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School of
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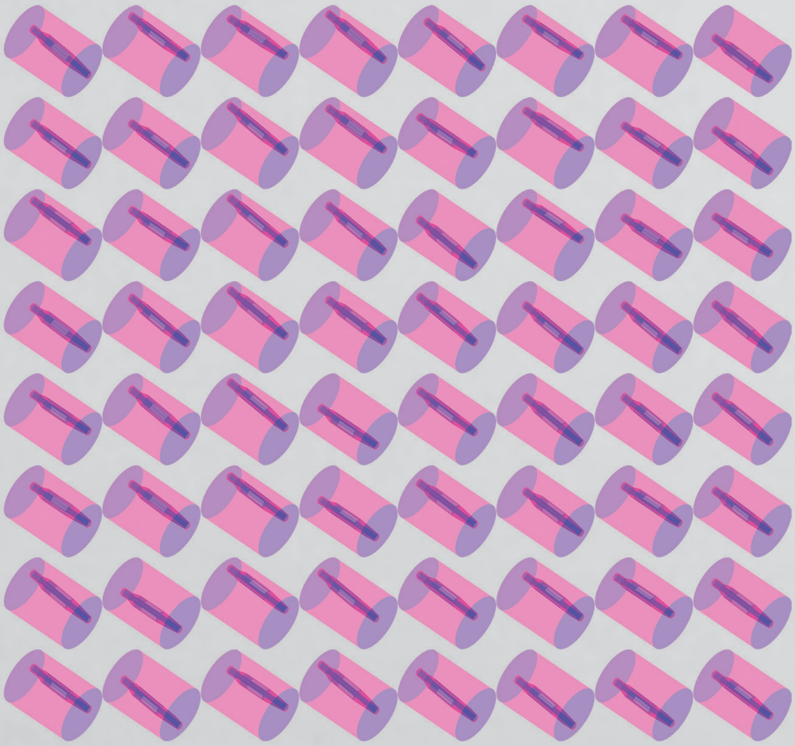
ICP Institute of
Computational Physics

Research Report 2024



www.zhaw.ch/icp

The cover graphic shows automatically generated simulation domains used to produce synthetic data for machine learning.

Contents

Preface

These introductory words were not generated by a large language model (apart from the support for translation and grammar checking). Artificial intelligence (AI) would have produced a nice and harmless greeting that can be optimized in a few minutes so that everything fits, and nobody is bothered by it.

In contrast, I'd like to share a thought with you here, which relates AI to our physics simulations, domain knowledge and entrepreneurial spirit, all three of which characterize the ICP. In my vision, AI does not replace physics simulations, but helps to repackage numerics and make it accessible to a wider range of users.

When the browser-based ChatGPT was released in 2022, I assumed that the wow effect would soon be over and that the impact on our research projects would be relatively small. I am now questioning this assumption. Still, no chatbot can reliably reproduce our expertise in multiphysics modeling or the knowledge from our R&D focus areas. But a new paradigm for interaction between humans and computers is currently being established. The question arises as to whether we will control simulation applications via a language model in the future. The rules that need to be observed here need to be worked out in a suitable way and the language model trained accordingly. A dialog-based interface to a simulation tool would have to ask questions, convey numerical know-how and support the visualization of simulation results. Unlike today's graphical user interfaces, there would no longer be any checkboxes or drop-down menus. Today, we at the ICP are building bridges between numerical modeling and the resulting innovations with our applied research projects. We should use this knowledge for the development of future AI-driven simulation tools. Our experience with knowledge transfer, as we practice it daily in teaching, would also flow into this.

However, we are already visionary in our diverse research projects, which are described in this institute report. I would like to thank all ICP staff, students and partners for their outstanding commitment and expertise, which have made a significant contribution to our success.

Andreas Witzig, Head of ICP

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, 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 the 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 allows us to successfully apply simulation-based optimization in many fields. We are familiar with a wide range of governing physical equations and find numerical solutions even when the effects are closely interrelated. We also develop single-purpose numerical tools tailored to the specific needs of our partners, and we use commercial software where it is more suitable.

Our specialties in this context include the application, extension and development of coupled models using our own finite element software SESES, the fluid dynamics software OpenFoam (open source) and commercially available products such as COMSOL.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1.1 Scalable Simulation-Based Design of Actively Controlled Magnetic Levitation Devices for Industrial Applications

This application presents a novel approach to the simulation-based scaling of actively controlled magnetic levitation devices designed for industrial applications. The study explores the intricate relationship between the size and weight of levitating objects, the magnetic force requirements, and the stabilizing mechanisms provided by a combination of permanent magnets and actively controlled electromagnetic coils. The focus is on developing a robust simulation methodology to handle variable scales and environmental disturbances such as flow forces, achieving minimal energy consumption while maintaining high precision and stability.

Contributors: M. Boldrini, V. Buff, G. Boiger
Partners: Confidential
Funding: Innosuisse
Duration: 2023-2025

Magnetic levitation technology offers significant potential for aseptic applications as it avoids any recesses and contact areas. A primary challenge in implementing maglev systems is scaling the technology to different sizes while ensuring precise control under dynamic conditions. This research addresses these challenges by developing a scalable simulation model that predicts and optimizes the performance of maglev systems under a range of operational conditions (Fig 1).

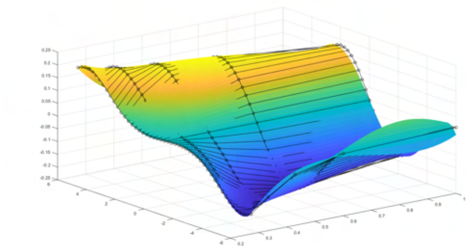

Fig. 1: Visualization of the fit function.

The simulation framework is developed using a combination of Multiphysics software tools to model the magnetic interactions and force dynamics within the maglev system. Initial models are constructed to represent various scales of maglev devices, incorporating elements such as permanent magnets and electromagnetic coils. Parametric studies are conducted to determine how variations in the device size and weight affect the required magnetic forces for stabilization (Fig 2). Simulations are then specifically designed to assess the impact of external flow forces on the stability of the levitating object, allowing for dynamic adjustments of magnetic forces. The optimization algorithms refine the magnetic field configurations to ensure efficient energy usage while maintaining stability and precision. These algorithms dynamically adjust coil currents and magnet placements based on real-time simulations.

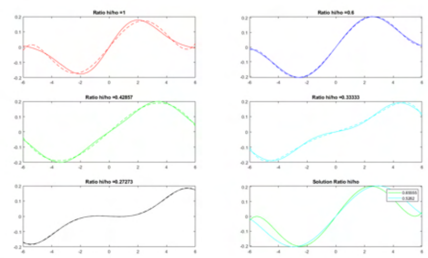

Fig. 2: Forces dependent on relative position of levitator magnet for different ratios.

The research highlights the importance of a simulation-based approach in scaling magnetic levitation technology for industrial use. The findings support the feasibility of adapting maglev systems to different scales, emphasizing the need for precise control mechanisms and energy efficiency in the face of external disturbances.

1.2 Position and acceleration control of a linear drive for generating vibration profiles

This project deals with the development of a control system for generating vibration profiles on a two-axis linear drive system. Non-linear friction effects and a narrow range of motion place high demands on the quality of the control. By separating the bandwidth of the position controller and the vibration profiles and the introduction of a feedforward control to compensate for the gravity of the test object the control system was successfully implemented and tested

Contributors: V. Buff, M. Hostettler, G. Boiger
Partners: Roche
Funding: Roche
Duration: 2021–2023

This project began with the need for a system to validate findings from fluid dynamic models on the behaviour of molecular solutions under shear stress. These stresses are generated by vibrations when the liquid is transported. To generate these test vibrations in the x and z directions, a smaller, vertical linear actuator was fixed to a larger, horizontal linear actuator. As a result of the set-up, the horizontal system is indifferently stable, the vertical system is unstable, which requires a position controller. This position controller is in concurrence with the control of the vibration profile.

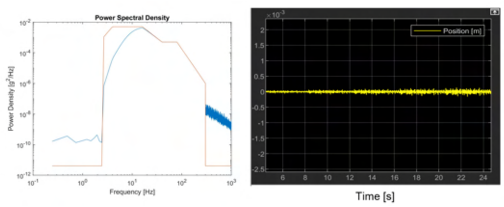

Fig. 1: Illustration of the problem Case 1: In the case of a high bandwidth for the position controller, low frequencies of the desired vibration profile are strongly damped. The graph on the left shows the target profile in red and the simulated profile after 100s in blue. The criteria for position stability ($|x| < 0.1m$) are met (graph on the right).

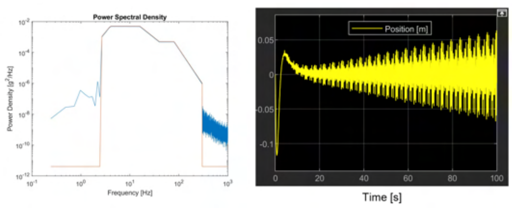

Fig. 2: In the second case with a lower bandwidth of the position controller, the target profile (graph on the left, red curve) is achieved (graph on the left, blue curve), but the position criteria cannot be met in the transient phase (graph on the right).

The deflection at the start of control occurs primarily with the vertical drive and is caused by the force of gravity acting on the sample. During the transition from position control, which brings the specimen into position, to vibration control, which performs the actual test, the information on the static gravity compensation is lost. As a result, the sample leaves the narrow spatial frame and the test is cancelled. The force-generating current required for gravity compensation is therefore determined by an identification routine during the start-up and used as feedforward in the subsequent vibration control. This feedforward can significantly slow down the initial deflection. This allows the use of a position controller with a smaller bandwidth.

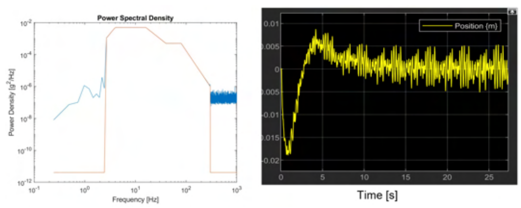

Fig. 3: Implementation of pre-control using gravity estimation. The left graph shows the target profile in red and the actual profile at T = 30s in blue. The graph on the right shows the initial outward movement, which has been significantly reduced and is within the position criteria.

The implementation of the present control system on the real system shows a high qualitative and quantitative consistency between the model and the system.

1.3 Thermal Design Lab - Measuring equipment for determining material properties

In our R&E projects, we support our project partners with physical computer simulations. Their accuracy requires reliable material data, which is often not available in the literature and therefore requires our own measurements.

Contributors: S. Ehrat, J. Santana de Castro, T. Hocker
Partners: IMPE - Adhesives and Polymer Materials, IMES - Applied Mechanics
Funding: ICP
Duration: Ongoing

Various measuring instruments are available in the Thermal Design Lab to evaluate the material properties of liquid and solid materials.
The portable density meter «DMA 35» can be used to reliably determine the density of liquids. Only a small sample of less than 50ml is required to determine a density between 0 g/cm^3 - 3 g/cm^3 at a measuring temperature between 0 °C - 40 °C.
A «ViscoQC 300 L» rotational viscosimeter with temperature control unit is available for determining dynamic viscosities. This allows viscosities between 0.1 mPa s - 6,000 Pa s to be analysed in the temperature range of 15 °C - 80 °C.

Fig. 1: The portable density meter «DMA 35» (left) [1] and the rotational viscometer «ViscoQC 300 L» with temperature control unit «PTD 80» (right) [2] from Anton Paar.

The portable thermal properties analyser «Tempos» is available for analysing the thermal conductivity of liquids and solids and is based on the transient line source measuring principle. A measurement takes 90 seconds. The minimum sample volume is approx. 50ml or a volume of 2x2x8cm for solids. Measurable thermal conductivities are between 0.02 W/(m K) - 6.0 W/(m K) for a temperature range of -50 °C - 150 °C. To increase accuracy, we also use our own model to extract thermal conductivities from the temperature measurement data obtained.
In addition, a «CORIO CP 1000F» temperature control bath from Julabo with an operating range of -50 °C - 100 °C is available for tempering the measurement sample.

Fig. 2: The portable Thermal Properties Analyser «TEMPOS» from METER (left) [3] and the measuring sensor «KS-3» for measurements in low-viscosity liquids for the determination of thermal conductivity.

For measurements of heat capacity and thermal conductivity at high temperatures, we work together with the IMPE and IMES.

Literature:

[1] DMA 35, https://www.anton-paar.com/corp-de/produkte/details/dma-35/7 (08.05.2024)
[2] ViscoQC 300 L, https://www.anton-paar.com/corp-de/produkte/details/viscoqc/ (08.05.2024)
[3] TEMPOS, https://metergroup.com/products/tempos/ (08.05.2024)

1.4 Model based optimization of complex microstructures

A Digital Materials Design (DMD) framework was established, allowing for a systematic and knowledge-based optimization of materials with complex microstructures, which is based on a combination of several methodological modules (tomography, image analysis, stochastic geometry, AI/NN, cloud computing, multiphysics modeling). In the present project, the DMD framework was used for optimization of solid oxide fuel cell electrodes (SOFC). In a broader context, the DMD toolbox can easily be adapted for design optimization of other functional materials, such as battery electrodes, filters or catalysts.

Contributors: P. Marmet, L. Holzer, T. Hocker, V. Muser, G. K. Boiger
Partners: HEXIS, Math2Market, University of Fribourg, ETHZ ScopeM
Funding: Swiss Federal Office of Energy, Eurostars
Duration: 2019–2024

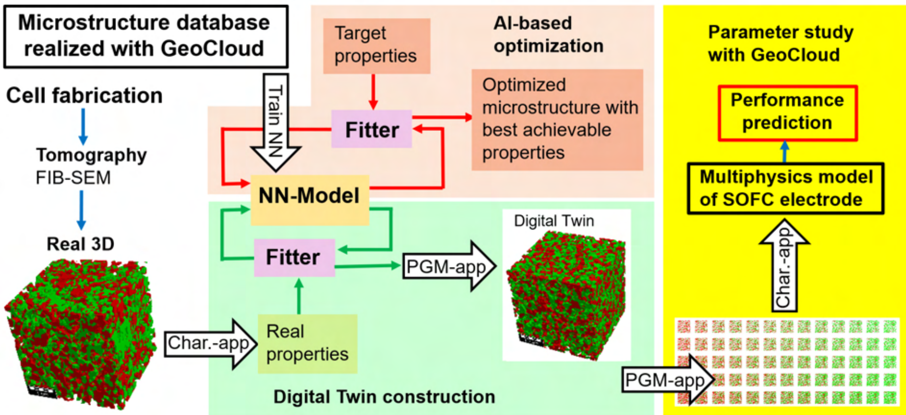

Fig. 1: Overview of the Digital Microstructure Design (DMD) methodologies.

Our DMD framework is the result of two complementary projects, one related to the methodologies (partner: Math2Market, funding: Eurostars) and one related to materials optimization of novel Ni-free SOFC electrodes (partner: HEXIS, funding: BFE). A detailed description of methods and results can be found in the Ph.D. thesis of Ph. Marmet (University of Fribourg) [1]. The workflow for the application of the DMD modules includes the following steps (Fig. 1):

→ Fabrication and testing of SOFC electrodes.

→ 3D imaging by FIB-SEM tomography.

→ 3D analysis of microstructure parameters and effective properties [2] using a fully automated characterization-app, now available in GeoDict [3].

→ Stochastic 3D database: Digital microstructure twins are constructed based on a pluri-Gaussian method (PGM) [4]. Stochastic twins have the same statistical properties as the real structures from tomography. A large number of 3D microstructures and their properties can efficiently be realized and analyzed by cloud computing. For this purpose, our stochastic modeling approach (PGM) and our automated characterization-app are integrated in a new cloud application of Math2Market (GeoCloud/GeoDict).

→ Using the 3D database as training data, a neural network is trained to establish a link between the PGM construction parameters and the effective microstructure properties. This allows for an automated construction of digital twins.

→ A trained network can also be used for AI-based optimization of a 3D-strucuture with predefined target properties (surface area, conductivity etc).

→ A multiphysics electrode model (experimentally calibrated) finally provides the link between the microstructure properties and the electrode performance. The cloud-based workflow for performance optimization thereby allows for extensive parametric studies covering a wide range of virtual microstructures and properties.

Literature:

[1] P. Marmet, PhD thesis, University of Fribourg, Switzerland, URL: https://doi.org/10.21256/zhaw-28430, 2023.
[2] L. Holzer et al., 1st ed. Springer Cham, 2023, ISBN: 978-3-031-30477-4.
[3] P. Marmet et al., Energy Adv., 2 (7), 980–1013, 2023.
[4] P. Marmet et al., Energy Adv., 2 (11), 1942–1967, 2023.

1.5 Laboratory Test Setup for the Characterization of Mechanosensitive Liposomes

This project focused on the characterization of the mechanosensitive behavior of Hard Shell Liposomes. These microscopic lipid membrane spheres enable the targeted release of medical agents at blood vessel constrictions, allowing precise treatment of blood clots without excessive drug dosing.

Contributors: M. Hostettler, G. Boiger
Partners: Acthera
Funding: Innosuisse
Duration: 2022–2024

In the treatment of arteriosclerotic narrowed blood vessels, the patient is injected with medication to combat the constriction. However, as these anticoagulant drugs pose a burden on the healthy body, it is important to keep the dosage low and apply them as locally as possible to the vessel wall affected by the stenosis.

The use of Hard Shell Liposomes (HSL) offers a promising solution. The active ingredient is encapsulated in microscopic lipid membrane spheres (see Fig. 1), which prevent it from coming into contact with healthy tissue. This allows for the medication to be injected intravenously without complication. Once they reach the stenosis, the lipid membranes rupture and release the drug locally.

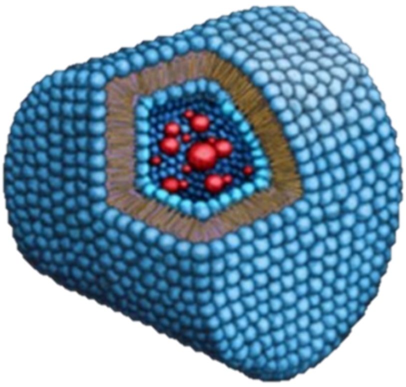

Fig. 1: Artist's rendering of an HSL particle: A lipid membrane (blue) forms a microscopic vessel that can be filled with an active substance (red).

The basis of this targeted release mechanism lies in the utilization of increased wall shear stresses in blood flow at the stenosis, which trigger the rupture of the lipid membranes. Numerical studies have shown that the shear forces in stenotic blood vessels are significantly higher than in healthy tissue [1].

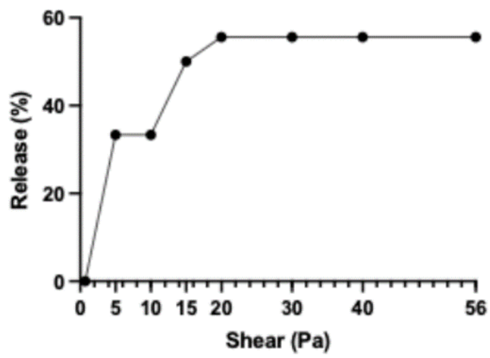

Fig. 2: Characteristic release curve of an HSL product. A pronounced increase in release is observed above a certain shear force.

