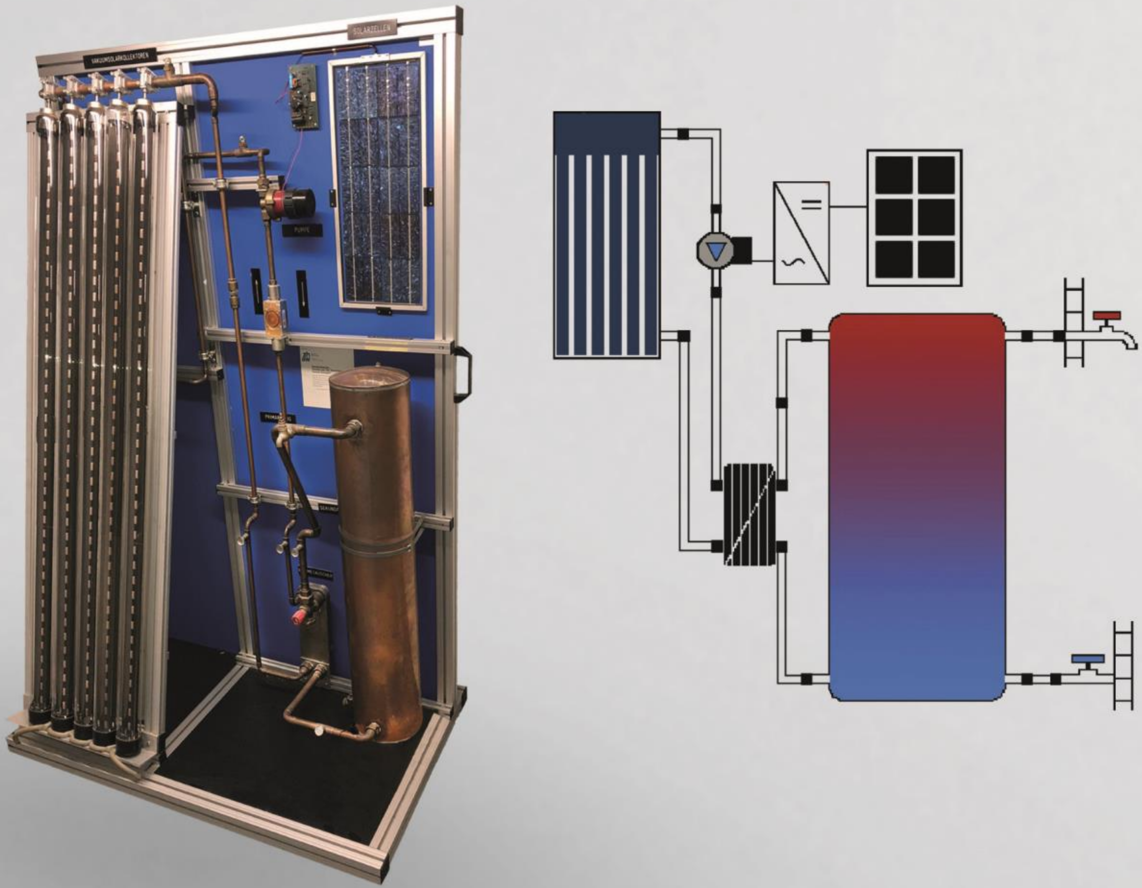
Zurich University
of Applied Sciences

School of
Engineering

ICP Institute of
Computational Physics

Institutsbericht 2019



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Der Vergleich von Simulation und Experiment ist im Bereich der Forschung gut etabliert. Mit der dargestellten Anlage wird auch in der Ausbildung die Abweichung von numerischer Berechnung und Messung thematisiert. Studierende im Studiengang *Energie und Umwelt* analysieren anhand des Versuchsaufbaus (links) die Wärmeflüsse in einer Solaranlage. In den Simulationsübungen nutzen sie das Planungstool Polysun, um dieselbe Anlage im numerischen Modell nachzubilden (rechts).

Vorwort

Der vorliegende Institutsbericht führt die Tradition des ICP weiter, die Forschungsprojekte in einem jährlich erscheinenden Report zusammenzufassen. Neu werden zusätzlich zu den Aktivitäten in den Forschungsschwerpunkten des ICP auch Projekte aus der Lehre dargestellt.

Die *Digitalisierung* verändert nicht nur Forschung und industrielles Engineering, sondern auch den Unterricht an der Fachhochschule. Wir beobachten, wie unsere Studierenden mit leistungsfähigen und handlichen Mobilgeräten in die Vorlesung kommen. Einerseits kommt man damit dem papierlosen Studium einen wesentlichen Schritt näher. Ein schönes Wandtafelbild wird fotografiert und findet sich nahtlos in den digitalen Notizen neben Unterrichtsmaterialien, die auf Moodle bereitgestellt werden. Andererseits wird ein alter ICP-Traum wahr: Simulationen sind im Unterricht angekommen! Anhand von numerischen Experimenten können wir den Studierenden physikalische Vorgänge zugänglich machen, die aufgrund ihrer Dimension sonst nicht greifbar sind. Die grosse Sammlung an analogen Experimenten – viele davon aus einer Zeit als unsere Schule noch *Technikum Winterthur* genannt wurde – wird ergänzt durch *digitale Experimente*. Simulationen können auf den mobilen Geräten der Studierenden durchgeführt werden, aktivieren die Studierenden, wecken ihre Neugierde und helfen beim Darstellen komplexer Zusammenhänge. Es freut uns, wenn wir vonseiten des ICP mit unseren Computerexperimenten einen aktiven Beitrag zur Erweiterung der Physiksammlung leisten können. Es ist uns bewusst, dass die Nutzung der mobilen Endgeräte für diese Zwecke neben den offensichtlichen Chancen auch didaktische Herausforderungen mit sich bringt. Ein grosses drittmittelgefördertes Projekt der Internationalen Bodenseehochschule IBH befasst sich unter dem Didaktik-Schlagwort *Seamless Learning* genau mit diesem Thema; es wird in Kapitel 5.2 beschrieben.

Wir sind zuversichtlich, dass wir mit unseren Simulationen die Qualität des Grundlagenunterrichts steigern und bei den Studierenden auch das Interesse an der angewandten und industrienahen Forschung wecken. Die Resultate aus diesen Projekten sind in den ersten vier Kapiteln dieses Berichts dargestellt. Ein Dankeschön an alle Forschenden für ihr Engagement in der Wissenschaft und für die hochinteressanten Artikel, die ihre Aktivitäten zusammenfassen.

Andreas Witzig, Institutsleiter ICP, April 2019

Inhaltsverzeichnis

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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Gernot Boiger


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Sebastian Spirig


Asier Zubiaga

1.1 Powder Coating: Simulation-based prototype development of a novel powder coating gun generation, based on targeted adaption of the coronal field

Imposed additional electric field near the nozzle outlet exploit the charge of powder particles to deflect particle trajectories without moving the coating gun itself. Simulation-based and experimental proof-of-concept are established. Parameter studies are being conducted and will lead to a functional pre-prototype as project deliverable.

Contributors: G. Boiger, M. Boldrini, V. Lienhard, B. Siyahhan, V. Buff, J. Gianotti
Partners: Wagner International AG
Funding: Direct
Duration: 2018–2019

Based on prior and ongoing Innosuisse Projects with Wagner, this independent project focuses on deflecting and directing a powder cloud without moving the coating gun itself. Within the scope of the Innosuisse projects, tailored powder coating simulation has been developed and still undergoes further development. Simulation-based corona shape prediction considering gun geometries and other influences, allow i) targeted modifications of corona shapes, ii) influence particle trajectories and iii) optimization of powder coating results. The project aims for targeted modification of the governing electric field between coating gun and substrate, solely by constructional means in and attached to the powder coating gun, thus i) varying the focus of local coating intensity without moving the gun, ii) minimize areas with low coating quality and iii) maximize coating efficiency.

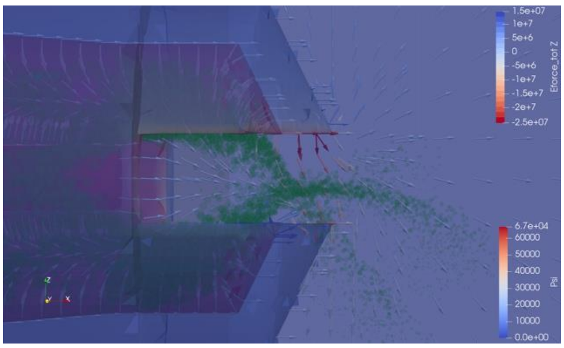


Fig. 1: Close up on coating gun nozzle. Concept simulation of particle (green) trajectories with imposed additional voltage between upper and lower part of the slit, resulting in a downward acceleration of the charged powder particles.

The main approach exploits particle charge, redirecting the trajectories by added electric fields. The deflection depends on strength and direction of the applied electric field. Initially, several concept studies have been performed in order to assess feasibility and governing forces in the relevant areas (see Fig.1). First, a capacitor model has been introduced, imposing variable electric potentials to upper and lower nozzle outlet areas. The deflection is proportional to the capacitor area and inversely proportional to capacitor distance. Prestudies showed that feasible deflecttion occurs in the range of 10-50kV, which is well within the order of magnitude of the overall coating operation voltages.

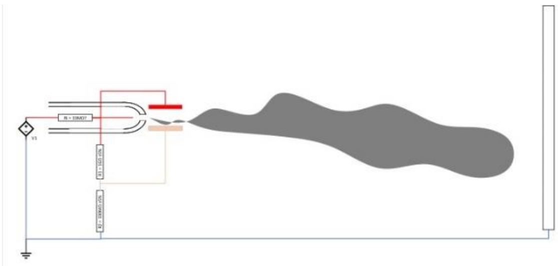


Fig. 2: Capacitor imposes additional electric field perpendicular to particle trajectory.

The simulation-based proof-of-concept is leveraged to a safely operational experimental setup. Nozzle attachments introducing isolated capacitor plates in the slit outlet area were constructed (see Fig. 2). Experimental proof-of-concept was established in internal experiments. Simulation-based and experimental parameter studies are being conducted, leading to a functional pre-prototype.

1.2 Entwicklung der Serienreife von neuartigen vollkeramischen Hochtemperatur-Heizelementen zur Heisslufterzeugung

Im Folgeprojekt zu Leister 1 wird das im vorgängigen Projekt entwickelte Heizelement zur Serienreife weiterentwickelt. Die Arbeiten umfassen die weitere Verbesserung der OpenFoam®-Modelle, den Abgleich mit verschiedenen Versuchs- und Messaufbauten, bis hin zum serienreifen Prototypen mit klarem Herstellungskonzept.

Contributors: M. Boldrini, J. Gianotti, G. Boiger
Partners: Leister Technologies AG
Funding: Innosuisse
Duration: 2015–2019

In diesem Entwicklungsprojekt mit Leister wird ein neuartiges Heizelement für industrielle Heissluftpistolen entwickelt. Die neuen Heizelemente sollen aus leitfähiger Keramik hergestellt werden. In Bezug auf Herstellungskosten und Zuverlässigkeit sollen die Keramikelemente den gegenwärtig gängigen Elementen, welche auf metallischen Heizdrähten basieren, überlegen sein. Die Entwicklung erfolgt als Zusammenarbeit zwischen dem IMPE und dem ICP. Hierbei fokussiert sich das IMPE auf die Entwicklung der Hochleistungskeramik. Das ICP entwickelt mehrere numerische Berechnungsmodelle, welche die Simulation und den Vergleich verschiedener Heizelement-Geometrievarianten ermöglichen. Dies führte bereits 2017 zur Entwicklung der Doppelhelix, was einem vollen Erfolg der ersten Projektphase gleichkam. In der nächsten Projektphase soll nun die Doppelhelix zur Serienreife geführt werden.

Illustration 1: Thermo-fluiddynamische Simulation des Heizelements in OpenFoam®.

Zur weiteren Entwicklung der Heizelemente wurde das ZPP als weiteres Kompetenzzentrum hinzugezogen. Das ZPP legt seinen Fokus auf die Entwicklung und Optimierung des Herstellungsprozesses.

Das ICP verfolgt in der aktuellen Phase zwei Hauptaufgaben. Einerseits werden auf Basis eines OpenFOAM®- sowie eines SESES-Modells Geometrieanpassungen überprüft, um Schwachstellen erkennen und Optimierungen realisieren zu können. Andererseits werden auch Messaufbauten realisiert, welche es erlauben einen genauen Einblick in die bestehenden Randbedingungen zu erhalten. Als erstes wurde hierzu ein Aufbau zur Messung des Volumenstroms umgesetzt. Hiermit können Anlagen- und Ventilatorkennlinien für verschiedene Geometrien ermittelt werden, welche zur genaueren Validierung und weiteren Verbesserung der Simulationsmodelle dienen.

In folgenden Schritten soll die Geometrie in Bezug auf Wärmeübergang, Druckverlust und Herstellbarkeit weiter verbessert werden, bis hin zum serienreifen Prototypen.

Illustration 2: Verschiedene Doppelhelix Geometrie-Varianten.

1.3 Wood Gasification – From ICP to Melides, Portugal

In search of a sustainable method to reduce the non-native Eucalyptus population in Melides, Portugal, the ICP has been laboring alongside the Aberta Nova foundation. We are developing a prototype wood gasification reactor, which will operate almost without any tar production. The novel, low-maintenance gasification system shall be versatile enough to turn any type of wood chips into thermal energy, combustible gas and electricity.

Contributors: G. Boiger, D. Neeser, A. Fassbind, P. Caels
Partners: Aberta Nova
Funding: Aberta Nova, internal
Duration: since 2016

Wood gasification is a potential core technology in the context of sustainable, decentralized heat and electricity supply for homeowners as well as small and medium businesses. For years, the ICP has conducted research in this field.

Since 2016 an ICP team has teamed up with the Portuguese Aberta Nova foundation to construct a prototype 20kWel- and recently a low-tar, low-maintenance 5kWel-gasifier at their site in Melides. While the aggregates from the beginning ran quite smoothly on Pine, Eucalyptus up until recently caused problems concerning long-term stationary operation. Among the main problems were (i) the high amount of excess thermal energy, released by the gasification reaction as well as (ii) unwanted tar condensation throughout the systems.

Figure 1: D. Neeser and G. Boiger (ICP) and P. Caels (Aberta Nova) working at prototype gasifier.

Since the summer of 2017, an ICP/ZPP gasification team, composed of D. Neeser, A. Fassbind and G. Boiger, has stayed at the Aberta Nova site for several weeks. Within this period the whole wood gasification system was mapped out, modeled [1], a gas-air-water heat exchanger was devised, tar condensation behavior was studied and a novel low-tar system was dimensioned. Based on this work and after careful planning and organizing necessary materials and tools, a prototype low-tar, low-maintenance 5kWel-gasifier was welded, assembled and put to operation. Figure 1 shows the ICP team, working with P. Caels at the Aberta Nova site, while Figure 2 presents the CAD drawing vs. final state of our novel heat exchanger.

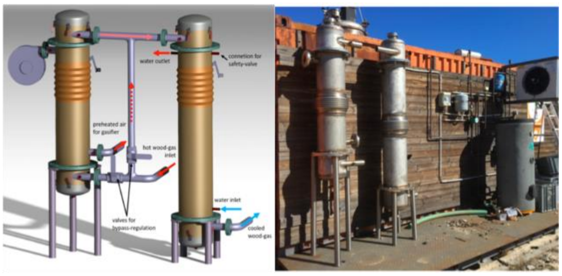


Figure 2: CAD scheme (left) of gasifier and actual result of our efforts (right).

Together with our Portuguese partners, lead by P. Caels, the ICP researchers were thus able to achieve (i) assertion of full functionality of the novel low-maintenance gasifier, (ii) successful test runs showing stable operation with Eucalyptus, (iii) hardly any tar condensation in various test modes and (iv) an increase of electrical power output due to higher system efficiency based on higher reactor temperatures and cooler wood gas.

Literature:

[1] Boiger, G. (2014). A thermo fluid dynamic model of wood particle gasification and combustion processes. IJM, Volume 8, Number 2. 203-230. Peer reviewed.

1.4 Impact of fouling on mechanical resonator-based viscosity sensors

This study discusses a state-of-the-art online viscosity sensor, which is used in an environment subject to fouling. A fouling layer can contaminate the measurement and is a potential source of error. The effect of a fouling layer has been studied on a simplified fouling model numerically and experimentally.

Contributors: D. Brunner, G. Boiger
Partners: Rheonics GmbH
Funding: Innosuisse
Duration: 2018–2020

Monitoring viscosity in a chemical, biological or another industrial process is essential to maintain the quality of the process. In many industrial processes, the viscosity of a fluid is strongly related to the fluid's composition, hence the viscosity can be used to detect changes and proper countermeasures can be taken.

Nowadays, online integrated viscosity measurements are possible by using mechanical resonators. However, there are issues when deposits are built on the resonating structure. Fouling or the formation of deposits on the resonator are a potential threat, which can contaminate the measurement and yield in a wrong prediction.

In the presented study, a probe style resonator has been coated with copper, which is a simplified, purely elastic deposit model. Figure 1 shows the copper deposit on the resonating tip of the sensor.

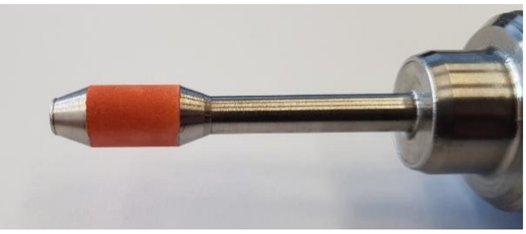


Figure 1: Resonator with fouling model (copper deposit).

The resonator has been mathematically approximated by a 2-mass 3-spring system. The fluid interaction has been modelled based on a 2-D model in COMSOL Multiphysics. Based on a flat surface, the viscous damping (represented by Γ) would be slightly decreased purely by inertial effects of the fouling layer. However, the experiments indicate that the damping increases. Furthermore, the relative increase is more pronounced for low viscosity which breaks the typical linear behavior of the sensor.

These effects could be explained by surface roughness. The fouling layer may be flat on a macroscopic level; however, it shows a roughness in the micrometer scale. This roughness is in the order of magnitude of the characteristic length scale of the flow, hence carries significance. The roughness has been modelled by two sinusoidal wavy surfaces and can explain the characteristics of the measurements, see Figure 2. However, further investigations on the surface structure and 3-D flow simulations are needed to fully understand the phenomenon and make reliable predictions. Future studies will involve deposits encountered in industry such as CaCo3 or paraffin.

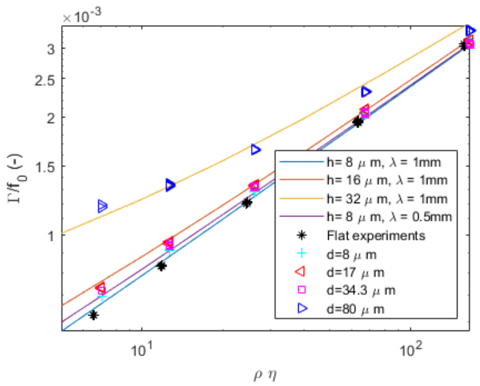


Figure 2: Comparison of experimental data to numerical predictions.

1.5 Model of a decanter centrifuge to predicte the settling behavior of particles in solid-liquid suspensions

Centrifuges are devices which employ a high rotational speed to separate components of different densities. Recently, Tilo Hühn and coworkers from ZHAW Wädenswil developed a completely new process for chocolate making where the chocolate beans are crushed, dissolved in water und then separated in a decanter centrifuge. To support the optimisation of this process, a yet simple, but powerful model has been developed.

