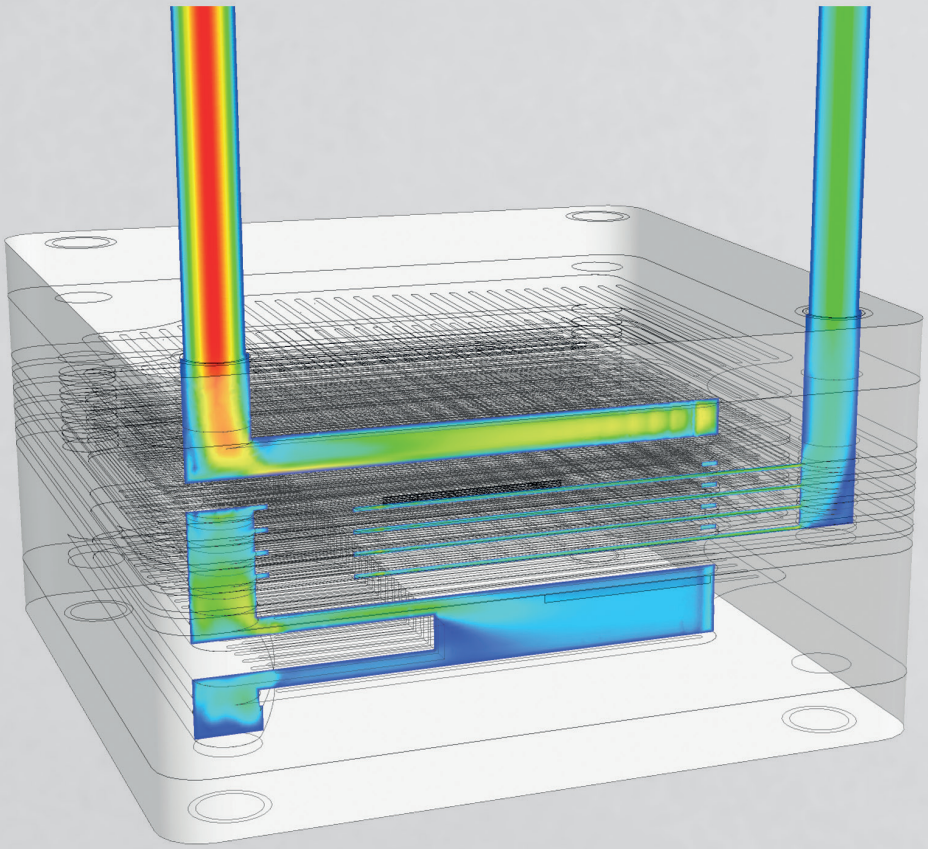
School of Engineering

ICP Institute of Computational Physics

Research Report 2023



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The cover graphic shows a velocity distribution within a solid oxide fuel cell system. To complement measurement data and perform design optimizations the ICP uses thermo-fluidic simulations.

Preface

At ICP, we specialize in advanced physics simulations and can thus offer innovative solutions in various application areas. We understand the industry-specific issues and can often present our results in the respective communities at conferences or publish them as scientific papers.

We usually verify our numerical models with laboratory measurements. In this way, first we ourselves and then our customers gain confidence in the simulation. The model parameters are validated or calibrated in the lab. In this year's research report, we would like to devote special attention to our laboratory activities. In chapter 6 we describe the various measurement facilities and draw a the direct link to research projects shown in the first five chapters.

By carrying out specific laboratory projects, our students acquire valuable skills and often establish a close contact to our industrial partners. By supervising these projects, we at the ICP make an important contribution to teaching. Laboratory work is often complementary to the rest of our teaching activities in the basic subjects of mathematics, physics and numerics.

Andreas Witzig,

Head of ICP

Table of Contents

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.

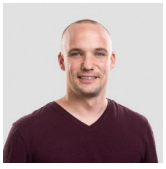
At the ICP, we perform applied research in the field of multiphysics modeling and develop finite element as well as finite volume simulation software.

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.


G. Boiger


M. Boldrini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1.1 Development of a fast cloud-based simulation workflow for the complete aerodynamic evaluation of airborne vehicles

The field of Computational Science is facing an increasing demand for data-intensive investigations. Engineering tasks such as parameter-, sensitivity- and optimisation studies need ensemble computing to an ever-increasing extent. At the same time, the field of artificial intelligence (AI) is pushing for ever more extensive, numerically derived learning-, testing-, and validation data.

Contributors: G. Boiger, D. v. Oerle, A. Schubiger
Funding: internal
Duration: 2022

With the cloud software Kaleidosim, hundreds of numerical simulations can be run simultaneously, allowing for the generation of large amounts of data in a short amount of time [1]. In our study, we focused on using OpenFOAM as the simulation tool and developing tools and routines to simplify, automate, and speed up the study of hundreds of simultaneous simulations in the cloud (Fig. 1). We conducted a complete 360° aerodynamic analysis of various airborne vehicles to test our toolbox, which included 420 OpenFOAM CFD cases. Each case was a steady-state, Reynolds Average Stress (RAS) turbulence model-based, single-phase flow simulation on a 1.5 million cell hexahedral finite volume grid, with drag and lift coefficients calculated for each scenario (Fig. 2).

The toolbox was developed using a combination of Python and Kaleidosim API routines, with the Python-based graphical user interface (GUI) enabling the switching between different CAD models to compare multiple aircraft. The GUI also allowed for mesh sensitivity analysis to identify optimized meshes for each aerodynamic shape, with a series of mesh sensitivity analyses performed using snappyHexMesh and CfMesh grids (Fig. 3).

The results of our work demonstrate that a combination of cloud computing via Kaleidosim-based API routines and Python scripting can speed up certain parameter study workflows by a factor of 50-100. The semi-automated workflow of the aerodynamic study with 420 cases could be performed and post-processed in under 45 minutes, whereas a comparable workflow had previously taken up to a full working week on local hardware. This approach offers a promising tool for accelerating research and development in various engineering and scientific fields beyond aerodynamic analysis.

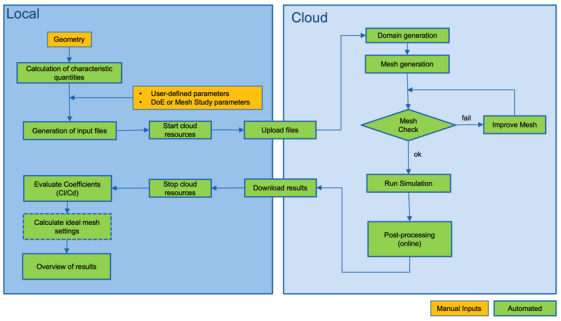

Fig. 1: Overview of the developed workflow.

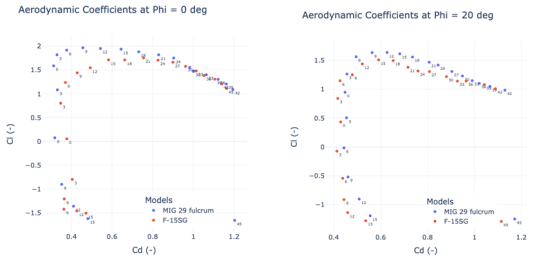

Fig. 2: Automatically generated comparison of the calculated lift (Cl) and drag (Cd) coefficients of two models for different pitch angles (alpha) and yaw angle (phi).

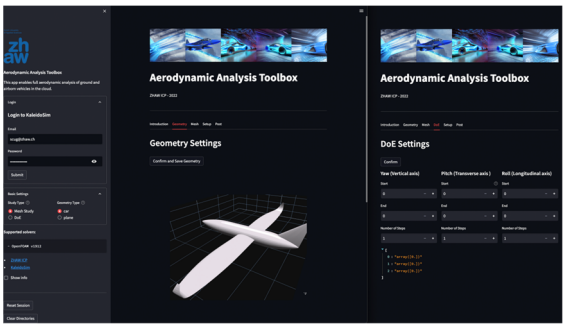

Fig. 3: Overview of the Aerodynamic Toolbox web application and its Design of Experiment (DoE) settings.