The aim of the project was to develop a method for characterizing HSL. For this purpose, a test rig was designed that enables HSL solution to be subjected to different shear stresses and to quantify the proportion of particles destroyed in the process.

It could be shown that the investigated HSL particles indeed exhibit a pronounced shear stress threshold, above which the release significantly increases (see Fig. 2). Based on these results, flow simulations can be used to determine how much of the active substance is released at the stenosis for a given dose, and how much is lost in the rest of the bloodstream.

Literature:

[1] D. L. Bark Jr., D. N. Ku, Wall shear over high degree stenoses pertinent to atherothrombosis, *Journal of Biomechanics*, 43 (15), 2010.

1.6 Modelling of Peristaltic Pumps with Respect to Viscoelastic Tube Material Properties and Fatigue Effects

Peristaltic pump technology is widely used wherever relatively low but highly-accurately dosed volumetric flow rates are required. Nevertheless, when applied in conjunction with polymer-based tubing material, supplied peristaltic flow rates are reported to be significantly lower than the expected set flow rates. In such cases, the dynamic behavior of the used tube material becomes non-negligible and must be taken into account. In the scope of an Innosuisse project, those effects have been investigated and a simulation method has been developed to correctly predict the pump behavior.

Contributors: M. Hostettler, G. Boiger
Partners: Confidential
Funding: Innosuisse
Duration: 2019–2022

The operating principle of peristaltic pumps is based on the cyclic motion of mechanical sliders or rollers, which forces a liquid through a flexible tube (see Fig. 1). The volume conveyed per pump cycle is determined by the geometry of that peristalsis and is therefore ideally constant. However, this requires that the tube constantly follows this motion and that the sliders do not lift off. Depending on the pumping frequency and the material properties of the tube, however, this cannot be ruled out. This can lead to a reduction of the conveyed fluid volume per cycle and thus of the resulting flow rate.

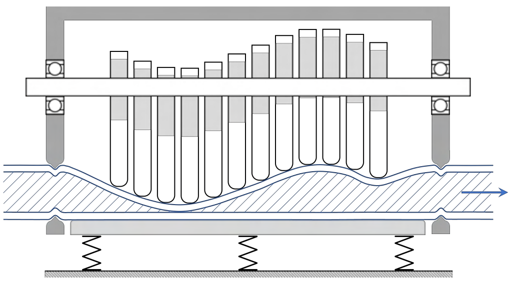

Fig. 1: Cross-sectional view of an exemplary peristaltic pump with a horizontal arrangement of vertically moving sliders that cyclically deform the tube.

This reduction in pumping capacity is strongly dependent on the viscoelastic properties of the selected tube material and can also change over the operating time due to fatigue effects of the tube. In order to ensure a precise flow rate, the puming frequency must therefore be continuously corrected, based on real time measurements of the instantaneous flow rate or, depending on the operating point and duration, by means of calibration data generated a priori.

Up to now, such calibration data has been determined experimentally from a large number of time-consuming measurements. An alternative to this is the use of numerical methods such as fully 3D dynamic fluid-structure-interaction simulations, which achieve good accuracies but are too costly to be economically viable.

In order to present an industrially applicable numerical calibration method, a drastically simplified, yet sufficiently accurate simulation model has been developed in this project.

It is based on a very simple structural representation of the tube using constitutive material models and includes straightforward geometric constraints to calculate the fluid flow. In addition, specific measurement methods have been developed to determine the relevant material properties for a given tube.

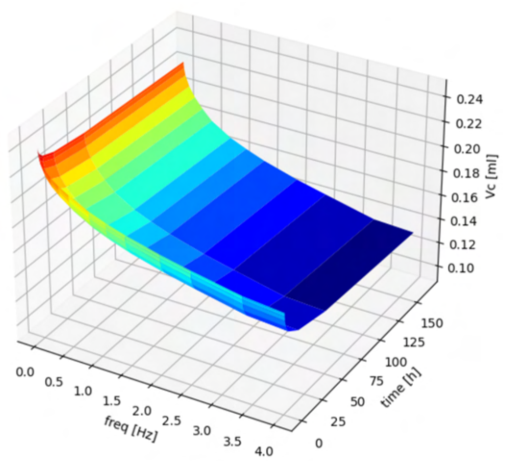

Fig. 2: Simulation results of the decreasing pump performance for a specific tube. It shows how the conveyed volume per cycle Vc decreases with higher pump frequencies (viscoelastic behavior) and over time (fatigue effect).

The simulation results (see Fig. 2) have been validated using flow measurements on real peristaltic pumps with different, pump frequencies, time scales and tube materials.

Literature:

[1] M. Hostettler et al., *Fluids*, 8 (9), 254, 2023.

1.7 Corrosion of multiphasic Titanium Alloy Implants

Titanium alloys are frequently used for implants in the human body. Despite the excellent corrosion resistance of these alloys, oxidizing species produced during inflammatory episodes can lead to a corrosive attack. In this project, a Swiss/French consortium will reveal the basic mechanisms of the corrosion of additive manufactured titanium implants using a combination of experimental methods and mathematical modelling.

Contributors: L. Holzer, Y. Safa, P. Marmet
Partners: Thermomechical Metalurgy Lab (EPFL), Institut de la Corrosion (Brest, France), Laboratoire de Réactivité de Surface (CNRS-Paris Sorbonne, France), tldr group (Imperial College London, UK)
Funding: SNSF, French National Research Agency
Duration: 2023–2026

Titanium and its alloys are among the most widely used biocompatible materials as implants in the human body. However, they may deteriorate under the influence of several electrochemical, mechanical and biological factors. The corrosion resistance of titanium is mainly attributed to the presence of a thin passive layer on its surface, but this layer degrades in the presence of oxidizing species produced during inflammatory episodes, such as hydrogen peroxide or radicals that alter the passive film, leading to corrosion of the metal. Moreover, the initiation of damage might be related to the stress corrosion cracking (SCC) phenomenon. Ti6Al4V alloy is a popular implant material because of its mechanical properties. Additive manufacturing has become a competitive alternative to conventional machining techniques with an obvious advantage in the field of biomedical implants for a custom fabrication of devices. Selective laser melting is particularly suitable for the manufacture of small parts with high geometric accuracy. Moreover, an optimization of local mechanical and electrochemical properties can be achieved through local heat treatments during additive manufacturing. In this project, a consortium of partners from France and Switzerland works together to reveal the basic mechanisms of the corrosion of additive manufactured Ti6Al4V implants using a combination of experimental methods and modelling. Extensive electrochemical and mechanical testing provides information on the macroscopic behavior, while local electrochemical measurements are needed to describe the local, microscopic phenomena in detail. The experimental methods are complemented with mechanical and electrochemical models in order to explain the observed phenomena on a fundamental level. Advanced imaging techniques allow to show the detailed microstructure of pristine and corroded samples. Fig. 1 shows the surface and cross section of a corroded Ti6Al4V sample exposed to a PBS solution with 3 % hydrogen peroxide for 5 days. The deep trenches visible in the FIB cross section originate from dissolution of the β-phase.

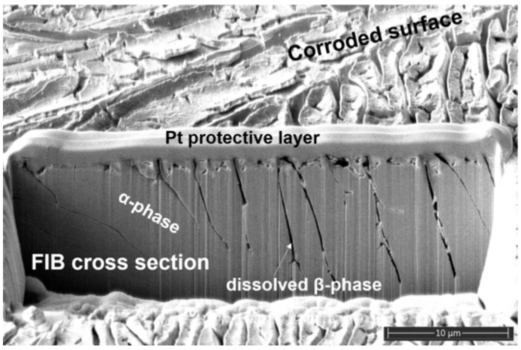

Fig. 1: Surface and cross section of a corroded Ti6Al4V sample exposed to a PBS solution with 3 % hydrogen peroxide for 5 days. The cross section is milled using a focused ion beam (FIB).

Moreover, a predictive approach will be developed based on a virtual materials testing (VMT) framework, which combines 3D digital microstructure representations with numerical simulations. In order to limit the time and cost of the fabrication and imaging process performed on a large number of samples, a virtual geometrical representation of the 3D microstructure will be established using generative adversarial networks (GAN's). This allows creating virtual microstructures with structural properties similar to those observed by tomography. The VMT framework then allows to perform extensive parametric studies to predict the SCC resistance for a wide range of Ti-samples and associated corrosive environmental settings. Hence, this project will elucidate the influence of microstructure, corrosion environment and mechanical load on the corrosion behavior of additive manufactured Ti6Al4V implants.

1.8 Corrosion prediction in multiphasic titanium alloy

In this project we adopt a model-based approach making a synergistic contribution with other partners' activities on additive manufacturing, corrosion and mechanical fatigue tests to investigate relationships between biological environment and titanium implant corrosion. A novel implementation of numerical model allowed a consistent analysis and prediction of corrosive activies in-between titanium alloy phases

Contributors: Y. Safa, P. Marmet, L. Holzer
Partners: Mechanical Metallurgy Lab (EPFL), Institut de la Corrosion (Brest, France), Laboratoire de Réactivité de Surface (CNRS-Paris Sorbonne, France)
Funding: SNSF, French National Research Agency (ANR)
Duration: 2023–2026

Degradation of titanium implant due to inflammation effects is generally described by an initiation of micro-cracks and propagating dissociation flaws inside and between titanium alloy phases. This is driven by an electrochemical process in the corrosive inflammatory medium of the human body. We adopt a model-based approach interrracting with other consortium partners activities (additive manufacturing, corrosion experiment, and mechanical fatigue test), to investigate relationships between biological corrosive environment, the mechanical load and the initial microstructure of the Ti6Al4V alloy.

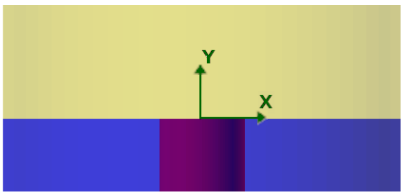

Fig. 1: Schematic of titanium alloy (Ti6Al4V) phases: β (red), α (blue) under electrolyte (yellow).

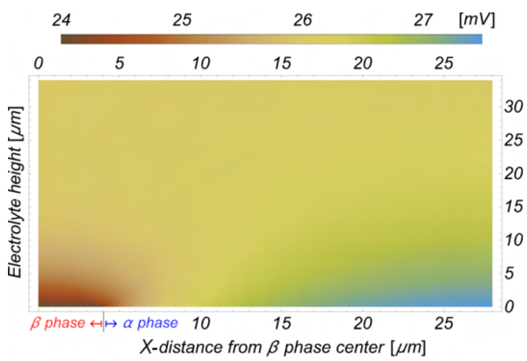

Fig. 2: Potential field in electrolyte domain. Model is implemented in Mathematica.

A new implementation of in-house numerical model of ADI Alternating Directional Implicte scheme is conducted at ICP demonstrating an advanced predictive capability to describe reactive transport of ionic charges inside the metallurgical structure of titanium phases. In the exemplar case shown in this report, we introduce the anodic contribution of α phase with respect to cathodic reaction of β phase involving oxygen reduction and metal dissociation Fig. 1. The potential distribution inside the electrolyte is shown in Fig. 2 and Fig. 3.

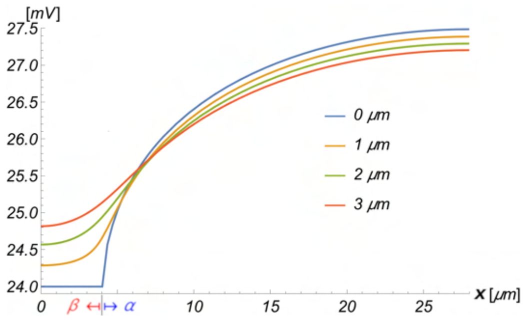

Fig. 3: Potential at different heights in electrolyte.

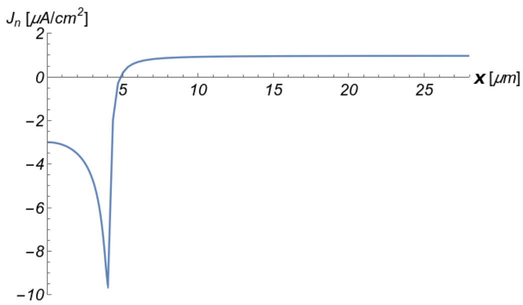

Fig. 4: Normal flux along electrode surfaces.

The model capability to satisfy charge conservation condition can be clearly concluded from Fig. 4 through a zero total integral of normal flux along the electrodes' surfaces. Here we should highlight the increase of normal fluxes in β phase close to the α-β interface. This makes a clear agreement with experimental observation that electrochemical corrosion of β phase is starting at that interface assuming passive behaviour in α phase.

1.9 Simulation-based Optimization of Key-Performance-Attributes by Variation of Powder-Parameters

An OpenFOAM based Eulerian-Lagrangian Multiphysics solver has been created in order to predict coating efficiency, homogeneity and coating patterns for industrial powder coating applications. Following meticulous experimental validation, a parameter study was conducted on U-profile-substrates in order to relate powder material parameters to optimized key-performance-attributes.

Contributors: G. Boiger, B. Siyahhan, A. Schubiger
Partners:
Funding: ICP
Duration: 2023–2024

While wet paint coating still dominates the coating sector, powder coating is described as emerging technology and accounted for approximately 15% of coating market share in 2021. In this context a Multiphysics simulation software has been developed to predict the key-performance-attributes of industrial powder coating applications based on applied process-parameter settings. The software is a Eulerian-Lagrangian finite-volume Multiphysics solver, based on OpenFOAM, capable of modelling mass transfer effects between powder-coating pistols and electrically grounded metallic substrates. It considers various factors such as fluid dynamics of process airflow, coating-particle-dynamics, particle-substrate interactions, and particle charging mechanisms within the corona. The software is fully compatible with Massive Simultaneous Cloud Computing technology, allowing hundreds of simulated coating scenarios to be computed simultaneously. Experimental validation efforts have been conducted by comparing software-based predictions of coating efficiency, homogeneity and coating patterns to real-life full-substrate-body scans of coating thickness distribution. The results indicate a high degree of practical relevance of the technology (see e.g. Fig.1).

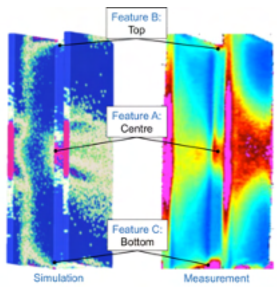

Fig. 1: Simulation based prediction (left) vs. experimentally derived (right) coating pattern of a powder coated U-profile.

The current simulation study aims to demonstrate the potential of the simulation software for adjusting coating lines and optimizing powder coating of U-profiles. Specifically, the study focuses on optimizing the key-performance-attributes of the powder coating application with respect to varying material parameters of the applied powder, namely mean particle diameter, standard deviation of Gaussian particle size distribution, and powder particle density. The software predicts and visualizes coating-patterns, coating-efficiencies, and the batch-based standard deviation of coating thickness on a U-shaped metallic substrate, resulting in concrete and optimized powder-settings. The obtained results (see e.g. Fig. 2 and Fig. 3) could be highly relevant for powder material suppliers.

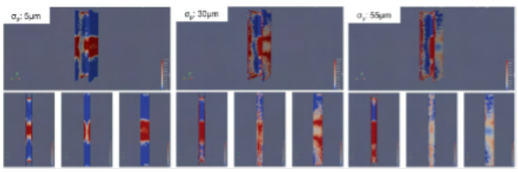

Fig. 2: Simulated coating patterns for varying Standard deviation of particle diameters: 5 µm (left), 30 µm (centre) and 55 µm (right).

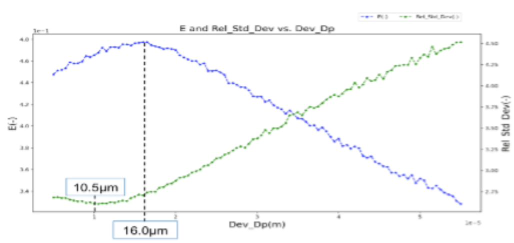

Fig. 3: Coating efficiency (E, blue) and relative Standard batch-based coating deviation (Rel_Std_Dev, green) against Standard deviation of particle diameters (Dev_Dp).

Literature:

G. Boiger et.al., Multiphysics Modelling of Powder Coating of U-Profiles: Towards Simulation-based Optimization of Key-Performance Attributes by Variation of Powder-Parameters, The International Journal of Multiphysics, 17 (2), 169–190, 2023.

1.10 Exploring Humidity, Pressure, and Temperature Effects on Water Droplet Evaporation Using OpenFOAM and DAKOTA

This study utilises the capabilities of DAKOTA (Design Analysis Kit for Optimization and Terascale Applications [1]) from Sandia National Laboratories. Focusing on the evaporation rates of water droplets, a critical process in various industrial and environmental applications, we employ a parameter study to investigate the influence of three key variables: humidity, temperature, and pressure. This study was conducted to test the capabilities of coupling DAKOTA with OpenFOAM, and assess its application for future projects. Utilising DAKOTA's Orthogonal Array Sampling and Main Effects analysis, this study seeks to identify the significant contributors to variations in evaporation rates, thereby optimising simulation practices and improving predictive accuracy.

Contributors: A. Schubiger, G. Boiger
Partners:
Funding: ICP
Duration: 2023–2024

The Dakota analysis employs a Design and Analysis of Computer Experiments (DACE) using Orthogonal Array Sampling (OAS) method focused on main effects. The simulation setup includes three continuous design variables: humidity (Y_{H2O}) ranging from 1e-6 to 0.35 (kg/kg), pressure (P) from 90 to 110 kPa, and temperature (T) from 290 to 390 Kelvin and a constant spray rate of 8.0e-4 kg/s. A total of 120 simulations were conducted.

The simpleReactingParcelFoam solver utilises a Lagrangian framework for the injection and tracking of discrete particles, such as droplets or particles, within a continuous Eulerian phase (gas or fluid flow). This coupling allows the simulation to capture complex interactions between the injected particles and the surrounding fluid, including heat and mass transfer effects, such as evaporation or chemical reactions. The solver's capability to model the dynamics of particle behaviour within the flow makes it particularly suited for studies involving spray dynamics, particle-laden flows, and multiphase reactions.

The ANOVA analysis of the three variables shows distinct effects on the dependent variable. Humidity and Temperature have both demonstrated significant impacts with extremely low p-values (1.21e-10 for Variable 1 and 1.57e-11 for Variable 3) and high F-values (8.95 for Y_{H2O} and 9.78 for T), suggesting that they contribute meaningfully to variations in the response. On the contrary, pressure shows no significant effect, indicating its influence on the dependent variable is statistically insignificant (p-value = 0.99), F-value = 0.128). The successful integration of DAKOTA with OpenFOAM in this study not only provided valuable insights into evaporative phenomena but also demonstrated the feasibility of using these tools in tandem for future projects, paving the way for more comprehensive and intricate simulations in upcoming research endeavours.

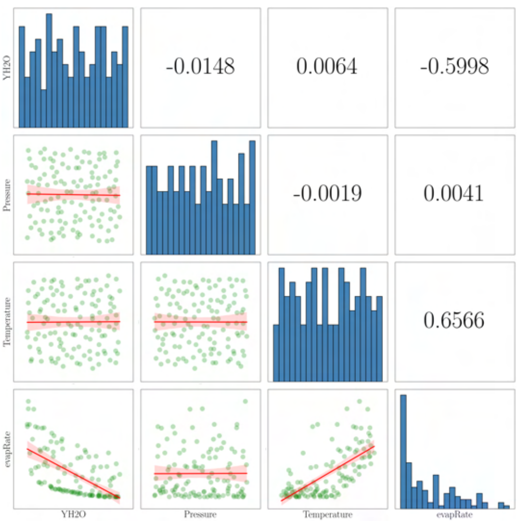

Fig. 1: This figure presents a linear regression plot demonstrating the relationships between variables, accompanied by histograms depicting the distribution of each variable and a heatmap showing pairwise correlations to highlight the strength and direction of their associations.