Contributors: T. Hocker, D. Wyss
Partners: T. Hühn, ZHAW Inhaltsstoff- und Getränkeforschung
Funding: preliminary study
Duration: 2018–2019

Separating the individual phases of suspensions by centrifuges is a common process in many industries. Often, solids and liquids are first merged together to perform some sort of extraction, i.e., dissolving certain components from the solid into the liquid phase. However, for further processing, these phases need to be separated again from each other. To run this separation process in a continuous mode, decanter centrifuges are particularly convenient. There, a screw drive is used to continuously discharge the collected solids. Fig. 1 provides a sketch of the main component of such a centrifuge.

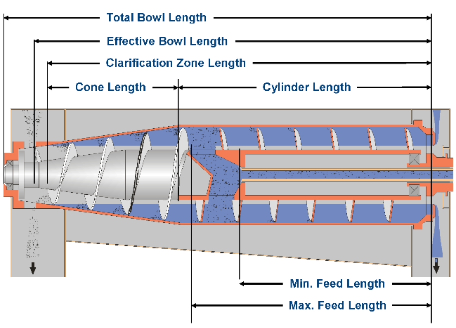


Fig 1: Sketch of a decanter centrifuge used to separate solids from liquids by exploiting their different densities.

To ensure a high degree of separation, bowl speeds of up to 5’000 rpm are used. Operating such centrifuges under steady-state conditions can be challenging, especially when the fed suspension changes its physical properties such as its viscosity or density. It therefore makes sense to use physical models to gain a better understanding of the settling process of solid particles from the suspension and how this is related to the properties of the feed as well as the geometry and operating parameters of the used centrifuge [1].

Fig. 2 shows a sketch of the simplified geometry on which our model is based. Here, the feed enters from the right. Due due to higher density of the contained solids they settle at the inner wall of the bowl – provided the flow velocity is not too large and the particles are not too small.

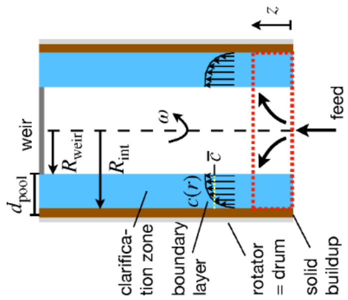


Fig 2: Simplified geometry for which the decanter model has been developed.

Using the well-known Stokes’ settling theory as basis, we were able to derive a yet simple, but powerful model to predict the settling behaviour as well as the solids buildup and subsequent discharge. Fig. 3 shows typical model results at a certain point in time. Here, a feed containing six different particle sizes has been assumed. Besides the settling paths, the model predicts the solids buildup at the bowl wall shown as grey area.

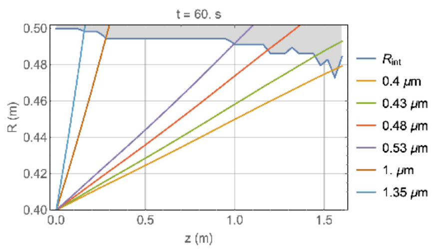


Fig 3: Particle settling paths and solids buildup predicted by the model for a feed containing six different particle sizes.

Literature:

[1] M. Gleiss, S. Hammerich, M. Kespe, H. Nirschl, Chemical Engineering Science, 163, pp. 167–178 (2017).

1.6 Analyzing the thermal behavior 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 create an improved model setup to better determine the influence of the sensor properties and dimensions on the thermal behavior.

Contributors: L. Ruckstuhl; Advisor: T. Hocker
Partners: Medyria AG, Winterthur, M. M. Sette, A. Di Iasio
Funding: Master thesis
Duration: 2018–2019

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. During a preliminary student project it was discovered that the set temperature of the sensor and the actual temperature on the surface are not identical. The surface temperature highly depends on the velocity of the flow and the isolation layer covering the heated area of the sensor. According to the sensor manufacturer layer variation of 10% (or 0.5 μm) can be expected within one batch of sensors. As illustrated in Fig. 1 these deviations lead to a surface temperature variation of up to 6% at2 $\frac{m}{}$

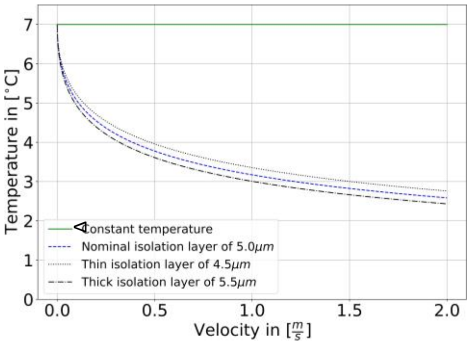


Fig. 1: The thermal behaviour of the sensor suface for different isolation thicknesses and flow velocities is illustrated.

In the preliminary model this surface temperature is a boundary condition, thus for each simulation first the occurring temperature needed to be calculated. This has disadvantages to use the model for predictions, because the velocity above the heating element might not be known or the heated area is changing in addition to the temperature. In order to improve that, a 2D CFD-model was developed, which in addition to the fluid includes the solid region of the sensor. Choosing a flat surface has the following advantages: firstly, the surface temperature correlation is simpler for flat surfaces; secondly, the validation of the flow profile over a flat plate can be done using literature and, lastly, the mesh generation is simplified. In a later step, a 2D-model representation of the sensor on a cylindric surface can be added if necessary. Fig. 2 shows a comparison between the calculated average surface temperature and the simulation results for two different flow velocities. The heated sensor area is indicated by the vertical red lines. The average surface temperatures correlate well with the simulation results.

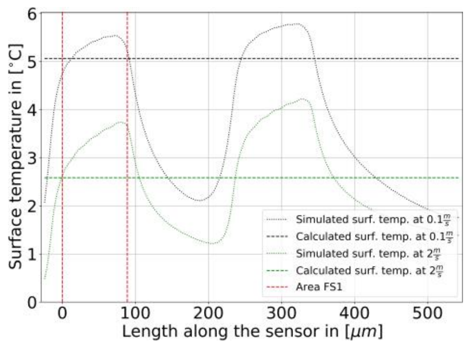


Fig. 2: A comparison between the calculated average surface temperature and the simulation results for two velocities are shown.

This supports the hypothesis that most of the variations observed between nominally identical catheters is due to their differences with respect to the isolation layer above the heated elements. As next steps, the thickness variations of the isolation layer will be further investigated by microscopy and resulting T-profiles will be assessed by thermal imaging.

1.7 Multi-scale model of crystal-polymorphism

In the casting process, crystals nucleat and grow in multiple forms affecting the thermo physical properties of the materials. At macro-scale observation, the quality of the solid is influenced by both the thermodynamic and mass kinetic effects during crystallization. However, several static and kinetic effects are micro-scale players, they affect the material through a departure from the local thermodynamic equilibrium and cause undercooling phenomena. A new predictive approach is built through a coupled solving of the macro-scale heat-mass transfer problem and the micro-scale problem of grain solidification in undercooled melt. The new model shows the influences of local cooling rate as well as the surface curvature of the seeding crystal grains and nuclei on the temperature of the bulk material. With the new approach, the post-recalescence solidification is computationally reproduced in agreement with the values from experimental measurements.

Contributors: Y. Safa, T. Hocker
Partners: IFNH ETH Zurich, and Swiss chocolate manufacturing partners
Funding: Innosuisse
Duration: 2016–2018

The formation of polycrystals materials from a melt phase at high cooling rate promotes the nucleation and the growth of unstable crystal forms with limited latent heat release. In contrary, a low cooling rate promotes the growth of stable crystal forms accompanied by a large release of latent heat. Interconversion between different crystal polymorph and between melt and crystal take place. One can simplify the analysis of this problem by adopting a macro-scale model of heat-mass transfer system of equations to obtain the time-space distribution of the temperature and crystals. In such a simplified macro-scale model, interconversion between different crystal polymorph is represented as reaction equations with kinetic parameters (e.g. reaction constants) depending on the transition temperatures between phases in melt-crystals mixture. This simplified analysis comes on the expense of a realistic representation of the role of the cooling rate how it affects produced materials during moulding process. Indeed, a high cooling rate, is accompanied with melt undercooling of liquid phase below the melting point. This undercooling reflects a departure from the local thermo-dynamic equilibrium and influences the crystal formation. Different scenarios of interface undercooling including attachment kinetic and solute trapping at the interface were analyzed. Only the curvature undercooling was found pertinent to the chocolate solidification problem due to small size values of nuclei and seeding grains at given surface tension. Undercooling can be an interfacial phenomena taking place on the surface of seeding crystal micro-grains and nuclei that are growing in a cooled or supercooled melt. The above simplified macro-scale model of heat-mass transfer cannot be a sufficient means to capture such an interface undercooling between micro-grain and surrounding melt. Indeed a restriction to a micro-scale model is needed to capture the effects of interface undercooling. Such micro-model is formulated through Stefan problem in a melt micro-domain containing a spherical grain where heat conservation expressed in both solid and liquid parts. Stefan condition of solid front advancement is imposed on the grain surface and curvature undercooling (Gibbs-Thomson relation) is also introduced as interface condition.

In this research works, we treat a phase change coupling energy transfer and mass transformation between different phases. 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, derive relationships that can aid in process design. On the other side, the undercooling caused by grain curvature are analyzed at micro scale to be taken into account through a new coupling model describing the interaction between macro and micro effects. Note that developed approach contributes an applicable predictive tool to many industrial applications, like for example, polymer processing, cement manufacture, food processing (chocolate) and pharmaceutical industries.

Patent: Y. Safa, *Une turbine éolienne bionique plus légère que l'air.*, Bern Switzerland. PAdmin Cr/00168/17.

1.8 Powder Coating: A Post Processing Tool to Analyze Powder Coating Thickness Data

Powder coating is an environmentally friendly alternative to other methods for providing surface finishes. A big challenge in the field has been the non-invasive assessment of the quality of a coating. To address this issue the Coatmaster 3D technology [1], based on advanced thermal optics, was used to gather thickness information from coated substrates. Subsequently a post processing tool was developed for the assessment of the data in terms of the coating performance parameters derived also in the scope of the project.

Contributors: Bercan Siyahhan, Marlon Boldrini, Gernot Boiger
Partners: Winterthur Instruments, Wagner International AG
Funding: Innosuisse
Duration: 2016–2019

A post processing tool was developed using Python and its TkInter GUI package. It also links to Paraview for data visualization functionalities. The tool comprises mainly of data filtering and statistical analysis frameworks. The data filtering procedures include: (i) elimination of geometric and measured value outliers, (ii) exclusion of specified geometric regions, and (iii) automatic noise elimination with a median filter-based masking procedure. The statistical operations directly yield the performance parameters of coating processes. The first performance parameter is the average coating thickness (ACT):

$$ACT = \frac{\sum_{i=1}^{N_{unfilter}} D_i}{N_{unfilter}}$$

The ACT is a direct indicator of the coating efficiency, as between two different coating procedures with the same amount of powder being used, the one with the higher ACT will have deposited a higher portion of the powder, hence a higher efficiency. The second performance parameter is a measure of how inhomogeneous (In) the coating on a substrate is:

$$\text{In} = \frac{\frac{1}{N_{bin}-1}\sqrt{\sum_{i=1}^{N_{bin}}(D_i - D_{max})^2 \frac{N_i}{N_{max}}}}{D_{max}}$$

The In is basically a weighted, normalized standard deviation of the thickness from the most frequently measured value on its discrete distribution graph illustrated in Fig. 1.

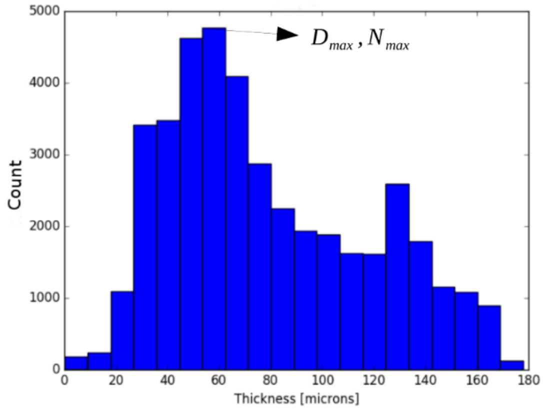


Fig. 1: Thickness measurent data as a discrete distribution.

A homogeneous coating is desired in most cases in practice hence a procedure with a lower In will be favoured.

The tool has the capability to apply the outlined procedures to large sets of data automatically, laying the groundwork for parameter optimization of coating processes and numerical simulation [2] comparisons.

Literature:

[1] A. Bariska, N. Reinke, Berührungslose thermische Schichtprüfung, ZHAW Winterthur, Switzerland. Swiss Engineering STZ, 2011.

[2] G. Boiger, Euler-Lagrangian Model of Particle Motion and Deposition Effects in Electro-Static Fields Based on OpenFoam, The International Journal of Multiphysics, 2016.

1.9 Prüfstand zum kontaktlosen Verschweissen von Kunststoffproben

Das Infrarot-Schweissverfahren ist in der Technik eine weitverbreitete Methode zum Verbinden von Kunststoffrohren. Die zu verbindenden Bauteile werden in einem bestimmten Abstand zum Heizspiegel gebracht, aufgewärmt und mit einer vordefinierten Kraft gefügt. Durch den Abstand zwischen Heizspiegel und den Rohrenden werden die Bauteile primär über Wärmestrahlung erwärmt. Dies führt zu einer konkaven Schmelzfront, welche die Qualität der Schweissnaht negativ beeinflussen kann. Auf einem Prüfstand soll die beste Heizsystemlösung, im Hinblick auf eine optimale Schweissnahtqualität, evaluiert werden.

Contributors: N. Jenal, M. Gorbar, S. Spirig, T. Hocker, C. Brändli
Partners: Institute of Materials and Process Engineering (IMPE), Georg Fischer Piping Systems
Funding: Innosuisse
Duration: 2018–2021

Beim Infrarot-Schweissverfahren werden die zu verbindenden Rohre in einem bestimmten Abstand zum Heizspiegel platziert. Durch den Abstand zwischen Heizspiegel und Rohr kann der Eintrag von Verunreinigungen in die Schweissnaht sehr gering gehalten werden. Dieses Verfahren wird dementsprechend häufig in technischen Bereichen verwendet, in denen ein hohes Mass an Reinheit vorausgesetzt wird. Es wird beispielsweise für die Fertigung von Rohrleitungen in Reinräumen angewendet.
Die Enden werden in erster Linie über Wärmestrahlung aufgeschmolzen, siehe Fig. 1. Dieses Aufheizverfahren führt zu einer konkaven Form der Schmelzfront, welche die Schweissnahtqualität negativ beeinflussen kann.

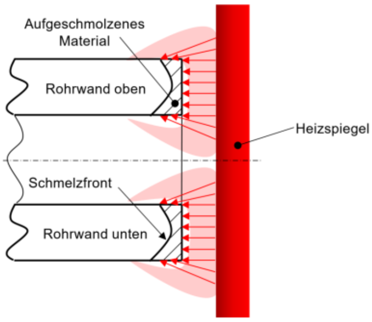


Fig. 1: Schematische Darstellung des Infrarot-Schweissprozesses.

Mit einem Prüfstand soll u. a. evaluiert werden, welche Einflüsse die Dynamik des Aufheizprozesses und die Fügekraft auf die Schweissnahtqualität haben. Damit unterschiedliche Heizelementdicken auf dem Prüfstand montiert werden können, werden die Elemente über eine Klemmvorrichtung auf dem Schwenkarm befestigt, siehe Fig. 2. Über Flügelmuttern kann das Heizelement manuell in vertikaler sowie horizontaler Richtung präzise platziert werden. Die Fügekraft wird über eine Druckfeder aufgebracht. Die Federkraft kann über eine Sechskantmutter variabel eingestellt werden. Ein zusätzlich eingebauter Kraftsensor dient zur Überprüfung der Federkraft.
Weiterhin soll der Prüfstand zur Validierung dienen, sobald mittels CFD-Untersuchungen ein Optimum für den Abstand Probe/Heizelement gefunden wurde.

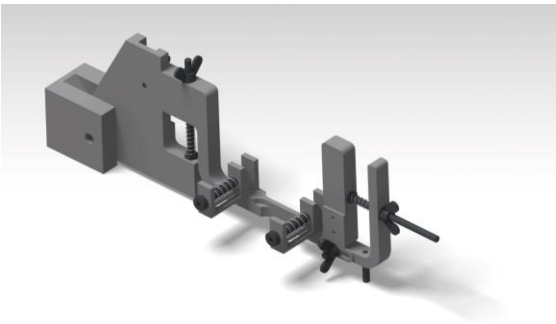


Fig. 2: Schwenkarm zur Aufnahme verschiedener Heizsysteme inklusive Mechanismen zur Feinjustierung.

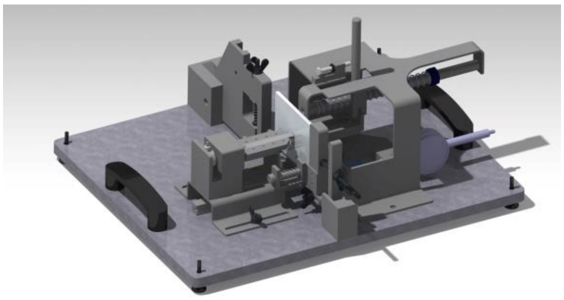


Fig. 3: Aktuelles Design des Prüfstands zum kontaktlosen Verschweissen von Kunststoffproben.

1.10 Dynamic delamination in morphing blades and wings

A numerical framework for the study of delamination in morphing composite blades and wings is introduced using eXtended Finite Element Method (XFEM), and nonlocal continuum mechanics (peridynamics (PD)) to study fracture in the stiffener used in conjunction with the blade. As for the composite morphing blade, cohesive elements are used to represent the interlaminar weak zone and delamination has been studied under dynamic pulse loads. Intraply damage is studied using peridynamics with capability to address the problem adequately for the necessary level of sophistication. Through the use of fracture energy alone the nonlocal model is capable of capturing intra- and interlaminar fractures. The proposed framework can thus have a major impact in design applications where dynamic pulse and impact loads of all natures (accidental, service, etc.) are to be considered and may therefore be utilised in design of lightweight morphing blades and wings.

Contributors: A. S. Fallah, M. Ghajari, Y. Safa
Funding: Swiss National Science Foundation
Duration: 2018

Advances in structural aerodynamics have given rise to constant evolution in novel blade designs of improved airfoil cross sections and wings with continuous shape morphing. This allows these flexible structures to adapt continuously their shapes with respect to aerodynamic conditions and applied loads. Under the action of dynamic pulse loads there could be fracture in the stiffener (Fig.1)

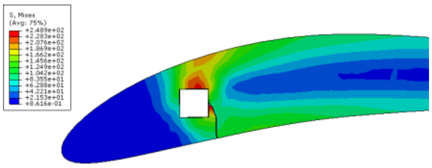


Fig. 1: XFEM crack in the stiffener and its propagation towards the boundaries.

In morphing blade, depending on the regime of pulse loading (impulsive, dynamic, quasi-static), the pattern of fracture would be different. Interlaminar fracture may be accurately captured using cohesive elements (Fig.' 2 and 3), but for intra-ply fracture peridynamics was used (Fig. 4)

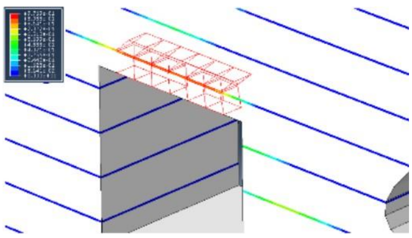


Fig. 2:Excessive shear distortion.