Literature

[1] Gernot Kurt Boiger, Darren Sharman, Bercan Siyahhan, Viktor Lienhard, Marlon Boldrini and Dominic Drew. A massive simultaneous cloud computing platform for openfoam. In 9th OpenFOAM Conference, online, 19-20 October 2021. ZHAW Zürcher Hochschule für Angewandte Wissenschaften, 2021.

1.2 coatSim: A Simulation Software for the Analysis of Processes Involving Particle Laden Flows

In the scope of this project, a software is developed with the ultimate goal of analysing any process that involves particle laden flows, with particular emphasis on powder coating applications. Previously the intuitive workflow encompassing geometry, automated meshing and cloud computing operations along with the interface to create parameter studies was introduced. In this report upgrade to the software interface and the capability to carry out post processing operations directly on the cloud is covered.

Contributors: B. Siyahhan, G. Boiger
Funding: Gebert Rüf Stiftung
Duration: 2021–2023

coatSim is a simulation software to replicate any process that involves particle laden flows, in a digital environment. Currently, the module specifically for powder coating applications, is developed. Powder coating is a surface finishing process where dry paint particles in the form of a powder cloud are electrically charged passing through a coating pistol and subsequently deposit on the surface of a grounded substrate upon contact. Since this is a complex multiphysics problem [1], the industry has traditionally relied on trial-and-error based methods for process development. coatSim alleviates the numerical expertise needed to simulate the process to serve as a predictive digital tool for the wider industry.

The main interface of the powder coating module has been updated incorporating a color-coding scheme as illustrated in Fig. 1. Here, the operations highlighted in yellow are the optional ones, while green indicates an operation that has been successfully carried out and red the pending operations. This serves as a simplification for the user to follow the sequential workflow. The optional operation of post processing directly on the cloud is the major update for the coatSim software, as it circumvents the necessity of downloading large data from the cloud to perform the post processing. This is essential, especially in parameter studies, where the user will typically be interested in certain key process parameters that can be derived from the sizeable simulation output data. Furthermore, time is spared on downloading data as well as carrying out post-processing operations locally. Two types of post processing operations have been incorporated. In one, called the default post-processing as illustrated in Fig. 2, the crucial parameter, namely the coating thickness and the homogeneity are evaluated. The second one allows the user to create a Paraview script(s) (currently in Paraview version 5.6) to be applied automatically after the simulation allowing the generation of snapshots or clips of the simulation results. In the default post-processing the coating thickness calculated on the substrate surface is used to generate the inhomogeneity field as in Equation (1). Then unified statistics operations are performed on both the thickness (t) and the inhomogeneity (In) in accordance with Equations (2) and (3), where $\varnothing$ represents either the t or the In field, and the subscript m stands for the median, $Q1$ the first quantile, $Q3$ the third quantile and av for the average values of the field.

$$\mathrm{In} = \frac{\left|\nabla t - \nabla t \cdot \overrightarrow{n_f}\overrightarrow{n_f}\right|}{t} \tag{1}$$

$$\delta_i = \begin{matrix} 0 \Rightarrow \phi_i < \phi_m\text{-}1.5(\phi_{Q3}\text{-}\phi_{Q1}) \vee \phi_i > \phi_m + 1.5(\phi_{Q3}\text{-}\phi_{Q1}) \\ 1 \Rightarrow \phi_i > \phi_m\text{-}1.5(\phi_{Q3}\text{-}\phi_{Q1}) \wedge \phi_i < \phi_m + 1.5(\phi_{Q3}\text{-}\phi_{Q1}) \end{matrix} \tag{2}$$

$$\phi_{av} = \frac{\sum_{i=1}^{N_{cell}} \phi_i \, \delta_i}{\sum_{i=1}^{N_{cell}} \delta_i} \tag{3}$$

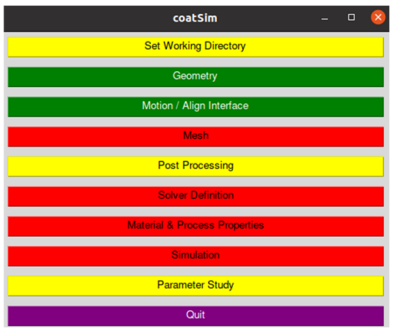

Fig. 1: The color-coded interface of the coatSim software.

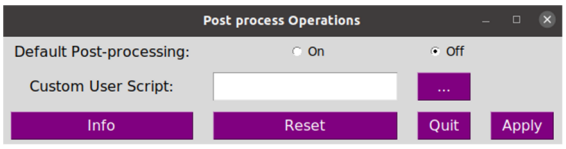

Fig. 2: The interface for the post-processing operations.

Source

[1] Boiger, G. (2016) Characterization of particle-laden flows and deposition behaviour in electro-static fields. Int. Journal of Multiphysics. 10(2), pp. 195–204. http://dx.doi.org/10.21152/1750-9548.10.2.195

1.3 The Effect of Particle-Surface Interactions on Powder Coating Patterns

In industrial processes, powder coating is widely utilized to attain functional or aesthetic surface properties on manufactured parts. Previously a Eulerian-Lagrangian Multiphysics solver has been developed within the OpenFOAM framework in order to simulate the powder coating process [1]. In this study, the powder particle-substrate and particle-particle interactions that occur on the surface of a substrate during the coating process are investigated. This is instigated by the observation that some particles glide over the substrate, rather than sticking to it upon first contact.

Contributors: B. Siyahhan, G. Boiger
Partner(s): Oslo Metropolitan University (OSLOMET)
Duration: 2021-2024

In powder coating micron range powder particles are electrically charged in a coating pistol as they are transported along with a carrier airflow through an electric field generated by an electrode. Once they emerge from the pistol, the particles are driven by a combination of electrostatic and fluid drag forces, towards the electrically grounded substrate, where they either get blown off or stick to the surface. To determine which of the two scenarios hold for a particle, the total force made up of the gravity $\vec{F}_{grav}$, pressure $\vec{F}_{pres}$, shear traction $\vec{F}_{shear}$, electrostatic $\vec{F}_{eStat}$ and particle-particle repulsion $\vec{F}_{rep}$ forces given in Equation (1) is split into it normal $\vec{F}_n$ and tangential $\vec{F}_t$ components as formulated in Equation (2). The ratio of the magnitude of these forces expressed in Equation (3) dictates whether a particle sticks to the substrate. The detailed calculations can be found in [2]. Of these forces, the gravity depends on the orientation of the substrate whereas the pressure and the shear traction depend on the flow field, and the electrostatic to its corresponding field as depicted in fig. 1. Distinct from these, the repulsion force depends on the actual distribution of the particles at a given time point. For a test case involving a 10X10 cm flat plate with a stationary pistol placed at a distance of 15 cm, the non-dimensionalized forces can be illustrated as in fig. 2. The resultant coating patterns have been investigated under two scenarios of stick upon impact (force ratio=0) and stick when the force ratio exceeds 10 as depicted in fig. 3. It can be concluded that the substrate interactions are crucial in determining the final coating pattern correctly and the method needs to be refined further for a closer match to the experimental data.

$$\vec{F}_{tot} = \vec{F}_{grav} + \vec{F}_{pres} + \vec{F}_{shear} + \vec{F}_{eStat} + \vec{F}_{rep} \quad (4)$$

$$\vec{F}_n = \vec{F}_{tot} \cdot \vec{n}\ \vec{F}_t = \vec{F}_{tot} - \vec{F}_n \quad (5)$$

$$r = \frac{|\vec{F}_n|}{|\vec{F}_t|} \quad (6)$$

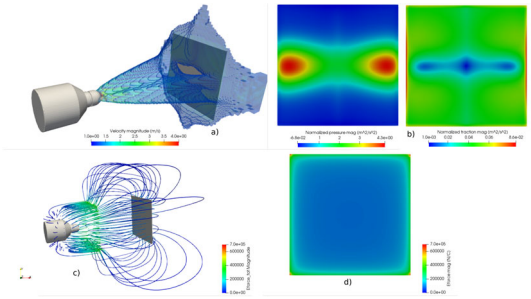

Fig. 1: The flow field in a) allows the calculation of the pressure and the shear traction b) on the substrate. The electrostatic field c) allows the calculation of its corresponding force d).

