova site (right).

During the summer and autumn months of 2017, the ICP/ZPP *gasification team*, composed of D. Neeser, A. Fassbind and G. Boiger stayed at the Aberta Nova site for several weeks. Within this period, the whole wood gasification system was mapped out, modeled [1] and a novel gas-air-water heat exchanger was dimensioned so that up to 20 kW of thermal energy could be drained and fed into Aberta Nova's internal heating system.

Later in the year, after carefully planning and organizing necessary materials and tools, the site was visited again, the prototype heat-exchanger was welded, assembled and added to the gasification system. Fig. 1 shows D. Neeser, a BSc student at ICP, working on assembling the heat exchanger featuring 52 individual exchange-pipes while Fig. 2 presents the CAD drawing vs. final state of the real-life heat exchanger.

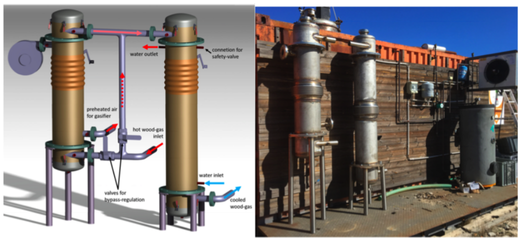

Fig. 2: CAD scheme (left) of gasifier and actual result of our efforts (right).

In very close cooperation with the Portuguese gasification development team, led by P. Caels, the ICP researchers were thus able to achieve (i) assertion of full functionality of the novel heat-exchanger, (ii) successful test-runs showing stable gasifier operation with Eucalyptus, (iii) significant energy feedback into the reactor due to air pre-heating and (iv) an increase of electrical power output due to higher system efficiency based on higher reactor temperatures and cooler wood gas.

Literature:

[1] G. Boiger, A thermo fluid dynamic model of wood particle gasification and combustion processes. *Int. J. Multiphys.*, Vol. 8 (2), 203–230, 2014.

4.2 Viscosity measurement based on torsional vibrations of circular structures

This study discusses a state-of-the-art online sensor, which can provide the means to measure the viscosity of the passing fluid. The sensor is composed of a tube resonator, excitation coils, and dampers and can be integrated into a piping system in a non-intrusive manner.

Contributors: D. Brunner, G. Boiger
Partners: Rheonics GmbH
Funding: KTI
Duration: 2016–2017

A novel type of viscosity sensor has been developed. It is composed of a tube resonator, excitation coils, and dampers. The novel tube-style sensors are different in comparison to ordinary ones. Typical viscosity sensors are probe-style and create obstruction within the piping system, disturbing the flow and creating a potential source of contamination in critical processes. The tube-style sensor, however, uses the tube as a sensing element and eliminates any intrusive parts. The schematic design is shown in Fig. 1. Viscosity is measured by determining the characteristic parameters of the resonator such as the damping and resonance frequency of the first torsional mode within the measuring section L in Fig. 1. The torsional mode is limited by two masses on each side, which act as a low pass filter and inhibit wave propagation near and above the resonance frequency.

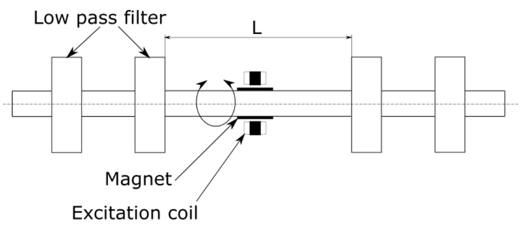

Fig. 1: Design concept of the tube sensor.

Experiments were conducted to develop a deeper understanding of the sensor. The goal was to determine the damping of the excited mode, which can be correlated to a viscosity-density product of the contained fluid. The damping parameter is represented by Δf, which is the frequency difference between excitation and angular velocity of the tube. Experimentally Δf is measured within a phase-lock control loop. In the mathematical models, the damping parameter can be determined analytically. The experimental results of the damping parameter were compared with two mathematical models for the fluid. One is based on a CFD simulation and the other one is based on an analytical approach for low viscous fluids. Both models were found in good agreement at low viscosities. The prediction of the damping by the models as well as the experimental data is shown in Fig. 2. The CFD model predicts slightly higher damping values than the analytical model with increasing viscosity-density product. This behavior can be explained by the curvature of the tube, which is neglected in the analytical model. At the bottom line, the experimental results were found to be in agreement with the model with reasonable accuracy.

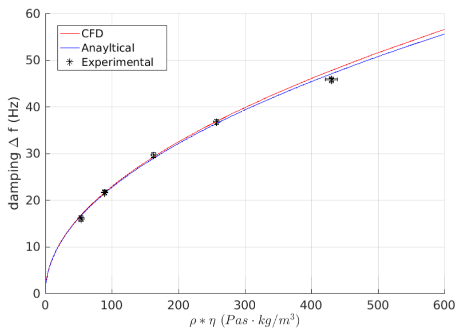

Fig. 2: Comparison of experimental data and derived models of tube sensor.