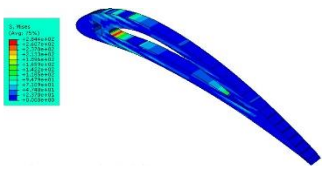


Fig. 3: Stress distribution and mismatch.

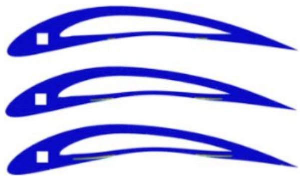


Fig. 4: Simulation under impulsive loading fracture using PD.

The differences and similarities between delamination patterns for impulsive, dynamic, and quasi-static loadings are appreciated with detailed analyses of delamination patterns. It is anticipated that in the case of an impulse higher modes of vibration are triggered and the delamination occurs throughout the blade in several locations simultaneously or sequentially, however, for quasi-static loading the pattern of fracture is more as propagation from a single location till complete separation and subsequent cracks are mostly geometric i.e. due to large deformations and change of initial configuration. For dynamic pulse a mixture of both phenomena may be encountered depending on whether the pulse is closer to an impulse or to a quasi-static load. It is shown the proposed framework is capable of capturing all major features of dynamic delamination in composite morphing blades through an accurate and consistent computational modelling scheme.

Paper:

A. Fallah, M. Ghajari, Y. Safa, *A computational framework for the study of dynamic delamination in morphing composite blades and wings*, Submitted to Journal Engineering Structures.

1.11 Spectral composition of the Faraday instability in small vessels

The agitation of liquids inside vessels is a source of problems for biological or pharmaceutical liquid solutions. One important aspect to understand the agitation of aqueous solutions is the stability threshold above which the free surface shows normal modes. The parametric instability under vertical vibration has been extensively studied theoretically and experimentally.

Contributors: A. Zubiaga, G. Boiger, D. Brunner, F. Sager, M. Clemens, E. Koepf
Partners: F. Hoffmann-La Roche Ltd. Basel
Funding: F. Hoffmann-La Roche Ltd. Basel
Duration: 2018–2019

Mechanical stress conditions, such as agitation during shipping, can result in denaturation and aggregation of biomolecules, thereby affecting the stability of the products profoundly. The transportation degradation is linked to the shear stress induced by the agitated fluid.

Exposed to vertical vibrations, liquids are prone to show Faraday instabilities when the acceleration grows above certain threshold value. These modes are stationary and can grow large inducing a high shear stress on the dissolved product. The vessel shape, its dimensions and the fluid characteristics (mass density, viscosity and surface tension) influence the formation of instabilities. The parametric instability under vertical vibration has been studied thoroughly by Kumar & Tuckerman [1] using a Floquet analysis for viscous fluids.

For this work, both theoretical and experimental studies for small vessels have been performed [2]. The mode components of the Faraday instability have been calculated with a Floquet analysis in a wide frequency range, ranging from 5 Hz to 150 Hz. The calculated Faraday instability threshold has then been validated experimentally by measuring water in small vials under vertical vibrations (Fig. 1). A qualitative agreement with the theory is observed, and the disagreement in the position of the stability tongues can be well explained by the non-linear viscosity effects exerted by the container walls.

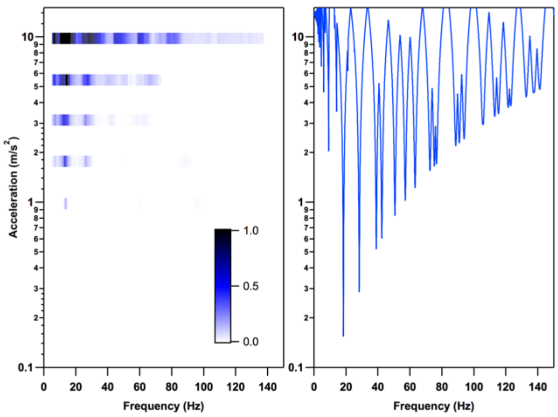


Fig. 1: The acceleration plotted versus frequency in the experiments (left panel) and in the stability analysis (right panel).

The lower k-momentum cut-off has a protective effect on the liquid against low-frequency instabilities. At frequencies larger than 20 Hz, the instability threshold increases steeply due to the intrinsic response of the liquid to high frequencies. The existence of a low stability region between 10 and 70 Hz has been confirmed by the experiments. Future studies will study the influence of fluid characteristics in the position of the stability threshold, as well as the increase on the shear stress caused by the Faraday instability.

Literature:

[1] Kumar K, Tuckerman LS. Parametric instability of the interface between two fluids. J Fluid Mech., 1994, 279, 49–68.

[2] A. Zubiaga, D. Brunner, F. Sager, M. Clemens, E. Koepf, G. Boiger. Faraday instability in small vessels under vertical vibration. Int. J. Multiph., 2019, submitted.

1.12 PVT-Hybridkollektoren: Wärme und Strom aus der Sonne

Die Kopplung von Photovoltaik und Solarthermie verspricht mit PVT-Hybridmodulen einen Zusatznutzen gegenüber der herkömmlichen Solarenergienutzung. Sowohl beim Bau dieser Module als auch in der Systemeinbindung liefert das ICP mit hochstehenden Computersimulationen einen wichtigen Beitrag.

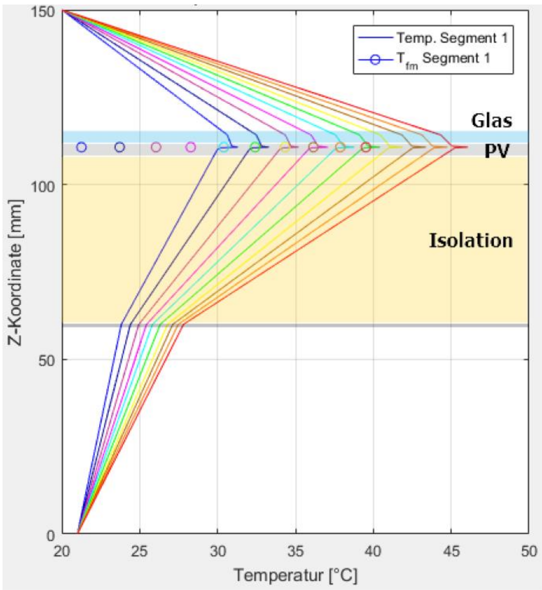
Contributors: T. Frei, D. Schaltegger, A. Witzig
Partners: Ponzio Solar SA, Institut für Energietechnik und Fluidengineering (IEFE)
Funding: Innosuisse
Duration: 2017–2019

Die Dachfläche für Solarenergienutzung wird knapp. Dies ist die grosse Chance der PVT-Hybridkollektoren: Auf jedem Quadratmeter wird gleichzeitig Solarstrom produziert und Energie in Form von Wärme geerntet.

PVT-Hybridkollektoren haben verschiedene Einsatzgebiete:

- Bei der Verwendung der Wärme für die Aufbereitung von Trinkwarmwasser wird das Temperaturniveau hochgehalten. Die Wärme über einen Wärmetauscher an den Warmwasserspeicher abgegeben. Im Vergleich zu anderen PVT-Systemen verspricht diese Konfiguration einen guten Kompromiss zwischen Effizienz und Energiekosten.
- Kombination mit Wärmepumpe und Erdsonden oder Eisspeicher: In dieser Situation kann sehr viel Energie geerntet werden. Nicht nur bei direktem Sonnenlicht, sondern auch bei Diffuslicht und hohen Aussentemperaturen bringt die Wärmenutzung noch hohe Erträge.
- Kombination mit Wärmepumpe als Ersatz für die Erdreichanbindung: Diese Konfiguration verspricht eine kostengünstige Lösung, da die teure Energiespeicherung im Erdreich wegfällt [2]. Der PVT-Hybridkollektor wird als Wärmetauscher gegenüber der Aussenluft betrieben. Eine sorgfältige Auslegung anhand von Simulationen ist jedoch Voraussetzung, da bei einer falschen Dimensionierung die nötige Wärmeleistung nicht bezogen werden kann.

Die Modellierungskompetenzen am ICP werden zur Unterstützung der Systemoptimierung und zur Erweiterung der Simulationsmodelle eingesetzt. Dafür wird einerseits die kommerziell erhältliche Software Polysun eingesetzt und erweitert [3], andererseits werden neue Computermodelle entwickelt und anhand von Messungen verifiziert [4, 5].



Figur: Simulation des PVT-Hybridkollektors. Temperaturverlauf an 10 Stellen entlang des mäanderförmigen Wärmetauscher-Rohrsystems.

Referenzen:

[2] Ch. Schmidt et. al. (Fraunhofer ISE): Quellseitig in Wärmepumpen-Heizsystem integrierte PVT-Kollektoren. Symposium Solarthermie, Bad Staffelstein, Juni 2018.

[3] www.polysunsoftware.com

[4] T. Frei: Herstellung und thermische Simulation von neuartigem Hybridkollektor. Studentenarbeit ICP-ZHAW, Februar 2017.

[5] T. Frei: Simulation eines Hybridkollektors im instationären Betrieb. Studentenarbeit ICP-ZHAW, September 2017

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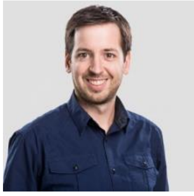
2 Fuel Cells and Microstructures

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 micro-structures 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


Robert Herrendörfer


Gaël Mourouga


Jürgen Schumacher


Jakub Wlodarczyk

2.1 Simulating the energy yield of next generation photovoltaics

Emerging 3rd generation photovoltaic technologies are characterized at standard test conditions in laboratory, yet it is uncertain how they perform in real outdoor installations. We have developed a model to simulate the energy yield of PV modules considering geographical position, local weather and characteristics of the device. We use the tool to analyze the performance loss of monolithically connected tandem solar cells caused by red/blue shift of the solar spectrum. For the promising silicon heterojunction perovskite tandem cell, we obtain a mismatch loss of 1.27% on the integrated annual module power.

Contributors: D. Bernhardsgrütter, M. Schmid
Partners: EPFL-LPI, EPFL PV-Lab, EMPA-TFPV
Funding: SNF
Duration: 2015–2018

We have developed a tool to simulate the energy yield of 3rd generation PV technologies including the promising silicon heterojunction perovskite tandem cell (SHJ-PSC). It allows us to assess the performance loss of tandem solar cells operating at real outdoor conditions compared to standard test conditions (STC), for which they are optimized. Additionally, the simulated power output provides data required for the analysis of the impact of novel PV technologies on the grid.

The model considers the geographical position, local weather, orientation and characteristics of the device, i.e. external quantum efficiency (EQE), current-voltage curve (IV) and temperature coefficients. To estimate the energy production of outdoor installations, synthetic clear-sky spectra are generated considering the atmospheric absorption and the red/blue shift of the spectrum. Then weather data consisting of integrated irradiance, temperature, wind, and pressure are used to rescale the spectra to the measured irradiance and to estimate the module temperature. EQE and IV data together with temperature coefficients are then used to predict the module power.

To validate the model, we have compared the predictions of our forecasting tool with simulation results generated with the commercial software PVsyst. The comparison has been conducted for a generic module and weather data of the year 2017, resulting in annual deviations of less than 5%, cf. Fig. 1.

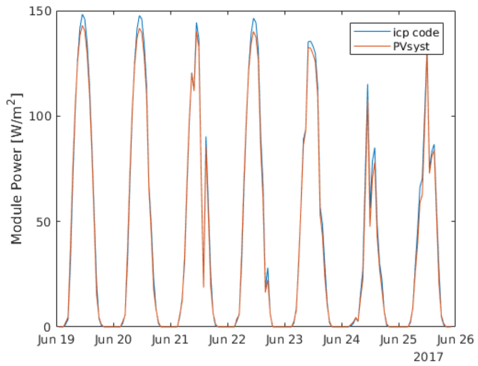


Fig. 1: Simulated power output of the module TSM-290DD05A.08(II) calculated with our model and with PVsyst.

We applied the validated model to quantify the current mismatch losses of monolithic two-terminal (2T) tandems caused by blue/ red shift of the solar spectrum. We used the simulation software SETFOS to generate the EQE and IV of a power-matched SHJ-PSC. The mismatch losses have been estimated by comparing the energy yield of the 2T tandem with the sum of the performances of each sub-cell operating independently. We obtained a mismatch loss of 1.27% on the integrated annual module power.

No mismatch losses arise for mechanically stacked four-terminal (4T) tandems, but an additional transparent electrode is necessary leading to increased parasitic optical absorption. We have thus calculated an upper limit for these absorption losses for the 4T tandem to be more efficient than its 2T counterpart.

2.2 Analyzing the dynamic response of perovskite solar cells

Within less than a decade since their advent, perovskite solar cells (PSCs) have reached efficiencies on a par with silicon-based cells. Numerical simulations provide insight into the physical processes within these novel cells, facilitating further optimization of the technology. When PSCs are excited by intensity-modulated light with varying frequency, they show a response at low frequency which is characteristic for these devices. We use a drift-diffusion model to link this unique feature to mobile ions within the cell.

Contributors: D. Bernhardsgrütter, M. Schmid
Partners: EPFL-LPI, EPFL PV-Lab, EMPA-TFPV
Funding: SNF
Duration: 2015–2018

Perovskite solar cells have attracted tremendous interest within the photovoltaic community over the last decade. The technology is regarded as a promising candidate to compete with silicon solar cells in the near future. The excellent optical and electrical properties of perovskite materials have boosted the efficiencies above 20% within less than 10 years of research. No other technology has achieved comparable results in such a short stretch and perovskite has the bonus of being a potential low-cost technology through low-temperature solution processing. Furthermore, their absorption properties make them an ideal candidate as top cell in combination with bottom silicon cells to form even more efficient tandem solar cells.

Intensity-modulated photocurrent spectroscopy (IMPS) and intensity-modulated photovoltage spectroscopy (IMVS) are important characterization techniques for solar cells. The cells are exposed to sinusoidally modulated light, while either the current (IMPS) or voltage (IMVS) response is measured. These techniques are applied to probe transport and recombination of charges within the cell. By measuring the response for a wide range of frequencies, varied processes at different time-scales are revealed.

Perovskite solar cells admit a distinct reponse at low frequency (< 10 Hz). We use numerical simulations to test the hypothesis, that mobile ions are responsible for this feature. Our model comprises one-dimensional drift-diffusion equations coupled with ion transport. Two complementary methods are used to compute the small signal response. The sinusoidal steady-state analysis (S3A) is based on linearization of the model equations around the stationary operating point. Typical results of the S3A-method are depicted in Figure 1.a, b). In contrast, Fourier decomposition (FD) entails the computation of the Fourier transform of the transient cell response to a light intensity step, cf. Figure 1.c). While the S3A-method is more efficient and accurate, the FD-method provides additional interpretation of IMPS and IMVS results by relating the time and frequency domains.

Our results indicate that the low-frequency response of PSCs is explicable by ion migration. As the ions are assumed to have low mobility, they respond to the excitation on different time-scales as electrons and holes. Simulated IMPS and IMVS responses therefore admit two separate time constants, cf. Figure 1.b). The origin of the high frequency response lies in the transport and recombination of electronic charges, while the low frequency response is associated with mobile ions.

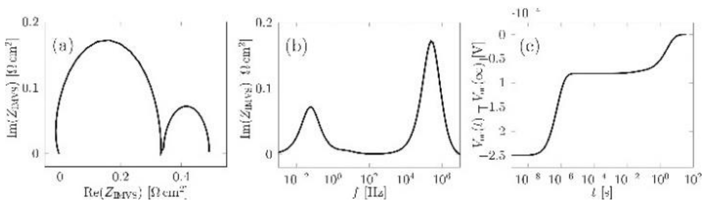


Fig. 1: Simulated IMVS response of a perovskite solar cell. Part a) shows the Nyquist plot and subfigure b) the imaginary part of the IMVS transfer function. The simulated photovoltage of a PSC excited by a small light intensity step is shown in subfigure c).

2.3 Advanced characterization of fuel cell stacks for automotive applications (ACTIF)

The project ACTIF aims at optimized operational strategies for fuel cell systems regarding the three main aspects efficiency, life-time and costs on the stack level. This will be enabled by enhanced understanding of fuel cell stacks on the basis of advanced time-resolved characteri-zation techniques and mathematical modeling.

Contributors: J. O. Schumacher, R. Herrendörfer
Partners: GreenGT
Funding: Swiss Federal Office of Energy SFOE
Duration: 2018–2021

During the initial phase of this project (October 2018 - December 2018), we have developed a time-dependent single-cell polymer electrolyte fuel cell (PEFC) model. On the basis of the fully parameterized, one-dimensional and steady-state two-phase model previously developed at ICP, we additionally account for the time-dependency in the governing equations for electrons, protons, heat, dissolved water, gas and liquid water. Implementation in COMSOL Multiphysics allows for accurate spatio-temporal numerical resolution and flexible model setups.

To test our new implementations, we have conducted time-dependent numerical experiments. In so-called jump experiments, during which boundary conditions are changed abruptly, we analysed the duration of the transients of each governing process. In agreement with theoretical values, the characteristic time scale is the longest for membrane hydration and the shortest for electrical double layer charging and discharging. We showed that the membrane hydration is therefore responsible for the hysteresis effect observed in cyclic voltammetry experiments (Figure 1). Furthermore, we proved the numerical stability of our approach by showing that the solution converged with increasing spatiotemporal resolution.

The next steps of this project are the extension of this time-dependent model on the stack level, model order reduction and implementation of fuel cell degradation mechanisms. We will apply the model to simulate the dynamic response of a fuel cell system of the Swiss company GreenGT and collaborate with the German partners Fraun-hofer ISE and DLR. This collaboration targets the validation of our model using experimental measurement data. This will be essential for using our models to characterize and optimize fuel cells systems with respect to performance and durability.

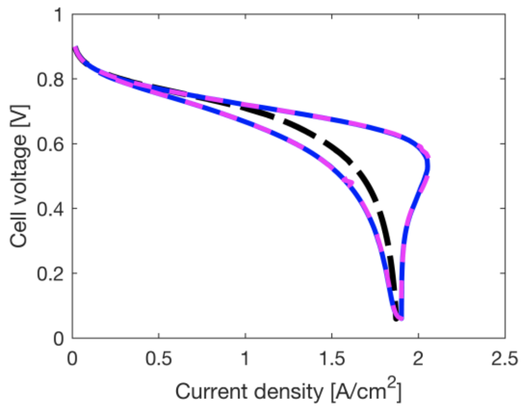


Figure 1: The figure shows the fuel cell polarization curve resulting from the simulation of a cyclic voltammetry experiment. The magenta line represents the solution obtained only with the accumulation term in the conservation equation of dissolved water (i.e., the membrane water content). The steady-water solution (black curve) is plotted for comparison.

2.4 Experimental parameter uncertainty in polymer exchange membrane fuel cell modeling

This project aims at determining the transport parameters of polymer exchange membrane fuel cells (PEMFC) whose uncertainties affect the performance prediction the most. The first part explores the scatter in material parameterization and its impact on the simulated polarization curves. The second part analyses the sensitivity of the model output to uncertainties in a robust way by introducing the concept of relative condition number to fuel cell modeling.

Contributors: R. Vetter, R. Herrendörfer, J. O. Schumacher
Partners: Swiss energy competence center (SCCER): Efficient technologies and systems for mobility (SCCER Mobility)
Funding: Innosuisse
Duration: 2014–2020

Predictability of PEMFC models has suffered from significant uncertainty in the parameterization of material properties. In this project the most critical transport parameters were determined for which a more accurate experimental characterization is required to enable reliable fuel cell performance prediction.