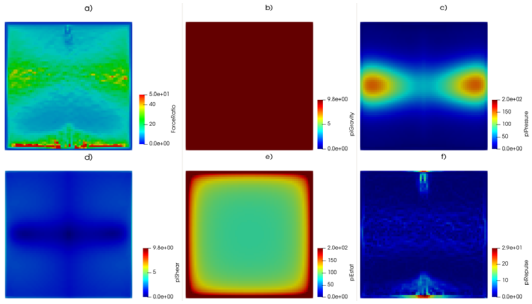

Fig. 2: The non-dimensionalized force components.

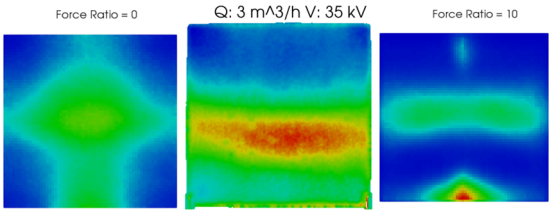

Fig. 3: The coating pattern with the scenario stick upon impact (left) the experimental one (middle) and stick upon force ratio of 10 (right).

Source

[1] Boiger, G. (2016) “Characterization of particle-laden flows and deposition behaviour in electro-static fields.” Int. Journal of Multiphysics. 10(2), pp. 195–204.
http://dx.doi.org/10.21152/1750-9548.10.2.195

[2] Siyahhan, B., Boiger, G., Fallah, A. S., Khawaja, H. and Moatamedi, M. (2023) “Multiphysics Simulation of Particle-Surface Interaction and its Effect on Powder Patterns and Process Optimization”, The International Journal of Multiphysics, 17(1), pp. 77-90. doi: 10.21152/1750-9548.17.1.77

1.4 Simulation of a magnetic sensor system for contactless measurement of absolute position

As part of the development of a linear actuator, a non-contact and cost-effective system for measuring the absolute position of the moving object was developed. The findings from the numerical simulations allow the generation of a model that adapts to magnetisation losses.

Contributors: G. Boiger, A. Schubiger, M. Boldrini, V. Buff
Funding: Innosuisse
Duration: 2023

The development was driven by the need for a cost-effective solution for measuring absolute position in a serial product. The main criteria are cost, precision, stability, complexity and size. The approach investigated uses magnetism and Hall sensors to determine the position. Fig. 1 describes the underlying idea. Permanent magnets are fixed in a magnetically conductive steel sheet. The magnets alternate the direction of their magnetisation. The opposite arrangement of magnets is shifted by a quarter of a periode.

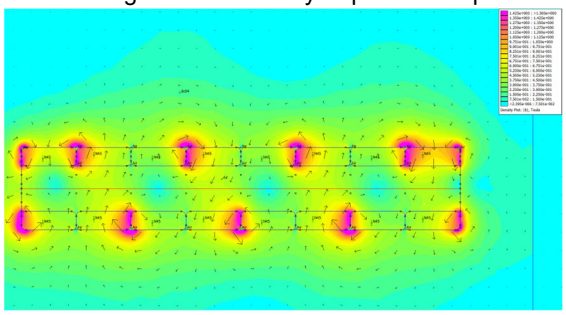

Fig. 1: Solution of the finite element model. The blue lines describe geometry boundaries. The red line describes the movement trajectory of the Hall sensors.

This arrangement produces a periodic signal on the red line. The period length (T) results from the distance between two magnets magnetised in the same direction. Ideally, the sensors move on the red line with the position x and thus measure a position-dependent quantity By(x) normal to the red line. By means of a Fast Fourier Transformation (FFT), it can be shown that the signal can be represented very accurately with the 2nd and 4th harmonic oscillation. A parallel shift of the red line in the direction of the magnets is shown by the shift of the phases of the two oscillations, which is π/2 in the middle and increases or decreases with increasing shift depending on the direction. Furthermore, it has been shown that both the ratio between the amplitudes of the 2nd and 4th harmonic and the difference between the phases of the 2nd and 4th harmonic oscillations remain the same with weaker or stronger magnetisations of the system. Fig. 2 shows this correlation graphically. If a model is formed from the two frequencies and the corresponding phases and amplitudes, this can be adapted to changes in the magnetisation by measuring the peak.

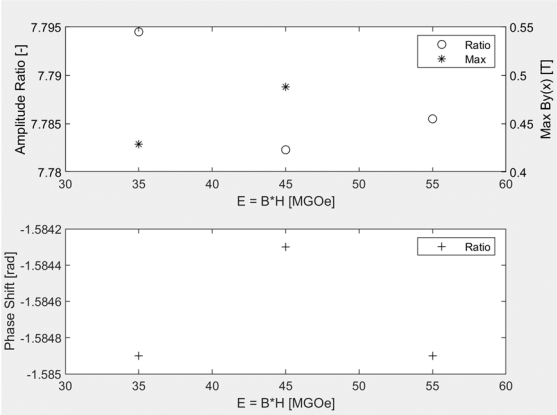

Fig. 2: Top: Influence of the magnetisation of the outer magnets on the ratio of the amplitudes of the 2nd and 4th harmonic oscillation of the signal (o). As well as the maximum of the field strength in y - direction over the entire trajectory (*). Below: Change in the phase of the 2nd and 4th harmonic oscillation of the signal with variable magnetisation.

The simulations and the sensitivity analysis show a promising sensor setup for the absolute position in the measuring range up to 15 mm. The setup is economical and a higher precision is conceivable with a suitable arrangement of additional measuring points. The precision that can finally be achieved depends to a large extent on the precision of the components and the magnetisation. These limits are being tested with an initial prototype.

1.5 Using Neural Networks to create digital twins of 3D tomography images

Digital Material Design (DMD) is a crucial part of developing and discovering new energy materials to tackle challenges such as degradation, efficiency, etc. As 3D tomography is an expensive and time-consuming process, DMD often relies on stochastic digital microstructure twins. We propose a method to create a digital twin based on 3D tomography images, using neural networks and evolutionary optimization algorithms.

Contributors: V. Muser, L. Holzer, P. Marmet, G. Boiger
Partner(s): Math2Market
Funding: Eurostars
Duration: 2022-2025

The development of energy materials is widely accepted to be crucial for tackling future challenges in climate change and population growth. Whether the focus is on storing or generating energy, energy materials play an important role. Unfortunately, the process of inventing or optimizing these materials is expensive and tedious because of the complexity of the fabrication processes, the imaging processes, and the evaluation of the materials. On the other hand, artificial intelligence has developed exponentially in the past decades and has proven to solve complex problems in various scientific areas. It is therefore only natural that Machine Learning (ML) has become an important part in the research of energy materials.

One possibility to apply ML is in the characterization of materials: In [1], a standard characterization for microstructure is developed using GeoDict. The problem with this characterization is that it is computationally expensive and takes a long time to complete. Using Artificial Neural Networks (ANN), a surrogate model for the characterization can be trained, which speeds up the calculations drastically.

In this project, we first created 500 stochastic digital microstructures, using a pluri-Gaussian method (PGM), and for each of these microstructures the standard characterization was calculated. This led to a sample set with the stochastic parameters of the PGM as features and the corresponding results from the standard characterization as labels. By training an ANN, we were able to accurately predict the standard characterization based on the stochastic parameters (Fig. 1).

In a second step, we implemented an evolutionary optimization algorithm to find the optimal set of stochastic parameters that minimize the L1 distance of the corresponding standard characterization values, predicted by the ANN, and a set of given values. This enables an automatic fitting of a stochastic model to a given 3D microstructure material: By calculating the standard characterization of the tomography images, a set of target values is obtained and the optimization algorithm will be able to calculate optimal stochastic parameters that result in very similar characteristics. These optimal parameters can then be used to create a digital twin of the material.