The study proved the validity of the proposed sensor. The CFD and analytical models were shown to be capable of accurately predicting the response of the sensor and hence can be applied as optimization- and design tools in ongoing development projects involving Rheonics and ICP.

4.3 Measuring thermal coating resistance of turbine blades

Thermal barrier coatings (TBC) protect turbine blades against heat and mechanical stress. Due to uncontrollable process parameters, the thermal coating resistance varies during the production of turbine blades. Currently, the resistance is measured by a visible inspection of microscopic cross-section images. This is very labour intensive and requires the destruction of production samples. Therefore, we investigated a new, fast and non-destructive measurement approach using impulse thermography. We showed that it's possible to reliably measure the thermal coating resistance if the effusivity of the substrate is known.

Contributors: A. Bariska, N. Reinke, S. Hauri
Partners: Winterthur Instruments AG, Oerlikon Metco AG
Funding: CTI
Duration: 2015–2017

TBC consist of two layers: first a bond coat (nickel alloy) is applied to the steel substrate and then the functional top coat (yttrium stabilized zirconia, YSZ) is applied onto the bond coat. The two most important factors governing the protective function are the porosity and the thickness of the YSZ coating. In order to compare the barrier properties of two different coatings these two parameters have to be quantitatively combined. This combination is, however, difficult as the influence of the porosity on the thermal barrier property is dependent on the microstructure of the porosity.

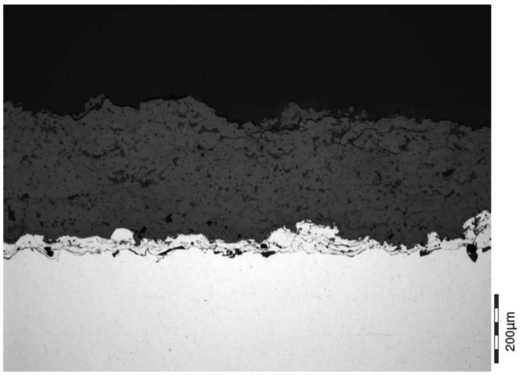

Fig. 1: Polished cross-section image of a TBC consisting of a bond coat (middle) and the top coat (top) on a steel substrate (bottom). Source: Oerlikon Metco AG, Wohlen.

Instead of using microscopic cross-section images to determine the porosity and the thickness, as shown in Fig. 1, we used the impulse-thermography-based CoatMaster measurement system to directly measure the thermal properties of the TBC. We assume, as a simple approximation, a constant heating power on the outside and a constant cooling power on the inside of the turbine blade. The temperature difference ΔT and the heat flow θ through the coating are constant and related, via a material parameter called thermal coating resistance R_{th}, with the formula $\theta = \Delta T / R_{th}$. To make the values independent of the area we have to use the heat flux density in W/m^2. The thermal coating resistance is therefore given in $(Km^2)/W$. With the CoatMaster measurement system, we can directly measure the thermal propagation time of a coating τ (unit: s). If the thermal effusivity ϵ (units: $J/(m^2 K \sqrt{s})$) of the coating is known and the thermal propagation time is measured, the thermal coating resistance can be calculated with $R_{th} = \sqrt{\tau}/\epsilon$.

In a series of measurements we could show that it is possible to reliably measure the thermal coating resistance with a fast and nondestructive measurement approach. A selection of measurements is given in Tab. 1.

Sample	Average Coat Thickness	Top Coat Porosity (image analysis)	Thermal Coating Resistance (absolute)	Thermal Coating Resistance (relative)
270	160µm			
284	140µm	4%	169 µKm²/W	75%
285	270µm	4%	225 µKm²/W	100%
286	328µm	1.9%	-	-
287	150µm	11.3%	221 µKm²/W	98%
288	228µm	11.1%	317 µKm²/W	141%
289	356µm	11%	-	-
290	75µm	15%	242 µKm²/W	108%
291	340µm	17.9%	-	-
292	280µm	15%	576 µKm²/W	256%

Tab. 1: Thermal coating resistance measured with the CoatMaster system.

4.4 kickAR – Tischfussball 4.0

kickAR ist die Integration von Anzeigeelementen wie Beamern oder Bildschirmen in ein traditionelles Spielgerät wie einem Kickertisch. Sensoren wie Kameras und Lichtschranken erfassen die Positionen des Balls und die Lage der Spielerstangen und ermöglichen eine Interaktion mit der integrierten Anzeige. Die Kombination von Anzeigeelementen und Sensoren erlaubt mannigfaltige Möglichkeiten zur Neugestaltung des Spielgeschehens.