In the first part, a comprehensive set of material parameterizations from the literature was incorporated into the recently developed macro-homogeneous two-phase membrane-electrode assembly model at ICP [1]. This numerical model demonstrated the large spread in performance prediction resulting from published experimental data on material properties. Membrane transport properties induced the largest spread in the fuel cell performance curve: the diffusivity of dissolved water, the protonic conductivity and the electro-osmotic drag coefficient [2].

To analyze the sensitivity of the model output to uncertainties in the model input in a robust way, the second part conducted extensive forward uncertainty propagation analyses for 26 input parameters (operating conditions and material parameters) and 12 output parameters (characteristics of the polarization curve and fuel cell state) [3]. By introducing the concept of condition numbers to fuel cell modeling, the propagation of uncertainty through the model is measured explicitly. Besides a local sensitivity analysis, a global sensitivity analysis was conducted that covers a broad range of operating conditions and material properties.

Among the most critical model parameters are the membrane transport properties (Figure 1): membrane hydration isotherm, the electro-osmotic drag coefficient, the membrane thickness and the diffusivity of dissolved water. As shown in first part, these parameters suffer from the largest scatter in available experimental data. This calls for a better characterization of the membrane properties.

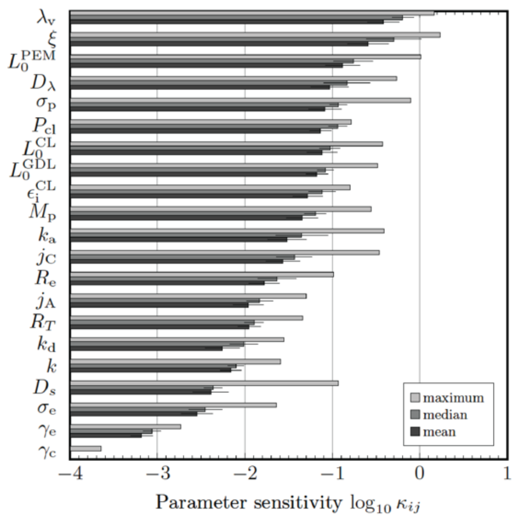


Figure 1: Global model sensitivity to parameter uncertainty. Material parameterizations are sorted by significance in decreasing order.

Literature:

[1] R. Vetter and Jürgen O. Schumacher, Computer Physics Communication, 234, 223–234, 2019

[2] R. Vetter and Jürgen O. Schumacher, 2019 arXiv:1811.10091

[3] R. Vetter and Jürgen O. Schumacher, 2019 arXiv:1811.10093

2.5 Modelling and simulation of an organic redox flow battery cell

Organic redox flow batteries show promises as a low-cost, sustainable energy storage device. It is still a very young technology, and a lot of work is required in optimizing materials and components. The aim of this work is to provide a macrohomegeneous model of the organic cells, in order to estimate the best compromise between performance and lifetime, and ultimately provide insights on various parameters of the cells. It is part of the project FlowCamp, a research and training project funded by the European Union's Marie-Sklodowska-Curie programme. FlowCamp involves 11 partner organisations from 8 different countries. Research in FlowCamp aims to improve materials for high-performance, low-cost next-generation redox-flow batteries.

Contributors: G. Mourouga, J. O. Schumacher
Partners: ETH Zürich, Hungarian Academy of Science, Univ. Grenoble-Alpes, JenaBatteries
Funding: European Commission, Horizon 2020, Marie Skłodowska-Curie Training Networks
Duration: 2018–2021

There are two organic chemistries under study in the FlowCamp project: all-quinone and all-polymer. The former consists of quinones – cheap, natural charge carriers, encountered in photosynthesis processes for example – dissolved in an aqueous sulfuric acid electrolyte. The latter consists of synthetized long-chain polymers – relatively cheap, and highly tunable – dissolved in sodium chloride. While the equations of the models are valid for both chemistries, our efforts have for now focused on the all-quinone chemistry, because of a greater amount of data available.

The redox active molecules for this system are 1,2-dihydrobenzoquinone-3,5-disulfonic acid on the positive side and anthraquinone-2-disulfonic acid on the negative side (left and right tank respectively, see figure below)

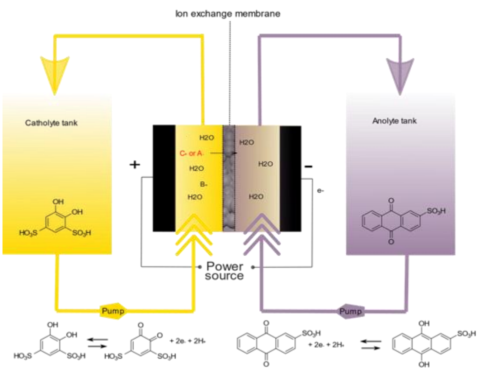
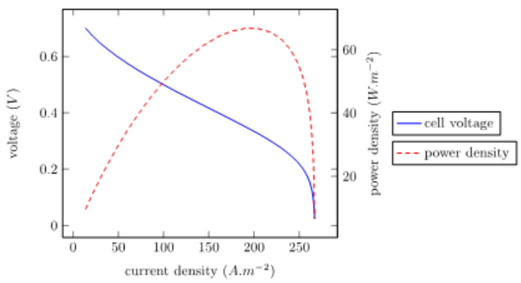


Figure 2. Illustration of an all-quinone organic redox flow cell.

These molecules yield a fast proton-coupled electron transfer process, and the absence of precious metal catalysts make the all-quinone chemistry an interesting candidate for green, low-cost energy storage [1].

The downside is that this chemistry yields a relatively low energy density compared to other chemistries, and solutions to overcome this may result in an increased crossover of the benzoquinones to the negative electrode, which in turn reduces the expected lifetime of the battery [1].



The aim of our work in the FlowCamp project is to provide a reliable model of the cells, which would allow us to tune properties such as electrolyte composition and viscosity, membrane properties and organic cell architecture [2].

The 1D macrohomegenous model of the cell was made using COMSOL Multiphysics and includes charge and mass transport phenomena in the electrodes and the membrane. We are working on a multicomponent diffusion model, in order to better model the transport phenomena in the ion-exchange membranes, which are a critical component of these cells.

Literature:

[1] B. Yang, L. Hoober-Burkhardt et al., Journal of The Electrochemical Society, vol. 161, no. 9, 2014.
[2] https://www.flowcamp-project.eu/

2.6 Modeling and Simulation of a Hydrogen-Bromine Redox Flow Battery Cell

The main issue of emerging technologies in renewable energy storage is their cost. It can be mitigated by utilizing cheap and abundant reactants such as hydrogen and bromine. This study describes a macrohomogeneous modeling approach to the hydrogen-bromine redox flow battery system as well as case studies to better understand the impact of key operating parameters on the overall cell performance. It is part of the FlowCamp project [1], a research and training project funded by the European Union's Maria Skłodowska-Curie program. FlowCamp involves 11 partner organizations from 8 different countries. Research in FlowCamp aims to improve materials for high-performance, low-cost next-generation redox-flow batteries.

Contributors: J. Włodarczyk, J. O. Schumacher
Partners: Elestor B.V., Fraunhofer Institute for Chemical Technology, University of Stuttgart
Funding: European Commission, Horizon 2020, Maria Skłodowska-Curie Training Networks
Duration: 2018–2021

One of the flow battery systems which utilizes abundantly available chemicals for electrolytes, characterized by high power density, is the hydrogen-bromine flow battery (HBRFB).

A typical setup of a HBRFB system consists of an electrolyte storage vessel and a pressurized hydrogen gas vessel, electrolyte circulation pump, and a cell stack, which is composed of current collectors, bipolar plates, porous electrodes (carbonaceous materials for the Br_2 side and platinum alloys for the H_2 side), and an ion-selective membrane.

On discharge, at the negative electrode, dissolved hydrogen gas diffuses to the catalyst surface and is oxidized to protons on discharge. At the same time, at the positive electrode, dissolved bromine gas diffuses to the catalyst surface and is reduced to bromide anions. In the processes of charging, both reactions are reversed with a relatively high efficiency of up to 80% [1] due to facile electrokinetics.

In the activities encompassed by the FlowCamp project we are developing a continuum-scale mathematical model of a single-cell hydrogen-bromine flow battery (HBFB). It comprises of the most relevant transport through-plane processes and electrochemical phenomena for the operation of the HBFB, that is, transport of charge, water, hydrogen, protons, bromine and bromide.

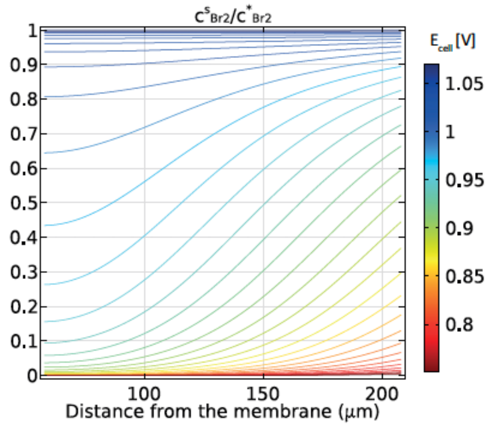


Fig. 1: Bromine surface concentration to bromine bulk concentration ratio distribution in the carbon felt electrode on discharge.

Furthermore, the model is enriched with supplementary phenomena such as: Nernstian losses due to reactant local surface concentration variations, Donnan potential on the HBr/Br_2 solution-membrane interface, and gas adsorption in the ionomer on the gaseous hydrogen side according to Henry's law.

The FlowCamp project promotes a strong collaboration amid the participants and creates a bond between empirical and modeling studies. This approach opens a spectrum of possibilities for experimental validation of the computer simulations, which then serve as guidelines to design recommendations implemented by experimentalists.

References:

[1] FlowCamp project website available at: www.flowcamp-project.eu

2.7 Microstructure evolution upon High Temperature Corrosion of Metallic Interconnector (MIC) for Solid Oxide Fuel Cells (SOFC)

Oxidation of metallic interconnectors (MIC) is a major source for performance loss, which limits the lifetime of SOFCs. Oxidation rate and associated contact resistance can be influenced by suitable choice of interconnector materials and coatings. In this project the microstructure evolution of oxide scales are investigated for two ferritic steels with and without coatings. A detailed characterization of the microstructure represents the basis for a fundamental under-standing of the underlying mechanism, which is necessary for purposeful materials improvement.

Contributors: L. Holzer, L. Keller, T. Hocker, D. Burnat, A. Heel, F. Fleischauer, J. Grolig, A. Mai
Partners: Hexis, ScopeM/ETHZ
Funding: BfE
Duration: 2015–2018

High temperature oxidation was investigated for two ferritic steels (Crofer22APU and 1.4509). Samples with different coatings (Co, MnCoFe) were oxidized at 850°C in air. The microstructure evolution was characterized by time-lapse microscopy at distinct time steps up to 5400 hours. Microstructure characterization at ETHZ (ScopeM). involved broad ion beam (BIB), SEM- and (S)TEM-EDX.

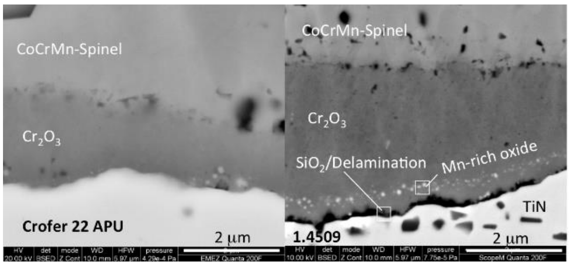


Fig. 1: Example of scale microstructures after oxidation for 500 hours at 850°C in air. Left: Crofer 22 APU with Co-coating, right: 1.4509 with Co-coating. Note difference of MIC -scale interface.

On both ferritic samples without coating a douplex scale is formed consisting of Cr_2O_3 and MnCr-spinel on top. For Crofer the MIC-scale interface is perfect. In contrast, 1.4509 shows high porosity and strong delamination at the MIC-scale interface. Subtile changes of the MIC composition induce significant differences in the microstructure. In particular, a slightly higher Si-content of 1.4509 leads to the formation of Si-oxide (ca. 10-20 nm needles) at the MIC-scale interface, which is responsible for the observed delamination. For 1.4509 with Spinel-coating, delamination can be suppressed at early oxidation stages. However, delamination is then even more complex at prolonged oxidation, where several delamination horizons can be detected at the MIC-scale interface and within the oxide layers. During the ongoing oxidation the composition of the spinel coating changes due to interdiffusion (i.e. enrichment with Cr, Mn). These compositional changes may lead to a drop of conductivity and to an increase of the contact resistance. In order to compensate such negative interdiffusion-effects the coating thickness must be increased.

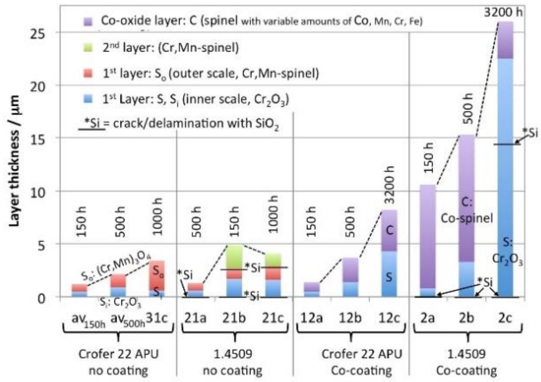


Fig. 2: Thickness of oxide layers for 4 materials.

The investigations also involved the quantification of oxidation rates and associated contact resistances. Delamination and spinel compositions are found to be more critical than the layer thicknesses. The results are promising in the sense that relatively cheap ferritic materials can be used in combination with coatings that are capable to suppress delamination and Cr-evaporation.

2.8 Model to predict degradation-optimized operation of high-temperature fuel cell stacks

Even though fuel cell stack developers have come a long way in reducing degradation that leads to power losses over time, a certain degree of ageing is considered to be unavoidable. It therefore makes sense to find out if a smart strategy to operate fuel cell stacks could be be used to minimise power losses. Here we present first results showing how varying stack operation temperatures affect stack degradation.

Contributors: T. Hocker
Partners: Hexis AG, Winterthur, J. Grolig, F. Vandercruysse
Funding: Swiss Federal Office of Energy
Duration: 2018–2019

Assessing, understanding and reducing losses in fuel cell systems is a task that has been tackled both experimentally [1] and theoretically [2] over many years. Even though many advances have been made and fuel cell systems are starting to become commercially available, a certain degree of ageing is considered to be unavoidable. Since the ageing of fuel cells – such as batteries – depends on how they are operated, it would be highly desirable to employ smart operation strategies that help reducing power losses. In this project we analysed how changes in the stack operation temperatures affect stack degradation. For this, we employed a simple, yet powerful approach for expressing the internal resistance of a fuel cell stack repeat unit ASR_{RU} in mΩ cm2 as a function of time and temperature. This approach is based on the complete differential of ASR_{RU} which in its integrated from is represented by

$$ASR_{RU}(t,T) = ASR_{RU}(t_0,T_0) + \int_{t_0}^{t} \frac{\partial ASR_{RU}}{\partial t}\bigg|_T dt + \int_{T_0}^{T} \frac{\partial ASR_{RU}}{\partial T}\bigg|_t dT$$

Based on Eq. 1, stack degradation data such as the synthetical data shown in Fig. 1 can be readily used to predict the time-dependent degradation for arbitrary T -profiles

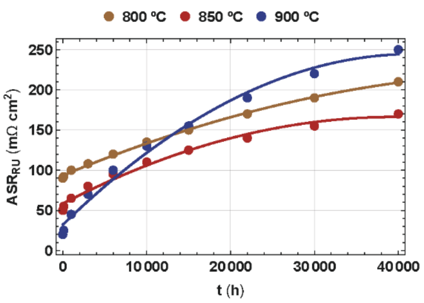


Fig 1: Synthetical data for the time- and temperature- dependent internal resistance of a fuel cell stack repeat unit.

The results of such an analysis is shown in Figs. 2 and 3. It turns out that increasing the stack temperature from 800 °C to 900 °C after 20’000 h decreases power losses compared with operation at constant temperatures of either 800 °C, or 900 °C.

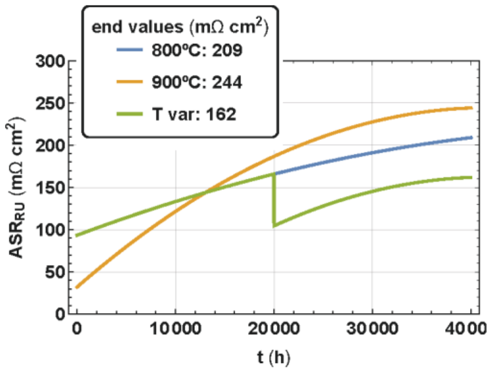


Fig 2: Evolution of the internal resistance of a fuel cell stack repeat unit for: T = 800°C T = 900°C and T increased from 800°C to 900°C after 20'000 h.

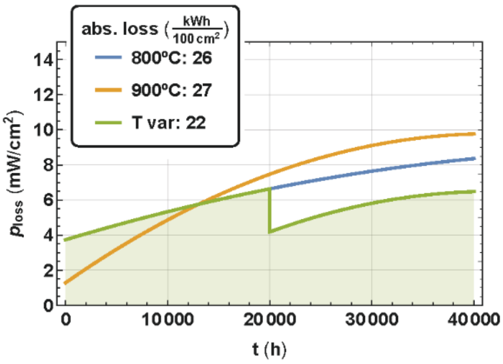


Fig 3: Power losses of a fuel cell stack repeat unit for the three different operation modes shown in Fig. 2.

Literature:

[1] A. Mai, B. Iwanschitz, J. A. Schuler, R. Den-zler, V. Nerlich, A. Schuler, ECS Transactions, 57, pp. 73–80 (2013).

[2] C. Meier, D. Meier, F. Vandercruysse, T. Hocker, *The International Journal of Multiphysics*, Vol. **12**, 393–411 (2018).

3 Organic Electronics and Photovoltaics

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 tera-hertz 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 measure-ment and simulation technology. This chapter gives an overview on ongoing R&D projects carried out in this interdisciplinary research field of the ICP.


Tobias Bach


Ennio Comi

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Simon Züfle

3.1 From Lab to Fab: Upscaling of Perovskite Solar Cells

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 and helps improving a software tool to predict the performance of large-area perovskite cells.

Contributors: E. Comi, E. Knapp, M. Neukom, B. Ruhstaller, A. Schiller
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 perovskite solar cells and organic light-emitting electrochemical cells. It is assumed that the two types of devices have, in addition to electron and hole transport, ion transport in common. Ion transport is relatively slow in comparsion with electron and hole transport. This behaviour requires an adaptation of the measurement system and simulation software. In previous years of the project the hardware was improved to fully characterize the devices. The numerical solver was complemented with the ionic transport equations to adequately describe the hysteresis in perovskite solar cells. These modifications were performed for small lab cells, sized a few mm^2. Besides the development of measurement and simulation tools for small lab cells, we applied the software LAOSS by Fluxim AG for simulating large-area perovskite cells. To keep simulation times and load at a minimum a compact 1+2D approach is pursued. Instead of simulating a full 3D device, we take advantage of the characterzation of the small cell and use this information to feed the large-area calculation as depicted in Fig 1. This configuration will account for the reduced conductivity of the transparent electrode and can include self-heating. We mimic small and large cells by covering the large cells with differently sized masks while shining light on them. The resulting current-voltage curves show an interesting shift of the open circuit voltage [1] which can partly be explained by simulation. Currently, we are testing algorithms for fitting large-area current-voltage curves.