Literature:

[1] Adams, B. M. et al., *Dakota 6.19.0 documentation. Technical Report SAND2023-13392O, Sandia National Laboratories*, 2023. Available online from http://snl-dakota.github.io.

2 Electrochemical Cells

The team Electrochemical Cells and Microstructures is working on the modelling and simulation of electrochemical flow cells for various applications:

- Proton exchange membrane fuel cells are being developed to power heavy-duty vehicles like trucks. The aim is to replace combustion engines that currently run on fossil fuels. Thereby, the key technical challenge is to increase the durability of membrane electrode assemblies (MEAs). We are currently addressing this topic in the European project PEMTASTIC with a combination of micro- and meso-scale MEA models that allow to simulate both the cell performance and durability at power load cycling.
- Redox flow batteries (RFBs) are a technology for the grid-scale energy storage of fluctuating renewable power from photovoltaics and windmills. Aqueous organic RFBs have the advantage of low solvent cost and relatively high conductivity, and water-based electrolytes allow for safe battery operation. As a result of the European project SONAR, we have recently published a computationally efficient physics-based model of an aqueous organic RFB. The model is suitable for application in computational high-throughput screening to identify new active materials.
- Electrochemical flow cells are a key component of the future synthesis technology in the chemical industry, where electrical energy is used to power electrochemical reactions. The use of flow cells for the electro-organic synthesis will allow to produce fine chemicals or pharmaceuticals by use of renewable energy. Our team participates in the European project MiEI, where we are working on the simulation of electrode structures and the model-based analysis and design of electrochemical flow cells.


Alessandro Cucchi


Edoardo Scoletta


Jürgen Schumacher


Roman Schärer


Axel Dullak


Lourenco C. Vieira

2.1 Meso and continuum scale flow cell modelling for electroorganic synthesis

MiEl is a research and training project funded by the European Union's Marie Skłodowska-Curie programme. Involving 9 partner organisations and 5 associated partners from 9 different countries, MiEl concerns the development of novel synthesis technologies for the chemical industries, combining the novel advantages of electrochemistry, microprocess engineering and flow chemistry to this effect. Through the joint effort of an international network of 12 doctoral candidates, the ambitious research objective is to upscale these flow cell technologies and assemble them in arrays for the safe, flexible and sustainable synthesis of chemical products for the future, namely in the pharmaceutical industry.

Contributors: A. Dullak, L. Vieira, J. Schumacher, R. Schärer
Partners: ICT, UvA, DTU, UWK, UCT Prague, SU, INO, ECHEM, JAN, ZHAW, KIT, USZ
Funding: European Union: Horizon-MSCA-2021-DN-01-01
Duration: 2023–2026

In the European doctoral network project MiEL, 12 doctoral candidates are developing electroorganic synthesis technology for the chemical industries of the 21st century, fusing the sustainable advantages of electrochemistry, microprocess engineering and flow chemistry. Electrochemical technologies have shown to offer high energy efficiency in production, while microfluidics increase safety and process control in a variety of chemical processes. As such, a merging of the two procedures in the form of electrochemical flow cells (Fig. 1) seems to be the logical step towards a more reliable and scalable, safer and greener chemical industry. The three distinct synthesis routes under investigation (two-phase, aqueous and non-aqueous electrosyntheses) can be regarded as relevant model processes for this aim.

Ultimately, the ambitious research objective is to upscale these novel flow cell technologies and electroorganic processes through integrated cell concepts, such as printed circuit board (PCB) technology with embedded sensors and in-situ yield control via machine learning optimization. The cells may then be assembled in arrays for the safe, scalable and sustainable synthesis of chemical products, which can also be used for catalytic screening. Lastly, a parallel techno-economical evaluation shall provide guidance across all modules of the project, and ensure that its economic and ecologic "sweet spots" are well defined, for the context of applied electrosynthesis.

As a fundamental partner of the MiEl consortium, ZHAW-ICP's role is to enable the systematic understanding of these electrochemical processes and their feasibility by conceiving multiphysics models of flow cells on different length scales (continuum and mesoscale), resorting to state-of-the-art numerical methods such as Lattice Boltzmann Method (LBM). Via the kinetics and mass transport simulation of electrode structures subject to multi-phase fluid flow and multi-electron step reactions, the mission is to assess the performance of the developed cells by solving for current-potential distributions, as well as concentration, velocity and pressure profiles. The subsequent optimization of these models with respect to key figures shall guarantee the right design and operating conditions for these technologies towards achieving the desired sustainability of industrial application, evidencing ZHAW-ICP's essential contribution to the overall project.

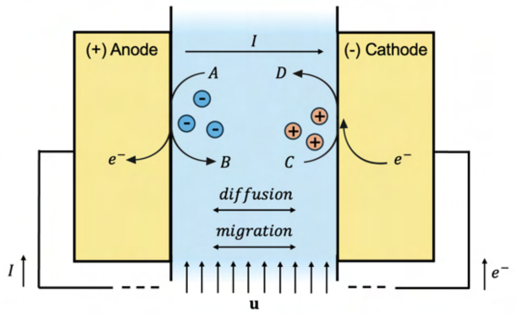

Fig. 1: Schematic of electrochemical flow cell.

Literature:
[1] MiEl project website: https://project-miel.eu/

2.2 Robust PEMFC membrane electrode assemblies derived from model-based unserstanding of durability limitations for heavy duty applications

The aim of this project is to meet the key technical challenges to increase the durability of membrane-electrode assemblies (MEA) for heavy-duty vehicles applications. These challenges are approached with a combination of model-based design and development of durable catalyst coated membranes by using materials tailored for heavy-duty operation at high temperature (up to 105° C). The quantitative target corresponds to a durability of 20,000 hours by maintaining a power density 1.2 W/cm^2 at a cell voltage of 0.65 V, with a platinum loading of 30 g/kW.

Contributors: J. O. Schumacher, A. Cucchi, E. Scoletta, R. P. Schärer
Partners: DLR, IRD, Imerys, CEA, Chemours, Heraeus, Symbio
Funding: European Union's Horizon Europe research and innovation programme
Duration: 2023–2026

The project aim is to overcome the durability limitations of polymer electrolyte membrane fuel cells (PEMFCs) by developing new application-tailored component materials, cell model-based designs, and operating strategies, in line with the Strategic Research and Innovation Agenda (SRIA) of the Clean Hydrogen Joint Undertaking. The main purpose is then to bring the highly innovative concept of durable heavy-duty membrane electrode assembly (MEA) to technology readiness level (TRL) 4.

Different institutes contribute to this project: DLR, CEA, ZHAW are responsible for MEA characterization, ex-situ analysis and model-based designs. Component suppliers (IRD) and material suppliers (IMERYS, Heraeus, Chemours) are responsible for providing the innovated and improved different sub-components of the catalyst coated membrane (CCM).

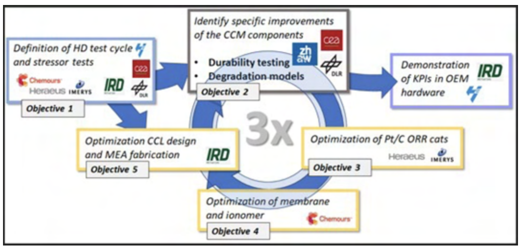

Fig. 1: Workflow methodology of the PEMTASTIC partners

ZHAW is responsible for developing models to describe the performance and degradation of MEAs. A first 1D performance model has been developed which describes the transport processes of mass, charge, heat, and the electrochemical reactions occurring within the MEA. We have parameterised the properties of MEA materials such as the membrane, ionomer, and the gas diffusion layers.

During operation the fuel cell catalyst layers are exposed to harsh conditions (elevated temperature and high electric potential) which lead to catalyst material degradation. This results in a significant decrease of fuel cell performance with load changes. We have implemented [1] a degradation model of catalyst layers with carbon-supported platinum (Pt/C) [2]. We use the model for simulating degradation stimuli, such as temperature and electric potential, in order to describe the loss of available electrochemical surface area (ECSA) of platinum nanoparticles. Coupled effects are considered such as platinum particle oxidation, particle dissolution and redeposition (namely Ostwald ripening), carbon oxidation and corrosion, platinum particle detachment and agglomeration, which lead to particle growth and the consequent loss of ECSA.

Due to computational limitations, it is difficult to apply numerical simulations with spatio-temporal resolution to reproduce the fuel cell dynamics caused by driving cycles with a duration of several hours. One main objective of the work in the PEMTASTIC project is to develop an efficient strategy of model-order-reduction in order to allow for model-based MEA health monitoring and fuel cell durability predictions.

Literature:

[1] COMSOL Multiphysics®, v. 6.2., www.comsol.com., COMSOL AB, Stockholm, Sweden.
[2] A. Kregar et al., *J. Power Sources*, 514, 230542, 2021.

2.3 Mesoscale Modelling of the Catalyst Layer in PEMFCs

Proton exchange membrane fuel cells (PEMFCs) are a promising technology contributing to the decarbonization of the industry and transport sector. The European funded PEMTASTIC project aims to increase the durability of membrane electrode assemblys (MEAs) for PEMFCs by a combined experimental and modelling approach. The Cathode Catalyst Layer (CCL) strongly impacts the overall performance due to the sluggish oxygen reduction reaction and longevity of the fuel cell by critical degradation phenomena, such as carbon corrosion, platinum dissolution, or ionomer degradation. At ICP we are developing mesoscale models with the aim to better understand the coupled processes at the mesoscale and develop improved parameterizations for macrohomogeneous cell models.

Contributors: R. P. Schärer, A. Cucchi, E. Scoletta, J. O. Schumacher
Partners: DLR, IRD, Imerys, CEA, Chemours, Heraeus, Symbio
Funding: European Union's Horizon Europe research and innovation programme
Duration: 2023–2026

The cathode catalyst layer is a thin layer sandwiched between a proton-exchange membrane and the microporous layer with a thickness of about $O(10\,\mu\mathrm{m})$. This layer is composed of carbon particles providing the overall structural support, catalytic platinum nanoparticles, and proton-conducting ionomer. The platinum acts as a catalyst for the sluggish oxygen reduction reaction $4\mathrm{H}^+ + 4\mathrm{e}^- + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O}$. Although written here as a single-step reaction, the oxygen reduction is known to proceed as a multi-step reaction generating multiple intermediate species. Understanding the formation of intermediate species on the platinum and carbon surfaces is of great importance as they can block the available active surface sites for further oxygen reduction. Furthermore, parasitic side-reactions, such as carbon corrosion or platinum dissolution degrades the material, leading to a reduction of the available electrochemical surface area (ECSA).

At the ICP we develop transient and spatially-resolved models that capture the multistep reaction pathways of surface reactions. To account for the dynamic local chemical conditions we investigate the usage of a modified Poisson-Boltzmann model to describe the electrolyte in the vicinity of the reactive surfaces. The chemical surface model will be coupled to mass transport equations for the mobile species driven by diffusion and migration. Additionally, we consider the dynamic evolution of the two-phasic liquid-gas mixture in the pore space, which plays a critical role in determining the local transport resistances.

For this we investigate a coupling of the species mass balance equations with the Lattice Boltzmann Method (LBM) to describe the two-phase dynamics. LBM is an attractive methodology for multi-phase and multi-component transport in porous materials. It is based on a spatial velocity discretization of the Boltzmann equation, which allows for a fully explicit time-stepping scheme that is highly parallelizable.

Finally, an up-scaling strategy will be developed, by consideration of a simplified representation of the catalyst layer structure. The simplified representation will be used to determine effective volume-averaged transport parameters, such as the saturation-dependent permeability, which will be integrated into a macrohomogeneous cell model.

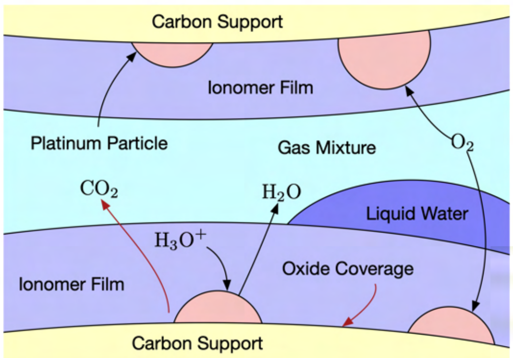

Fig. 1: Simplified model geometry of a mesopore in the CCL.

Literature:

[1] PEMTASTIC project web site: https://pemtastic-project.eu/

2.4 Macroscopic Cell Models for Organic Flow Batteries

Flow batteries (FBs) are a promising technology for the stationary storage of energy derived from renewable energy sources. Organic molecules are an attractive alternative to conventional metal-based electrolytes because they can be synthesised locally. Within the European Horizon 2020 project SONAR, a multiscale modelling and optimisation framework is being developed that will enable high-throughput screening of chemical compounds as well as optimisation of FB components and the overall system design. For this purpose, macroscopic cell models are being developed at the ICP, which allow efficient simulations of the coupled physicochemical transport processes.

Contributors: R. P. Schärer, G. Mourouga, J. Wlodarczyk, J. O. Schumacher
Partners: ICT, SCAI, DTU, LRCS, KIT, UNSW
Funding: European Union's Horizon 2020 research and innovation programme
Duration: 2020–2023

FBs store energy in the form of dissolved electroactive molecules, which are stored in tanks. These molecules are pumped through electrochemical flow cells, where they react electrochemically on the electrode surface during a charging or discharging process. In this process, electrons are exchanged between the electroactive molecules and the electrode in the two half-cells through redox reactions. At the ICP, macroscopic cell models are developed to calculate important performance indicators of an electrochemical flow cell. These include, among others, the cell voltage, the power density, or the efficiency. These models make it possible to determine the influence of the operating conditions, the cell geometry, and material properties on the cell performance.

The RfbScFVM model is a macroscopic description of the spatially and temporally resolved balance equations of the charge, mass, momentum, and energy densities within a cell. Fig. 1 shows a simplified cell geometry described by this model. The modelled cell components include the electrically conducting end plates, the porous electrodes, as well as a separator domain consisting of a semi-permeable membrane. To validate the model predictions, performance measurements were carried out on a laboratory cell with the organic MV/TEMPTMA system from JenaBatteries. Fig. 2 shows the polarisation curve and power density of the FB cell as a function of the electric current density as predicted by the model, together with the experimental measurement results. The results show a promising agreement between the model and the experimental data even at very high current densities. The model implementation in Julia is available as open-source software on our GitHub repository [2].

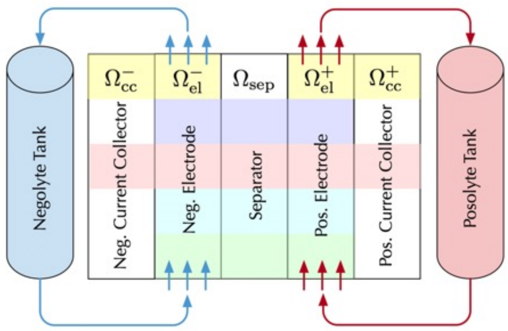

Fig. 1: Simplified model geometry of a flow cell.

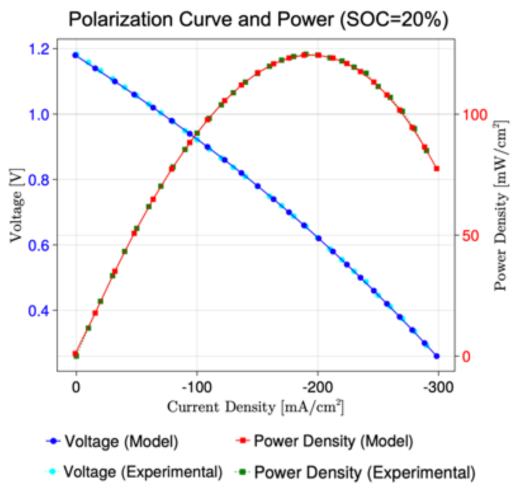

Fig. 2: Cell voltage and power density of a lab sized cell at state of charge 20%.

Literature:
[1] SONAR project web site: https://www.sonar-redox.eu
[2] GitHub repository: https://github.com/Isomorph-Electrochemical-Cells

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 more than 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 are 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 and memristor applications, too. Luminescent quantum dots are important ingredients in novel displays and thus are also subject of our research. Further into the invisible range of electromagnetic waves, terahertz photonics is a growing technological field for non-invasive diagnostics applications.

The ICP carries out R&D in the field of OLED, OPV, perovskite PV and non-linear optical crystals for terahertz photonics technology by employing multi-physics computer models and devising novel measurement systems. In the laboratory of the ICP, we fabricate OLEDs and novel solar cells on a small scale for R&D purposes and have set up a novel terahertz photonics measurement system for diagnostic purposes. We focus on device and material characterization methods by a combination of advanced measurement and simulation technology and have gained experience with machine learning. This chapter gives an overview on ongoing R&D projects carried out in this interdisciplinary research field of the ICP.


Amit Sachan


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S. Parayil Shaji


Simon Zeder


Tabea Krucker


Fuxiang Ji

3.1 Ultra-broadband terahertz optical characteristics of semiconducting materials upon optical excitation

The aim of this project was to measure different semiconductors with terahertz (THz) time-domain spectroscopy (TDS) in a photoexcited and a non-photoexcited state, to calculate the change in parameters such as the sample conductivity, induced by the photoexcitation and to identify the major challenges for reliable parameter extraction upon optical excitation.

Contributors: M. Auer, M. Jazbinsek, U. Puc
Partners:
Funding: Master Thesis, MSE Photonics
Duration: 2023

The THz TDS measurement system at ZHAW is capable to generate and measure THz radiation over a wide frequency range. It was used to measure different photoexcited semiconductors (silicon, germanium, indium phosphide) and compare them with a corresponding reference measurement of the material without photoexcitation. The photoexcitation introduces a thin film with altered parameters on the surface of the sample. Based on these measurements, material parameters such as the induced conductivity of the thin film, were calculated with different approximations. Figure 1 shows the measured transmission THz spectra of a silicon sample at different laser powers used for photoexcitation, from a continuous wave 975 nm laser diode. Since the spectra depend on the transmitted radiation at each THz frequency, they depend on the refractive index and absorption coefficient of the sample, which are related to the complex dielectric function and therefore also to the the electrical properties such as the conductivity of the sample. The amplitude transmission spectra in Fig. 1 show that the photoexcitation significantly increases the sample conductivity, which results in THz absorption. At low photoexcitation power, the conductivity increases mainly in the lower THz frequency range, while at higher powers, a complete ultra-broadband optical conductivity can be achieved. The widely used thin film approximation for parameter extraction is however not valid for such dramatic changes and therefore a more advanced numerical parameter extraction method is required for higher power measurements.