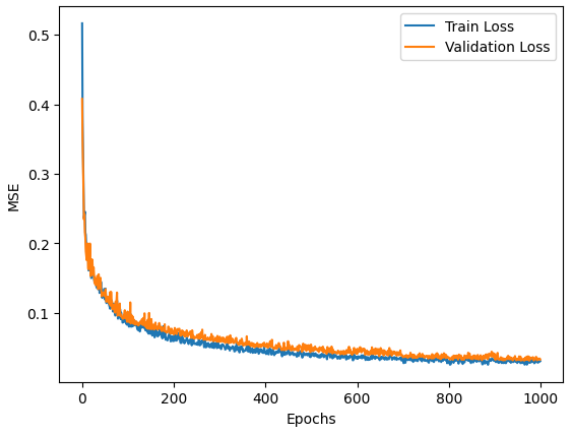

Fig. 1: Train and Validation MSE losses of the ANN over 1000 epochs

Literature:

[1] Marmet, P., Holzer, L., Hocker, T., Boiger, G., Bausinger, H., Mai, A., Fingerle, M., Reeb, S., Michel, D., & Brader, J. (2023). Standardized microstructure characterization of SOC electrodes as a key element for Digital Materials Design. *Energy Advances*

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, highly-accurately dosed volumetric flow rates are required and where fluid contamination must be excluded. Nevertheless, when applied in conjunction with hoses not recommended by the manufacturer, supplied peristaltic flow rates are reported to deviate from expected set flow rates relevantly. In such cases, the dynamic behavior of the used hose material becomes non-negligible and must be taken into account. In the scope of an Innosuisse project, those material effects have been investigated and a simulation method has been developed to correctly predict the pump rate in consideration of the dynamic properties of the hose material.

Contributors: M. Hostettler, G. Boiger
Partner(s): confidential
Funding: Innosuisse
Duration: 2019-2022

The operating principle of peristaltic pumps is based on the cyclic movement of mechanical sliders or rollers, which forces a liquid through a flexible hose (see Fig. 1). Theoretically, the volume conveyed per pump cycle is constant and is determined only by the geometry of the peristalsis. However, this requires that the tube constantly follows this motion and that there is no lift-off of the sliders. Depending on the pumping frequency and the material properties of the hose, however, this cannot be ruled out. This results in a reduction of the conveyed fluid volume per cycle and thus of the effective flow rate.

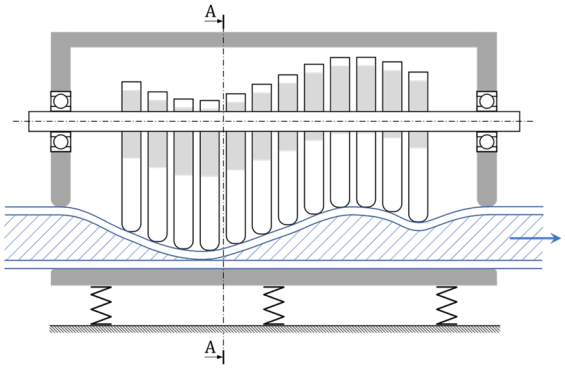

Fig. 1: Cross-sectional view of an exemplary peristaltic pump with a horizontal arrangement of sliders that cyclically deform the hose.

This reduction in pumping capacity is strongly dependent on the viscoelastic properties of the selected hose material and can also change over the operating time due to fatigue effects of the hose. 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 hose 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 hose.

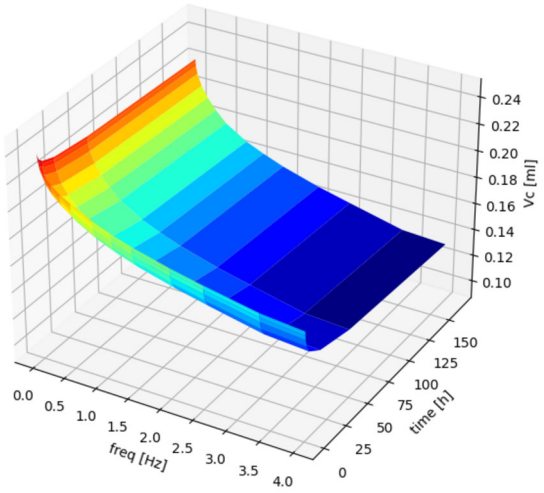

Fig. 2: Simulation results of the decreasing pump performance for a specific hose material. It shows how the conveyed volume per cycle Vc decreases with higher pump frequencies (viscous behavior) as well as over time (fatigue effect).

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

1.7 PhysioCath: CFD-Simulation for therm. Microcatheter blood flow sensor

Cardiovascular diseases (CVD) are the leading cause of death globally, affecting 422.7M people per year. Ischemia with non-obstructive coronary artery (INOCA) increases the risk of major cardiac events, with a 1.5x increased mortality rate. The lack of effective and accurate tools for timely evaluation of coronary impairments creates a great need with a substantial market opportunity. This project aims to develop the PhysioCath microcatheter to measure pressure and mean flow velocity in blood vessels and to be used for effective diagnosis of INOCA.

Contributors: M. Battaglia, S. Ehrat, T. Hocker, C. Kirsch, E. Knapp, J. Sant. de Castro, G. Sartoris
Partner(s): Medyria AG, Ente Ospedaliero Cantonale (EOC), Universitätsspital Zürich (USZ)
Funding: Innosuisse
Duration: 2021–2023

Medyria is developing a proprietary sensor for measuring local, time-resolved blood flow velocities based on the thermal convection principle. The sensor can be small enough for a micro endovascular device and it is combined with an off-the-shelf pressure sensor in a specifically developed microcatheter, the socalled PhysioCath. The system is simple enough to be used during an angiography allowing the operator to see the various cardiac indexes in real time on a portable monitor.
In order to investigate different effects and influences of the PhysioCath geometry on the flow and thermal propagation in a more effective way, CFD simulations support the physical measurements of Medyria. Fig shows the simulation environment of such a geometry. Here, the outer contour of the catheter is reproduced in detail and the interior as precisely as necessary.

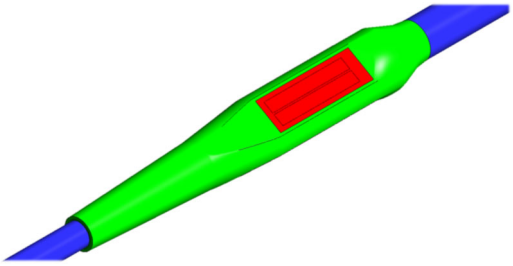

Fig. 1: Illustration of the simulation environment of the PhysioCath without surrounding fluid area (blue: guide wire, green: housing of the PhysioCath, red: heated zone).

Fig. shows the surface temperatures of two simulations with water at different average flow velocities at the inlet. Here the effect of the flow velocity on the temperature distribution at the surface is clearly visible.
Furthermore, in addition to the geometric effect of the PhysioCath, the influence of the fluid used can also be investigated. This is of extreme importance because the material properties of blood differ significantly from water and the handling of such is not pleasant.

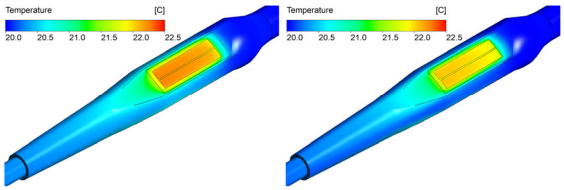

Fig. 2: Temperature distribution on the surface of the PhysioCath at different mean flow velocities of water and the same heating temperature (left: $\bar{v} = 0.1m/s$, right: $\bar{v} = 0.5m/s$).

Fig. compares the required heating power over the average flow velocity of 4 different fluids. It is obvious that the heating power is clearly dependent on the fluid used.
In the future, further CFD simulations will be used to assess the influences of different arrangements of the heating zones, the PhysioCath geometry or the flow channel on the heating performance. In addition, the alignment of the catheter in the flow channel and the difference between a stationary, sinusoidal pulsating and real "blood" flow will be investigated.