The collaboration with the ICP spin-off Fluxim allows for the implementation of the new tools into the simulation software Setfos and LAOSS and the integrated measurement solution Paios. All of them 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 ICP contributes to an emerging field in academic and industrial research.

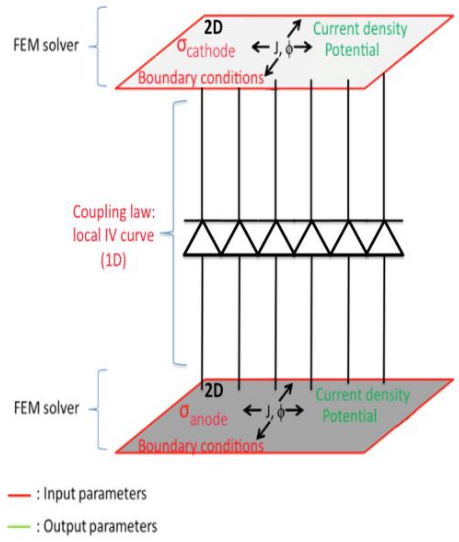


Fig. 1: Interplay of 1D model or measurement of lab cell and 2D model for electrodes.

Literature:

[1] Kiermasch et al., Effects of Masking on Open-Circuit Voltage and Fill Factor in Solar Cells, Joule (2018), ttps://doi.org/10.1016/j.joule.2018.10.016

3.2 Ultrabroadband THz photonics based on organic crystals

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

Contributors: U. Puc, T. Bach, V. Michel, M. Jazbinsek
Partners: Rainbow Photonics AG
Funding: Innosuisse
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 femtosecond (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 wave-lengths.

We characterized the refractive indices in the broadband THz range of various starte-of-the-art organic electro-optic crystals, DAST, DSTMS, OH1 and HMQ-TMS, which allowed us to evaluate theo-retically their best application ranges for ultra-broad THz-wave generation and coherent THz electric-field detection, depending on the available pump laser wavelength and the desired generated THz frequencies (see Fig. 1). For our pump fs laser source operating at the central frequency of 1560 nm, the best choice is DSTMS, which we also confirmed experimentally.

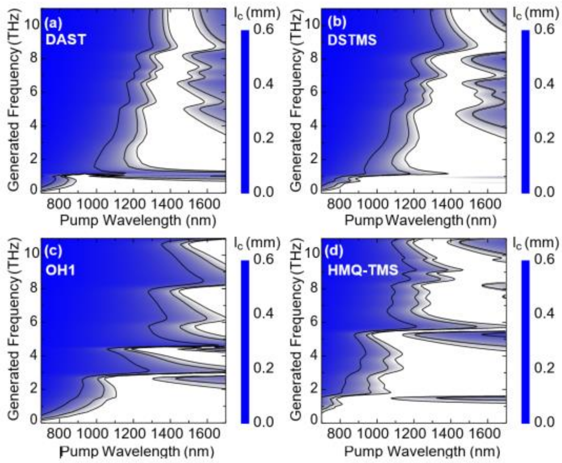


Fig 4: Coherence length lc for THz-wave generation in (a) DAST, (b) DSTMS, (c) OH1 and (d) HMQ-TMS as a function of the pump optical wavelength and the generated THz frequency f. The white area represents coherence lengths larger than 0.6 mm and therefore best for efficient THz-wave generation and/or detection.

We employ a very compact (19.5x9.5x7.5 cm3) commercial fs laser from Menlo Systems with pulse length of 40 fs, 190 mW average power, 100 MHz repetition rate as pump beam. Figure 2 shows the acquired THz time-domain electric field and the corresponding power spectrum obtained in dry air atmosphere using DSTMS crystals for both THz-wave generation and detection. We achieve a very large frequency bandwidth extending beyond 15 THz, with a high dynamic range of up to 60 dB.

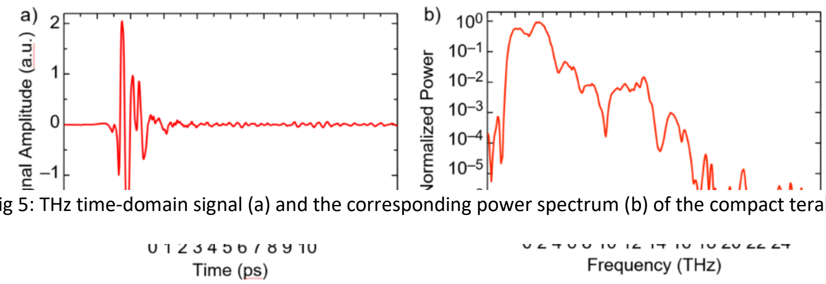


Fig 5: THz time-domain signal (a) and the corresponding power spectrum (b) of the compact terahertz setup.

3.3 Dye-Sensitized Solar Cells: Simulation of the Impedance, Experimental Validation and Parameter Extraction

In this bachelor thesis, impedance spectra of six different dye-sensitized solar cells (DSCs) provided by the industrial partner H. Glass were measured at different bias voltages and compared with each other. In addition, a simulation model for electrochemical impedance spectroscopy (EIS) was formulated based on differential equations (describing a diffusion model) and RC elements (representing a transmission line model). Subsequently, this model was implemented into PECSIM, a software for the simulation of DSCs, in order to extract the cells' parameters.

Students: L. Basler, E. Comi Category: Bachelor Thesis
Mentoring: D. Bernhardsgrütter, M. Schmid
Handed in: 08.06.2018

DSCs represent an alternative technology to conventional silicon-based devices. The potential advantage of DSCs lies in their low production costs due to cheap raw materials. Especially for niche applications they are considered a promising solution.

Electrochemical impedance spectroscopy (EIS) is a measurement technique that has proven to be extremely useful for the characterization of DSCs. EIS allows to determine the impedance of a device at different frequencies. With the help of the measured impedances, charge transport and undesired recombination processes inside a DSC can be investigated and consequently optimized.

In the context of this work, a simulation model for impedance spectroscopy is developed and implemented in PECSIM. It is based on diffusion and transmission line models of the dye-sensitized solar cell. Additionally, DSCs with different material properties are examined via EIS measurements and compared to each other. This is done using a measuring device, Paios which was developed by the company Fluxim AG at the ZHAW. The main goal of this work is to simulate the measured data in PECSIM and to extract the key properties of the cells.

Using extensive parameter fitting it could be demonstrated that the EIS simulation tool is able to accurately match measured spectra. Through this process, the new version of PECSIM was not only validated, but also shown to be capable of deriving informative properties of DSCs, such as transport and recombination resistances. This work sets the foundation for further simulation-based optimization of the DSC technology, with the prospect that these cells can be produced commercially in the near future.

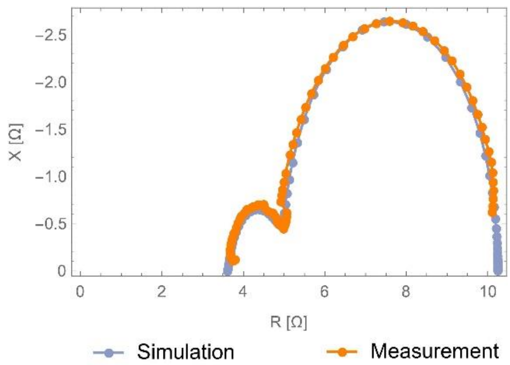


Fig. 1: EIS simulation and measurement of a DSC shown in a Nyquist plot. The PECSIM simulation yields a curve that perfectly matches the measurement result.

Student Project:

L. Basler, E. Comi, Dye-Sensitized Solar Cells: Simulation of the Impedance, Experimental Validation and Parameter Extraction, Supervisors: D. Bernhardsgrütter, M. Schmid, Bachelor Thesis in Energy and Environmental Engineering.

3.4 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.

3.5 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.

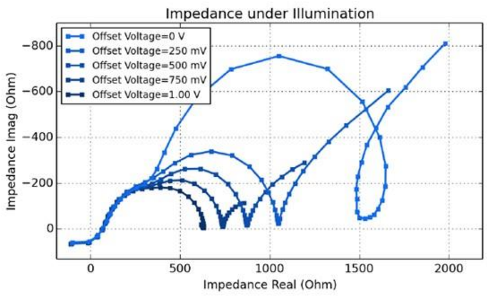


Fig. 1: Measurement of the impedenca spectra. At midfrequency an inductive loop occurs.

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.

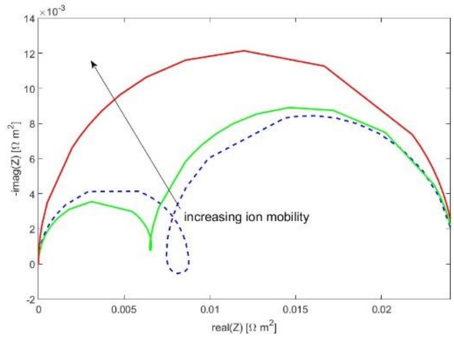


Fig. 2: Simulation of the impedance spectra in qualitative agreement with measurements shown in Fig. 1. A variation of the ion mobility shows an significant impact on the inductive loop.

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.

3.6 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: 2016–2019

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.

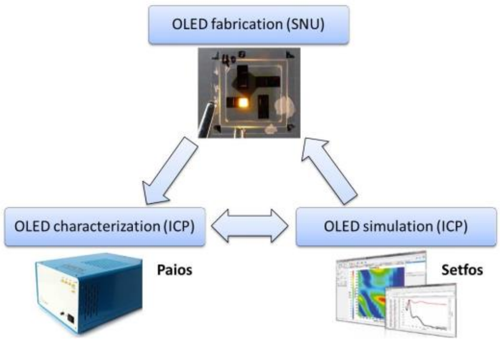


Fig. 1: Project approach for the investigation of high efficient state-of-the-art fluorescent exciplex OLEDs.

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 electrooptical 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.

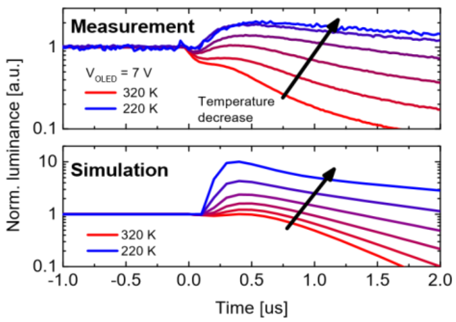


Fig. 2: Measured and simulated temperature-dependent transient EL decay behavior of the OLED after voltage turnoff (t = 0 us).

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.

M. Regnat, K.P. Pernstich, S. Züfle, B. Ruhstaller, *Analysis of the bias-dependent split emission zone in phosphorescent OLEDs*. ACS Applied Materials & Interfaces 10 (37), 31552 (2018)

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.


Andreas Bachmann


Mathias Bonmarin


Daniel Fehr


Lorenz Holzer


David Schaltegger


Matthias Schmid


Andreas Witzig

4.1 Skinobi – an affordable sensor to track skin condition and age

Skinobi is an affordable sensor that tracks skin condition and age. It can be used at home by everyone to improve their skin condition over time. The sensor is based on the measurement of the skin surface temperature over time during active cooling.

Contributors: Ch. Kirsch, A. Zubiaga, G. Boiger, M. Bonmarin
Partners: opus néoi GmbH
Funding: Innosuisse
Duration: 2018–2020

The skin is the first barrier of our organism and plays therefore a very important role. Like every other organ, the skin can be affected by a variety of diseases. Although very few of them are lethal, they can have a dramatic psychological impact for those affected. In addition, in our modern society, the skin reflects our health and youth and plays a very important social role. Today, thousands of different products are available over the counter to either treat specific skin disorders or to simply preserve the skin from aging and external aggressions.

Our goal is to help every customer assessing the efficacy of his or her skin treatment or preferred daily lotion. The measuring instrument will be wirelessly connected to a smartphone or tablet, and it will allow the user to easily retrieve important skin parameters. To achieve this task, we will use an innovative sensor developed specifically for measuring the thermal characteristics of human skin. Thermal conductivity, heat capacity or density are very good markers of the skin condition and they correlate with physiological parameters like the hydration or the epidermis thickness. Up to now, the few apparatus on the market are either reserved to trained professionals or they are closer to "lifestyle gadgets" than to scientific-based devices. We want to close this gap and offer an affordable yet reliable device for home use.

While some preliminary work has already been achieved within the framework of an SATW project, substantial scientific and technical developments are still required to reach the poof-of-concept stage. The goal of this project is to develop a fully working prototype in terms of both hardware and software, that can be used as a demonstrator. Technical developments will be achieved in close collaboration with ZHAW while the experimental validation will take place at the University Hospital Basel. Finally, a first batch of 100 devices will be produced by opus néoi GmbH and delivered to key opinion leaders and potential strategic partners.

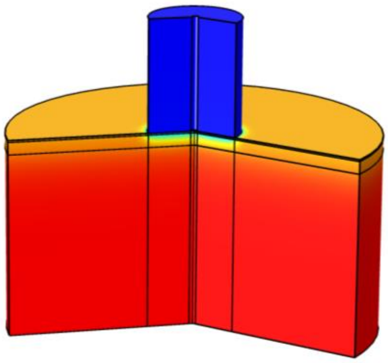


Fig. 1: Computational simulation of the measurement process. A cold aluminum block is brought into contact with the skin surface whereas the transient skin surface temperature is monitored using a thermopile sensor.

4.2 3D-Thermografie für Medizinalanwendungen

Mit Thermografie können lokale Wärme-Anomalien in der Haut detektiert und klassifiziert werden. In diesem Projekt wurde die konventionelle 2D-Thermografie erweitert für 3D-Untersuchungen. Die 3D-Rekonstruktion basiert dann auf einer geometrischen Analyse von 2D-Stereo-Bildpaaren, wobei unterschiedliche Algorithmen implementiert und verglichen wurden. Für die Bild-Akquisition wurde ein Versuchsaufbau erstellt, welcher gleichzeitig Aufnahmen im sichtbaren Spektrum (vis: ca. 380 – 780 nm) als auch im langwelligen Infrarotbereich (IR: ca. 7 – 14 µm) aufzeichnen kann. Die Kombination von vis- und IR-Daten erhöht die Qualität der 3D-Wärmebilder signifikant.

Contributors: C. Bader, L. Holzer, M. Bonmarin
Partners: Prof. A. Navarini, Uni Basel
Funding: -
Duration: 2018–2019

Um 3D-Körperoberflächen rekonstruieren zu können, werden (multiple) 2D Stereo-Bilder benötigt, welche dasselbe Objekt jeweils aus unterschiedlichen Winkeln erfassen. In diesem Pilotprojekt wurde ein Thermografie-Versuchsaufbau derart ausgelegt, dass unterschiedliche 3D-Rekonstruktionsmethoden mit demselben Setup durchgeführt werden können. Gegenwärtig enthält der Versuchsaufbau zwei RGB-Kameras (Logitech C270) und zwei Longwave-Infrarotkameras (FLIR Lepton 3.5), welche unter einem konstanten Winkel auf einem Schwenkarm fixiert sind. Die Bildakquisition kann über ein beliebiges Drittgerät gesteuert werden (Python-Interpreter). Dank der flexiblen Steuerungssoftware wäre es auch möglich, den Versuchsaufbau mit zusätzlichen Sensoren auszustatten um die Oberflächen von grösseren Körpern vollständig abbilden zu können.

Die 3D-Rekonstruktion unter Verwendung von Matlab, ReCap, Fiji und OpenCV basiert auf der Identifizierung identischer Punkte in Stereo-Bildpaaren. Aufgrund der geometrischen Beziehung können mittels Triangulation die entsprechenden 3D-Koordinaten von markanten Bildpunkten berechnet werden. Aus zahlreichen Punkten wird dann eine sog. point-cloud, welche in eine polygonale 3D-Oberfläche umgewandelt werden kann (Abbildung 1a). Für herkömmliche vis-Bilder kann diese 3D-Rekonstruktion zuverlässig durchgeführt werden. Verschiedene Algorithmen wie 'structure from motion' und 'multi view stereo vision' kommen dabei zum Einsatz.

Im Gegensatz dazu stellt die 3D-Rekonstruktion von IR-Wärmebildern wegen der relativ kleinen Zahl an markanten Bildmerkmalen eine grosse Herausforderung dar. Die 3D-Rekonstruktion von Wärmebildern wird deshalb in zwei Teilschritten durchgeführt. In einem ersten Schritt wird eine herkömmliche 3D-Rekonstruktion mit vis-Bilddaten generiert (Abbildung 1a). In einem zweiten Schritt werden die IR-Bilder dann auf die bereits erstellte 3D-Rekonstruktion überlagert (Abbildung 1b).

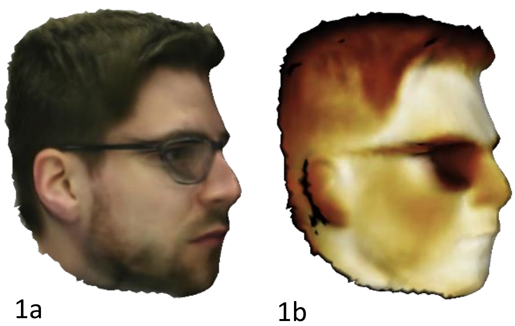


Abbildung A: 3D-Rekonstruktion von vis- (1a) und IR-Bilddaten (1b)

In Zukunft können solche 3D-Wärmebilder verwendet werden für grundlegende Untersuchungen von thermischen Hautanomalien basierend auf modernsten Methoden zur Datenanalyse (Big Data / Künstliche Intelligenz).

4.3 Tragbares Gerät zur Frühdiagnose von Lymphödemen

Contributors: D. Fehr, A. Bachmann, B. Bonmarin
Funding: Innosuisse
Duration: 2018–2019

Die Wahrscheinlichkeit, bis ans Lebensende ein Lymphödem zu entwickeln, liegt nach einer Brustkrebsbehandlung bei ca. 30 % – und das ist nur einer der möglichen Risikofaktoren. Millionen von Menschen müssen daher mit einem erhöhten Risiko rechnen, an einem Lymphödem zu erkranken. Bei dieser Krankheit ist die Funktion des Lymphsystems dauerhaft gestört, wodurch z. B. die Arme irreversibel anschwellen, wenn nicht rechtzeig eine geeignete Behandlung eingeleitet wird. Diese verlangsamt die Schwellung oder stoppt sie sogar komplett. Eine frühe Diagnose der Krankheit ist somit zentral. Dennoch gibt es zurzeit keine standardisierte, breit verfügbare Methode, die bei Menschen mit erhöhtem Risiko ein regelmässiges und zuverlässiges Monitoring erlaubt.

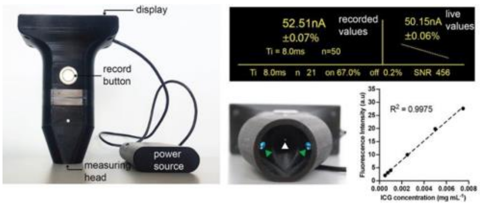


Abb. 1: Links: Autarkes Handgerät mit Batterie. Oben rechts: Display. Mitte: Messöffung. Unten rechts: Gemessener Wert versus tatsachlicher Markerkonzentration.