Contributors: U. Vögeli, S. Hauri, N. Reinke
Partners: Winterthur Instruments AG
Funding: ZHAW
Duration: 2017 – 2018

Tischfussball ist eine Sportart, die auf einem Spielgerät gespielt wird, das Kickertisch genannt wird. Ziel des Spiels ist es, mit an drehbaren Griffstangen über einer rechteckigen Spielfläche angebrachten (Fussball)spielerfiguren eine oft vorgegebene Anzahl von Bällen ins gegnerische Tor zu schiessen. Spielfläche und Anordnung der Spielfiguren sind dabei dem Fussballspiel nachempfunden. Ein Kickertisch hat normalerweise je vier Griffstangen an den beiden Längsseiten der Spielfläche, an denen pro Spieler insgesamt elf Spielfiguren verteilt angebracht sind. Tischfussball wird seit Jahrzehnten in der Pädagogik als Kommunikations- und Rehabilitationsmittel genutzt. Millionen Kickertische stehen daher in Jugendeinrichtungen, Schulen, Pfadfinderheimen, in Spielzimmern von Kinderkrankenhäusern sowie in vielen Kinderzimmern. Aufgrund der niedrigen Einstiegsschwelle werden Kickertische zudem auch häufig in Gaststätten aufgestellt.

Insbesondere für Anfänger dieser Sportart ist das rasche Spielgeschehen oft nicht nachvollziehbar. Der Lerneffekt und damit die Motivation insbesondere im Spiel gegen erheblich stärkere Spielpartner ist damit begrenzt. kickAR löst dieses Spiel einerseits durch Visualisierung der Ballbewegung (Tracing) sowie durch virtuelle Verkleinerung der Torbreite (Game-Balancing). kickAR gibt darüberhinaus zahlreiche Zusatzinformationen wie die aktuelle Ballgeschwindigkeit, Statistiken zum Ballbesitz und zählt automatisiert den Spielstand. Eine interaktive Tonausgabe lässt den Spieler noch tiefer in das Spielgeschehen eintauchen.

kickAR nutzt Highspeed-Kameras, welche mit bis zu 500 Bildern pro Sekunde die Position von Ball und Spielerstangen verfolgen. Die Datenauswertung erfolgt GPU-basiert auf einer hochperformanten Grafikkarte. Die grafische Anzeige erfolgt auf einem hochauflösenden 4k-Bildschirm, welcher in Echtzeit Spielinformationen einblendet. Der Tischfussball hat zahlreiche Fans auf verschiedenen Anlässen wie der tun Ostschweiz und tun Luzern gewonnen und wird auch auf dem Winterthurer Oberflächentag und der Nacht der Technik zum Einsatz kommen. kickAR wird im Rahmen von Projekt- und Bachelorarbeiten weiterentwickelt.

Weitere Informationen auch auf kickAR.ch

Abb. 1: Begeisterte Besucher auf der tun Ostschweiz bei der Erprobung des kickAR.

4.5 Technologien zur Viskositäts-Regelung für die kontrollierte Applikation von Beschichtungsmaterialien

Die Steuerelektronik und die darauf ausgeführten DSP-Algorithmen zur Auswertung von Viskositätssensoren wurden an eine neuartige Inline-Sensortechnologie angepasst. Danach ist ein Flow-Loop-System entwickelt und aufgebaut worden, um die Inline-Sensoren unter definierten Bedingungen zu testen und eine vollständige Charakterisierung der Sensoren durchzuführen. Der um eine automatisierte Verdünner-Dosierung erweiterte Flow-Loop wird zum automatischen Viskositäts-Regelsystem, das eine konstant hohe Beschichtungsqualität gewährleistet, und ermöglicht dadurch dem Anwender massive Einsparungen an Material, Anlagen- und Arbeitszeit.

Contributors: D. Fehr, U. Vögeli, A. Bariska, S. Hauri, N. Reinke
Partners: Rheonics GmbH
Funding: KTI
Duration: 2016–2017

Zur Auswertung der Sensorsignale eines neuartigen Inline-Viskositätsmeters wurde eine Auswerteeinheit auf Basis eines DSP (Digitaler Signalprozessor) entwickelt. Als Ausgangslage diente eine Elektronik mit zugehöriger Software, die von einem vorgängigen Projekt stammt. Das Analog-Front-End und die Algorithmen wurden an die neuen Inline-Viskositätssensoren adaptiert.

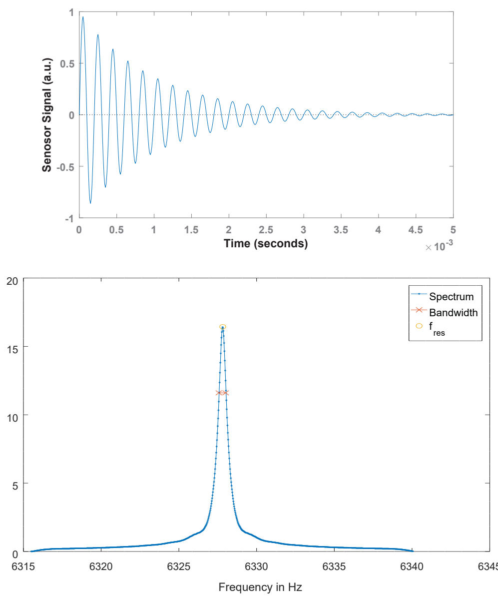

Abb. 1: Charakteristischer Ausschwingvorgang eines mechanischen Schwingers zur Viskositätsbestimmung (oben) und das zugehörige Spektrum, aus dem durch Bestimmung von Mittenfrequenz und Bandbreite auf die Viskosität des Fluids rückgeschlossen werden kann (unten).