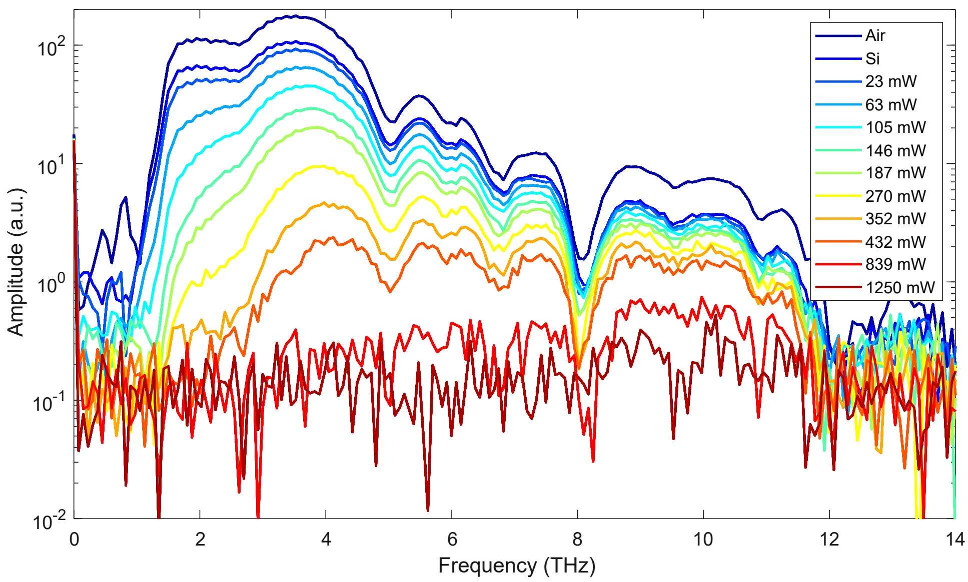


Fig. 1: Different spectra measured on the same silicon sample at different excitation laser powers. The spectrum amplitude decreases with increasing power over the whole measured frequency range. At the highest excitation power, the amplitude was practically zero. Therefore, this silicon in combination with the laser diode could be used as an efficient optical THz modulator with a modulation depth of almost 100 % at the highest optical power.

Literature:

[1] M. Auer, Ultra-broadband terahertz optical characteristics of semiconducting materials upon optical excitation, ZHAW School of Engineering, Master Thesis MSE, 2023.

3.2 Investigating charge transport in organic semiconductors with electrochemical methods and modelling

Today organic semiconductors are used in many technological applications. However, these materials must be thoroughly studied in order to design even better products. Our project aims to improve the characterization of organic semiconductors using electrochemical measurements in combination with computer simulations.

Contributors: Ş. C. Cevher, G. Kissling, B. Ruhstaller, K. P. Pernstich
Partners:
Funding: SNSF
Duration: 2020–2024

Nowadays organic semiconductors are widely used in display and lighting applications (OLED TVs and light panels) and in the fabrication of novel transistors, sensors, data storage elements and solar cells. In order to produce better devices, the understanding of the physical processes and the materials properties of organic semiconductors needs to be improved. In this interdisciplinary project we investigate organic semiconductor materials using electrochemical methods and multi-physics modelling. The project combines the ICP department's computer modelling-expertise with fundamental electrochemistry research.

The aim of the project is the development of a reliable method for the characterization of a range of organic semiconductor properties and materials parameters. The experiments will give us insight into some properties which have so far been very hard or almost impossible to measure. Common numerical models can then be optimized using our experimental results.

We are using electrochemical methods to characterize organic semiconductor materials. The molecules will either be electrochemically studied in solution or as thin films adsorbed onto substrates. The stability and the semiconductor properties of the materials, such as the positions of the valence and conduction bands and of defect states, will be investigated.

The positions of the valence and conduction bands were analysed in detail using electrochemical experiments in solution, as illustrated with exemplary voltammograms in Figure 1, and correlate well with literature data.

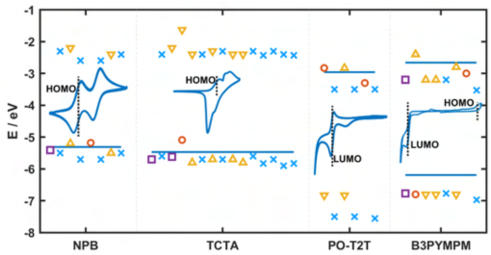


Fig. 1: Exemplary cyclic voltammetry measurements of the various OLED materials and comparison of measured HOMO/LUMO (lines) energies with literature data (markers).

Measurements in solution have the disadvantage that the energy levels differ from those in thin films. Therefore, we have developed a novel electrode structure that enables measuring the energy levels in thin films. Figure 2 shows a cyclic voltammetry measurement of a thin NPB film. The measured HOMO position agrees well with literature values, and we hope to establish this measurement technique as a standard in the organic electronics research community.

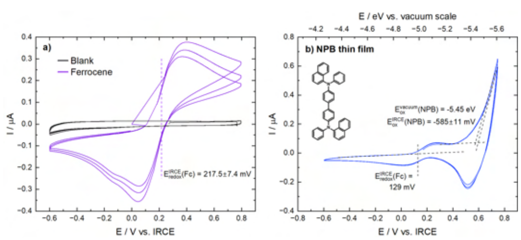


Fig. 2: Voltammograms of blank ITO and ITO/ferrocene (panel a) and of the ITO/PEDOT:PSS/NPB thin film (panel b).

3.3 New tools for characterizing quantum-dot displays

Quantum dots are a promising technology for use in modern displays. With the help of quantum dots, the background illumination can be improved, resulting in more brilliant colors and at the same time simplifying the internal structure. In this project, we are extending existing simulation software and developing new measurement equipment to support research and development in this area.

Contributors: K. P. Pernstich, M. Frioud, A. Bachmann, C. Kirsch, B. Ruhstaller
Partners: Fluxim AG
Funding: Innosuisse
Duration: 2021–2024

In modern displays, the backlight no longer consists of a light source that emits white light, e.g., a white LED, but of a combination of a blue LED or a blue OLED and a quantum dot (QD) film. The QD film absorbs the blue light and emits it in one of the other primary colors, i.e., red or green, resulting in a more brilliant color reproduction. Figure 1 illustrates the improved color gamut and the spectral output when using a blue backlight plus QD film compared to only a white backlight unit.

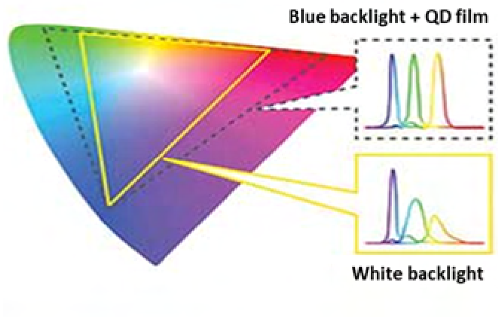


Abb. 1: Color gamut and spectral output of a display using a blue backlight plus QD film or just a white backlight unit. Source: Photonics.com.

To benefit from this new technology, Korean and Swiss partner organizations have joined forces in this international Innosuisse project. The Swiss partner company Fluxim is expanding its products in the areas of measuring instruments and simulation software. The Korean partner company is developing a process to encapsulate the quantum dots and thus make them more durable. The academic partners in Korea are working on the fabrication and optimization of blue OLEDs and on an inkjet printing process to selectively deposit the QD films over individual OLEDs.

At the ICP, we are involved in the further development of an accurate optical QD model to calculate the propagation of light as a function of its polarization direction and in the development of a measuring device for the detailed investigation of QD films and QD-OLEDs.

The development of the optical model is essentially finished, and it is now implemented in the commercial software packages Setfos and LAOSS. Once implemented, we can proceed with final evaluation of the model.

To characterize the down-conversion films, it is best to perform angular dependent measurement. In this work we discovered that the measurement geometry has a large influence on the results. Figure 2 shows the measurement setups to analyze the influence of the illumination geometry to determine a key-characteristics called light conversion efficiency.

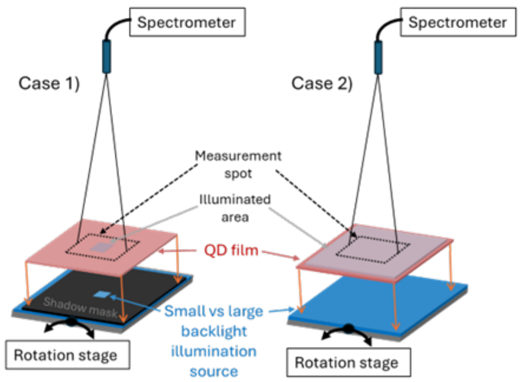


Fig. 2: Measurement setups to analyze the influence of the illumination geometry on the light conversion efficiency.

The light conversion efficiency using the two measurement setups and different emission profiles of the light source varies by up to 20%. In [1] we describe the mechanism behind these changes and suggest a method to make precise measurements of the light conversion efficiency.

Literature:

[1] M. Regnat, et. al., International Conference of Display Technology, Hefei, China, 2024

3.4 Multispectral image analysis and machine learning for PV quality assurance

The reproducible production of homogeneous and defect-free layers is crucial for the up-scaling of perovskite solar cells. In order to achieve this goal, perovskite solar cells are being investigated in this project using a new type of measurement setup and are optimised and improved with the help of a digital twin.

Contributors: M. Battaglia, E. Comi, R. Wirth, C. Kirsch, E. Knapp, B. Ruhstaller
Partners: Fluxim AG, Solaronix AG
Funding: Innosuisse
Duration: 2022–2025

The measurement setup developed in this project uses various imaging methods such as electroluminescence (EL), photoluminescence (PL) and dark lock-in thermography (DLIT) to analyze and characterize perovskite solar cells. In addition, classic current-voltage characteristics and impedance spectroscopy data can also be measured.
The typical workflow is visualized in Fig. 1: The process begins with a perovskite solar cell, which in our case was manufactured by our partner Solaronix. It is measured in our novel setup, which is developed as a compact device for use in a glovebox. The resulting images and curves are used to train a Physics-Informed Neural Network (PINN), which determines the unknown model and material parameters. Using the values found, we can create a digital twin of the original cell.
Fig. 1 contains a CAD drawing of the planned final measurement setup. The SMU, the LED panels for illuminating the solar cell and the cameras for the imaging processes are installed in the blue blackout shell. This measurement setup was planned in collaboration with the Institute of Product Development and Production Technologies (IPP) and is scheduled to be produced in small series for further tests in 2024.
The structure of a PINN is also shown in Fig. 1. A PINN extends the loss function of a regular neural network with additional terms that are based on the physical laws of the solar cell. This means that the physical model is integrated into the neural network and less measurement data is required for training to determine the unknown parameters.

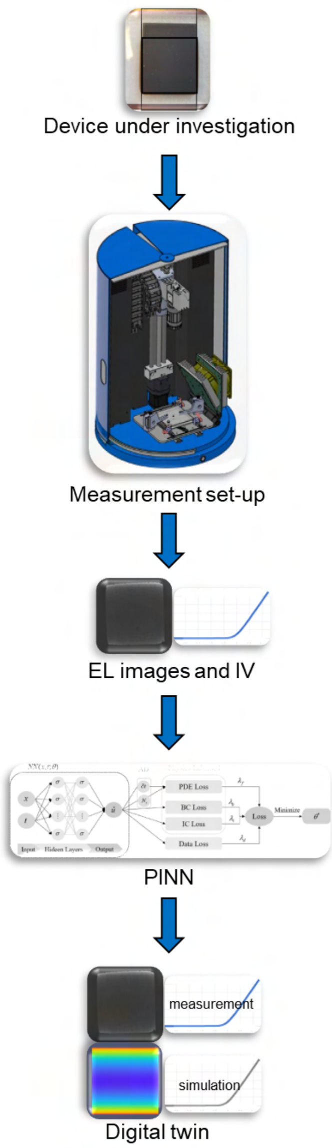


Fig. 1: Workflow for the generation of the digital twin

3.5 Characterizing and exploiting mobile ions in perovskite solar cells and memristors

We are working on the device physics of various emerging semiconductor devices. In this project our focus is on better understanding of the mixed ionicelectronic conductivity of perovskite semiconductors in different device architectures including perovskite solar cells and memristors. We are currently investigating characterization techniques that aim to extract essential ionic parameters from perovskite solar cells, with the goal of gaining a deeper understanding of the effects of mobile ions, developing effective mitigation strategies, and identifying any exploitable opportunities arising from these unique properties. Furthermore, by fabrication and characterization of different memristors devices we are trying to focus on better understanding filaments formation and rupture as the main suggested switching mechanism in perovskite memristors to improve the memristor's properties.

Contributors: M.A. Torre, M. Mohammadi, F. Ebadi, N. Kabir, W. Tress
Partners:
Funding: ERC
Duration: 2021–2025

Solar cells based on metal-halide perovskite absorbers became the rising star in photovoltaics research. Their outstanding opto-electronic properties enabled a power conversion efficiency higher than 25%. While developing these solar cells, a hysteresis in the current-voltage curve was observed. Further studies scrutinized the hysteresis and found a slow transient response and a strong dependence on voltage sweep rate. The findings of these studies provide strong evidence for ion migration being the reason for the hysteresis. These observations and the importance of charge transport layers show the complexity of the interplay between the collection and recombination of photogenerated charges and the movement of ions.

In the context of solar cells, the slow response of mobile ionic defects can lead to significant performance fluctuations in both the short and long term. The internal energy level landscape of a perovskite solar cell is affected by the distribution of mobile ions, which in turn can either enhance or impair its performance. These changes can be reversible or irreversible, depending on whether mobile ions just accumulate in the bulk material, are involved in unwanted chemical reactions, or penetrate through different layers of the solar cell stack. To ensure the stability and reliability of solar cells, it is crucial to comprehend and learn to tune or control the dynamics of mobile ions under different operating conditions.

Beyond solar cells there are other electronic devices that can be fabricated with lead-halide perovskites to exploit the effect of mobile ions. Devices where perovskite is sandwiched between asymmetric contacts can be turned on and off by moderate (<1 V) forward and reverse voltages, respectively, making them interesting candidates for resistive switches (Fig. 1). The state can be probed by smaller read voltages, which give a rather ohmic response with low (on) or high (off) resistance.

Given the hysteresis, also memristors can be fabricated. A memristor is a 2-terminal circuit element characterized by a constitutive relation between two variables q (charge) and φ (magnetic flux) representing the time integral of the element's current i(t), and voltage v(t) that displays a pinched hysteresis loop in its i-v characteristics. A potential future application for memristors is neuromorphic computing.

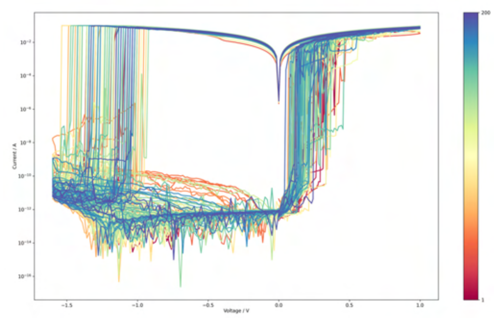


Fig. 1: Current-voltage curve of a resistive switch fabricated in our labs.

3.6 Accelerated aging and modeling of perovskite solar cells

In this SNSF funded research project in collaboration with Saule Research Institute, Poland, we aim to understand, model and predict the degradation of perovskite solar cells quickly and reliably by employing accelerated aging with non-destructive in-situ characterization. We have developed an in house accelerated aging setup which can vary intensity and temperature, and keep it in maximum power point as well in other key points of solar cells.

Contributors: Sharun Parayil Shaji, Kazem Meraji, Wolfgang Tress
Partners: Saule Research Institute, Wroclaw, Poland
Funding: SNSF
Duration: 2023–2027

Perovskite solar cells are one of the fastest growing photovoltaic technology which has grown in power conversion efficiencies than any other kind of solar cells. But these have been in lab for almost two decades and have reached efficiencies over 26%. The major reason for keeping this technology away from commercialization is the lack of stability. Accelerated aging gives the life-time of the devices under operating conditions quickly and accurately. [1] This project aims to address this issue by utilizing accelerated stress factors to understand the degradation pathways using in situ characterization under real-world conditions with the help of big data and machine learning. [2] We have developed a setup for accelerated aging of solar cells, which allows us to vary the light intensity from 0.1 to 10 sun intensity and set the temperature between 10 ℃ to 100 ℃. Additionally, we have designed the setup to be modular, enabling placement in the glove box for exposure to different controlled environments. We are also developing a machine learning algorithm which can analyse the data generated during the accelerated aging process, which would simplify and even give insights into the changes in charge transport in a quick manner. In the long run, the outcomes from this project should facilitate a faster development of stable perovskite-based PV, helping this technology to penetrate more easily the energy market. This would help to accelerate the decarbonization of the economy, thus reducing the disastrous impact of global warming on our society.

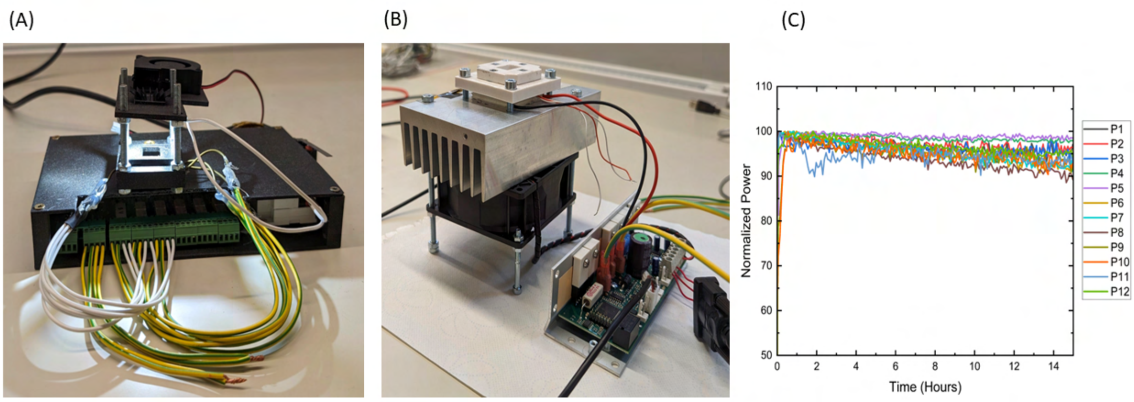


Fig. 1: (A) Aging setup with Maximum power point tracker running under one sun illumination. (B) The Temperature controllable stage which can be paired to the maximum power point tracker and illumination unit. (C) Stability data of some perovskite cells which were fabricated in our lab.

Literature:

[1] X. Zhao, T. Liu, Q. C. Burlingame, T. Liu, R. Holley III, G. Cheng, , N. Yao, F. Gao, Y. L. Loo, Accelerated aging of all-inorganic, interface-stabilized perovskite solar cells. Science, 377 (6603), 307–310, 2022.

[2] O. Zbinden, E. Knapp, W. Tress, Identifying Performance Limiting Parameters in Perovskite Solar Cells Using Machine Learning, Solar RRL, 2024.

3.7 Stable & non-toxic lead-free perovskite for light emission

Lead halide perovskites have emerged as a new generation of light-emission materials. However, the toxicity of lead and intrinsic instability issues significantly hinder their further devel-opment and commercialization. This motivates us to develop novel stable and non-toxic lead-free perovskites for light emission.