In dieser Arbeit wird, zusammen mit dem Institut für Pharmazeutische Wissenschaften der ETH Zürich, eine geeignete Methode zur Frühdiagnose von Lymphödemen entwickelt. Sie besteht aus einem fluoreszierendem Marker, der in die Haut des Patienten injiziert wird, und aus einem, für medizinische Verhältnisse, einfachen Messgerät, welches die Abbaurate des Markers mittels der Fluoreszenzintensität bestimmen kann. Bei einer reduzierten Abbaurate besteht der Verdacht auf ein sich entwickelndes Lymphödem. Im Idealfall werden die Patienten mit dieser Methode ihr Lymphsystem selbständig und regelmässig überwachen können und im Verdachtsfall frühzeitig einen Spezialisten aufsuchen können. In verschiedenen Vorprojekten wurde ein geeigneter fluoreszierender Marker und ein erstes portables Messgerät mit optischer Sensorik zur Quantifizierung des Fluoreszenzsignals entwickelt. Dazu wurde die bestehende Optik (Abb. 2) um eine autarke Steuerelektronik und Bedienelemente ergänzt und in einem kompakten Gehäuse verbaut (Abb. 1). Mit diesem Handgerät konnte die Methode bereits in verschiedenen Versuchen validiert werden.

Momentan wird das Messgerät überarbeitet und als tragbarer Sensor realisiert, d. h. das bisherige Handgerät schrumpft auf die Grösse einer Armbanduhr. Dazu wird die Optik von Grund auf neu Entwickelt, weil die bestehende prinzipbedingt nicht weiter verkleinert werden kann. Erste Versuche sind vielsprechend. Bei vergleichbarer Empfindlichkeit konnte die Optik beträchtlich verkleinert werden. Parallel wird eine passende Smartphone-App implementiert, die neben der Bedienung des Sensors auch eine modellbasierte Messdatenauswertung erlaubt. Das Modell:

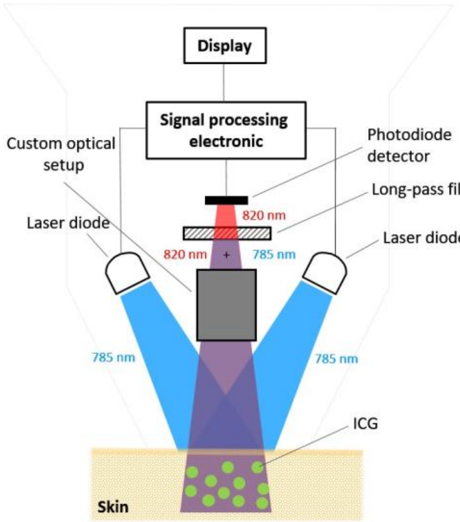


Abb. 2: Optische und elektronische Komponenten des Handgeräts.

Literature:

[1] A. Polomska et al., *Minimally invasive method for the point-of-care quantification of lymphatic vessel function*, JCI Insight, 4(4), 2019.

Paper:

A. Fallah, M. Ghajari, Y. Safa, *A computational framework for the study of dynamic delamination in morphing composite blades and wings*, Submitted to Journal Engineering Structures.

4.4 DermaIR – Increasing the capabilities of dermatoscopy using thermal imaging sensors

We want to extend the abilities of standard epiluminescence microscopy by adding dynamic thermal imaging capabilities. Giving the physicians additional information about the temperature of the lesion will drastically improve the differential diagnostic of various skin disease. This project will deliver a fully working, clinically tested diagnostic device, ready to enter the market and increase Fotofinder products portfolio

Contributors:	Ch. Bader, A. Bachmann, M. Bonmarin
Partners:	FotoFinder Systems GmbH
Funding:	EUROSTARS
Duration:	2018–2021

The project content is confidential.

4.5 Modellierung von Erdregisterspeichern zur thermischen Analyse

Zur Planung von Wärmepumpen-Heizungssystemen mit Erdreichankopplung wird oft dynamische Simulation eingesetzt. Auf dieser Grundlage werden Variantenentscheide getroffen und Regelparameter optimiert. Die vorliegende Arbeit hilft, komplexe Erdregister adäquat abbilden zu können und der digitalen Planung zugänglich zu machen.

Contributors: T. Frei, A. Witzig
Partners: E-Zeit Ingenieure, NM Numerical Modeling GmbH, Vela Solaris AG
Funding: Masterarbeit
Duration: 2018–2019

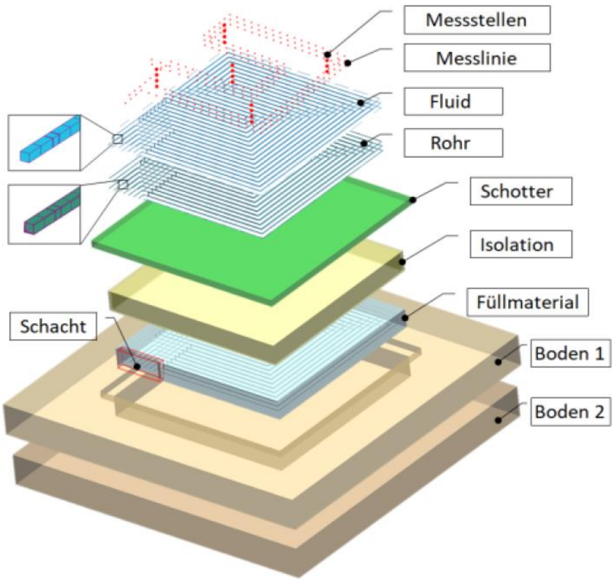
Wärmepumpen-Heizungssysteme nutzen häufig das Erdreich als Wärmequelle. Neben Erdsonden gibt es auch das Konzept des Erdregisters, wozu auch der im Jahr 2016 patentierten Erdwärmespeicher "E-Tank" zählt. Je nach Grösse und Auslegung sind Erdregister-Speicher geeignet zur saisonalen Speicherung.

Beim thermisch aktivierten Erdreich handelt es sich um einen Speicher mit sehr grosser Masse und Trägheit. Eine einfache Langzeitberechnung des E-Tanks ist bereits möglich mit dem kommerziellen Planungstool Polysun [1]. Darin werden jedoch die kurzfristigen Wärmetauscher-Effekte und die detaillierte Geometrie des Erdregisters nicht abgebildet. Um das vorausgesagte Systemverhalten zu verbessern, ist ein dreidimensionales Simulationsmodell auf Basis der Finit-Element-Methode erstellt werden. Dabei kommt die am ICP entwickelte Multiphysik Software SESES zum Einsatz. Anhand eines einfachen instationären Versuchsmodells wurden die physikalischen Formeln und Parameter implementiert. Daran konnte getestet werden, wie sich der Einfluss des Berechnungszeitschritts und die Finite-Elementgrösse auf das Simulationsergebnis auswirken [2].

An unterschiedlichen Bereichen des Modells, sowie in einer Rohrleitung wurden die Temperaturen und Energieströme aufgezeichnet. Anhand der Feldmessdaten einer Versuchsanordnung in Chemnitz, könnte das Simulationsmodell kalibriert werden. Es wurde eine gute Übereinstimmung mit den Messdaten aus dem Jahr 2016 gefunden.

Die gewonnenen Kenntnisse werden in der dynamischen Jahressimulation nicht laufend mitgeführt, da sie in der aktuellen Implementierung noch viel Rechenpower beanspruchen. Das vollständig parametrisierbare Simulationsmodell besteht derzeit aus 33 Millionen Elementen. Ein Lösungsweg für die Reduktion des Rechenaufwands wurde theoretisch aufgezeigt aber noch nicht umgesetzt.

Der Erfolg dieser Arbeit liegt darin, dass solche grosse Simulationsgebiete abbildbar sind. Das neue Simulationsmodell ist ein hervorragendes Werkzeug für die Weiterentwicklung und Optimierung des E-Tanks und anderer Systeme mit Erdregister.



Figur: E-Tank Erdregisters in Explosionsansicht. Rohrführung und Schichtaufbau des Erdreichs werden für die Simulation detailliert abgebildet.

Referenzen:

[1] www.polysunsoftware.com

[2] T. Frei: Modellierung und Simulation eines neuartigen Erdregisterspeichers (E-Tank) zur thermischen Analyse. Masterarbeit ICP-ZHAW, Juli 2018.

4.6 Digitaler Zwilling: Building Information Modeling (BIM) nutzen für Simulation von gebäudeintegrierten Energiesystemen

Abstract

Contributors: A. Witzig, D. Schaltegger
Partners: Swisscom Industrial IoT, Meier Tobler AG, BS2 AG, Vela Solaris AG
Funding: Innosuisse
Duration: 2018–2020

Die Digitalisierung hat die Baubranche erreicht: Building Information Modeling (BIM) bedeutet in einem ersten Schritt die geometrische Erfassung von Bauwerksdaten und bietet in Kombination mit veränderten Planungsabläufen ein grosses Potential für eine umfassende optimierte Planung. Aufgrund der technologischen Möglichkeiten werden ausserdem viele Geräte ans Internet angeschlossen (Internet of Things, IoT). Digitale Pläne wie auch IoT-Logdaten bleiben aber für die energetische Optimierung der Gebäude weitgehend ungenutzt.

Für die Simulation bietet sowohl BIM wie auch IoT grosse Erfolgsaussichten: Neue internationale Standards und offene Schnittstellen erlauben die Verwendung von Geometriedaten als Input für die numerischen Modelle. Messdaten von Sensoren stehen für die Validierung der Berechnungen und für die Kalibrierung von Simulationsparametern zur Verfügung. Letztlich verspricht die Übertragung der in der Simulation ermittelten optimalen Regelung auf das Heizungssystem sowohl Zeitersparnis wie auch eine Reduktion von Unsicherheiten. Der technologische Fortschritt erlaubt die Optimierung von Arbeitsabläufen, wie beispielsweise die extensive Nutzung von Fernwartung für Wärmepumpensysteme.

Am ICP laufen mehrere Projekte, die sich mit der konkreten Umsetzung des digitalen Zwillings im Gebäudebereich befassen. Einerseits werden dabei die numerischen Modelle entwickelt, welche die Heizungs- bzw. Kühlsysteme hinreichend genau abbilden und aufgrund der Einbindung von Messresultaten die Simulationsparameter bestimmt. Andererseits werden organisatorische Herausforderungen adressiert: So wird beobachtet, dass die Steuerung und Regelung von Wärmepumpensystemen in der Praxis oft nicht den ursprünglich geplanten Regelalgorithmen folgen. Aus diesem Grund können Planungswerte für den Energieverbrauch und dem Eigennutzungsgrad der Photovoltaikanlage nicht erreicht werden. Zur Lösung können technische Neuerungen beitragen (direkte Programmierung der Regler aus den Planungsdaten [1]) oder eine Anpassung der Abläufe und Geschäftsmodelle [2].

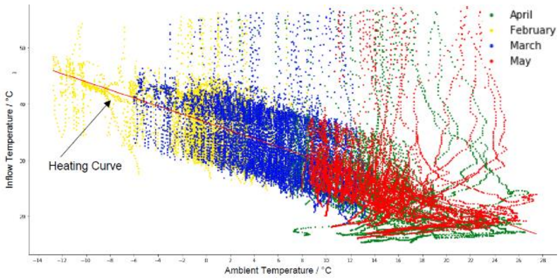


Fig. 1: Figure Caption.

Das übergeordnete Ziel f die Forscher am ICP sowie auch die involvierten Industriepartner ist die energetische Optimierung. Aus den verschärften Energiegesetzen ergeben sich aber auch finanzielle Anreize: Die im Baugesuch versprochene energetische Performance muss durch Messungen im fertiggestellten Gebäude nachgeprüft werden. Abweichungen werden durch Simulationen mit BIM-Daten bereits während der Bauphase erkannt. Damit werden Risiken minimiert und Geld eingespart.

Referenzen:

[1] R. Grosskopf: Wärmepumpen direkt angeseuert via Simulationssoftware. Bachelor Thesis ICP-ZHAW, Juni 2017.

[2] H. Sotnikova: Predictive IoT-maintenance for heat pump systems. Master Thesis ICP-ZHAW, Oktober 2018.

4.7 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 de-struction of production samples. Therefore, we investigated a new, fast and non-destructive measurement approach using impulse thermography. We showed that it is 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: 2015–2018

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.

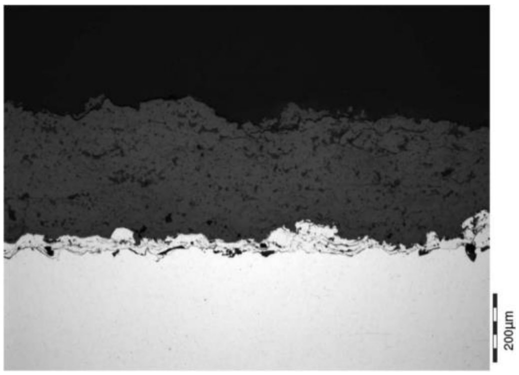


Fig. 1: Polished cross-section image of a TBC consisting of a bond coat (middle) and the top coat (top) on a steel substrate (bottom). Source: Oerlikon Metco AG, Wohlen.

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 $\vartheta = \Delta T/R_{th}$. 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 E (units: $J/(m^2K\sqrt{s})$) of the coating is known and the thermal effusivity E (units: $J/(m^2K\sqrt{s})$) of the coating is known and the thermal propagation time is measured, the thermal coating resistance can be calculated with $R_{th} = \sqrt{\tau}/\varepsilon$.

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 µKm^2/W	75%
285	270µm	4%	225 µKm^2/W	100%
286	328µm	1.9%	-	-
287	150µm	11.3%	221 µKm^2/W	98%
288	228µm	11.1%	317 µKm^2/W	141%
289	356µm	11%	-	-
290	75µm	15%	242 µKm^2/W	108%
291	340µm	17.9%	-	-
292	280µm	15%	576 µKm^2/W	256%

Tab. 1: Thermal coating resistance measured with the Coat-Master system.

5 Lehre

5.1 Gamification in der Lehre

Die zunehmende Digitalisierung ist in vielen Bereichen des Alltags bemerkbar und hat auch den Bereich der Lehre nachhaltig verändert. Eine weitere Zunahme in diesem Bereich ist zu erwarten und wird in der Strategie «Bildung und digitale Transformation» der ZHAW aktiv gefördert.

Als Ersatz oder Ergänzung für klassischen Frontalunterricht haben sich verschiedene Methoden etabliert, etwa die Unterstützung von Vorlesungen mittels digitaler Medien (Videos, Wiki, MOOCs, Klicker, Quizzes etc.) und Lernplattformen wie Moodle, OLAT, oder Mahara. Besonders in technischen Fachgebieten ist es üblich, neben der Vorlesung auch noch Übungsstunden abzuhalten, in denen die Studierenden Übungsbeispiele lösen müssen. In diesem Bereich gibt es noch kaum Ansätze, den Präsenzunterricht durch digitale Methoden zu ergänzen und unterstützen.

In einem Pilotprojekt über «digitale Lehrformen» wurde eine Web-Applikation entwickelt, welche die Digitalisierungslücke im Bereich der Übungsstunden schliessen soll. Die Web-Applikation verwendet Elemente, die sich auch in Computerspielen wiederfinden und dort zu einem positiven Erlebnis führen, wie zum Beispiel das Sammeln von Punkten oder besonderen Medaillen.

Ausgangspunkt für die Entwicklung der App war, dass im Physikunterricht ein Grossteil der Übungen im Selbststudium stattfindet und dass man als Dozent kaum Kontrolle über den Lernfortschritt der Studierenden hat. Diese Situation wird durch die zunehmende Digitalisierung der Lehre verstärkt werden. Studierende konsultieren auch häufig die Musterlösung und meinen, die Aufgabe gemeistert zu haben, doch die Erfahrung zeigt, dass die Konzepte der Musterlösungen selten auf andere Problemstellungen übertragen werden können. Auch wirken die oftmals schwierigen Aufgaben demotivierend.

Mit der entwickelten Web-Applikation werden die Übungsaufgaben online verteilt. Es werden Punkte für korrekte Lösungen vergeben und ein Hilfesystem unterstützt das Lösen der Aufgaben, wobei jeder Hinweis Punkte kostet. Durch das Punktesystem erhalten Studierende live Feedback über den persönlichen Lernerfolg und Dozierende über den Lernerfolg der Klasse. Ein zentrales Feature der App ist die Möglichkeit, die Musterlösung zu kommentieren, falls man die Aufgabe nicht lösen konnte. Durch dieses Verschriftlichen findet vertieftes Lernen statt. Dieses Feature ist ein Alleinstellungsmerkmal der App, da eine vertiefte Auseinandersetzung mit der Musterlösung im Präsenzunterricht praktisch nicht vorkommt.

Ein erster Probelauf während des laufenden Semesters verlief erfolgreich. Erste Rückmeldungen stellen der App ein gutes Zeugnis aus. Eine umfangreiche Evaluation wurde in Zusammenarbeit mit dem Zentrum für Evaluation der PHZH entworfen und die Durchführung ist für das Frühjahrssemester 2019 geplant.

Die von uns entwickelte Web-Applikation ist ein neuartiges und einzigartiges Tool in der e-Didaktik-Landschaft und bietet einen echten Mehrwert für digitale Lehrformen. Die App lässt sich in vielen Fächern einsetzen, insbesondere in Physik und Statistik mit R, sowie in allen Fächern in dem die Übungsaufgaben ein numerisches Resultat liefern. Anpassungen an die Anforderungen für Mathematik sind geplant und sollen in einer laufenden Bachelorarbeit implementiert werden.

Aufbau der Web-App

Abbildung B zeigt einen Screenshot der Web-App, wie sie in dem Semesterwochen 13 und 14 im Fach PHSVS1 eingesetzt wurde. Diese Seite erscheint nach dem Einloggen eines Studierenden und zeigt den sogenannten *Live Lernfortschritt* als Key Performance Indicator. In den Boxen oben sieht man die bereits erzielten *Punkte* (in diesem Fall 7 Punkte); die *Medaillen* und *Kudos* (= a score of honorary degrees) sind weitere Features, die noch nicht implementiert sind. Links befindet sich ein Auswahlmenu, welches zu den Aufgaben der einzelnen Wochen führt.

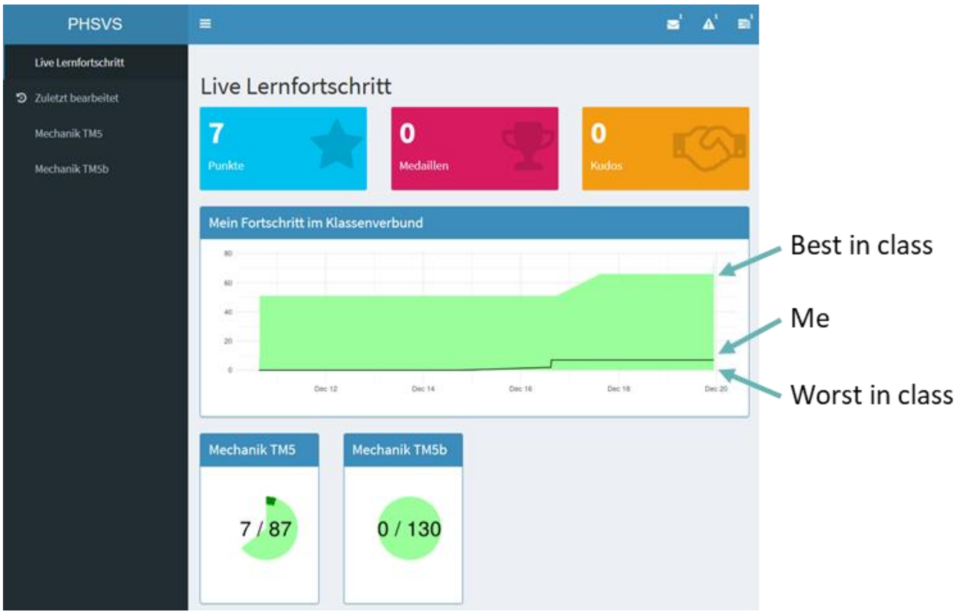


Abbildung B Screenshot der Seite "Live Lernerfolg". Neben den bereits erzielten Punkten sieht man den eigenen Lernerfolg im Vergleich zu seinen Kommilitonen sowie den Lernerfolg und die noch offenen Aufgaben für jede Woche.