Das zugrundeliegende Messprinzip kann wie folgt beschrieben werden: Der mit Fluid umspülte mechanische Schwinger des Viskositätssensors wird durch die Elektronik in Schwingung versetzt. Dabei hängen Resonanzfrequenz und Dämpfung des mechanischen Schwingers von der Dichte und Viskosität des Fluids ab. Abbildung 1 zeigt einen charakteristischen Ausschwingvorgang, der die Form einer exponentiell abfallenden Schwingung aufweist. Die DSP-Elektronik bestimmt die Resonanzfrequenz und Dämpfung anhand des Spektrums des Ausschwingvorgangs, welcher ebenfalls in Abildung 1 zu sehen ist.

Parallel zur Auswerteelektronik ist auch eine Teststrecke (Flow-Loop) entworfen und realisiert worden (Abbildung 2). Sie ist wie ein typischer Nassbeschichtungsprozess aufgebaut: Förderung von Beschichtungsmaterial und Verdünner, Mischer, Zirkulation mit dem Inline-Viskositätssensor und einem Abgriff, der die Applikation des Beschichtungsmaterials simuliert.

Mit dem Flow-Loop und der oben beschriebenen Auswerteelektronik können die Viskositätssensoren unter typischen Betriebsbedingungen getestet und charakterisiert werden. Weiterhin ermöglicht das System die Entwicklung einer Inline-Viskositäts-Regelung zur automatisierten Mischung von Verdünner und Beschichtungsmaterialen, die in verschiedenen industriellen Beschichtungsanwendungen eingesetzt werden kann.

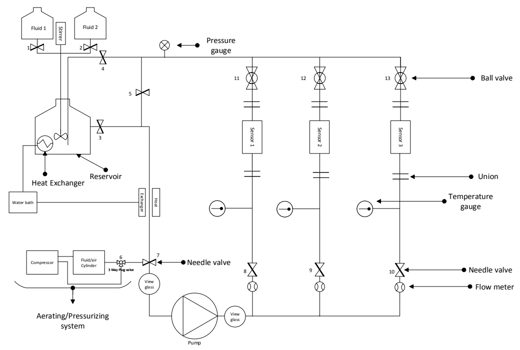

Abb. 2: Flow-Loop-Testsystem.

4.6 Prüfstand zur Analyse der Erstarrung von Schokolade

Neben dem Temperieren, also dem gezielten Züchten von stabilen Fettkristallen, haben die transienten Wärmetransportprozesse während der Erstarrung der flüssigen Schokolade in der Form einen markanten Einfluss auf ihre Optik, Konsistenz und Haltbarkeit. Mithilfe eines designierten Prüfstands soll das Abkühlverhalten der Schokolade unter kontrollierten Bedingungen optimiert werden. Ziel ist es, die daraus gewonnenen Erkenntnisse für die Entwicklung eines optimalen Kühlverfahrens zum Einsatz in Confiserien zu nutzen.

Students: S. Ehrat, J. Frigil, T. Mesarec
Category: Master of Science, Semesterprojekt
Mentoring: T. Hocker
Handed In: December 2017

Confiserien produzieren verschiedenste Schokoladeprodukte in einer grossen Vielfalt unterschiedlicher Formen und Grössen. Diese Erzeugnisse werden häufig ohne Verpackung in der Auslage präsentiert. Flecken und ein ungleichmässiger Glanz stören jedoch das optische Erscheinungsbild. Sie sind aber auch Ausdruck einer nicht optimalen Konsistenz mit negativem Einfluss auf das Mundgefühl und die Haltbarkeit. Solche Fehler entstehen durch falsches Temperieren und ungleichmässiges Abkühlen. Sie treten besonders bei grösseren Schokoladentafeln auf. Peter Abegglen, ein pensionierter Confiseurmeister aus Bern, konnte in Kühlversuchen zeigen, dass sich die Bildung von Flecken beim Erstarren der Schokolade in Tafeln unter Verwendung von Coolpacks vermeiden lässt.