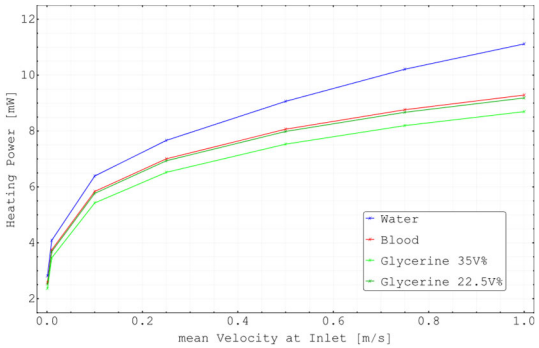

Fig. 3: Required heating power of the PhysioCath above mean flow velocity at the inlet when using different liquids.

1.8 LILLY: Model-based process optimisation of a solid oxide fuel cell

In high-temperature fuel cells (SOFC), the chemical reaction energy from the oxidation of a fuel is converted into thermal and electrical energy. Due to its high overall efficiency and various applications, this technology can make an important contribution to a sustainable energy supply. In the Innosuisse project "LILLY", an interdisciplinary team develops a mobile SOFC system with 50-150 W power. The system can guarantee a low-maintenance and reliable energy supply in remote measuring stations.

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Funding: Innosuisse
Duration: 2022–2024

Three process steps are required to guarantee reliable operation of a SOFC. Reforming (1) produces H2 and CO from hydrocarbons such as propane. Both molecules can be converted into electricity and heat on the cell (2). Subsequently, unconverted fuel is oxidized in the post-combustion (3). Heat is released in all three steps. At the same time, heat is dissipated via the insulation and the exhaust gases. A thermodynamic equilibrium is created, which has a significant influence on the operation of the cell.

To complement measurements and the material development of the project partners, a thermo-fluidic model was created of the reformer, cell and post combustion. With this model, we could show that the thermal conductivity of the housing is an important material parameter. A high thermal conductivity leads to a uniform temperature distribution. This reduces thermo-mechanical stresses in the housing. At the same time, the risk of local temperature minima is reduced. This prevents soot deposition from the gas, which can lead to deactivation of the cell. From these results, a minimum thermal conductivity of the housing material was determined (Fig. 1).

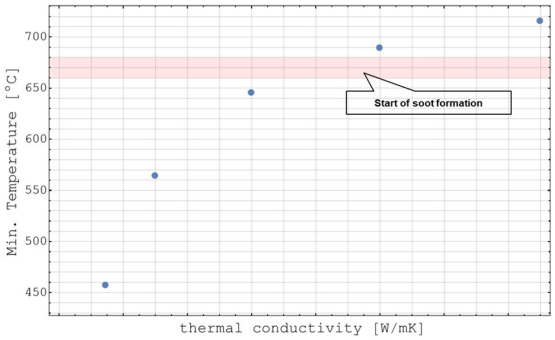

Fig. 1: Minimum temperature in the enclosure for different thermal conductivities

To calculate the boundary conditions for the CFD simulations, a 0D model with global mass, species and energy balances was built. This model can also be used to analyze different operating states with little effort and therewith support process optimization.

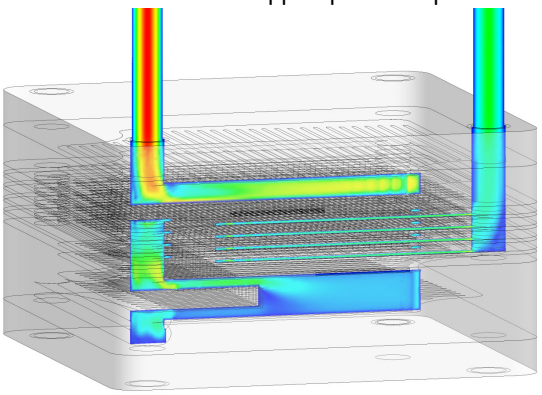

Fig. 2: Velocity distribution in the overall model of the SOFC from Inergio

In the further course of the project, the oxidation reactions will be included in the model of the post combustion. In this way, it can be determined more precisely where the combustion heat is released and how the temperature is distributed in the housing.

In a further step, the flow distribution on the cell can be optimized. For this purpose, we have to couple the CFD simulation with a model for the simulation of current-voltage characteristics. This approach allows us to calculate and visualize the current density on the cell and estimate the influence of design adjustments.

1.9 Massive mesh generation for PhysioCath

Cardiovascular diseases are the leading cause of death globally, affecting 422.7M people per year and the PhysioCath project aims to develop a blood flow velocity sensor for the effective diagnosis of ischemia with non-obstructive coronary artery. Among others, the project requires robust mesh generation to produce massive numerical\&synthetic data to train neural networks by AI.

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Partner(s): Medyria AG
Funding: Innosuisse
Duration: 2021-2023

Medyria is developing a proprietary sensor for measuring local, time-resolved blood flow velocities based on the thermal convection principle. The sensor can be small enough for a micro endovascular device and it is combined with an off-the-shelf pressure sensor in a specifically developed microcatheter, the so-called PhysioCath. The system is simple enough to be used during an angiography allowing the operator to see the various cardiac indexes in real time on a portable monitor.

At ICP, the initial phase of the project was devoted to develop a FE/CFD-model of the PhysioCath system in order to produce large amount of simulation data for AI machine learning. At the beginning, we were using the open-source software (salome); a generic platform for pre- and post-processing. For mesh generation and available out-of-the box are the packages (netgen) and (gmsh). The latter does not really support mesh boundary layers so that all meshing was done with (netgen). Although (salome) GUI interface it not particularly user friendly, it has the advantage that it can be fully driven by python scripts, hence we wrote first scripts to run the CAD construction for parameterized geometries, the meshing and afterwards the numerical simulations all in batch mode. It was more or less working but we were largely unhappy due to the large number of errors showing up everywhere in this pretty large software bundle and the complexity of the scripting. We then decided to remove this bottle-neck.

For these reasons, we have developed our own mesh generator based on a mixture of (netgen), (tetgen) and (seses) software together with the openCASCADE libraries for the CAD construction; the mesh generator uses a python interface. The software is written in C++ and for the CAD construction, basically it just interfaces the various library calls. For the constructed CAD geometry, the library yields the lists of edges, faces and solids which are then meshed singularly. The meshing of edges and faces defined by charts is robust&fast and the major problems arise in the tetrahedralization of solids with a prescribed and beforehand computed triangular surface mesh. There are not yet fail-proof numerical algorithms to run a constrained Delaunay tetrahedralization, however, in practice, the (tetgen) based generator is pretty robust, much less the one based on (netgen). On success, however, this latter yields better shaped tetrahedra, whereas the former generates more flat also called sliver tetrahedra.

To these basic software components, which have been rewritten to fit our data structures, we have added additional features e.g. for boundary layers and the possibility the define the mesh size functionally on input, thus allowing to finely tune edge&surface&volume meshing. The just-in-time compiler for a fast evaluation has been taken from (seses). The next Fig. shows a mesh of ca. 2.2M tetraheda generated in ca. 40 s using the mesh size function MaxH*((1-0.10)/6.25*(z*z-5*z)+1) on a z-axis cylinder of length 5 and with MaxH=0.3.

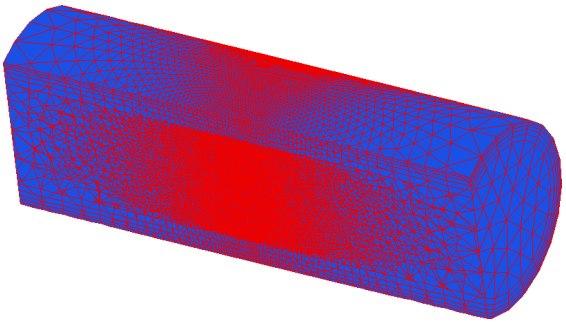

Fig. 1: Tetrahedral mesh with boundary layer and of variable size

1.10 Digital Materials Design of Ceramic Solid Oxide Fuel Cell Anodes

In an industrial PhD project, a Digital Materials Design (DMD) framework was established, allowing for a systematic and knowledge-based materials and microstructure optimization of novel solid oxide fuel cell (SOFC) anodes. In our DMD approach we combine stochastic microstructure modeling, virtual testing of 3D microstructures and a multiscale-multiphysics electrode model to explore the available design space by performing parametric studies.