Zentral ist auch die Darstellung der eigenen Punkte verglichen mit den Punkten der Mitstudierenden. Dies erzeugt einen gewissen Gruppendruck, der motivierend wirken soll. Durch die Verschleierung der einzelnen Identitäten sollte der Gruppendruck nicht zu gross werden.

Für jede Woche sieht man in dieser Darstellung auch die bereits erreichten Punkte sowie die Punkte, die man noch erzielen kann. Diese übersichtliche Darstellung sollte ebenfalls einen gewissen Leidensdruck erzeugen, da man jederzeit sieht, wie viel Arbeit noch bis zum Ende der Woche zu erledigen ist. Es ist aber auch eine Belohnung, wenn man sieht, dass man eine Woche vollständig bearbeitet hat.

Abbildung C zeigt die Wochenansicht für das Thema «Mechanik TM5». Es sind vier Aufgaben zu lösen und zu jeder Aufgabe wird der Punktestand übersichtlich dargestellt. In der ersten Aufgabe wurden bereits 5 Punkte erzielt (dunkelgrüner Balken). In der zweiten Aufgabe wurde ein Hinweis benutzt, wodurch die Zahl der zu erreichenden Punkte gesunken ist (fehlendes Tortenstück in Aufgabe 2).

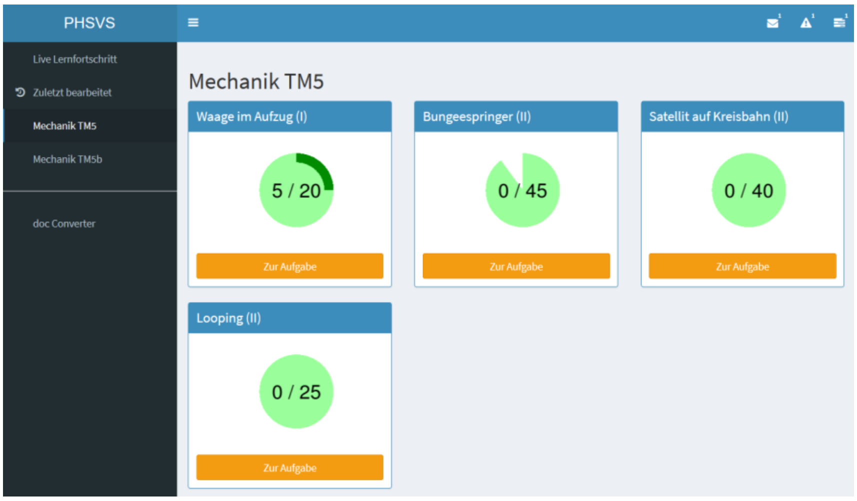


Abbildung C Wochenansicht mit den einzelnen Übungsaufgaben. Für jede Übung wird deutlich, wie viele Punkte man bereits erreicht hat (dunkelgrüner Balken), wie viele Punkte noch erzielt werden können (hellgrüne Fläche) und wie viele Punkte man durch die Benutzung von Hinweisen vergeben hat (fehlendes Tortenstück in Aufgabe Bungeespringer).

Abbildung D zeigt die Ansicht einer Übungsaufgabe, wobei der einleitende Text auch ein Bild oder Video beinhalten kann. Eine Übung kann beliebig viele Teilaufgaben (a), b), c), …) beinhalten. Jede Teilaufgabe besitzt ihren eigenen Text sowie ein Feld zur Übermittlung der eigenen Lösung. Gibt der Nutzer oder die Nutzerin die korrekte Lösung ein, werden die Punkte gutgeschrieben, in diesem Fall 30 Punkte.

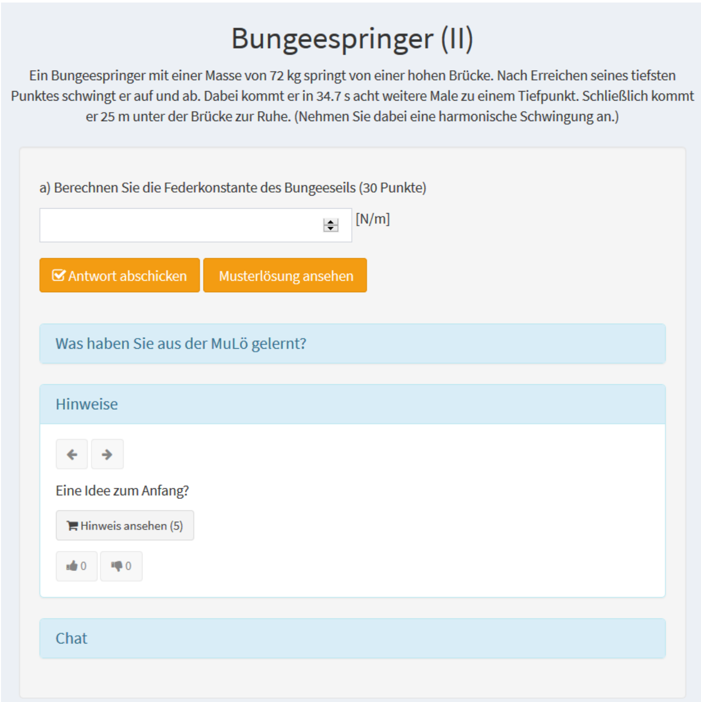


Abbildung D: Ansicht einer Übungsaufgabe, wobei der einleitende Text auch ein Bild oder ein Video beinhalten kann. Eine Übung kann aus beliebig vielen Teilaufgaben (a), b), …) bestehen. Jede Teilaufgabe hat ihren eigenen Text, sowie ein Feld zur Übermittlung der eigenen Lösung. Wird die Musterlösung angesehen, wird ein Feld zur Übermittlung der Reflektion über die Musterlösung eingeblendet. Sind für die Aufgabe Hinweise definiert, werden Sie angezeigt. Ein Chat innerhalb der Klasse ist auch für jede Teilaufgabe verfügbar.

Wurden für diese Teilaufgabe Hinweise definiert, werden diese angezeigt. Jeder Hinweis ist mit Kosten verbunden, in diesem Beispiel 5 Punkte. Die Hinweise sind gratis, nachdem die Aufgabe korrekt gelöst oder die Musterlösung gekauft wurde. Die Hinweise können von Studierenden auch positiv oder negative bewertet werden und helfen der Lehrperson, die Hinweise zu verbessern.

Für jede Teilaufgabe ist ein Chat verfügbar, in dem sich die Studierenden gegenseitig helfen können. Für hilfreiche Antworten im Chat sollen Kudos (= a score of honorary degrees) vergeben werden; derzeit ist dieses Feature noch nicht implementiert.

Kann die Lösung trotz Hinweisen und Chat nicht gelöst werden, kann man sich die Musterlösung ansehen. Dadurch erhält man natürlich keine weiteren Punkte mehr für diese Aufgabe, es sein denn, man beschreibt detailliert was man aus der Musterlösung gelernt hat. Die Lehrperson liest den Text und kann dafür Punkte vergeben oder Fehler in der Reflexion der Musterlösung zurückmelden. Diese vertiefte Reflexion findet im Präsenzunterricht praktisch nicht statt, und ist ein Alleinstellungsmerkmal der App.

Der Mechanismus zur Reflexion über die Musterlösung verspricht eine wesentliche Steigerung des Lernerfolgs. Durch das Verschriftlichen fasst man oft lose Gedanken in konkrete Worte und da die Lehrperson die Reflexion liest, können Fehlkonzepte erkannt und ausgebessert werden.

Neben dem soeben beschriebenen Fragetypus, bei dem Teilaufgaben gestellt werden und ein numerisches Resultat abgefragt wird, stehen weitere Fragetypen zur Verfügung. So gibt es beispielsweise Multiple-Choice-Fragen, Freitextfragen (die derzeit nicht automatisiert überprüfbar sind) sowie komplexe Fragetypen, bei denen die Studierenden R-Code eingeben und ausführen können. Der R-Code wird automatisiert überprüft und insbesondere im Fach Statistik eingesetzt. Nachdem die Web-App, basierend auf einem bestehenden Projekt (tguishiny, entwickelt von G. De Cilia, B. Meindl, M. Templ), selbst programmiert wurde, lässt sich die App auch leicht auf andere Fragetypen erweitern, um den jeweiligen Wünschen und Ansprüchen gerecht zu werden.

Fazit

Aus der bisherigen Arbeit mit der Web-Applikation bin ich zu der Überzeugung gelangt, dass sich die Web-App für meinen Unterricht bewähren wird, d. h. die Studierenden einerseits dazu ermuntert, mehr Aufgaben zu lösen und andererseits wird sie vertieftes Lernen ermöglichen. Auch im Kollegium stösst die App auf breites Interesse.

Kurt Pernstich, ICP

5.2 Seamless Learning: Projektcluster und Leitung des IBH-Labs

Im Rahmen des Hochschulverbunds Internationale Bodensee-Hochschule IBH werden seit 2016 sogenannte Labs angeboten. Dies sind in sich vernetzte Projekte, die eine inhaltliche Verknüpfung haben und in einem grösseren themenspezifischen Forschungskonsortium durchgeführt werden. Das ICP leitet gemeinsam mit dem Zentrum für Innovative Didaktik (ZID) der ZHAW School of Management and Law das «Seamless Learning Lab». Das auf vier Jahre angelegte Projekt umfasst die Erarbeitung, Implementierung und Evaluation eines Seamless-Learning-Konzepts in verschiedenen Disziplinen mit Hochschul- und Industriepartnern.

Abbildung 1: Gruppenfoto beim internen Jahrestreffen des Seamless Learning Labs.

Folgende Partner gehören zum Projektkonsortium:

- ZHAW mit den Instituten ICP und IAMP aus der School of Engineering, ZID aus der School of Management and Law und LCC aus der Angewandten Linguistik
- HTWG Konstanz mit den Fakultäten Informatik und Life Science sowie dem Fachbereich Gesundheitsinformatik
- Hochschule Albstadt-Sigmaringen, Fakultät für Life Sciences
- FHS St. Gallen, Institut für Modellbildung und Simulation
- Universität St. Gallen, Institut für Wirtschaftspädagogik
- Interstaatliche Hochschule für Technik Buchs (NTB), Institut für Produktionsmesstechnik, Werkstoffe und Optik
- Duale Hochschule Baden-Württemberg, Ravensburg
- Universität Konstanz, Referat Lehre, Schreibzentrum
- Universität Liechtenstein, Fachstelle Didaktik und angewandte Linguistik
- Pädagogische Hochschule Vorarlberg, Fachdidaktik Naturwissenschaften

Gemeinsam werden Konzepte für grenz- und kontextüberschreitendes Lehren und Lernen erarbeitet. Dies geschieht vor dem Hintergrund des technologischen Fortschritts, der neue Anforderungen an Lehr- und Lernszenarien stellt. Es werden regelmässig Veranstaltungen durchgeführt, in denen Zwischenresultate präsentiert werden und die weitergehende Vernetzung gepflegt wird. Im vergangenen Jahr wurde in Winterthur die Seamless Learning Tagung 2018 durchgeführt und derzeit laufen die Vorbereitungen für den «Tag der Lehre» geplant mit dem Thema «Flexibles Lernen an Hochschulen gestalten».

Nutzung moderner Technologien

Lernen und Lehren befindet sich in einem tiefgreifenden Wandel. Lernende brauchen nicht viel mehr als ein mobiles Endgerät mit Internetzugang sowie ein Blatt und einen Stift, um überall und zu jedem Zeitpunkt zu lernen. Lernressourcen sind allgegenwärtig verfügbar (z. B. als OERs1, MOOCs2). Computergestütztes gemeinsames Lernen ist einfacher denn je (European Commission 2012: 9). Die Grenzen zwischen formalem und informellem Lernen verwischen zusehends. Die Technologien, die diesen Wandel befeuern, entwickeln sich rasant weiter. Die Anforderungen des lebenslangen Lernens stellen Herausforderungen für die Gestaltung adäquater technologieunterstützter Lehr-/Lernszenarien.

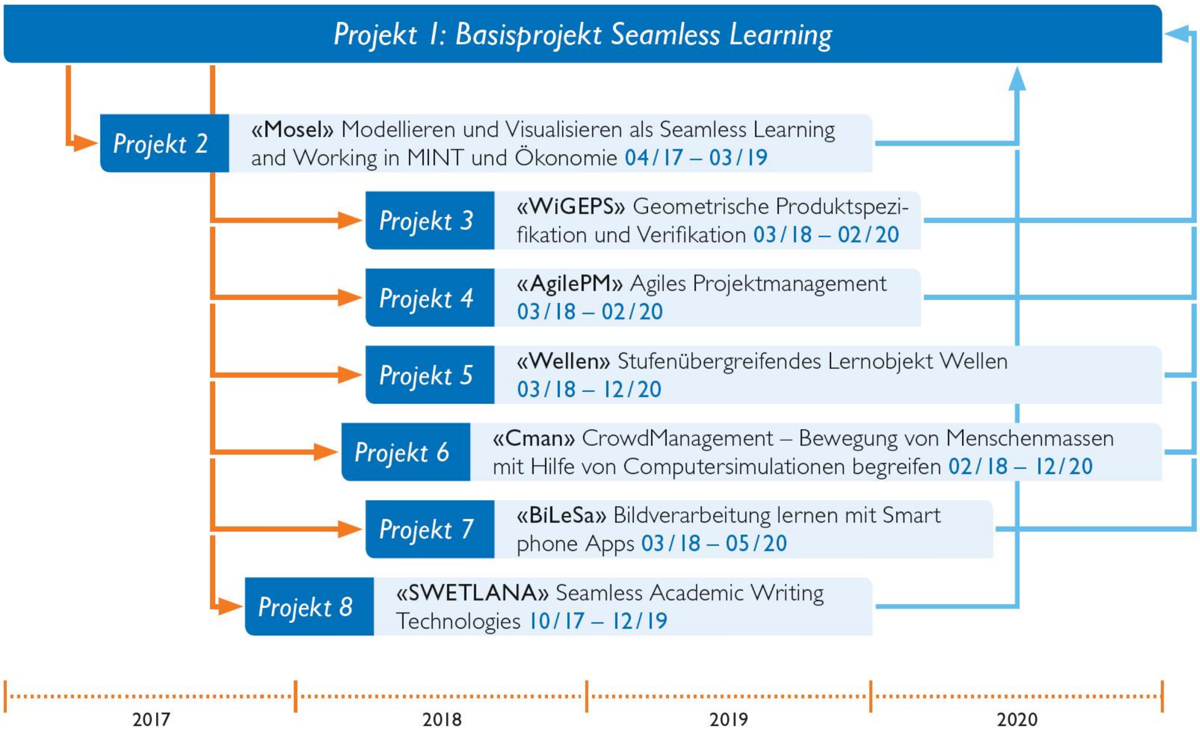


Abbildung 2: Projektübersicht. Das ICP ist im übergeordneten Steuerungsausschuss sowie in den Projekten 2, 5, 6 und 7 aktiv beteiligt.

Angepasste didaktische Konzepte

Aus Theorie und Praxis ist bekannt, dass zur Verfügung gestellte Technologie an sich noch wenig bewirkt. Sowohl Lehrende als Lernende müssen lernen, damit umzugehen, d. h. müssen befähigt werden. Ebenso bedarf es eines schlüssigen (fach-)didaktischen Konzepts. Ein weiteres, oftmals noch größeres Hindernis in der Karriere als (lebenslange) Lernende im 21. Jahrhundert stellen immer noch vorhandene Brüche in der Lernbiografie dar – exemplarisch von der Schule zur Ausbildung bzw. Hochschule und im Beruf mit entsprechender Weiterbildung. Der Transfer und die Übergänge gelingen eingeschränkt.

Das Konzept des «Seamless Learning» bietet einen Rahmen, die skizzierten technologischen und didaktischen Herausforderungen zu adressieren und ein lebenslanges, nahtloses Lernen über Bildungskontexte hinweg zu ermöglichen. Ziel dieses Labs ist daher, Seamless Learning für verschiedene Bereiche (in Einzelprojekten zu den Bereichen MINT, Sozialwissenschaften und zu Schlüsselqualifikationen, wie beispielsweise Projektmanagement) zu konzeptualisieren, entwickeln, implementieren, evaluieren und optimieren. Während einzelne Dimensionen von Nahtstellen für Seamless Learning bereits identifiziert sind, fehlt es bisher vor allem an erfolgreichen Piloten in verschiedenen Feldern. Das IBH Lab ermöglicht gerade dies und zwar grenzüberschreitend in Bezug auf Bildungskontexte, Bildungsphasen und Bildungsstufen und dies zu den verschiedenen Anwendungsfeldern in der Praxis.

Matthias Schmid, ICP

https://www.seamless-learning.eu

Appendix

A.1 Students Projects

D. Baumann, F. Hoernlimann, *Erhöhung der Energieeffizienz eines neuartigen Holzvergasungs-systems für Eukalyptus bei Melides, Portugal*. Betreuer: G. Boiger, A. Fassbind, Firmenpartner: Stiftung Alberta Nova, Projektarbeit Systemtechnik.

J. Baumgartner, A. Morgado, *Smartwatch for optical detection of impaired lymphatic vessel function*. Betreuer: M. Bonmarin, N. Reinke, Firmenpartner: Institute of Pharmaceutical Sciences at ETH Zurich, Bachelorarbeit Systemtechnik.

D. Bee, J. Giger, *A new hand-held imaging device to investigate the thermal properties of the human skin.* Betreuer: G. Boiger, M. Bonmarin, Firmenpartner: Dermolockin GmbH, Projektarbeit System-technik.

N. Boateng, M. Flüeler, *Android-Based Medical Image Processing.* Betreuer: M. Löser, M. Bonmarin, Firmenpartner: Dermolockin GmbH, Bachelorarbeit Electrotechnik.

C. Brändle, A. Schönenberger, *Temperaturüberwachung an Blattoberflächen von Pflanzkulturen durch Infrarotdetektoren.* Betreuer: T. Hocker, T. Bergmann, Projektpartner: Meyer Orchideen AG, Projektarbeit Maschinentechnik.

Y. Cornaz, *Weiterentwicklung eines neuartigen Holzvergasungssystems in Grandola (Portugal) zur Vergasung des lokalen Eukalyptus*. Betreuer: G. Boiger, A. Fassbind, Firmenpartner: Stiftung Alberta Nova, Bachelorarbeit Maschinentechnik.

S. Ehrat, *Theoretische und experimentelle Untersuchungen von Abkühlprozessen im sub-kW Bereich*. Betreuer: T. Hocker, Projektpartner: Wöhner AG, Vertiefungsarbeit Masterstudiengang.

A. Friedrich, M. Lauria, *Development and characterization of 3D skin tissue models with optical methods.* Betreuer: M. Bonmarin, M. Jazbinsek, Firmenpartner: Rainbow Photonics, Bachelorarbeit Systemtechnik.

J. Gianotti, *CFD basierte Optimierung eines Oel-Tanks.* Betreuer: G. Boiger, Firmenpartner: Regloplas AG, Bachelorarbeit Maschinentechnik.

R. Haldemann, F. Heuberger, *Erhöhung der Energieeffizienz eines Holzvergasungssystems in Portu-gal, durch thermo-dynamische 1D Modellierung.* Betreuer: G. Boiger, Firmenpartner: Stiftung Alberta Nova, Bachelorarbeit Maschinentechnik.