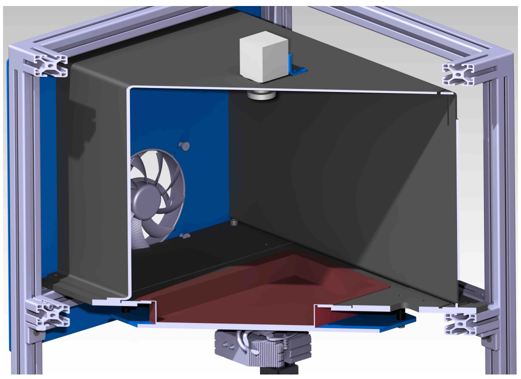

Abb. 1: Prüfstand zur Optimierung des Abkühlverhaltens von Schokolade über verschiedene Kühlmethoden.

Aus diesen Erfahrungen entstand die Idee für einen designierten Prüfstand zum kontrollierten Kühlen von Schokoladeprodukten. Abb. 1 zeigt den Aufbau des Prüfstands. Hierbei wird die Wärmeenergie der Schokolade einerseits durch erzwungene Konvektion an die Luft und andererseits durch Wärmeleitung an einen CPU-Kühler abgegeben. Letzterer erzeugt also eine zusätzliche Kühlwirkung gegenüber der üblichen, reinen Luftkühlung.

Um mögliche thermische Widerstände im Wärmeleitpfad an den CPU-Kühler zu detektieren, wurde ein 1D-Modell basierend auf der Wärmeleitungsgleichung in *Mathematica* implementiert. Zur Validierung des Modells wurden Kühlversuche mit einer 2 kg Schokoladenform der Confiserie Vollenweider durchgeführt, die in mehreren Messreihen mit aufgewärmtem Olivenöl und Wasser befüllt wurde. Aufgrund der nicht ausreichend genau bekannten thermischen Stoffdaten des Olivenöls waren diese Versuche für die Validierung nicht brauchbar.

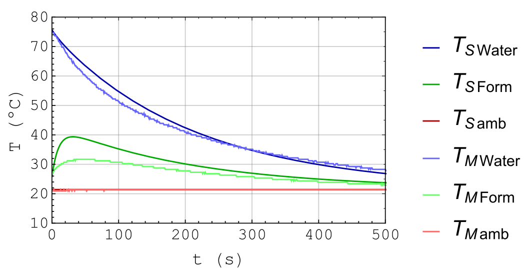

Abb. 2: Erster Abkühltest für eine mit Wasser gefüllte Schokoladenform: Vergleich der T-Messungen in Wasser und Formwand mit Lösungen der 1D-Wärmeleitungsgleichung.

Abb. 2 zeigt einen Vergleich zwischen den simulierten S- und den gemessenen M-Abkühlkurven von erhitztem Wasser. Im Modell wurde angenommen, dass es aufgrund der Verdunstung des Wassers zu einem verbesserten Wärmeübergang hin zur Luft kommt. Er konnte über Literaturdaten abgeschätzt werden. Die Diskrepanz zwischen Messung und Simulation hat mehrere Ursachen. Zum einen treten im Prüfstand laterale Wärmeströme auf, die im 1D-Modell nicht berücksichtigt wurden. Zum anderen lieferte der T-Sensor unter der Form je nach Position und Befestigungsmethode unterschiedliche Resultate.

4.7 Prüfstand für akkurate Oberflächentemperaturmessungen durch optimale Platzierung der T-Sensoren

Kontakttemperatur-Sensoren sind in einer grossen Anzahl verschiedener Ausführungen und Genauigkeiten zu meist moderaten Preisen verfügbar. Bei ihrer Verwendung zur Messung von Oberflächentemperaturen stellt sich meist die Frage, wie ein bestimmter Sensor am besten platziert werden sollte bzw. welcher Sensor für eine bestimmte Anwendung am besten geeignet ist. Datenblätter der Sensorlieferanten geben darüber keine Auskunft. Durch eine suboptimale Platzierung bzw. Befestigung können jedoch erhebliche Messfehler entstehen. Ziel dieser Arbeit ist es, an einem designierten Prüfstand in Kombination mit thermisch-fluidischen Computermodellen Richtlinien für eine optimale Anordnung von T-Sensoren zu erarbeiten.

Students: S. Spirig
Category: Master of Science, Semesterprojekt
Mentoring: T. Hocker
Handed In: December 2017

Die Temperatur gilt als die am häufigsten gemessene physikalische Messgrösse [1]. Die Gründe für diesen hohen Anteil sind vielfältig. Grundsätzlich sind die meisten Stoffeigenschaften temperaturabhängig. Zudem werden Temperaturmessungen für Energiebilanzanwendungen verwendet. Die fortschreitende Digitalisierung (Industrie 4.0, Internet of Things) wird dazu führen, dass Temperaturmessung zum Monitoring von Prozessen zukünftig noch an Bedeutung gewinnen wird. Trotz der grossen Auswahl an verfügbarem Messequipment sind akkurate Oberflächentemperaturerfassungen bisher nur wenig erforscht.