Contributors: P. Marmet, L. Holzer, T. Hocker, V. Muser, G. K. Boiger
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Funding: Swiss Federal Office of Energy, Eurostars
Duration: 2019–2023

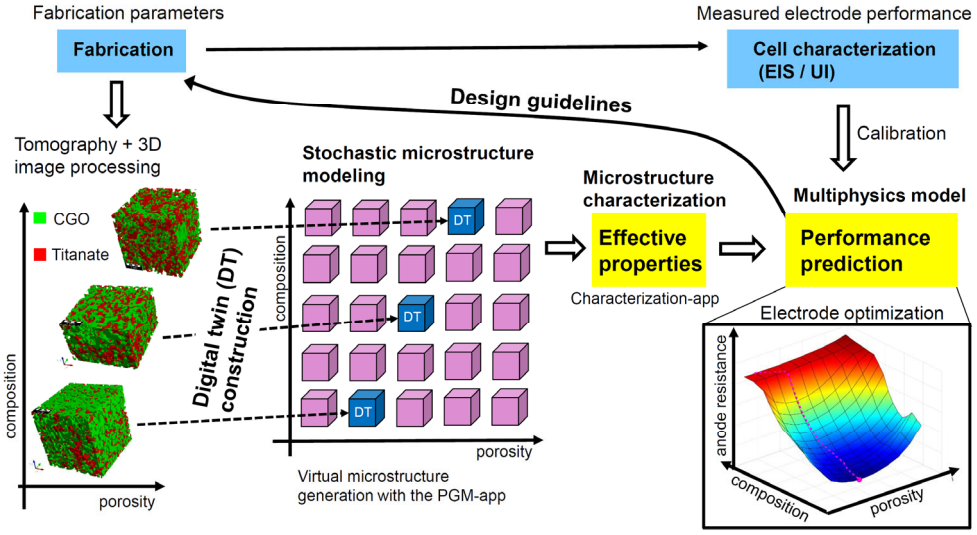

Fig. 1: Simplified overview of Digital Microstructure Design (DMD) methodologies: Stochastic microstructure modeling including virtual structure generation based on a pluri-Gaussian method (PGM-app), standardized microstructure characterization automated with the characterization-app and calibrated multiphysics model for electrode performance prediction. The DMD workflow can be used for a systematic material and microstructure optimization, resulting in design guidelines for the fabrication of electrodes with improved performance.

Solid oxide fuel cell (SOFC) technology is a promising solution for the on-demand supply of electrical energy using synthetic gas or biogas (or natural gas) as input. To significantly improve state-of-the-art anodes like Ni-YSZ, we elaborate on new nickel-free electrode concepts, which are based on mixed ionic and electronic conductors (MIEC) like doped ceria and perovskite (e.g., titanate) materials. However, there are numerous conflicting requirements complicating the development and optimization process with conventional methods of materials processing. To address these challenges a Digital Materials Design (DMD) framework for the systematic and model-based optimization of MIEC SOC-electrodes is elaborated. In our DMD approach we combine stochastic microstructure modeling, virtual testing of 3D microstructures and a multiscale-multiphysics electrode model to explore the available design space by performing parametric studies. The basis for the DMD process is a set of fabricated solid oxide cells. Their real microstructures are reconstructed using FIB-SEM tomography. Stochastic digital microstructure twins with matching microstructure properties are then constructed for each real structure using a pluri-Gaussian method. On that basis, the microstructure can be virtually varied for a large parameter space in a realistic way. A multiphysics continuum simulation model, calibrated to the experimental performance characterization of the cells, is then used to predict the impact of the microstructure variation on the electrode performance. This model-based approach enables to establish the relationship between materials choices and compositions, fabrication parameters, microstructure properties and cell-performance. This approach is thus capable to explore a much larger design space than it would be possible with experimental methods only. On this basis, design guidelines for the fabrication of electrodes with improved performances can be provided.

Literature:

[1] P. Marmet, PhD thesis, Digital Materials Design of Solid Oxide Fuel Cell Anodes, University of Fribourg, Switzerland, 2023.
[2] L. Holzer et al., Tortuosity and microstructure effects in porous media: classical theories, empirical data and modern methods, 1st ed. Springer Cham, 2023, ISBN: 978-3-031-30477-4.

1.11 Standardized Microstructure Characterization of SOC Electrodes

A software tool for 3D image processing and modeling was developed, which enables the analysis of microstructure properties of solid oxide cell (SOC) electrodes. A large number of microstructure characteristics can be determined, which are relevant for the performance of conventional electrodes like Ni-YSZ as well as for more modern electrodes that are based on mixed ionic and electronic conductor (MIEC) like Ni-CGO or titanate-CGO anodes. This 3D characterization tool is a key element for Digital Microstructure Design and open science concepts, as it provides automated and standardized microstructure characteristics in an efficient way. The tool is integrated into the commercial microstructure modeling software GeoDict from Math2Market.

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Partner(s): Math2Market, HEXIS, University of Fribourg
Funding: Swiss Federal Office of Energy, Eurostars
Duration: 2019–2023

Performance and durability of solid oxide cell (SOC) electrodes are closely linked to their microstructure properties. Thus, the comprehensive characterization of 3D microstructures, as e.g., obtained by FIB-SEM tomography, is essential for SOC electrode optimization. Recent advances and trends call for a standardized and automated microstructure characterization. Advances in FIB-SEM tomography enable the acquisition of more samples. Moreover, it is expected that the open science concepts will result in a tremendous increase of publicly available 3D-microstructure data from tomography of energy materials. In order to make reasonable comparisons of these 3D microstructures from different sources and to make reliable statistical analyses, these structures need to be analyzed with standardized 3D image processing tools. In addition, the emerging methods for Digital Materials Design (DMD) enable to create numerous virtual but realistic microstructure variations using stochastic microstructure modeling and to test them with multiphysics electrode simulations. For such a DMD workflow, many virtual microstructures need to be characterized. Thus, the availability of a standardized, efficient and automated microstructure characterization tool is a crucial prerequisite for the data-driven optimization of energy materials.

The standardized microstructure characterization tool for SOC electrodes is implemented as a Python app for the GeoDict software-package, which is published on Zenodo public repository [1] and described in a separate publication in detail [2]. A large number of microstructure characteristics can be determined with this app, which are relevant for the performance of conventional electrodes like Ni-YSZ and for more recent MIEC-based electrodes like Ni-CGO or titanate-CGO anodes. The list of 3D characteristics that can be determined selectively is long. An overview of the characterized microstructure properties is provided in Fig. 1. It includes morphological characteristics (e.g., tortuosity, constrictivity, effective volume fraction and size distributions for solid and for pore phases separately), interface properties (i.e., interface areas and three-phase boundary length) and effective transport properties deduced from morphological predictions and from numerical simulations (also for each phase and/or for each transported species separately). The standardized and automated microstructure characterization is a key element to exploit the full potential of open science, Digital Materials Design (DMD) and artificial intelligence (AI) for the data-driven optimization of SOC electrodes by providing standardized high quality microstructure property data.

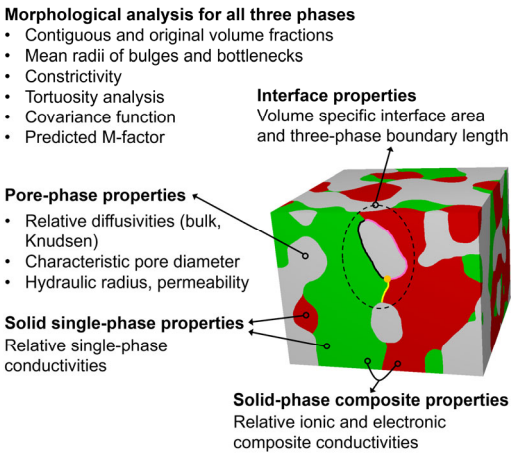

Fig. 1: Overview of the characterized microstructure properties for the two solid-phases, the total composite solid-phase, the pore-phase and the interface properties.