Contributors: W. Tress, F. Ji
Partners:
Funding: SNSF (Swiss Postdoctoral Fellowships)
Duration: 2023–2025

The energy crisis is a severe challenge facing the world today, in which lighting is one of the largest sources of energy consumption and accounts for one fifth of global electricity consumption. A promising way to save energy is to develop a new generation of high-efficiency and low-cost lighting technology, such as light-emitting diodes (LEDs). In recent years, organic-inorganic hybrid lead halide perovskite LEDs have drawn vigorous scientific interest due to their high efficiency above 20% and simple manufacturing processes. However, the toxicity of lead and intrinsic instability issues significantly hinder their further development and commercialization. Therefore, it is highly desirable to develop novel non-toxic, and stable light-emitting materials to fundamentally solve these issues.

This project aims to develop high-stability, non-toxic and low-cost LEDs with lead-free halide perovskites. Currently, the main challenge of lead-free perovskite LEDs is the absence of satisfactory materials and a lack of deep understanding of the device structure and carrier injection process of lead-free materials. Based on this thinking, we will first design and synthesize some novel lead-free perovskite materials with high photoluminescence quantum yield. One of the most attractive lead-free candidates is double perovskites (A2B+B3+X6), where divalent Pb2+ is replaced by monovalent B+ and trivalent B3+ metal ions, in terms of non-toxic, stable, and a wide range of possible combinations (Figure 1a). [1] More interestingly, lead-free halide double perovskites usually exhibit broadband and large Stokes shift emission derived from self-trapped excitons (STEs), [2] which is very attractive for single-emissive-layer white light-emitting diodes (WLED) (Figure 1b). Meanwhile, these STEs-related emissions could be further modified by introducing a suitable large A-site cation to reduce the three-dimensional crystal structure to a low-dimensional structure. In the end, based on the specific properties of the designed material, we will try to screen out an appropriate device structure to fabricate electroluminescence or photoluminescence LED devices. We aim to achieve high-stability and low-cost lead-free perovskite LEDs with an expected external quantum efficiency exceeding 5% (for electroluminescence devices), which is attractive for future commercialization. However, considering the huge challenge of fabricating highly efficient lead-free perovskite electroluminescent devices, down-conversion LEDs that utilize lead-free perovskites as phosphors will also be considered.

This project involves fundamental research that will provide a new understanding of the material design, key challenges, and light emission mechanisms for lead-free perovskites. These results will be beneficial to further explore the full potential of lead-free halide perovskite for light emission.

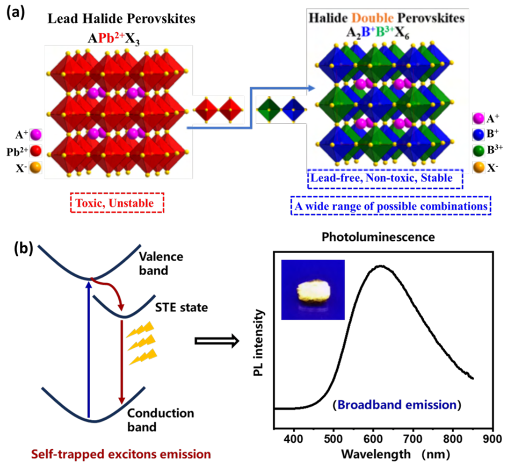


Fig. 1: (a) Schematic view of B+/B3+ cation substitution from lead halide perovskites (APbX3) to double perovskites (A2B+B3+X6). (b) Schematic of the energy level structure and mechanism of STE emission. The PL spectra and optical image are one example of STE emission in lead-free perovskite.

Literature:

[1] Sol. RRL 2023,7, 2201112.
[2] J. Phys. Chem. Lett., 10, 1999–2007, 2019.

3.8 Perovskite Solar Cells & Machine Learning

Perovskite Solar Cells are a type of solar cells with promising properties that make them a good candidate to help to reach the goal of a sustainable society. We use Machine Learning techniques to help to improve the efficiency of Perovskite Solar Cells and understand processes of degradation.

Contributors: O. Zbinden, E. Knapp, W. Tress
Partners:
Funding: DIZH, ERC Starting Grant
Duration: 2021–2025

The efficiency of perovskite solar cells (PSCs) has almost doubled to more than 26% in the last decade [1]. This development, together with a plethora of favorable properties, as well as easy and cheap production, makes them a very interesting candidate for future applications. However, the theoretically possible efficiency limit has not been reached yet, and stability issues must be overcome as well. Besides this, the efficiency of PSC devices highly depends on the experience of individual researchers/manufacturers. There are many reported applications of machine learning (ML) in the field of PSCs. We extend the application of ML in this field with a novel approach [2]. It seems to be common that increasing performance is often based on trial and error, which is not only time-consuming, but also resource intensive. By detecting limiting parameters in a PSC, our algorithm can be understood as an assistant in the lab to guide the manufacturer to changes in the recipe or procedure towards devices with higher efficiencies. Furthermore, it can be used to test if changes, for example passivation layers, lead to the desired result, or to see how degradation has changed the device.Because it is not possible to make enough to have sufficient data for the ML modelsto train the models, we simulated devices with Setfos [3]. For each device, different parameters are varied, one at a time, leading to a large data set representing many PSCs. The goal of these simulations is not to reach theoretically perfect, but realistic results that are close to what is commonly reached and reported. With the simulation results in hand, we want to find out if it is possible to identify the one parameter that changed with respect to the initial "standard" device. As an input we take the generated results, which are different points on the J-V curve, fill factor (ff), and the power conversion efficiency (pce). The targets we want to classify for are the changed parameters. It is important to mention that we do not want to make predictions about performance or stability, e.g. forecast the device's lifetime, but say which parameter contributed most to a detected loss in performance, or what limits a freshly made cell most, compared to a similar device without such a drawback. We tested different algorithms and

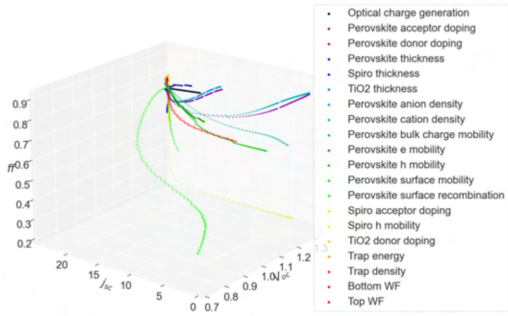


Fig. 1: 3D $\mathrm{V_{oc}} - \mathrm{J_{sc}} - \mathrm{ff}$ plot of the different parameters

compared their accuracies, with the result that random forests are suited most for our problem, with a classification accuracy on the test set of (86.59 ± 0.02) %. This high accuracy can be explained by looking in the 3D $\mathrm{V_{oc}} - \mathrm{J_{sc}} - \mathrm{ff}$ space, where $\mathrm{V_{oc}}$ is the voltage at open circuit, J_{sc} the short circuit current-density, and ff the fill factor of the J-V curve. Different changes of parameters lead to paths in this diagram that are often very characteristic. The curves that are harder to distinguish are caused by parameters that have a similar influence on the device performance. Therefore, some restrictions that are clearly specified have to be considered when the model is used. We applied our model to data in publications and can get satisfying results that can be physically explained.

Literature:

[1] NREL. Best research-cell efficiency chart plotted by national renewable energy laboratory, USA, 2023.

[2] Zbinden, O., Knapp, E. and Tress, W. (2024), Identifying Performance Limiting Parameters in Perovskite Solar Cells Using Machine Learning. Sol. RRL, 8: 2300999.

[3] Fluxim AG. Semiconductor simulator (setfos) https://www.fluxim.com/

4 Sensor and Measuring Systems

Our team of talented ZHAW engineers and scientists has been applying for more than ten years well established and emerging measurement methods to relevant medical and biological problems. We collaborate with startups, international companies as well as leading academic partners and bring our engineering expertise to projects requiring state-of-the-art technical development.

We have been dedicated to creating impact by cultivating an entrepreneurial mindset and thinking beyond academic publishing, focusing on technology transfer from the laboratory to industry. Our funding sources include the Swiss Innovation Agency (Innosuisse), the EU (Eurostars, Horizon 2020), the Swiss National Science Foundation (SNSF) and various private foundations as well as direct funding from industry.

Our core competence is the development of new sensors and measurement methods in biomedical engineering. In particular, we are experienced in skin science and technology: artificial skin models, computer simulations, development of new sensors, etc We benefit from the state-of-the-art infrastructure of the Optoelectronic Research Laboratory (OLAB) that allows the development of demanding prototypes.


C. Grossmann Ayber


Daniel Fehr


Dardan Bajrami


Davide Paparo


Fabrizio Spano


Ian Häusler


Jan Zwicky


Mathias Bonmarin

4.1 Artificial Skin Models

Artificial skin models for various applications mimicking the functionalities and the properties of the human skin are designed and developed in our laboratories.

Contributors: F. Spano, D. Fehr & M. Bonmarin
Partners: Various partners
Funding: Various fundings and student projects
Duration: 2019–2024

Artificial skin models have gained attention in the last years. They are mainly design to mimic the human skin and more recently as an alternative to animal testing. In our lab, we developed various skin models mimicking the functionalities and/or the properties of the human skin. For example, models mimicking the mechanical, thermal and optical properties of the human skin have been designed and fabricated. For mimicking the properties of the human skin, we designed specific combination of materials in stacking layers obtaining the same structure and the same properties of the human skin. And theses properties are function of the skin location to mimic (hand, palm, forearm, forehead, leg . . .). As an example, a specific skin model made of various layers and integrating various sensors measuring the temperature changes in real time has been developed. In parallel, the use of thermochromic powders can be implemented to fabricate a very cost-effective and simple skin model illustrating variations of temperature by a simple change in color without employing any electronics. In addition to the skin models related to heat mechanics, computational models of human skin have been developed which allow to study how different electrodes measure the moisture level of the outermost layer of skin, designed in particular to study the stratum corneum. The model shows how the stratum corneum changes its thickness and electrical properties depending on the skin hydration. The work also compares different types of electrodes and how they respond to these changes.

In parallel to the mimicking of the human skin properties, we developed even models mimicking certain functionalities such as the conductivity, the behaviour of the human skin suggested to radio frequency and the tactile sensitivity of the human skin as illustrated in Fig.1.

In addition, multi-layered skin models simulating the sweating functionality of the human skin have been designed and fabricated based on the use of solid liquid composite materials. To comply to the particular properties of the human skin, these materials, sometimes blends of hydrogels and elastomers are used. More recently, 3D printing techniques have been implemented. The 3D printing tecniques bring new potentialities and allow development of more complex skin models. As an example, we started recently developing 3D biohybrid skin model via 3D bio printing to be as close as possible to real human skin. Such technique will allow implementing cells or hair follicles or sweat glands directly into the hybrid skin models.

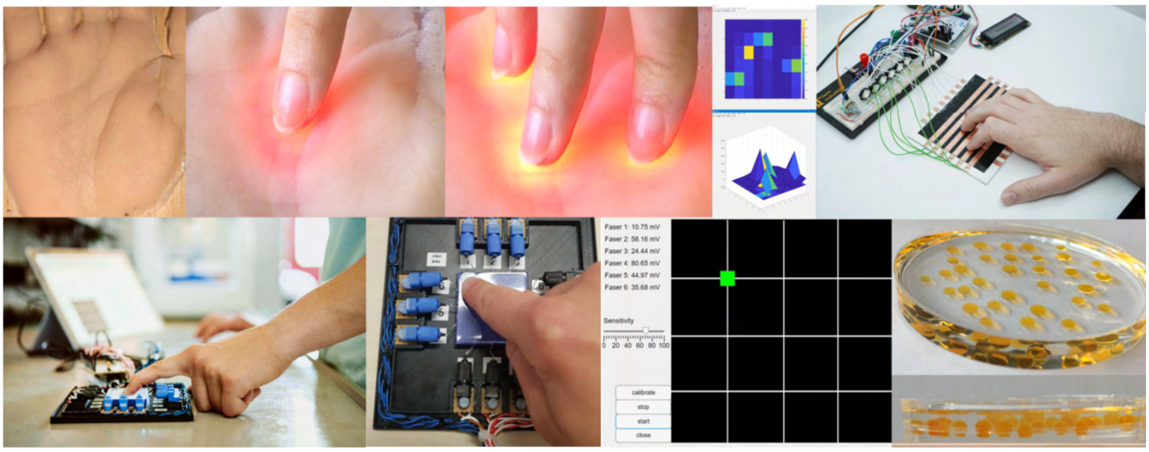


Fig. 1: Illustrations of various artificial skin models mimicking properties and functions of the human skin.

4.2 Thermal analysis of new transdermal devices for power transfer to ventricular assist devices

Contributors: C. Grossmann, R. Hagen, F. Spano, D. Fehr, M. Bonmarin
Partners: ETH Zürich
Funding: InnoSuisse
Duration: 2022–2024

We designed and simulated in COMSOL a ventricular assist device driveline that reduces infections by embedding thin copper wires with a polyurethane coating into a polymer-based material.

The gold-standard approach of Ventricular Assist Devices (VADs) involves using insulated transcutaneous metallic drivelines to deliver power from the external battery through the abdominal wall to the pump in the upper abdomen (Fig. 1.A). However, VAD drivelines can negatively affect wound healing, leading to driveline infections (DLI) in about 1 out of 5 patients within the first year of implantation [1], due to biofilm formation in the skin's upper layers.

To promote healing of small wounds by minimizing wire impact on the skin interface and reduce DLI, we propose a novel approach involving embedding a set of 0.2 mm diameter copper wires with polyurethane (PU) coating into a polymer-based material for VAD drivelines. We investigated the electrothermal implications of conductive wires on the human body through 3D COMSOL skin model simulations (Fig. 1.B) representing the epidermis, dermis, fat, and muscle [2]. Additionally, a PDMS layer was included in the model to represent the silicon-based material of the conductive skin. Various PU insulating coating thicknesses were tested on a 0.2 mm diameter copper wire. Increasing the insulation layer did not yield a significant improvement in the performance of the skin model. The observed temperature difference across the model can be primarily attributed to the temperature gradient within the skin layer, rather than to variations in the electric current.

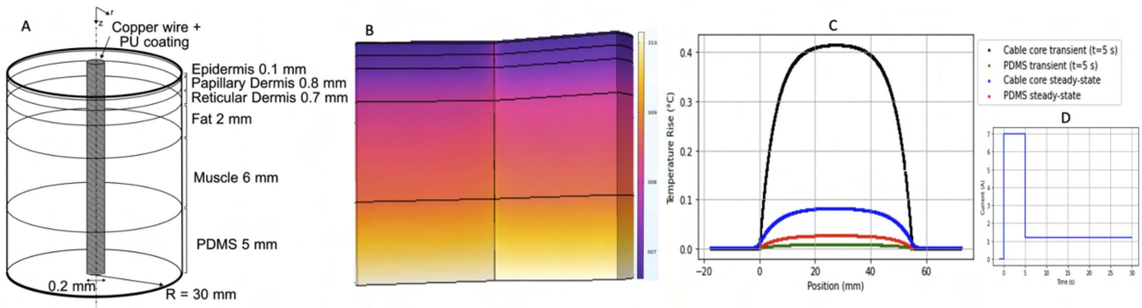


Fig. 1: A) Graphical representation of the 2D axisymmetric skin multilayered model [2]. B) Thermal distribution in COMSOL Multiphysics. Units: degrees Kelvin. C) Temperature rise in the core of the copper wire and in the PDMS due to inrush current and in the steady-state. D) Electrical conditions of the model.

Literature:

[1] A. P. Kourouklis, J. Kaemmel, X. Wu, Systems of conductive skin for power transfer in clinical applications, *Eur Biophys J 51*, 171–184, 2022.

[2] M. Bonmarin, F. A. Le Gal, Lock-in thermal imaging for the early-stage detection of cutaneous melanoma: A feasibility study, *Comput. Biol. Med.*, 47, 36–43, 2014.

4.3 Development of an efficient amplifier for thermotherapy applications on the skin

Contributors: I. Häusler, D. Paparo
Partners:
Funding: Gebert Ruf
Duration: 2023

The in-house developed thermotherapy device for treating cutaneous leishmaniasis initially featured a functional but inefficient power amplifier, posing issues for its battery-operated design necessary for field use. To enhance battery life, the output stage was redesigned. The new Class D topology circuit now shows an efficiency improvement of approximately 100%.

Cutaneous leishmaniasis, a skin disease caused by parasites, leads to lesions treatable with heat. The treatment involves applying electromagnetic energy to locally heat the skin to 50 ℃ and maintain it for 30 seconds, requiring devices capable of delivering up to 6W of power to heat quickly and maintain 1W for temperature stability. Designing an amplifier to manage this, accommodating the variability in skin characteristics, poses significant challenges.

Our team's earlier device for this treatment used an ADA4870 IC-based amplifier from Analog Devices, with an overall efficiency below 0.35. This low efficiency was problematic for a battery-operated device needing to maximize applications per charge, prompting a redesign of the final stage, shown in Figure 1.

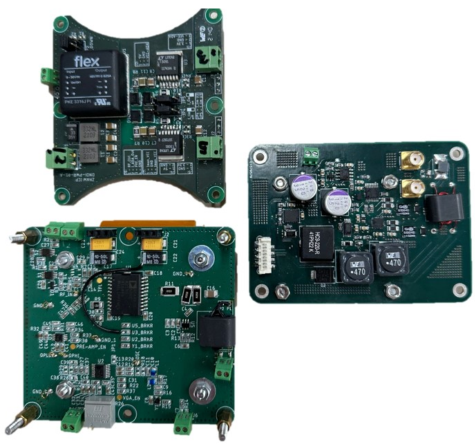


Fig. 1: Image of the circuit boards of the amplifiers: the old ones on the left and the new one on the right.

The new amplifier, using a current mode Class D topology with GaN transistors (GS61004B from Infineon), aims to reduce switching losses. The circuit was simulated in LtSpice, with the reflection of component parasitics. The results are detailed in Image 2. Notably, the simulation did not account for the DC-DC converter's efficiency, explaining the slightly higher simulated efficiency. Component values were optimized for maximum efficiency across the measured impedance range.[1]

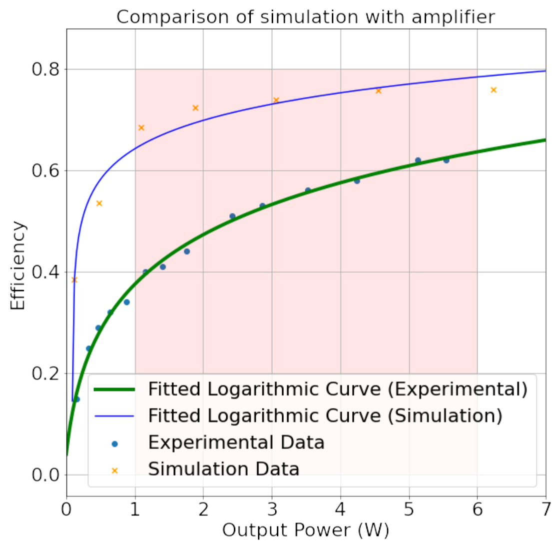


Fig. 2: Comparison between simulation and measurements on the implemented amplifier shows lower measured efficiency than simulated. Key reasons for this discrepancy include unaccounted losses from the DC-DC converter and the use of a suboptimal transformer core that increases losses.

Literature:
[1] I. C. Rodrigues Häusler, D. Paparo, D. Fehr, R. Hagen, M. S. Velez Mestre, M. Bonmarin, Assessment of Skin Impedance in Radiofrequency Therapy: A Study Utilizing Unique Electrode Form for Cutaneous Leishmaniasis Treatment, *2023 IEEE International Humanitarian Technology Conference*, 1–5, Nov 2023.