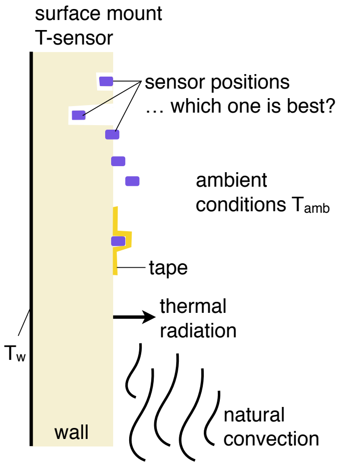

Abb. 1: Grundidee hinter einem designierten Prüfstand zur präzisen Messung von Oberflächentemperaturen mit verschiedenen Varianten, T-Sensoren zu positionieren.

So ergab sich die Idee, einen designierten Prüfstand für die Messung von Oberflächentemperaturen und parallel dazu Computermodelle zu entwickeln, um Richtlinien für optimale Sensoranordnungen abzuleiten. Dazu sollen Temperaturmessungen mit unterschiedlichen Sensortypen und -anordnungen vollzogen werden, siehe Abb. 1. Zunächst wurden die am häufigsten verwendeten T-Sensoren evaluiert und der in Abb. 2 gezeigte Prüfstand entwickelt.

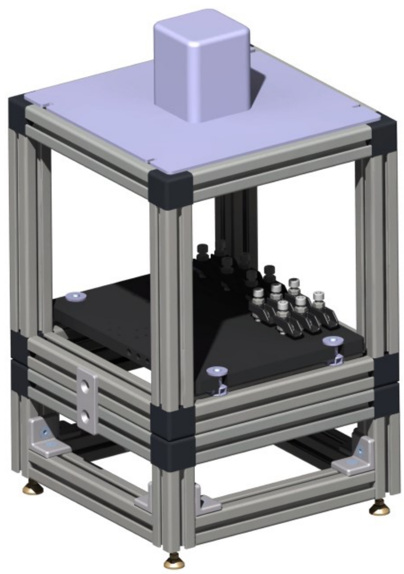

Abb. 2: Aktuelles Design des Prüfstands zur präzisen Messung von Oberflächentemperaturen über Kontakt T-Fühlern und Wärmebildaufnahmen.

Der Prüfstand ist mit einer Heizmatte mit Temperaturregelung ausgestattet, über die sich verschiedene T-Niveaus einstellen lassen. Ausserdem können die T-Sensoren an horizontalen und vertikalen Oberflächen aus verschiedenen Materialien angebracht werden. Parallel zu den geplanten Messungen sollen thermisch-fluidische Computermodelle entwickelt werden, die u. U. die Korrektur von unvermeidlichen Messfehlern erlauben.

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Appendix

A.1 Student Projects

D. NEESER, *Weiterentwicklung eines neuartigen Holzvergasungsreaktors in Thalwil und oder bei F&E Partner in Portugal*, Betreuer: G. Boiger, Firmenpartner: Stiftung Alberta Nova, Projektarbeit Energie- und Umwelttechnik.

S. LANDOLT, P. KHODADUST, *Einsatz Neuronaler Netzwerke zur Lösung Ingenieurtechnischer Probleme*, Betreuer: G. Boiger, Firmenpartner: ICP intern, Projektarbeit IT.

F. DANIEL, *Prozedurale Generierung von Template-basierten Graphen*, Betreuer: G. Boiger, Bachelorarbeit IT.

P. KAUFMANN, *Koppelung von "Maschine-Learning" Technologie mit Numerischen Modellierungsverfahren*, Betreuer: G. Boiger, Bachelorarbeit IT.

V. BUFF, L. PANGIONE, *Weiterentwicklung eines neuartigen Holzvergasungsreaktors*, Betreuer: G. Boiger, Firmenpartner: Stiftung Alberta Nova, Bachelorarbeit Energie- und Umwelttechnik.

K. BAUR, P. KAELIN, *Aerodynamic Characterization of Winged Aerostat for an Efficient Lighter Than Air Airship*, Betreuer: G. Boiger, Y. Safa, Firmenpartner: ICP intern, Bachelorarbeit Aviatik.

M. JANSEN, R. SCHELBERT, *Wind tunnel testing of small scale rotor for a new airborne wind power system*, Betreuer: G. Boiger, Y. Safa, Firmenpartner: ICP intern, Bachelorarbeit Aviatik.

T. OTT, *Development of a Thermodynamic Model of the Human Skin*, Betreuer: G. Boiger, Firmenpartner: Dermolockin AG, Masterarbeit Masterstudiengang.

J. DUNST, *Electrochemical Characterisation of NPB Organic Semiconductor Films*, Mentoring: K. Pernstich, B. Ruhstaller, Master Thesis.

J. DUNST, *Zyklische Voltammetrie zur Bestimmung der Energieniveaus von organischen Halbleitern*, Betreuer: K. Pernstich, Vertiefungsarbeit Masterstudiengang.