Literature:

[1] P. Marmet et al., “Characterization-app: Standardized microstructure characterization of SOC electrodes as a key element for Digital Materials Design,” Zenodo, 2023, doi: https://doi.org/10.5281/zenodo.7741305.
[2] P. Marmet et al., “Standardized microstructure characterization of SOC electrodes as a key element for Digital Materials Design”, Energy Advances, 2023, doi: 10.1039/D3YA00132F.
[3] L. Holzer et al., Tortuosity and microstructure effects in porous media: classical theories, empirical data and modern methods, 1st ed. Springer Cham, 2023, ISBN: 978-3-031-30477-4.

1.12 Stochastic Microstructure Modeling of Solid Oxide Cell Electrodes based on a Pluri-Gaussian Method

A tool for the stochastic microstructure modeling of solid oxide cell (SOC) electrodes based on a pluri-Gaussian method (PGM) was developed. The PGM-app allows for an efficient construction of virtual but realistic 3D microstructures consisting of three phases (two solid-phases and one pore-phase). The app is integrated into the commercial GeoDict software package. This approach allows for a systematic materials and microstructure optimization of SOC electrodes by exploring a much larger design space than it would be possible with experimental methods only.

Contributors: P. Marmet, L. Holzer, T. Hocker, V. Muser, G. K. Boiger
Partner(s): Math2Market, HEXIS, University of Fribourg
Funding: Swiss Federal Office of Energy, Eurostars
Duration: 2019–2023

Digital Materials Design (DMD) offers new possibilities for data-driven microstructure optimization of solid oxide cells (SOC). Despite the progress in imaging technology, 3D-imaging still represents a bottleneck for data driven optimization. Experimental microstructure variation studies are typically limited to a few 3D tomographies. Thus, a workflow for the virtual but realistic microstructure variation based on real tomography data is presented using stochastic microstructure modeling. The basis for this workflow is a suitable virtual structure generator. The pluri-Gaussian method (PGM) has shown to provide realistic virtual microstructures with well matching microstructure properties for SOC electrodes (e.g., [2]). As illustrated in Fig. 1, three-phase microstructures (two solid phases and one pore-phase) can be constructed in a very efficient way. The virtual structure generation based on the PGM is available on Zenodo public repository [1] as a Python app for the GeoDict software package. Moreover, a slightly adapted version is also implemented as a so-called GeoApp in the GeoDict release 2023. Fig. 2 illustrates examples for stochastic digital microstructure twins, which are constructed with the PGM-app for a set of three real 3D microstructures. The real structures are captured with FIB-tomography from LSTN-CGO anodes with different compositions and porosities. In order to match the microstructure properties of the real structures, the construction parameters for the PGM-model are determined by interpolation of a database of virtual structures. Moreover, the relative conductivities of the phases are optimized using morphological operations. The three stochastic digital microstructure twins can then be used as anchor points for a virtual microstructure variation for LSTN-CGO composition and porosity.

For all the virtual structures of the parameter study, the corresponding microstructure properties can be determined using our new software tool for automated microstructure characterization (see separate report in this volume). The resulting set of microstructure properties for the whole parameter space represents the basis for performance predictions with a multiphysics electrode model, which then enables to postulate design guidelines of an electrode with improved performance.

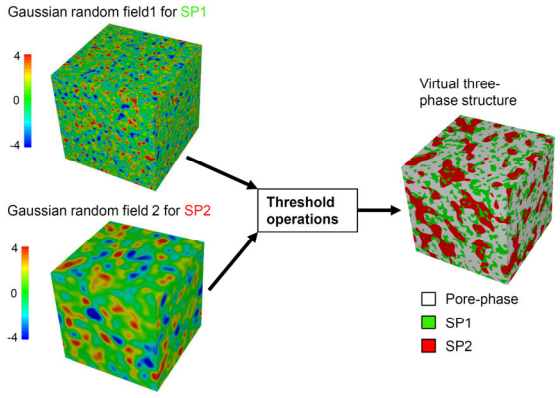

Fig. 1: Illustration of the virtual structure generation with pluri-Gaussian method. Two Gaussian random fields are combined with threshold operations to achieve three phases (two solid phases SP1 and SP2 and one pore-phase) with defined phase volume fractions and wetting behavior.

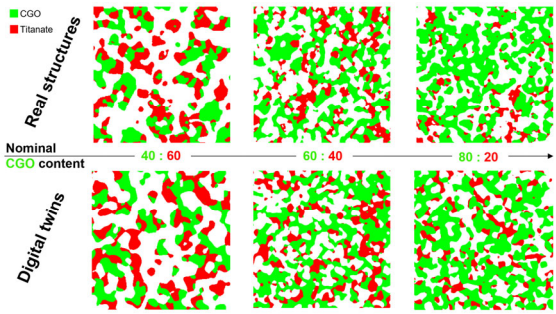

Fig. 2: Visual comparison of the real microstructures and their corresponding digital microstructure twin's.

Literature:

[1] P. Marmet et al., "Python app for stochastic microstructure modeling of SOC electrodes based on a pluri-Gaussian method," Zenodo, 2023, doi: https://doi.org/10.5281/zenodo.7744110.
[2] H. Moussaoui et al., "Stochastic geometrical modeling of solid oxide cells electrodes validated on 3D reconstructions," Comput. Mater. Sci., vol. 143, pp. 262–276, 2018, doi: 10.1016/j.commatsci.2017.11.015.

1.13 Digital Wolfram: optimizing Tungsten Inert-Gas (TIG) welding processes

In this multidisciplinary Innosuisse project we aim at developing Digital Wolfram (DW), an embedded hardware- and software-based expert system tailored to TIG-welders for monitoring and optimizing their processes. DW uses live current- voltage-, optical and acoustic data to forecast process irregularities and provide actionable recommendations.

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Funding: Innosuisse
Duration: 2023–2025

Even though Tungsten Inert Gas (TIG) welding is the premium metal joining technology, aspects critical to both the weld quality and the costs such as the timely replacement of the degrading tungsten electrode to date purely rely on empirical knowledge. Despite the broad range of available sensor technologies, in-line data collection and real-time signal processing capabilities available monitoring tools generally lack built-in "intelligence" to, e. g., use live current-voltage data to detect bad arc strikes to indicate a worn-out electrode.

This deficiency motivated Wolfram Industrie Switzerland (WIS) who optimizes TIG-welding processes for customers in the aerospace, nuclear, and semiconductor industries, to investigate them in their in-house lab on a more fundamental, science-based level. In collaboration with their partners from BFH and ZHAW, they could detect various process irregularities by combining current-voltage with optical and acoustic emission analyses.

This triggered the idea of Digital Wolfram (DW), a hardware- and software-based expert system tailored to TIG-welders for monitoring and optimizing their processes. DW will use data- and rule-based machine learning models to analyze live sensor data, detect irregularities and suggest actions to be taken. Concerning the latter, to reach a success rate of above 90 %, the employed models will be trained with in-house sensor data under well-controlled conditions in combination with extensive weld quality and electrode aging characterizations performed by our academic partners. For maximum reliability, DW will provide unique features such as measuring the voltage during the arc ignition phase by proprietary hardware.

Three key clients will act as beta testers and early adopters. Since DW can be retrofitted to TIG-welding machines at a competitive price it has a huge potential to reach broad market acceptance.

Fig. 1 gives an overview about DW's hardware and software components. The control unit collects data from an internal current-voltage sensor and optional external optical and acoustic emission sensors placed close to the weld head. This data is processed and fed to an expert system that identifies process irregularities and provides actionable recommendations to the operator.

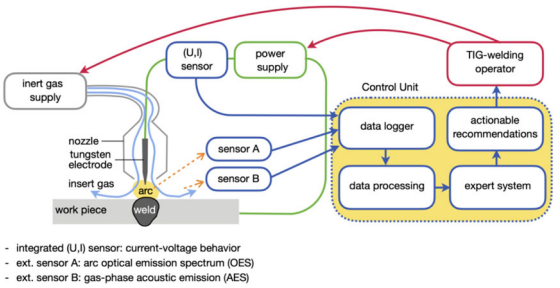

Fig. 1: Digital Wolfram's hardware and software components.