4.4 Modular and Portable Time-Resolved Fluorescence Measurement System

Contributors: R. Hagen, F. Spano, D. Fehr, M. Bonmarin
Partners:
Funding: Student Project
Duration: 2022–2024

We designed a portable, low-cost demonstration device that can perform time-resolved fluorescence measurements in the frequency domain. The device combines the flexibility and advanced measurement modes of a desktop sensor system with the small form factor of a portable point-of-care device.

The developed measuring device consists of two components, the excitation module and the detection module. Both modules are controlled and powered by a computer via a standard USB Type C port. The system configuration is shown in Fig. 1.

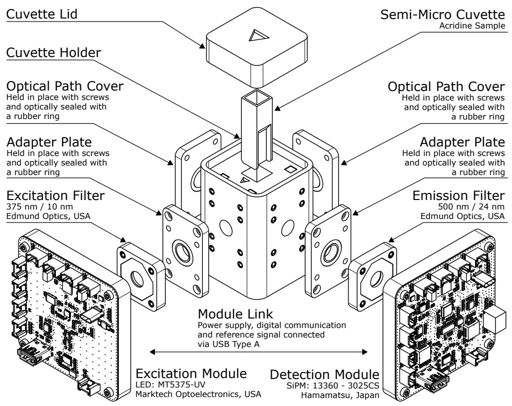


Fig. 1. Possible device architecture that can be used to characterize liquid samples in a semimicrocuvette.

The pulse generator of the excitation module is capable of generating pulses with a FWHM of 100 ps up to 5 ns with a resolution of 1 ps. The repetition rate (0-25 MHz) of the pulses is controlled by local signal generator.

The SiPM detector on the detection module combines a series of SPAD microcells. The system supports SiPMs with a bias voltage of 0-80 V. The detection module uses the heterodyning technique, which multiplies the HF input signals f_{Ref} and f_{Smp} with a signal f_{LO} from the local signal generator, resulting in synchronized output signals with frequencies $f_{\text{Ref}} \pm f_{\text{LO}}$ and $f_{\text{Smp}} \pm f_{\text{LO}}$. Low-pass filtering of the output signals suppresses the HF sum and allows only the ULF difference to pass. The phase delay between the two down-converted signals is proportional to the apparent lifetime of the sample.

The apparent lifetime measured of acridine (pH marker) with the developed device shows a decrease as a function of pH, see Fig. 2. At a pH of 6, the emission is dominated by AcH^+, resulting in an apparent lifetime of almost 31 ns. As the pH value increases, the ratio between [Ac^-] and [AcH^+] changes, decreasing the apparent lifetime of the sample. In the measured range of pH 6-8, the change in lifetime corresponds to a 2^{nd} polynomial and allows the calculation of pH based on the measured apparent lifetime. Based on the measured standard deviation of each point, one could predict an accuracy of pH $\pm$ 0.032 (95 % probability interval of $\pm\ 2\sigma$).

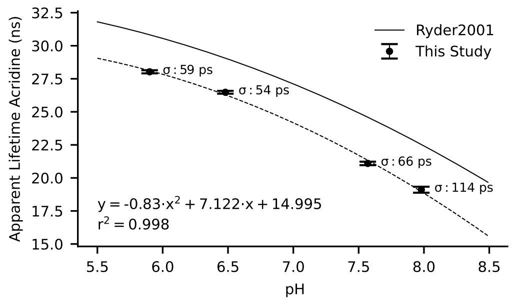


Fig. 2. Measurements of apparent lifetime of at different pH. The samples consist of 1 ml of 0.1 M aqueous K-phosphate buffer at different pH values with an acridine concentration of 0.001 M.

Literature:

[1] R. Hagen, F. Spano, M. Bonmarin, D. Fehr, Modular and Portable Time-Resolved Fluorescence Measurement System, Precision Photonic Systems ’23, Buchs SG, November 14, 2023.

4.5 Variations of skin thermal diffusivity on different skin regions

In this study, the relationship between thermal diffusivity of the skin and the melanin content and reddening of the skin (erythema) was investigated. The thermal diffusivity, melanin content, and erythema indices of 102 patients were measured. Thermal diffusivity was measured using a device developed in-house for transient temperature measurement. The measured data were analysed for correlation with thermal diffusivity.

Contributors: D. Bajrami, M. Bonmarin, F. Spano, D. Fehr, C. Kirsch, A. Zubiaga, P. Schulthess
Partners: Empa , University Hospital Basel
Funding: Leo Foundation, Innosuisse
Duration:

The thermal properties of the skin play an important role in clinical dermatology, personalised skin treatments or the efficacy of skin care products. In order to better understand the thermal processes and to analyse the influence of individual skin properties such as skin colour or erythema on the thermal properties, we measured the above-mentioned properties in this study and analysed them for correlations. An in-house device was developed to measure the thermal diffusivity of the skin. The device is composed of a handpiece and a base station connected to a computer (Fig. 1). The device uses a transient temperature measurement with a thermocouple embedded in a cooled metal cylinder. Calibration using a material (PDMS) with known diffusivity was performed to validate the functionality of the device. An algorithm considering the 1D bio-heat conduction equation was used to extract the thermal diffusivity. The model took into account the lateral heat flow near the skin surface and improved the accuracy of parameter extraction. Skin pigmentation and erythema (redness of the skin) were measured with a colorimeter. Melanin content and erythema index were determined based on diffuse reflectance measurements. A total of 102 participants were measured and statistical correlations between thermal diffusivity and pigmentation/erythema were analysed.

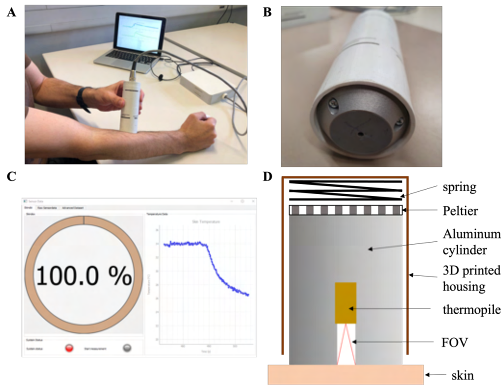


Fig. 1: A) Image of the device. B) Zoomed image of the hand-held device to illustrate the measuring opening of the device. C) User interface of the software. D) Diagram of the thermopile for measuring the transient temperature, which is installed in the hollow Peltier metal cylinder of the hand-held device.

Thermal diffusivity values were consistent with previous studies and showed variations across different body sites (Fig 2). Despite expectations, no significant correlation was found between thermal diffusivity and melanin content or erythema.

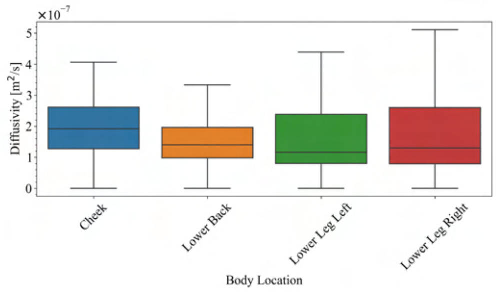


Fig. 2: Thermal diffusivity measured at different skin locations

4.6 Highly-Sensitive Fluorometer for Point-of-Care Testing

Contributors: J. Zwicky, C. Grossmann, D. Fehr, M. Bonmarin
Partners: University of Montréal
Funding: Student project
Duration: 2023–2024

We design and build a highly sensitive and compact point-of-care fluoromter to evaluate novel assays developed by our partners.

In this project, we design, build, and experimentally validate a portable yet sensitive fluorometer measuring fluorescence of a sample at a predetermined, but easily adaptable wavelength (excitation & emission). Goal is to develop a point-of-care (POC) device capable of running specific assays directly at the patients bedside. Specifically, the fluorometer is optimized to evaluate a novel assay for lactate quantification [1].

By the use of a the current integrating IVC102 (Transimpedance aplifier with capacitive feedback), the sensitivity of the module can be adjusted by software to match the sample concentrations. Using off the shelf filter cubes, the wavebands can be adjusted with no changes to the sensor design. The excitation LED can be changed and the driving current can be adjusted by the use of two resistors.

The optical path is optimised to match the needs of the sensor and reduce the complexity as well as the price. With a second diode sensor, the excitation intensity is measured to compute a ratiometric sensor value. This reduces instability issues of the excitation source as well as drifts.

The sensor is incorporated in a POC device, featuring a user interface. This allows the user to make measurements by the press of a button and gives also the possibility's to manually adjust the integration time and further measurement settings.

The project is an ongoing collaboration with the University of Montréal.

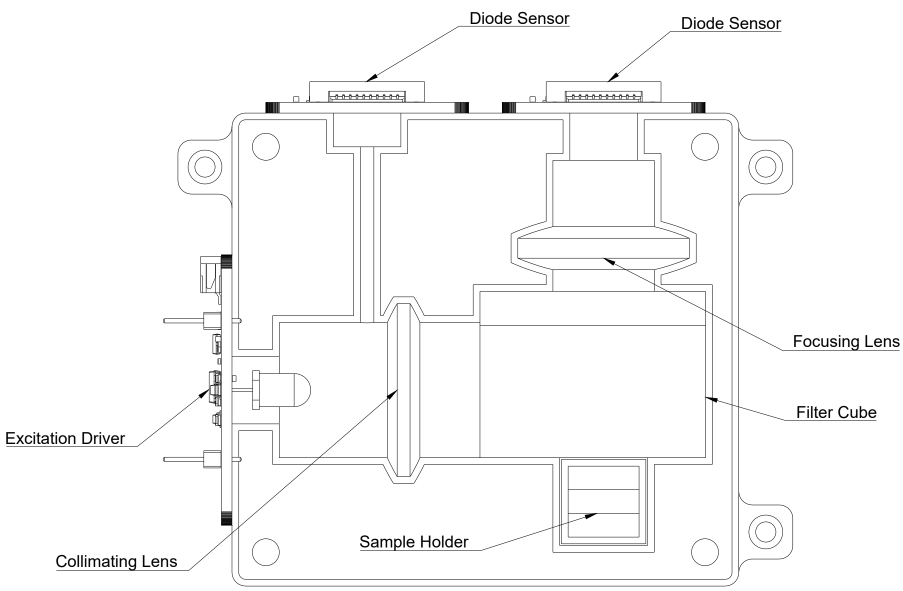


Fig. 1. Sensor module, showing the optical path of the sensor.

Literature:
[1] N. Guirguis, A. I. Machuca-Parra, and S. Matoori, Portable Near-Infrared Fluorometer for a Liposomal Blood Lactate Assay, *ACS pharmacology & translational science*, 6 (6), 907–912, 2023.

5 Building Simulation

Buildings affect our well-being, productivity, and various social interactions. Much of our energy is used in buildings, and through utilization of solar energy and environmental heat, modern buildings have become energy producers themselves. Large volumes of information, goods and people move around buildings. Data is continuously collected using sensors and measurement technology; simulations and control technology are used to ensure that all these processes can be optimally supported and controlled in an increasingly digital world.

At ICP, we support the digitalization in the building sector with computer simulations for physical-technical processes. Our contributions extend from the early through to the detailed planning phase all the way to the operation of the buildings. We have access to a large number of simulation tools and design our own algorithms where necessary. We use measurement technology to validate the simulations, determine material parameters and generate output data for predictive simulations.

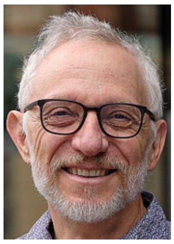
In 2022, the Swiss Building Simulation Association was established, which has transferred its management to the ICP (www.gebaeudesimulation.ch). The association brings together leading planning offices from the fields of construction and energy planning to jointly promote physical simulations in the construction industry. It currently has around 50 members.

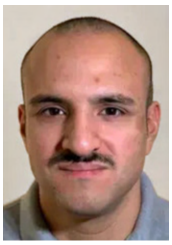

Franziska Schranz


Matthias Schmid


Andreas Witzig


D. Bernhardsgrütter


Markus Roos


Camilo Tello Fachin


Zoi Bratsos


David Kemf

5.1 Dimensioning of Gas Burners for a Fire Test Furnace

As part of the project *CPC construction method for load-bearing structures in building construction*, simulations were created to support the construction of a test facility for the strength testing of CPC panels in the event of fire.

Contributors: C. Tello, A. Witzig
Partners: ZHAW Institute Construction Technologies and Processes, R. Lutz
Funding: Innosuisse, CPC AG
Duration: 2023

The building materials developed in this project are based on the patented carbon prestressed concrete (CPC) technology [1]. It allows concrete to be used as a building material and still be lightweight. Because less concrete is required while maintaining the same strength, the technology is suitable for reducing costs and CO2 emissions in building construction. It must be experimentally proven that CPC panels also have sufficient strength in the event of a fire. In the subproject, a corresponding furnace was simulated in which the components can be tested in accordance with the standard [2].

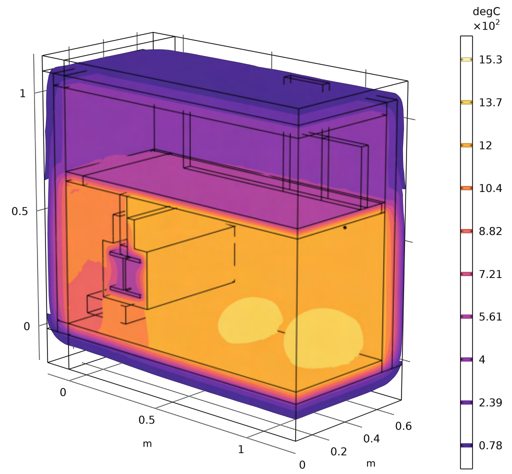


Fig. 1: A quarter of the vertical test furnace with symmetric boundary conditions for all simulated physical phenomena. The boundary separating the upper and lower combustion chambers is the component being tested, with associated temperature profiles shown in Fig. 2. The transparent structure depicted vertically in the upper cold combustion chamber transfers the load to the test object. In the lower combustion chamber, the gas burners are visible as well as a small part of the source term beneath the steel beam, which simulates the outlet of the chamber.

The simulation is used to determine the required output of the gas burners. The challenge of the modelling lies in the fact that many different effects are coupled with each other. The first step was to estimate how much of the gas burner output is emitted radiatively and how much convectively. As a result, the transient temperature development in the first 180 minutes was calculated (Fig. 2).

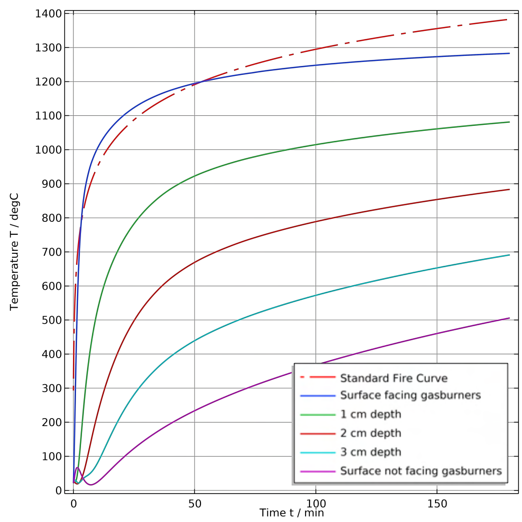


Fig. 2: Temperature profiles of the component being tested. The surface temperature of the component corresponds with satisfactory accuracy to the temperature profile prescribed by the regulatory bodies.

The primary benefit of this test is that the combustion chamber is not oversized. In addition, the understanding of the processes in the combustion chamber and the temperature conditions in the tested material increases.

Literature:

[1] http://www.cpcag.ch
[2] ISO 834 Fire Resistance Tests.

5.2 Indoor Night Cooling

To reduce overheating indoors in summer, it would be useful if thermal energy could be released into the environment during cool summer nights. The benefits of this passive cooling are often underestimated. In this simulation study, this type of resource-saving cooling is simulated and its benefits are quantified.

Contributors: C. Tello, A. Witzig
Partners: ICP
Funding: ICP
Duration: 2023

Many office buildings are actively cooled with heat pump cooling systems. The electricity consumption required for this results in high CO2 emissions and considerable costs. In this project, a transient 2D simulation with COMSOL Multiphysics was used to show the benefits of cooling with cold night air. The thermal behaviour of the walls, floor and ceiling is important here. After the room air has been quickly exchanged with a fan, the solid bodies continue to give off heat for a long time. It is crucial for the simulation that the heat transfer between the solid and the air is modelled realistically and that the radiation equilibrium between the walls, the floor and the ceiling is represented accurately.

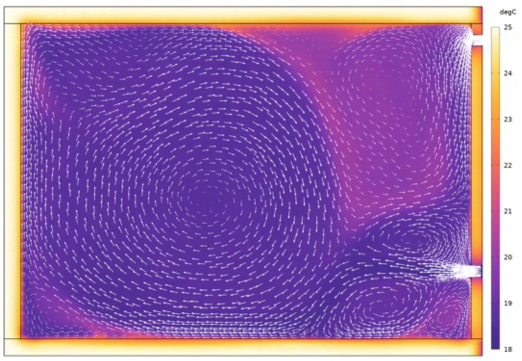


Fig. 1: Velocity field in the fluid flow domain and temperature distribution in all domains after 2 hours at 80 m^3/h inlet volume flux. Temporally constant inlet velocity and temperature are assigned as well as zero pressure and heat flux outlet conditions at the outlet. One large vortex and several smaller vortices in the corners occur. The lower temperature in the structure within the domain adjacent to the fluid flow boundaries shows that convective heat transfer is taking place.

The results show that a large effect can be achieved with a simple fan that consumes little energy. The dynamic simulations show that not only the air but also the building structure cools down and that comfort can be maintained for longer the following day. Measurements were also carried out in the project. However, the comparison between measurement and simulation will only be carried out in a follow-up project. It is also a challenge to disseminate the project results appropriately in order to use the findings to ensure that less energy is consumed when cooling indoor spaces in future.

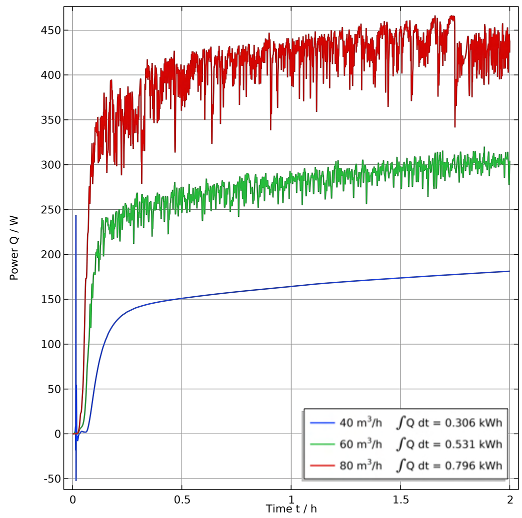


Fig. 2: Power and energy evaluated at the outlet. The laminar nature of the flow is evident at the lowest flow rate, shown by the blue curve. The more turbulent flow at the highest flow rate, red curve, corresponds to the flow shown in Fig. 1.