F. JOHN, *Optimierung des Kristallisationsverhaltens von Schokoladenprodukten durch eine geeignete Kühlmethode*, Betreuer: T. Hocker, Projektpartner P. Abegglen sowie H. U. Vollenweider, Bachelorarbeit im Studiengang Maschinentechnik.

D. KEMPF, J.-P. PÉCLARD, S. MORGENTHALER, *Entwicklung einer Virtual Reality Umgebung zur Darstellung von Flugsimulationen*, Betreuer: T. Hocker, , Projektarbeit im Studiengang Informatik.

D. MEIER, *Thermo-Fluidic Modelling of Chocolate Moulds in a Pilot Cooling Channel*, Betreuer: T. Hocker, Projektpartner ETH Laboratory of Food Process Engineering, Vertiefungsarbeit Masterstudiengang.

A. MEIER, R. ROPELATO, *OLED Lifetime-Tester*, Betreuer: K. Pernstich, O. Fluder (IMS), Bachelorarbeit.

T. MESAREC, *Optimierung von industriellen Abkühlprozessen mithilfe von theoretischen und praktischen Analysen*, Betreuer: T. Hocker, Projektpartner Wöhner AG, Rödental, Masterarbeit.

T. MESAREC, *Simulation von Wärmeleitung, Naturkonvektion und thermischer Strahlung in Ansys CFX*, Betreuer: T. Hocker, Projektpartner Wöhner AG, Rödental, Vertiefungsarbeit Masterstudiengang.

S. SPIRIG, *Grundlagen der numerischen Strömungssimulation anhand einer Rohrströmung*, Betreuer: T. Hocker, Vertiefungsarbeit Masterstudiengang.

A.2 Scientific Publications

G. BOIGER, T. OTT, L. HOLZER, D. PENNER, M. GORBAR, Y. DEHAZAN, *Multi-parameter improvement method for (micro-) structural properties of high performance ceramics*, Int. Journal of Multiphysics 11 (1), 49–69, 2017.

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A.6 Patents

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A.7 Teaching

A. BARISKA, *Lineare Algebra für Ingenieure, FS17, HS17*, Bachelor of Science.

G. BOIGER, *Fluid- & Thermodynamik I für MT - Vorlesung & Praktikum FS17*, Bachelor of Science.

G. BOIGER, *Numerik für IT I – Vorlesung & Praktikum, HS17*, Bachelor of Science.

G. BOIGER, *Physik und Systemwissenschaften für AV II – Praktikum, FS17*, Bachelor of Science.

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G. BOIGER, *Advanced Thermodynamics, HS17*, Master of Science in Engineering.