S. Helfenstein, S. Satkunaraja, *Numerical thermal model of the human skin.* Betreuer: M. Bonmarin, G. Boiger, Firmenpartner: Dermolockin GmbH, Bachelorarbeit IT.

I. Herzig, F. Scholpp, *Simulation und Experimentelle Validierung von Elektro-Statischen Beschichtungsprozessen.* Betreuer: G. Boiger, Firmenpartner: Wagner International AG, Projekt-arbeit Systemtechnik.

C. Hoch, *Entwicklung und Prototypbau eines neuartigen Konservierungsverfahrens für Fluide*. Betreuer: G. Boiger, Bachelorarbeit Maschinentechnik.

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

P. Khodadust, *Neuartige Kombination von CFD und Machine Learning Technologie*. Betreuer: G. Boiger, Bachelorarbeit IT.

S. LANDOLT, *Application of Novel Machine Learning Software to Predict Powder Coating Phenomena.* Betreuer: G. Boiger, Bachelorarbeit IT.

D. MEIER, *Modellierung von Uj-Kennlinien für Festoxidbrennstoffzellen unter Berücksichtigung der Brenngasverweilzeit*. Betreuer: T. Hocker, Projektpartner: Hexis AG, Masterarbeit Masterstudien-gang.

G. QUADRI, A. BACHMANN, *A new hand-held imaging device to investigate the thermal properties of the human skin.* Betreuer: M. Bonmarin, M. Löser, Firmenpartner: Dermolockin GmbH, Bachelor-arbeit Systemtechnik.

L. RUCKSTUHL, *Analysis of the calibration procedure of the Medyria velocity sensor based on thermo-fluidic CFD-models*. Betreuer: T. Hocker, Projektpartner: Medyria AG, Vertiefungsarbeit Master-studiengang.

S. SPIRIG, *Untersuchung der optimalen Platzierung von Temperatursensoren zur akkuraten Oberflächentemperaturmessung.* Betreuer: T. Hocker, Vertiefungsarbeit Masterstudiengang.

J. STOLL, F. ZIMMERLI, *Weiterentwicklung des thermischen Managements einer neuartigen Holzvergasungsanlage*. Betreuer: G. Boiger, Projektarbeit Energie- und Umwelttechnik.

A.2 Scientific Publications

S. ALTAZIN, C. KIRSCH, E. KNAPP, A. STOUS, B. RUHSTALLER, *Refined drift-diffusion model for the simulation of charge transport across layer interfaces in organic semiconductor devices*. J. of Appl. Phys. 124 (13), 135501, 2018.

S. ALTAZIN, L. STEPANOVA, J. WERNER, B. NIESEN, C. BALLIF, B. RUHSTALLER, *Design of perovskite/crystalline-silicon monolithic tandem solar cells*. Optics express 26 (10), A579-A590, 2018.

F. ANZENGRUBER, F. ALOITAIBI, A. GHOSH, L. KAUFMANN, B. MEIER, L. FRENCH, M. BONMARIN, A. NAVARINI, *Thermography: High sensitivity and specificity diagnosing contact dermatitis in patch testing*. Allergology International, in press (2018).

D. BRUNNER, H. KHAWAJA, M. MOATAMEDI, G. BOIGER, *CFD modelling of pressure and shear rate in torsionally vibrating structures using ANSYS CFX and COMSOL multiphysics*. Int. Journal of Multi-physics, 12 (4), 349-358, 2018.

D. BURNAT, G. NURK, L. HOLZER, M. KOPECKI, A. HEEL, *Lanthanum doped strontium titanate-ceria anodes: deconvolution of impedance spectra and relationship with composition and microstructure*. J. Power Sources. 385 (2018) 62–75. doi:10.1016/j.jpowsour.2018.03.024.

L. CAPONE, P. MARMET, L. HOLZER, J. DUJC, J. O. SCHUMACHER, A. LAMIBRAC, F. N. BUECHI, J. BECKER, *An ensemble Monte Carlo simulation study of water distribution in porous gas diffusion layers for proton exchange membrane fuel cells.* ASME Journal of Electrochemical Energy Conversion and Storage, 15 (2018) 031005 https://doi.org/10.1115/1.4038627.

P. CENDULA, L. STEIER, P. LOSIO, M. GRÄTZEL, J. O. SCHUMACHER, *Analysis of optical losses in a photoelectrochemical cell : a tool for precise absorptance estimation*. Advanced Functional Materials. 28(1), pp. 1702768, 2018. Available from: https://doi.org/10.1002/adfm.201702768.

M. DIETHELM, L. PENNINCK, S. ALTAZIN, R. HIESTAND, C. KIRSCH, B. RUHSTALLER, *Quantitative analysis of pixel crosstalk in AMOLED displays*. J. of Information Display, 1-9, 2018.

J. Dujc, A. Forner-Cuenca, P. Marmet, M. Cochet, R. Vetter, J. O. Schumacher, P. Boillat, *Modelling the effects of using gas diffusion layers with patterned wettability for advanced water management in*

proton exchange membrane fuel cells. Journal of Electrochemical Energy Conversion and Storage 15(2), 2018. Available from: https://doi.org/10.1115/1.4038626.

D. Fluhr, S. Züfle, B. Muhsin, R. Öttking, M. Seeland, R. Roesch, U. S. Schubert, B. Ruhstaller, S. Krischok, H. Hoppe, *Aluminum electrode insulation dynamics via interface oxidation by reactant diffusion in organic layers*. physica status solidi (a) 125, 23, 1800474, 2018.

S. Jenatsch, S. Altazin, P.-A. Will, M. Neukom, E. Knapp, S. Züfle, S. Lenk, S. Reineke, B. Ruhstaller, *Quantitative analysis of charge transport in intrinsic and doped organic semiconductors combining steady-state and frequency-domain data*. J. App. Phys. 124, 10, 105501, (2018)

S. Jenatsch, M. Regnat, R. Hany, M. Diethelm, F. A. Nüesch, B. Ruhstaller, *Time-dependent pin structure and emission zone in sandwich-type light-emitting electrochemical cells*. ACS Photonics, 2018.

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M. Neukom, S. Züfle, S. Jenatsch, B. Ruhstaller, *Opto-electronic characterization of third-generation solar cells*. Science and technology of advanced materials 19 (1), 291-316, 2018.

M. Neumann, O. Furat, D. Hlushkou, U. Tallarek, L. Holzer, V. Schmidt, *On microstructure-property relationships derived by virtual materials testing with an emphasis on effective conductivity*. 2018, Sim. Sci./Commun. Comput. Inf. Sci. (CCIS), Springer. 145–158. doi:10.1007/978-3-319-96271-9_9.

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M. Prestat, J. Soares Costa, B. Lescop, S. Rioual, L. Holzer and D. Thierry , *Cathodic Corrosion of Zinc under Potentiostatic Conditions in NaCl Solutions*. ChemElectroChem, 5, 1203-1211, doi: 10.1002/celc.201701325.

U. Puc, A. Abina, A. Jeglic, A. Zidansek, I. Kasalynas, R. Venckevicius, G. Valusis, *Spectroscopic analysis of melatonin in the terahertz frequency range*. Sensors 18, 4098, 2018.

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M. H. Shin, S. H. Lee, B. J. Kang, M. Jazbinsek, W. Yoon, H. Yun, F. Rotermund, O. P. Kwon, *Organic Three-Component Single Crystals with Pseudo-Isomorphic Cocrystallization for Nonlinear Optics and THz Photonics*. Advanced Functional Materials 28, 1805257, 2018.

B. Siyahhan, M. Boldrini, S. Hauri, N. Reinke, G. Boiger, *Procedure for experimental data assessment for numerical solver validation in the context of model based prediction of powder coating patterns*. Int. Journal of Multiphysics, 12 (4), 373--292, 2018.

L. Wang, S. Jenatsch, B. Ruhstaller, C. Hinderling, D. Gesevičius, R. Hany, F. Nüesch, *Organic Salt Semiconductor with High Photoconductivity and Long Carrier Lifetime*. Adv. Func. Materials 28, 16, 1705724, 2018.

A.3 Book Chapters

S. Altazin, L. Penninck, B. Ruhstaller, *OLED Outcoupling technologies: concepts, simulation, and implementation*. Handbook of Organic Light-Emitting Diodes, Springer Japan, 2018

A.4 News Articles

D. Neeser, G. Boiger, Tüftler macht Strom aus Holz. In: *Der Landbote*, August 2018.

A.5 Conferences and Workshops

S. Altazin, T. Beierlein, M. Diethelm, R. Ferrini, R. Hiestand, C. Kirsch, T. Offermans, L. Penninck, M. Regnat, B. Ruhstaller, *Electrothermal simulation of large-area semiconductor devices*. International Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP 2018), Winterthur, Switzerland.

S. Altazin, C. Kirsch, E. Knapp, A. Stous, B. Ruhstaller, *Refined drift-diffusion model for the simulation of charge transport across layer interfaces in organic semiconductor devices.* Applied Mathematics and Simulation for Semiconductors (AMaSIS 2018), Berlin, Germany.

G. Boiger, *Eliminating anomalies of CFD model results of the powder coating process by refining aerodynamic flow-particle interaction and by introducing a dynamic particle charging model*. 3rd International Conference on Fluid Dynamics & Aerodynamics, Berlin, 2018.

G. Boiger, B. Siyahhan, M. Boldrini, *Enhancing the understanding of complex phenomena in powder coating, by applying Eulerian-Lagrangian simulation methodology*. 13th International Conference of Multiphysics, Krakow, 2018.

D. Brunner, K. Haeuseler, S. Kumar, H. Khawaja, M. Moatamedi, G. Boiger, *Impact of fouling on mechanical resonator-based viscosity sensors: comparison of experiments and numerical models.* 13th International Conference of Multiphysics, Krakow, 2018.

D. FEHR, *Early diagnostics of lymphedema using a near-infrared fluorescent marker and custom portable detection device.* Swiss Society for Biomedical Engineering Annual Meeting, Biel, 2018.

E. KNAPP, *Physical model for inductive loop and negative capacitance in perovskite solar cells*. Asia-Pacific Hybrid and Organic Photovoltaics Conference (AP-HOPV), Kitakyushu, Japan, January 29, 2018.

E. KNAPP, *Modeling negative capacitance and inductive loop in perovskite solar cells*. Intl. Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP'18), Winterthur, Switzerland, Sept 4-6, 2018.

E. KNAPP, *Physical model for inductive loop and negative capacitance in perovskite solar cells*. Intl. Conference on Perovskite Solar Cells and Optoelectronics (PSCO), Lausanne, Switzerland, September 30, 2018.

M. NEUKOM, *Opto-Electronic Characterization of Third Generation Solar Cells.* Intl. Summer School on Nanosciences & Nanotechnologies (ISSON), Thessaloniki, Greece, June 30, 2018.

J. PIOTROWSKI, A. HÄFFELIN, R. VETTER, J. O. Schumacher, *Analysis and extension of a PEMFC model*, 15th Symposium on Modeling and Validation of Electrochemical Energy Devices (ModVal 2018), Aarau, Switzerland, April 12-13, 2018. Available from: https://doi.org/10.21256/zhaw-3599.

U. PUC, T. BACH, M. KRAJEWSKI, C. MEDRANO, M. JAZBINSEK, *Ultrabroadband terahertz time domain spectroscopy based on organic crystals.* 8th International Workshop on Terahertz Technology and Applications, Kaiserslautern, Germany, March 20-21, 2018.

B. RUHSTALLER, *Modeling Pixel Crosstalk through Common Semiconducting Layers in AMOLED Displays.* DFF Work Group Meeting, Gundersheim, Germany, Jan 25, 2018.

B. RUHSTALLER, *Reliable electrical characterization and modelling of organic LEDs and solar cells with doped layers and internal interfaces*. Intl. Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP'18), Winterthur, Switzerland, Sept 4-6, 2018.

B. RUHSTALLER, *Electronic, ionic and optical perovskite solar cell modeling and experimental validation*. NanoGe Fall'18 Meeting PeroMod, Torremolinos, Spain, Oct 22-26, 2018.

J. O. SCHUMACHER, *Elektromobilität mit Brennstoffzellen*, Podium Nachhaltige Mobilität, Hochschule Rapperswil, Switzerland, March 2018.

R. VETTER, J. O. SCHUMACHER, *An open implementation of a two-phase PEMFC model in MATLAB,* 15th Symposium on Modeling and Validation of Electrochemical Energy Devices (ModVal 2018), Aarau, Switzerland, April 12-13, 2018.

R. VETTER, J. O. SCHUMACHER, *A new open-source PEMFC simualtion tool for easy assessment of material parameterizations,* 15th Symposium on Modeling and Validation of Electrochemical Energy Devices (ModVal 2018), Aarau, Switzerland, April 12-13, 2018. Available from: https://doi.org/10.21256/zhaw-3621.k

A.6 Teaching

T. BERGMANN, T. HOCKER, *Thermische Energiesysteme, FS18*, Bachelor of Science.

G. BOIGER, *Fluid- & Thermodynamik I für EU - Vorlesung & Praktikum FS18*, Bachelor of Science.

G. BOIGER, *Numerik für IT II – Vorlesung & Praktikum, FS18*, Bachelor of Science.

G. BOIGER, *Numerik für IT I – Vorlesung & Praktikum, HS18*, Bachelor of Science.

G. BOIGER, *Physik und Systemwissenschaften für AV II – Praktikum, FS18,* Bachelor of Science

G. BOIGER, *Advanced Thermodynamics, HS18,* Master of Science in Engineering.

G. BOIGER, *Thermofluiddynamik Modellentwicklung mit OpenFoam I, HS18*, Master of Science in Engineering

G. BOIGER, *Two Phase Flow with Heat and Mass Transfer, FS18,* Master of Science in Engineering.

M. BONMARIN, *Numerik für IT I – Vorlesung* & *Praktikum, FS18*, Bachelor of Science.

M. BONMARIN, *Physik für Systemtechnik II – Vorlesung & Praktikum*, *FS18,* Bachelor of Science.

D. FEHR, *Mathematik: Analysis 1 für IT, FS18*, Bachelor of Science.

A. HEEL, T. HOCKER, *Abgas- und Abwasserbehandlung, HS18,* Bachelor of Science.

T. HOCKER, *Fluid- und Thermodynamik 1 – Vorlesung und Praktikum, FS18*, Bachelor of Science.

T. HOCKER, *Fluid- und Thermodynamik 2 – Vorlesung und Praktikum, HS18,* Bachelor of Science.

T. HOCKER, *Systemphysik für Aviatik 1 – Praktikum, HS18*, Bachelor of Science.

T. HOCKER, *Systemphysik für Aviatik 2 – Praktikum, FS18*, Bachelor of Science.

M. JAZBINSEK, *Physik für Energie und Umwelttechnik 1 – Vorlesung & Praktikum, FS18*, Bachelor of Science.

M. JAZBINSEK, *Physik für Energie und Umwelttechnik 2 – Vorlesung und Praktikum, HS18*, Bachelor of Science.

E. KNAPP, *Math for Aviation - Applied Numerics - FS18*, Bachelor of Science.

E. KNAPP, *Mathematik: Numerik für Energie- und Umwelttechnik- FS18*, Bachelor of Science.

C. KIRSCH, *MND2 – Mathematik: Numerik und Differenzialgleichungen 2* – FS18, Bachelor of Science.

C. KIRSCH, *MAE2 – Mathematik: Analysis für Ingenieure 2* – FS18, Bachelor of Science.

C. KIRSCH, *MANIT1 – Mathematik: Analysis 1* – HS18, Bachelor of Science.

C. KIRSCH, *MNUM – Mathematik: Numerische Methoden* – HS18, Bachelor of Science.

K P. PERNSTICH, *Physik und Systemwissenschaften für Verkehrsingenieure 1 - HS18*, Bachelor of Science.

K P. PERNSTICH, *Physik und Systemwissenschaften für Verkehrsingenieure 2 - FS18*, Bachelor of Science.

B. RUHSTALLER, *Applied Photonics - HS18*, Master of Science in Engineering.

B. RUHSTALLER, *Physik und Systemwissenschaften für Verkehrsingenieure 1 - HS18*, Bachelor of Science.

B. RUHSTALLER, *Physik und Systemwissenschaften für Verkehrsingenieure 2 - FS18*, Bachelor of Science.

J. O. SCHUMACHER, *Analysis für Ingenieure 4 - FS18*, Bachelor of Science.

J. O. SCHUMACHER, *Analysis für Ingenieure 3 - HS18*, Bachelor of Science.

J. O. SCHUMACHER, *Multiphysics Modelling and Simulation HS18*, Master of Science in Engineering.

J.O. SCHUMACHER, *Numerical Simulation of Solar Cells FS18*, Master Online Photovoltaics.

A.7 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.

Nano Lockin

www.nanolockin.com

NanoLockin is developing the new benchmark technology for the detection and analysis of nanoparticles in all kinds of products. The company won the Fribourg Innovation Awards in 2018.

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.

www.zarawind.com

Zarawind is a Winterthur-based ZHAW spin-off company involved in the development of an airborne wind energy system

Feature:
Zarawind technology aims to produce a renewable cost effective electricity from the strong and consistent wind power at high altitude. This is reachable using a rotor lifted by an aerostat at several handled meters.

Advantages:
wind power is permanently available with a strong capacity. Zarawind model insures continuous operation avoiding noisy problems, flickering , NIMBY clams and bird crash.

Benefit:
Insuring a renewable electrification of off-grid regions at effective cost.

Customers:
One-billion persons in off-grid.

A.8 ICP Team

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A.9 Location

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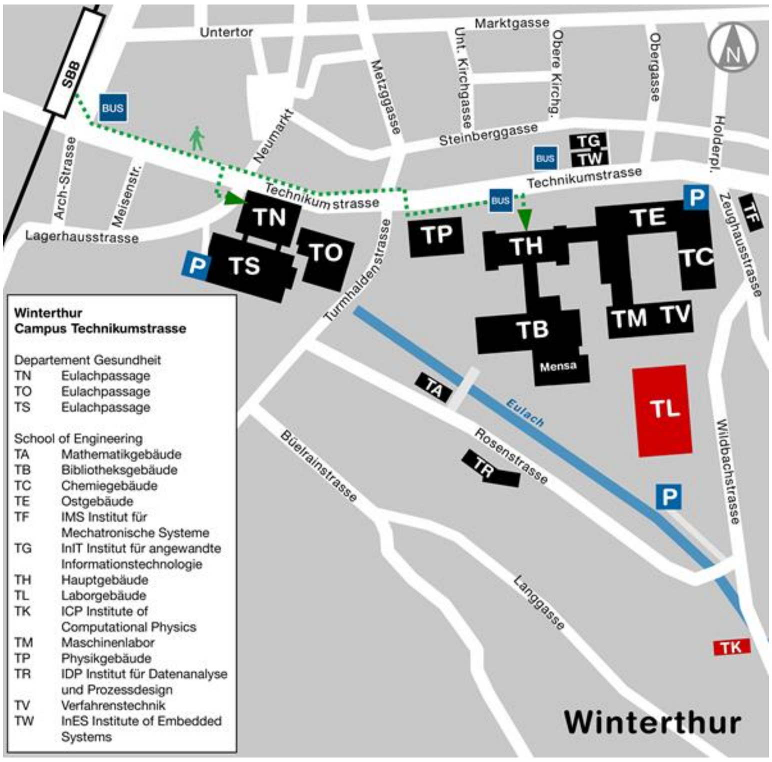

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