5.3 Massive parallelization for the simulation of decentralized energy systems

Heating systems are now often combined with solar systems. When designing these systems, it is often not just a single system configuration that is considered, but the input parameters are varied. In a research project together with the provider of the simulation software Polysun, a scheme was implemented that offers users massive parallelization and helps them to keep track of the parameter variation. If realistic examples are simulated, the limits of the physically possible solutions become apparent. An optimal system lies on this boundary. If the user selects the ecological benefit according to which he wants to optimize the system, it can automatically be shown how to achieve this goal with the least possible financial effort.

Contributors: A. Witzig, F. Schranz. M. Battaglia
Partners: Vela Solaris AG
Funding: Innosuisse
Duration: 2023–2025

The Polysun simulation software can be used to simulate decentralized energy systems. It turns out that in daily use, the users of the software define an energy system and stick with the first plausibly functioning system since the optimization must essentially be done manually. As a new paradigm, a larger number of simulations with different parameter settings are now started on the basis of user-defined start settings. To keep the waiting times short, the simulations are run in parallel on a computer farm with many CPUs.

The many simulations of the parameterized energy system are also suitable for automatic optimization. It is sufficient for the user to select a financial and an ecological dimension for optimization. As a result, a given ecological target can be achieved with less financial effort. The money saved in this way makes energy systems that use solar energy or environmental heat more cost-effective.

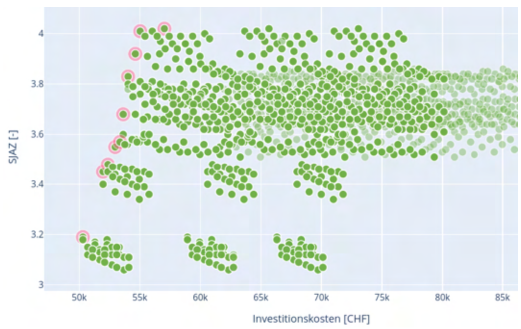


Illustration of a large number of simulations with a financial dimension on the horizontal axis and an ecological dimension on the vertical axis. Each green dot shows the result of one simulation. The simulations marked in orange show the boundary line at which maximum ecological benefit is achieved with minimum financial outlay.

5.4 Thermal Ground Activation

In the quest to harness sustainable and efficient energy solutions, thermal ground activation emerges as a promising technology. Floor heating infrastructure can also be used to cool the indoor atmosphere in summer. This extracted energy can be stored and used in winter for heating. In this numerical study, a sand heat tank with embedded heat coils is submerged in soil and the transient response of the outlet water is analyzed for later use in a reduced-order model setting. The COMSOL Multiphysics pipes environment allows modelling of non-isothermal fluid flow in pipes in 1D where the soil is modelled with plain 3D heat transfer.

Contributors: A. Witzig, C. Tello
Partners: ICP
Funding: ICP
Duration: 2023–2024

When one thinks of energy storage solutions, thermal ground activation is not among the ones thought of first. However, in recent years, several companies have been founded that make use of this underestimated possibility. A promising approach is to embed PE heating pipes that are used for floor heating installation in sand and shield the sand with an insulating layer that is open towards the bottom. This is done to allow the tank to interact with deeper soil and minimize losses to low ambient surface temperatures.

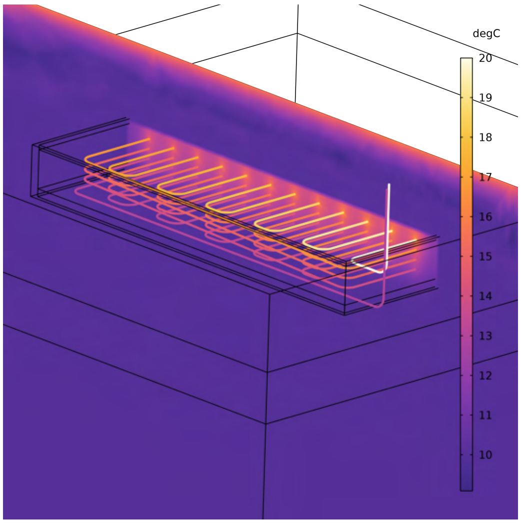


Fig. 1: Thermally activated ground with a downward-opening insulation jacket of 24 cm thickness. The top part of the soil, warmed by the sun, is visible. The temperature of the sand within the insulation is raised by the installed PE pipes, making it capable of storing energy. The glycol-water liquid enters heated into the topmost layer of heating pipes and flows along the pipes down the tank.

The heating pipes in this study are modelled as a 1D line in 3D space and meshed first, the rest of the mesh inside the tank's insulation grows from the line, such that the heat flux coupling of the two modelled phenomena happens at vertices and edges only.

Since obtaining such a solution is computationally expensive, simulating several decades is not feasible with Multiphysics FEM. The obtained curve shown in Fig. 2 is a result that is used to derive a reduced order model in e.g. MATLAB Simulink to be able to simulate and analyze the tank's behaviour over several decades. The procedure of obtaining a reduced order model involves advanced optimization techniques and is currently in progress.

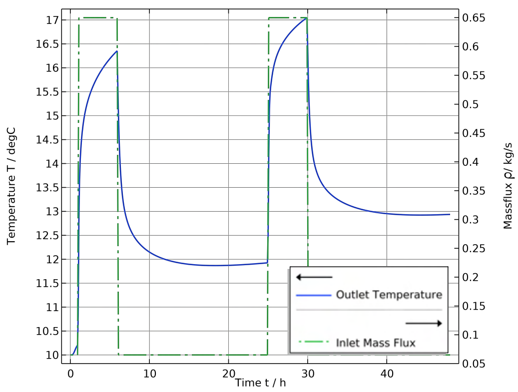


Fig. 2: Temperature at the outlet and mass flux at the inlet. Energy storage capabilities are shown in the offset of the two response peaks in the y-direction.

5.5 Thermal Simulation for Reducing the Energy Consumption

The digital platform ZHELIO was developed in a cross-departmental project with the involvement of Life Science and Facility Management and several institutes from the School of Engineering. The Swiss company Leicom AG actively participated with expertise and their software ELIONA to build a comprehensive digital twin for the building sector. This article reports the use case dedicated to reducing the energy consumption of office buildings.

Contributors: A. Witzig, F. Schranz, D. Schmid, V. Phimmasane, A. Rüst
Partners: Leicom AG
Funding: Innosuisse
Duration: 2020–2023

Modern buildings have a large number of isolated control and measurement systems. Transferring these heterogeneous applications into the digital world is challenging. In the Innosuisse project ZHELIO, a novel User Assistance System for Smart Commercial Buildings has been developed [1] which aims to become a platform for integrating data collection, signal processing and automation control. The demonstrated proof-of-concept on an existing building seamlessly integrates data from various building technologies and validates selected use cases. A wireless Internet of Things (IoT) sensor network enables the system's services by collecting indoor climate data and tracking assets. Integrated Digital Twins for thermal predictions and modelling of photovoltaic systems (PVS) facilitate dynamic energy optimisation. The results show how to reduce subsystems' operation hours and PVS payback time by providing intelligent, adaptable services.

One important Use Case of the project dealt with the reduction of the energy consumption of big office buildings. As a demonstrator, the RA building of ZHAW in Wädenswil has been modelled with the simulation software IDA ICE (see Figure) and the energy demand has been evaluated. The results have been in agreement with earlier investigations of this building [2]. An existing method for the automated import of architectural plans exists and has been tested and compared to the use of the built-in software capability for generating a building structure. In conclusion, a digital twin needs to offer various views on the building which arise from the planning and construction process as well as from maintenance. Eliona is well suited to support this requirement and offers a useful model integration that produces added value for several of the involved parties.

Literature:

[1] F. Schranz, V. Phimmasane, A. Witzig, A. Rüst, and D. Schmid, *User Assistance System for Smart Commercial Buildings*, 2024 European Conference on Computing in Construction, Greece, July 2024.

[2] R. Burgy, M. Hubbuch, R. Obrist *Energetische Betriebsoptimierung Minergiegebäude Seifen-Sträuli der ZHAW in Wädenswil*, Project Report, BFE, November 2016.

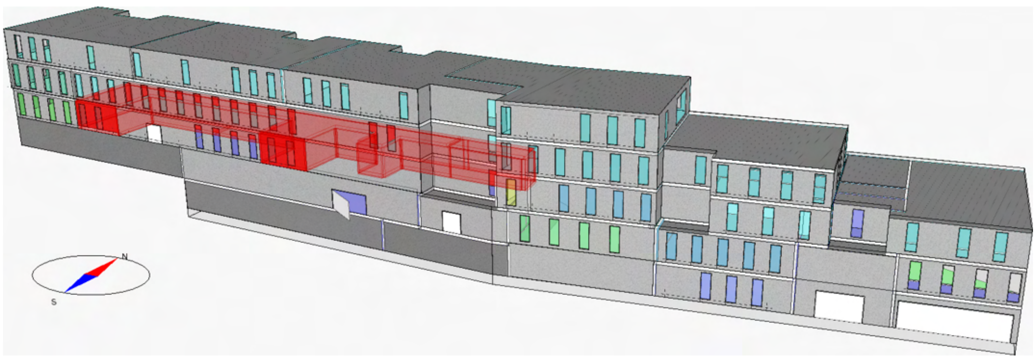


Fig. 1: IDA ICE simulation results. The heat demand is color-coded in the windows. A corridor zone is highlighted in red.

5.6 Development of a controlled nucleation method for supercooled PCM

The Swiss Federal Office of Energy's (SFOE) "Energy Perspectives 2050+" foresees a significant shift towards greater sustainability in Switzerland. By 2050, 1.5 million heat pumps are to be installed and the installed power of photovoltaic systems is to be increased to 40% of the country's total energy production. However, the plan faces challenges as electricity demand rises in winter and solar energy is unreliable. SeasonCell, a start-up founded by ZHAW and HSLU in 2023, is developing a seasonal heat storage system using supercooled phase change material (PCM) to overcome these challenges. This Master's thesis developed a method for nucleation triggering of the supercooled PCM, which contributes to the development of the SeasonCell STES system and supports Switzerland's sustainability goals in the energy sector.

Contributors: S. Pfyffer, K. P. Pernstich, A. Witzig
Partners: SeasonCell AG
Funding:
Duration: HS 2023/24

Phase change materials (PCMs) store thermal energy during their phase transition, usually from solid to liquid and back again, maintaining a relatively constant temperature, despite the absorption or release of heat. This property makes PCMs particularly useful for achieving high energy densities and storing thermal energy with minimal losses over long periods of time. Figure 1 illustrates the behavior of a PCM.

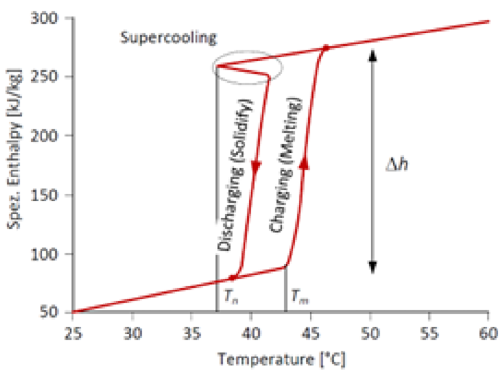


Fig. 1: Enthalpy vs. temperature diagram with melting and solidification hysteresis.

The process of nucleation triggering, or solidification, is critical to the use of PCMs for heat storage, as it initiates nucleation at the desired time for efficient release of stored heat energy.

A controllable mechanism for triggering the phase transition is essential for the effectiveness and reliability of a seasonal heat storage system based on supercooled PCMs.

This Master's thesis focused on the development of a controlled nucleation triggering method for supercooled sodium acetate trihydrate (SAT) in a seasonal thermal storage system. The project investigated nucleation theories, analysed different nucleation triggering mechanisms and finally designed and implemented a practical nucleation device tailored to the SeasonCell storage concept. This method successfully induces nucleation in supercooled SAT, demonstrating a 100% probability of nucleation.

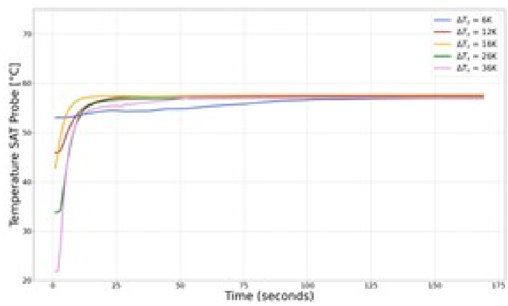


Fig. 2: Temperature curves of the nucleation tests with different subcooling temperatures of the SAT samples.

In addition, this thesis has developed an automated thermal cycling device that allows multiple SAT samples to be tested simultaneously and fully automatically, greatly enhancing SeasonCell's experimental capabilities for future research.

5.7 ThermoPlaner3D - Detailed building energy evaluation from large-area 3D thermography

ThermoPlaner3D develops large-scale, detailed 3D building energy assessments from multiperspective thermographic images, creating a new quantitative planning basis as well as a marketing tool for energy suppliers.

Contributors: M. Battaglia, E. Comi
Partners: FHNW, Considerate AG, BSF Swissphoto
Funding: Innosuisse
Duration: 2021–2024

The increase of the renovation rate in the building sector is a central component in the reduction of the energy demand of Switzerland. The ThermoPlaner3D project is developing an innovative product that enables energy supply companies (EVUs) to support the energy transition and profit from it at the same time.

While today energetic assessments of buildings are mainly done for single objects, there is a lack of tools to offer owners a low-threshold initial assessment of their building and to show them the potential of a refurbishment. The ThermoPlaner3D project aims to provide the necessary quantitative basis for an entire urban area with a single measurement flight using multiperspective thermal images from a remote sensing aircraft.

A first test flight was carried out in Grenchen before the start of the project in late winter 2021. With SWG, the utility company of Grenchen, a pilot customer for feedback is involved. Valuable insights were gained from the first test flight, which could be further refined in a second test flight in the winter of 2023 in Aalen in Baden-Württemberg.

Fig. 1: Roof temperatures and microclimate of a district.

The ICP is responsible for the scientific monitoring of data acquisition using infrared measurement technology and attempts to improve the evaluation and correction of the data using known and new approaches. We are also contributing our expertise in building simulation in order to be able to make statements about the annual consumption of the respective buildings from point measurements of the external temperatures of the building envelope.

Fig. 1 shows the roof temperatures of buildings including the microclimate temperature ranges. A heat transmission value is then estimated from the averaged roof temperature using a simple thermal model of the roof. The microclimate can be calculated as a by-product of a thermography flight using the TURN algorithm (Thermal Urban Road Normalization). The so-called TURN map of an urban area is shown in Fig. 2.

The test flight in winter 2023 was carried out with the system developed specifically for the project, which includes oblique cameras for capturing the facades in addition to the vertical images of the roofs. In the final part of the project, the potential of such a multi-perspective system will be analyzed and the evaluation further developed. Another focus is on developing a business model for our industrial partners.

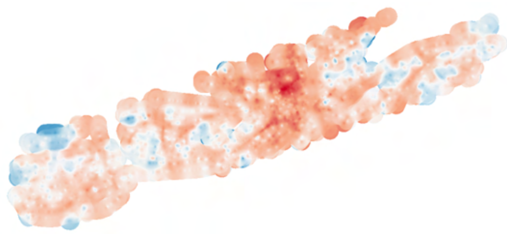


Fig. 2: The microclimate map of a city shows heat and cold islands at the time of the measurement flight.

Appendix

A.1 Student Projects

D. ACKERMANN & M. GABRIEL, *Building a Portable Multi-Wavelength Fluorescence Spectrometer*, Betreuer: M. Bonmarin, D. Fehr, Bachelorarbeit im Studiengang Systemtechnik.

M. AUER, *Ultra-broadband terahertz optical characteristics of semiconducting materials upon optical excitation*, Betreuer: M. Jazbinsek, Masterarbeit MSE Photonics.

G. BURGER, C. MÜNTENER, *Modellierung eines Wohnraums in Matlab/Simscpae für die Optimierung von Energiesystemen*, Betreuer: A. Witzig, Projektpartner Belimo AG, Bachelor Thesis.

D. BELUSKY, *Quality testing of advanced ceramic materials*, Betreuer: M. Jazbinsek, U. Puc, Projektarbeit Elektrotechnik.

G. BURGER, C. MÜNTENER, *Modellidentifikation für Energieoptimierung im Gebäude*, Betreuer: A. Witzig, K. Pernstich, Projektarbeit im Studiengang Systemtechnik.

A. FERREIRA, *Fully Solution Processed Distributed Bragg Reflectors for Colored Building-Integrated Photovoltaics*, Betreuer: K. Pernstich, B. Ruhstaller, Summer Internship "ThinkSwiss", Georgia Tech.

F. FURKAN & C. STEINER, *Neuartiges MOF-basiertes atmosphärisches Wassergewinnungssystem mittels Hydrogel*, Betreuer: M. Bonmarin, V. Buff, G. Boiger, Bachelorarbeit im Studiengang Systemtechnik.

C. GROSSMANN, *Development of an Innovative Neural Interface*, Betreuer: F. Spano, Vertiefungsarbeit Masterstudiengang.

C. GROSSMANN, *Digital Biomarkers for Cardiovascular Diseases and Neuroscience*, Betreuer: M. Bonmarin, Vertiefungsarbeit Masterstudiengang.

I. HÄUSLER, *3D Printing of conductive PDMS Material*, Betreuer: F. Spano,, Vertiefungsarbeit Masterstudiengang.

I. HÄUSLER, *Development and Characterization of Skin Phantoms for Electromagnetic Radiation Interaction and Thermotherapy Applications*, Betreuer: F. Spano,, Vertiefungsarbeit Masterstudiengang.

J. HINNEN, M.H. ANDRES, *Aufbau und Design eines LED-basierten Sonnensimulators für die Solarzellenforschung*, Betreuer: K. Pernstich, B. Ruhstaller, Bachelorarbeit im Studiengang Systemtechnik.

J. HINNEN, *Aufbau und Design eines LED-basierten Sonnensimulators für die Solarzellenforschung*, Betreuer: K. Pernstich, B. Ruhstaller, Projektarbeit im Studiengang Systemtechnik.

J. KÄPPLER & J. ZAUGG, *Development and Implementation of a Robotic Tactile Skin*, Betreuer: F.Spano, M. Bonmarin, D. Fehr, Bachelorarbeit im Studiengang Systemtechnik.

F. KÄSER & Y. WALDSPURGER, *Atmosphärisches Wassergewinnungssystem durch Strahlungskühlung*, Betreuer: M. Bonmarin, V. Buff, G. Boiger, Bachelorarbeit im Studiengang Systemtechnik.

G-L. LIBERATO, *Entwicklung von Drucksensoren basierend auf Fest-Flüssig Kompositionen*, Betreuer: F. Spano, Projektarbeit im Studiengang Systemtechnik.

M. GNOS, M. WICKIHALDER, *Effiziente Heizungsanlage in einer Kirche*, Betreuer: A. Witzig, Projektpartner Kegel Klimasysteme, Bachelor Thesis.

F. MEISSNER & D. MORF, *Development and implementation of an ultrasonic temperature measurement for dermatological applications*, Betreuer: M. Bonmarin, D. Fehr, Bachelorarbeit im Studiengang Systemtechnik.

M. MIJATOVIC, R. OSWALD, *Ein PowerPoint Add-In für zeitgesteuerte Aufgaben in der e-Exercises App*, Betreuer: K. Pernstich, Bachelorarbeit im Studiengang Informatik.