G. BOIGER, *Thermofluiddynamik Modellentwicklung mit OpenFoam I, HS17*, Master of Science in Engineering.

G. BOIGER, *Thermofluiddynamik Modellentwicklung mit OpenFoam II, FS17*, Master of Science in Engineering.

G. BOIGER, *Two Phase Flow with Heat and Mass Transfer, FS17*, Master of Science in Engineering.

G. BOIGER, *Numerik für IT II – Vorlesung & Praktikum1, FS17*, Bachelor of Science.

A. HEEL, T. HOCKER, *Abgas- und Abwasserbehandlung, HS17*, Bachelor of Science.

T. BERGMANN, T. HOCKER, *Thermische Energiesysteme, FS17*, Bachelor of Science.

T. HOCKER, *Fluid- und Thermodynamik 1 – Vorlesung und Praktikum, FS17*, Bachelor of Science.

T. HOCKER, *Fluid- und Thermodynamik 2 – Vorlesung und Praktikum, HS17*, Bachelor of Science.

T. HOCKER, *Systemphysik für Aviatik 1 – Praktikum, HS17*, Bachelor of Science.

T. HOCKER, *Systemphysik für Aviatik 2 – Praktikum, FS17*, Bachelor of Science.

M. JAZBINSEK, *Physik für Energie und Umwelttechnik 1 – Vorlesung & Praktikum*, Bachelor of Science.

M. JAZBINSEK, *Physik für Energie und Umwelttechnik 2 – Vorlesung & Praktikum*, Bachelor of Science.

C. KIRSCH, *Mathematik: Analysis für Ingenieure 2, FS17*, Bachelor of Science.

C. KIRSCH, *Mathematik: Analysis für Ingenieure 4, FS17*, Bachelor of Science.

C. KIRSCH, *Mathematik: Analysis für Ingenieure 1, HS17*, Bachelor of Science.

C. KIRSCH, *Mathematik: Numerische Methoden, HS17*, Bachelor of Science.

E. KNAPP, *Math for Aviation: Applied Numerics, FS17*, Bachelor of Science.

E. KNAPP, *Mathematik: Numerik für Energie- und Umwelttechnik , HS17*, Bachelor of Science.

K. PERNSTICH, *Physik und Systemwissenschaften für Verkehrssysteme 1 - Vorlesung und Praktikum*, Bachelor of Science.

K. PERNSTICH, *Physik und Systemwissenschaften für Verkehrssysteme 2 - Vorlesung und Praktikum*, Bachelor of Science.

N. REINKE, *Lineare Algebra für Ingenieure, HS17*, Bachelor of Science.

R. RUHSTALLER, *Physik für Verkehrsysteme Studiengang – Praktikum*, Bachelor of Science.

J. SCHUMACHER, *Analysis für Ingenieure 3 - HS17*, Bachelor of Science.

J. SCHUMACHER, *Multiphysics Modelling and Simulation FS17*, Master of Science in Engineering.

J. SCHUMACHER, *Numerical Simulation of Solar Cells FS17*, Master Online Photovoltaics.

J. SCHUMACHER, *Technologiepotentiale: Antriebs-/Fahrzeugtechnik und Energieträger im Bezug auf Wasserstofftechnologie HS17*, Master of Advanced Studies in Efficient Mobility ETHZ.

A.8 Spin-off Companies

NM Numerical Modelling GmbH
The engineering company, CH-Thalwil

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 where 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 support your product development cycle and to conform to yours time and budget constraints. 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

www.fluxim.com

Fluxim is a provider of device simulation software and measurement hardware to the display, lighting and photovoltaics community worldwide. Our principal activity is the development and the marketing of the simulation software SETFOS and LAOSS, as well as the all-in-one characterization platform PAIOS. SETFOS was designed to simulate light propagation and charge transport in large-area opto-electronic devices such as organic light-emitting diodes (OLEDs) and solar cells while PAIOS measures the dynamic opto-electrical response in time and frequency domain which supports the determination of material parameters. Our R&D tools are used worldwide in industrial and academic research labs for the development of devices and semiconducting materials with improved performance as well as the study of device physics.

WinterthurInstruments
noncontact and nondestructive testing of coatings

www.winterthurinstruments.ch

Winterthur Instruments AG 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.

DERMOLOCKIN

www.dermolockin.com

Dermolockin GmbH is a recently founded spin-off company developing active thermography-based setups for dermatological applications. The main focus lies in the detection and characterization of cutaneous cancerous lesions with lock-in thermal imaging methods.

opus néoi

www.skinobi.com

Opus Néoi is a spin-off company founded in 2016 developing Skinobi, the first reliable skin hydration sensor for end consumers. Skinobi allows the customer to monitor the skin condition at home and recommends the ideal, customized skin care solution utilizing a sophisticated neural network for the analysis and extraction of the parameters. The innovative measurement method specifically measures the thermal transport characteristics of the skin by optical means. Thermal conductivity, heat capacity or density are very good markers of the skin's condition and correlate with physiological parameters like hydration or epidermal thickness.

A.9 ICP-Team

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A.10 Location

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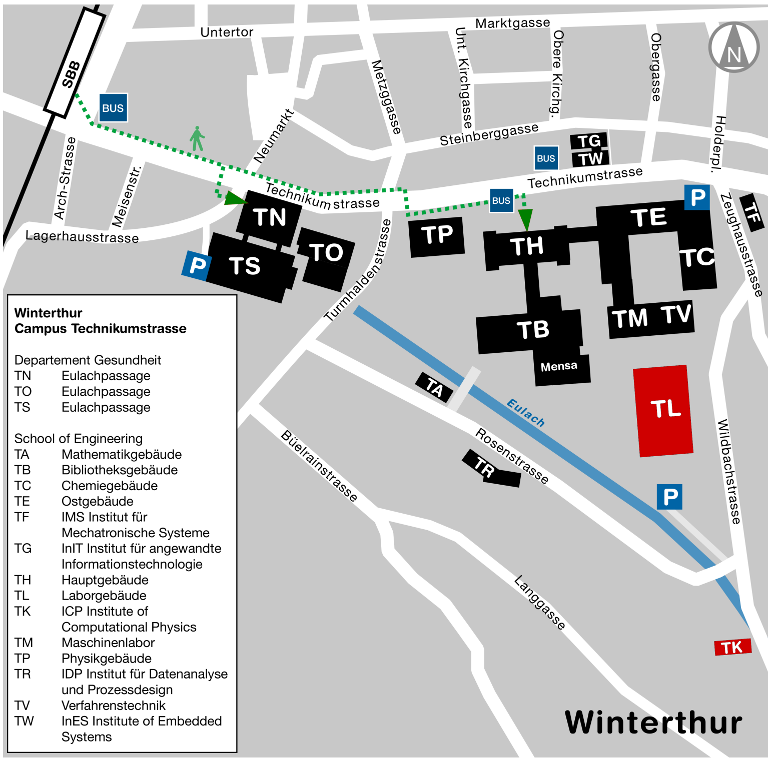

TK building

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