S. PFYFFER, *Development of a controlled nucleation method for supercooled PCM*, Betreuer: K. Pernstich, Masterarbeit.

L. PREVOTEL, *Design and Simulation of an LED-based Solar Simulator*, Betreuer: K. Pernstich, B. Ruhstaller, Mandatory training for Masters Course, University Paris-Saclay.

J. SCHWERTFEGER, *Kapazitiver Sensor zur Messung des Blutvolumens in einer kapillaren Transferpipette*, Betreuer: D. Fehr & M. Bonmarin, Projektarbeit im Studiengang Elektrotechnik.

A. SOUSSI, J. H. PARK, *Motivation durch Belohnung: Konzeption und Umsetzung eines Belohnungssystems in der e-Exercises App*, Betreuer: K. Pernstich, Bachelorarbeit im Studiengang Informatik.

R. WIRTH, *Cell Size Determination and Mapping of Local Resistance and Dark Saturation Current in Perovskite Solar Cells*, Supervisors: E. Knapp, M. Battaglia, Projektpartner: Fluxim AG, Solaronix S.A., Master's Specialization Thesis.

R. WIRTH, *Use of Physics Informed Neural Networks to Extract Solar Cell Parameters from Local Voltage Measurements*, Supervisors: E. Knapp, M. Battaglia, Projektpartner: Fluxim AG, Solaronix S.A., Master's Thesis.

M. YASSIN, *Evaluation of the impact of a new sterilization method on material interaction between implant and packaging material*, Betreuer: M. Bonmarin, D. Fehr, Projektpartner Zimmer Biomet, Winterthur, Masterarbeit.

J. ZWICKY, *Compact Multi-Wavelength Filter Module for Low-Light Fluorometry*, Betreuer: D. Fehr, Vertiefungsarbeit Masterstudiengang.

J. ZWICKY, *Optimized Detection Electronics for a Ratiometric Point-of-Care Fluorometer*, Betreuer: D. Fehr, Vertiefungsarbeit Masterstudiengang.

A.2 Scientific Publications

A. ABINA, T. KOROSEC, U. PUC, M. JAZBINSEK, A. ZIDANSEK, *Urinary metabolic biomarker profiling for cancer ciagnosis by terahertz spectroscopy : review and perspective*, Photonics, 9 (10), 2023.

A. Abina, U. Puc, M. Jazbinsek, A. Zidansek, *Analytical gas sensing in the terahertz spectral range*, Micromachines, 14 (11), 2023.

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A.3 Book Chapters

L. HOLZER, P. MARMET, M. FINGERLE, A. WIEGMANN, M. NEUMANN, V. SCHMIDT, *Introduction. In: Tortuosity and Microstructure Effects in Porous Media*, Springer Series in Materials Science, 333, 2023.

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L. HOLZER, P. MARMET, M. FINGERLE, A. WIEGMANN, M. NEUMANN, V. SCHMIDT, *Summary and Conclusions. In: Tortuosity and Microstructure Effects in Porous Media*, Springer Series in Materials Science, 333, 2023.

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A.4 Conferences and Workshops

G. K. BOIGER, B. SIYAHHANN, A. SCHUBIGER, M. HOSTETTLER, A. S. FALLAH, H. KHAWAJA, M. MOATAMEDI, *Multiphysics simulation-based investigation of electro-static precipitation phenomena in the context of coating standard automotive rims*, 18th International Conference of Multiphysics, Graz, Austria, December 2023.

V. BUFF, M. BOLDRINI, G. K. BOIGER, *Synergistic integration of multiphysics modelling and control engineering paradigms : a novel approach to dynamic algorithm formulation*, 18th International Conference of Multiphysics, Graz, Austria, December 2023.

E. COMI, S. JENATSCH, B. BLÜLLE, M. BATTAGLIA C. M. TORRE, C. KIRSCH, R. HIESTAND, U. AEBERHARD, B. RUHSTALLER, E. KNAPP, *Investigation of time and location dependent variations in electroluminescence images of perovskite solar cells*, 40th European Photovoltaic Solar Energy Conference and Exhibition (EU PVSEC), Lisbon, Portugal, September 2023.

F. EBADI, *In-Operando PL Measurements on Perovskite Solar Cells with and without Phase-Segregation*, E-MRS Spring, Strasburg, 31 May 2023.

L. HOLZER, *Review of Tortuosity and prediction of effective transport properties in porous media*, Data-driven modeling of porous, composite and polycrystalline microstructures for predicting their mechanical and transport properties, European Mechanics Society, Colloquium 632, September

2023, Ulm, Germany.

M. HOSTETTLER, G. K. BOIGER, *Calibration and numerical modelling of a peristaltic pump for accurate fluid transport in complex tube setups*, 18th International Conference of Multiphysics, Graz, Austria, December 2023.

F. VUCKO, G. RINGOT, P. MARMET, L. HOLZER, M. DUMOUCHEL, M. PRESTAT, *In vitro corrosion and stress corrosion cracking of Ti6Al4V alloy in H2O2-containing physiological solutions*, The Annual Congress of the European Federation of Corrosion (EuroCorr), Brussels, Belgium, August 2023.

P. MARMET, L. HOLZER, T. HOCKER, G. K. BOIGER, *Multiscale-multiphysics model for novel ceramic solid oxide fuel cell electrodes*, 18th International Conference of Multiphysics, Graz, Austria, December 2023.

M. MOHAMMADI, *Performance boosting polymeric finish layer for perovskite solar cells*, E-MRS Spring, Strasburg, 29 May 2023.

K. PERNSTICH, L. MESSENZEHL-KÖLBL, *Wie integrieren wir KI in die berufliche und akademische Schreibpraxis?*, LeLa Webinar-Reihe «AI or what the ChatGPT?» Implikationen für die Gestaltung der Lehre an Hochschulen,Winterthur, 2023.

K. PERNSTICH, *KI in der Lehre - Schriftliche Arbeiten*, Impuls Reihe SoE, Winterthur, 2023.

K. PERNSTICH, *Advanced Materials and Characterization Tools for Quantum-Dot enhanced Displays*, Photonics Lunch, Winterthur, 2023.

M. REGNAT, K. P. PERNSTICH, B. BLÜLLE, S. JENATSCH, M. K. HEO, B. RUHSTALLER, *Modeling the Impact of the Illumination Geometry on the Light Conversion Efficiency in Quantum Dot Down-Conversion Films*, International Conference on Display Technology, Hefei, China, 2024.

B. RUHSTALLER, *Enabling R&D tools for emerging display technologies from device simulation to stress testing*, OLEDs: Innovations, Manufacturing, Markets, TechBlick Online Conference, April 2024.

S. SEM, S. JENATSCH, S. ZÜFLE, A. GADOLA, D. HUDSON, C. PFLUMM, B. RUHSTALLER, *Accelerated lifetime testing and degradation mechanisms of a blue TADF OLED*, SID Display Week, Los Angeles, May 2023.

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R. P. SCHÄRER, J. O. SCHUMACHER, *A transient non-isothermal cell performance model for organic redox flow batteries*, 19th Symposium on Fuel Cell and Battery Modelling and Experimental Validation, Duisburg, 2023.

B. SIYAHHANN, G. K. BOIGER, A. FALLAH, H. KHAWAJA, M. MOATAMEDI, *A semi transient methodology for dual time stepping of particle and flow field simulations of an Eulerian-Lagrangian multiphysics solver*, 18th International Conference of Multiphysics, Graz, Austria, December 2023.

M. A. TORRE CACHAFEIRO, *Simulating the transient luminescence of perovskite light-emitting diodes under pulsed operation*, E-MRS Spring, Strasburg, 29 May 2023.

W. TRESS, *Characterization and Modelling of Perovskite Solar Cells*, E-MRS Fall, Warsaw, 18 September 2023.

W. TRESS, *Characterization and Modelling of Perovskite Solar Cells*, International Young Scientists Salon on Future Technologies for Carbon Neutrality, Tianjin, 13 October 2023.

W. TRESS, *Multidimensional Characterization and Modelling of Perovskite Solar Cells*, HOPV23, London, 14 June 2023.

W. TRESS, *Perovskite Solar Cells under Real World Conditions*, Workshop on Stable Hybrid Perovskite Materials for Photovoltaics Under Real-World Conditions, Fribourg, 23 February 2023.

A. WITZIG, *Künstliche Intelligenz in Wämrepumpen*, Fachtagung der Fachvereinigung Wärmepumpen Schweiz (FWS), Spreitenbach, November 2023.

A.5 Teaching

D. BAJRAMI, *Physik für Systemtechnik 2 – Praktikum, FS23*, Bachelor of Science.

M. BATTAGLIA, *Physics Engines, FS23, FS24*, Bachelor of Science.

M. BONMARIN, *Physik für Systemtechnik 2 – Vorlesung, FS23*, Bachelor of Science.

M. BONMARIN & D. FEHR, *Thermal Devices in Medicine – Vorlesung & Praktikum, FS23*, Bachelor of Science.

M. BONMARIN, *Höhere Mathematik für IT – Vorlesung & Praktikum, FS23*, Bachelor of Science.

M. BONMARIN, *Swiss Biodesign – Inventing next generation medical devices: From clinic immersion to MVP & business plan, FS23*, Master of Science in Engineering.

M. BONMARIN, *Medical Market Access, HS23*, Master of Science in Engineering.

D. FEHR, *Grundlagen der Elektrotechnik und Digitaltechnik für Informatik – Praktikum, HS23*, Bachelor of Science.

D. FEHR, *Physikalische Grundlagen der Sensorik – Thema Elektronik, HS23*, Bachelor of Science.

D. FEHR, *Photonics EVA – Thermography, FS24*, Master of Science in Engineering.

M. JAZBINSEK, *Physik 1 für Maschinentechnik und Energie- und Umwelttechnik – Vorlesung & Praktikum HS23*, Bachelor of Science.

M. JAZBINSEK, *Physik 2 für Maschinentechnik und Energie- und Umwelttechnik – Vorlesung & Praktikum FS24*, Bachelor of Science.

C. KIRSCH, *Analysis 1 für Systemtechnik, HS23*, Bachelor of Science.

C. KIRSCH, *Analysis 2 für Systemtechnik, FS24*, Bachelor of Science.

C. KIRSCH, *Analysis 3 für Systemtechnik, HS23*, Bachelor of Science.

C. KIRSCH, *Numerik für Systemtechnik und Elektrotechnik, FS24*, Bachelor of Science.

E. KNAPP, *Modellierung komplexer Systeme MKS, HS23*, Bachelor of Science.

P. MARMET, *Mathematik: Analysis 1 für Aviatik und Verkehrsysteme, Vorlesung und Praktikum, HS23*, Bachelor of Science.

P. MARMET, *Mathematik: Analysis 2 für Aviatik und Verkehrsysteme, Vorlesung und Praktikum, FS24*, Bachelor of Science.

K. PERNSTICH, *Physik: Grundlagenprojekt 1 für Verkehrssysteme, HS23*, Bachelor of Science.

K. PERNSTICH, *Physik: Grundlagen der Elektrotechnik und Digitaltechnik, Vorlesung und Praktikum, Studiengang Informatik, HS23*, Bachelor of Science.

K. PERNSTICH, *Physik: Grundlagenprojekt 2 für Verkehrssysteme, FS24*, Bachelor of Science.

K. PERNSTICH, *Data Science: Internet of Things for Data Science, FS24*, Bachelor of Science.

K. PERNSTICH, *Physik: Physics Engines, Studiengang Informatik, FS24*, Bachelor of Science.

B. RUHSTALLER, *Applied Photonics - HS23*, Master of Science and Engineering.

B. RUHSTALLER, *EVA Introductory Optics for Photonics - HS23*, Master of Science and Engineering.

B. RUHSTALLER, *Advanced Thin Films - FS24*, Master of Science and Engineering.

J. O. SCHUMACHER, *Lineare Algebra 1, HS23*, Bachelor of Science.

J. O. SCHUMACHER, *Lineare Algebra 2, FS23*, Bachelor of Science.

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J. O. SCHUMACHER, *Multiphysics Modelling and Simulation, FS23*, Master of Science in Engineering, Switzerland.

W. TRESS, *Physik 1 für Maschinentechnik, HS23*, Bachelor of Science.

W. TRESS, *Physik 2 für Maschinentechnik, FS24*, Bachelor of Science.

W. TRESS, *Physics on Micro and Nano Scale, HS23*, Master of Science.

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A.6 Spin-off Companies

NM Numerical Modelling GmbH
The engineering company, CH-Thalwil

NM Numerical Modelling GmbH, a spinoff company of ICP merged with the company maglab AG www.maglab.ch at the beginning of 2023. In February 2023, both companies were fully integrated into the American company CTS Corporation www.ctscorp.com. The worldwide actively CTS develops and produces sensors and actuators for the automobile industries. The knowhow in the form of IPs by NM GmbH is now exploited in product development.

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.

DermatoTherma

www.dermatotherma.com

DermatoTherma is developing a safe and intelligent thermotherapy device for treating cutaneous leishmaniasis. This neglected skin disease puts 350 million people worldwide at risk, and established drug treatments can have severe side effects. The start-up's goal is to make thermotherapy accessible and thus improve the quality of life of those affected. Data collected during the treatments will also be used to establish a more representative database of electrical skin properties, supporting research in neglected regions of the world. The start-up is in close collaboration with the Drugs for Neglected Diseases initiative (DNDi) and is supported by the Gebert Rüf Foundation and the BRIDGE programme of the SNF.

coatmaster

www.coatmaster.ch

Coatmaster AG (formerly known as Winterthur Instruments) 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, to detect delamination, for example. 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.

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 Award in 2018.

www.reorbis.ch

Reorbis GmbH, based in Winterthur, Switzerland, aims to provide services for the manufacturing industry in the form of life cycle analysis (LCA). In the aluminum industry there is great interest in LCA due to a new standard (Aluminum Stewardship Initiative, ASI). The offer is directed first and foremost towards achieving certification to the ASI standard. The recycling management is applied to other raw materials besides aluminum.

A.7 Laboratory Infrastructure

An often underestimated aspect of the development of physical simulation models is their validation and the associated improvement cycle. In terms of effort, this is often much more than *a few simple experiments to match the simulation*. Instead, this part of the multiphysics development process is the actual link between theoretical development and operational reality. Validation efforts and the associated necessary model improvement cycle can account for up to 60% of the project scope. Accordingly, it is important to give this area its appropriate strategic importance. Maintaining or expanding the capabilities of a validation laboratory is therefore important.

Process laboratory for organic electronics

Since 2012, the centerpiece of this laboratory has been a glove box with nitrogen atmosphere and integrated vacuum chamber for device fabrication by means of thermal evaporation of organic semiconductors and metals. A second box was installed in 2020. Thin films can also be produced from solutions using the spin-on process, and chemistry chambers are available for measurement and sample preparation. The laboratory has measuring methods for determining the optical, electrical and thermal properties of the components.

Electronics laboratory

The electronics lab allows us to efficiently develop, fabricate, and characterize prototypes for R&D projects with our industrial partners. It allows us to validate our simulation models on real systems and it enables us to use specialized instrumentation and sensor technology for the experimental setups in our other laboratories. Last but not least, students also benefit from the capabilities of our electronics lab, with a focus on rapid prototyping. Our lab meets these demands with a well-balanced basic equipment, such as SMD-capable soldering workstations with a basic set of components, a workstation for simple mechanical tasks, and various lab equipment such as power supplies, frequency generators, multimeters, oscilloscopes, DAQs, impedance analyzers, and debugging tools for embedded systems.

Laser and THz-Photonics laboratory

In this lab spectroscopy systems for visible (UV/Vis) and invisible (THz) range are available or under further development. Using fs-laser pulses, THz beams are generated via nonlinear effects in an organic crystal, which are sent through a sample under investigation to determine its properties non-invasively. Visible spectroscopy on temperature-dependent samples is measured in a vacuum chamber. A supercontinuum laser system was acquired in 2022 with co-funding from the Swiss National Science Foundation.

Thin film characterization laboratory

In this laboratory, various instrumentation is available to study thin film samples with angle-dependent ellipsometry, profilometry, 3D optical microscopy, FTIR spectroscopy.

Nano-Imaging laboratory

Current research on perovskite semiconductors requires information on the nanoscale. For this purpose, an atomic force microscope (AFM) combined with an optical spectrometer was acquired in 2022. It is a highly technical complex device that allows confocal optical microscopy such as luminescence and Raman, which can be combined with AFM techniques to allow near-field measurements (see project description on p. 23). The investment was paid by the ERC Grant OptEIon (grant agreement no. 851676).

Electroplating laboratory

The heart of the electroplating laboratory is an experimental copper refining electrolysis cell. In this electrolysis cell, controlled experiments on flow-coupled ion transport phenomena can be carried out under high current but low voltage. Although originally developed for copper refining, the system can also be used to simulate alternative ion transfer processes (e.g. for galvanic coating methods). The system is fully electronically controlled, has a highly developed interface, a self-cleaning system and corresponding ventilation systems.

Soft Materials Lab

We have a fully equipped laboratory in which we can work with various soft materials (such as polymers, hydrogels, etc.) under safe conditions. Examples of available devices: 3D bioprinter (liquid printing), rod coater, ultrasonic cleaner, centrifuge, magnetic stirrer, hot plates, pH meter, etc. With these devices we can develop sophisticated prototypes for biomedical applications.

Thermal Design Lab

Physicochemical computer models are valuable tools for developing new functional materials and industrial processes. However, their reliability and practical use depends heavily on the material data used. In addition, extensive calibrations and validations are usually necessary before use. With the Thermal Design Lab, we pursue the goal of generating as precise inputs as possible for our computer models using temperature and heat flow measurement technology in combination with thermal material data determination. The Thermal Design Lab currently includes a wide range of contact temperature sensors and thermal imaging cameras with different spectral ranges. We also use various methods to determine the thermal conductivities of liquids and solids.

Medizininformatiklabor

While the new medical informatics course is being set up, the laboratory will initially be used primarily for regular internships. Later, more and more experiments from project and bachelor theses will be carried out. As in the other thematic focuses, students in medical informatics and medical technology are also welcome to serve as assistants during the semester break in valuable support of the ICP's research projects.

A.8 ICP-Team

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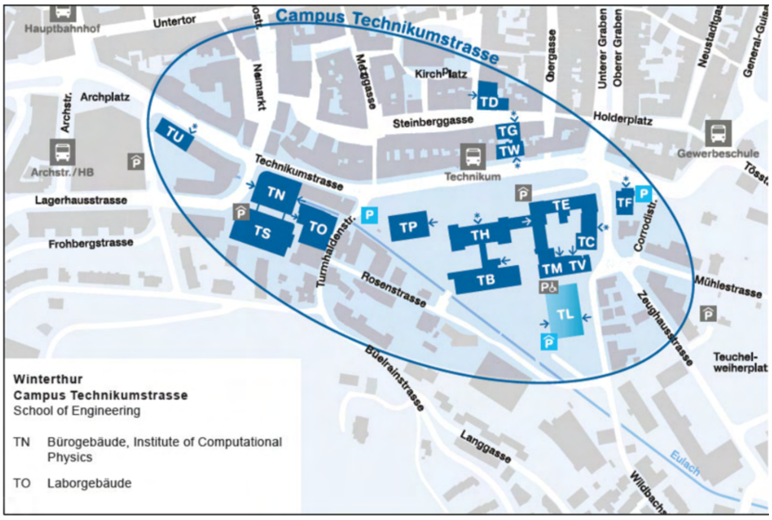
A.9 Location



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