To reach broad market acceptance a key feature of DW is the simplicity with which it can be combined with any existing TIG-welding equipment. This is illustrated in Fig. 2 which shows a mockup of the DW control unit placed underneath a typical TIG-welding power supply. The control unit will contain standard connectors for placing it in between the power supply and the closed or open weld head. And since DW will come with appropriate connector cables our customers will be able to put it into operation in a plug-and-play manner.

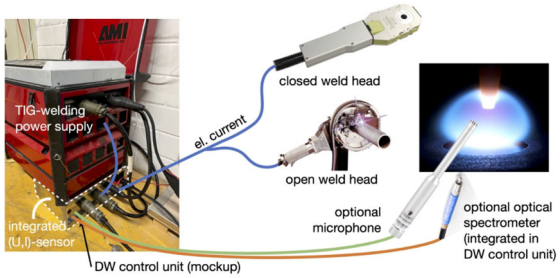

Fig. 2: mockup of the Digital Wolfram control unit.

2 Electrochemical Cells and Microstructures

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 mesoscale 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 MiEl, where we are working on the simulation of electrode structures and the model-based analysis and design of electrochemical flow cells.

We are mainly active in the modelling and simulation of electrochemical flow cells on three length scales, that is, the electrochemical double layer, mesoscale models to link processes that occur on the double layer scale and the continuum representation of porous electrodes, and on cell scale models. Thereby, we account for the coupling of electrochemical reactions and transport phenomena of momentum, mass, heat, and charge. We use these models to simulate cell performance and degradation phenomena but also to perform parameter sensitivity studies, and uncertainty propagation analysis.


D. Bernhardsgrütter


A. Cucchi


R. Schärer


J. Schumacher

2.1 Freely Available Web Application to Simulate Pedestrian Flow and the Associated Spread of Infectious Diseases

How can public spaces be designed to minimize the risk of infection during an epidemic? Within this project, a freely available web application is created, which allows the analysis of epidemic events at local level such as educational institutions or pedestrian zones. The simulations are based on a model describing the movement of pedestrians and are coupled with an epidemiological model.

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Financing: Interreg Alpenrhein-Bodensee-Hochrhein
Duration: 2021–2023

In a pandemic situation, protective measures are needed that severely restrict social life and the economy. The consequences of the interventions are often difficult to assess and there is a lack of knowledge to determine the optimal level of restrictions.
The question arises whether, for example, business closures can be avoided if the probability of spreading an infectious disease can be reduced by optimal room design. The aim of the project is to develop a software tool that can be used to simulate pedestrian movement and the associated probability of infection with various infectious diseases. The basis is the simulation software pFlow, which calculates the pedestrian flow of evacuation scenarios. pFlow has been developed at the ICP and at the HTWG in the past years [1].
The description of pedestrian flow is now coupled with an epidemiological model in the current project. With the possibility to simulate the spread of infections in a moving crowd, we obtain a novel tool that can be used to deduce design rules for spaces from an epidemiological point of view.
The simulation tool is available as an intuitive web application on our project website [2]. The users have the possibility to design spaces and to set numerous parameters that define the behavior of pedestrians and the associated spread of infectious diseases.

For example, the question can be investigated whether it is advantageous for a safe school operation during an epidemic to remove tables from classrooms. The simulation of both room configurations (a conventional room versus a room with fewer tables) is shown in Figure 1. The removal of the tables is advantageous only at the beginning of the evacuation. People can move faster and freely, which is why they reach the exit quickly. Consequently a jam is developed at the exit in this room configuration with fewer tables, which results in a higher rate of infection.
The web application can be used to analyze rooms in terms of crowd management and minimizing the risk of infection during an epidemic.

Literature:

[1] R. Axthelm, “Finite Element Simulation of a Macroscopic Model for Pedestrian Flow”, Traffic and Granular Flow ’15, Springer, 2015.
[2] Project website: http://www-home.htwg-konstanz.de/~raxthelm/eFlow/

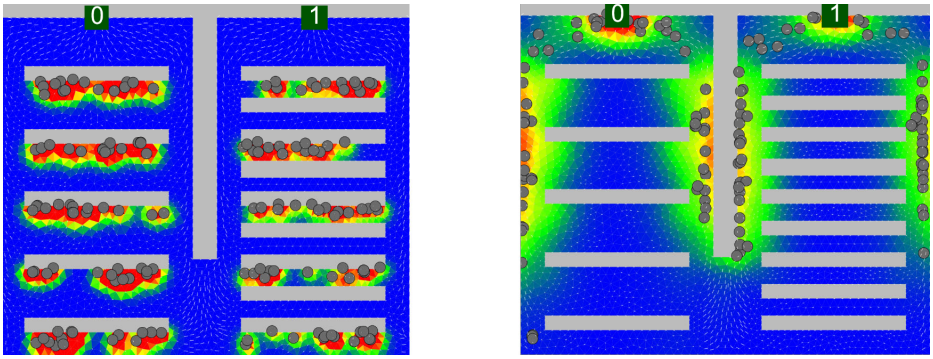

Fig. 1: Simulation of the evacuation of a classroom with removed tables (left half of the room) and a conventional room (right half). The exits are marked with numbers. The starting situation is shown on the left, the end of the evacuation is shown on the right. The removal of tables leads to a jam at the exit, which has a negative effect on the infection rate.

2.2 Modelling of Effective Transport Parameters in Porous Electrodes

Porous electrodes are a central component of electrochemical cells in redox flow batteries (RFBs) for stationary energy storage. In RFBs, dissolved electroactive molecules flow through porous electrodes where they react electrochemically at the electrode surface. Due to the complex geometry of technical electrodes, homogenised models are often used in macroscale descriptions, which consider the influence of geometry and transport processes on the pore scale by effective transport parameters. Within the SONAR project, a model for the calculation of effective transport parameters is being developed at the ICP. In particular, the model allows for the calculation of the electrolyte permeability as well as the effective diffusion, dispersion, and reaction rate of electroactive molecules for macrohomogeneous cell models of RFBs.

Contributors: R. P. Schärer, G. Mourouga, J. Wlodarczyk, J. O. Schumacher
Partner(s): ICT (DE), SCAI (DE), DTU (DK), LRCS (FR), KIT (DE), UNSW (AU)
Funding: European Union's Horizon 2020 research and innovation programme
Duration: Jan. 2020 – Dec. 2023

Macrohomogeneous cell models enable an efficient description of the macroscopic transport processes in electrochemical cells. Since the macrohomogeneous models are based on a local averaging of the pore scale description, the influence of the porous electrode geometry on the macroscopic transport processes must be modelled by effective parameters.

The macroscopic description can be derived from a pore scale description using the volume averaging method (VAM), among other methods. This allows the numerical calculation of the effective transport parameters for macrohomogeneous cell models.

The porous electrode is described simplistically as a periodic structure generated by a periodic continuation of a unit cell. To investigate the relationship between the geometry and the effective parameters, we consider different unit cells of the porous electrode which are shown in Fig. 1. The cylinders represent the simplified geometry of carbon fibres used in porous felts.

Fig. 2 shows as an example the predicted total dispersion, which is the sum of the effective diffusion and dispersion, for different geometries with a porosity of 90% as a function of the Péclet number. Fig. 3 shows a verification of the porous electrode model (VAM) in which the concentration profile of an electroactive molecule predicted using a macrohomogeneous description with the corresponding transport parameters evaluated for the SCd-2D unit cell geometry is compared with a direct simulation on the pore scale (DNS).

A reduced model for evaluating the effective parameters is published as open-source software on our GitHub repository [2].

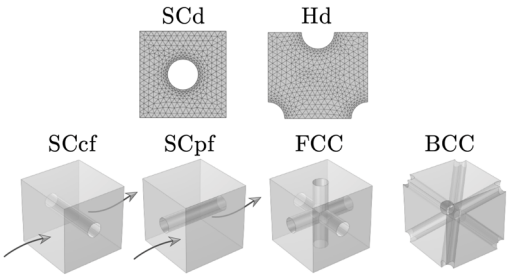

Fig. 1: Simplified unit cell geometries of porous electrodes, where the cylinders represent carbon fibres of porous felt materials.

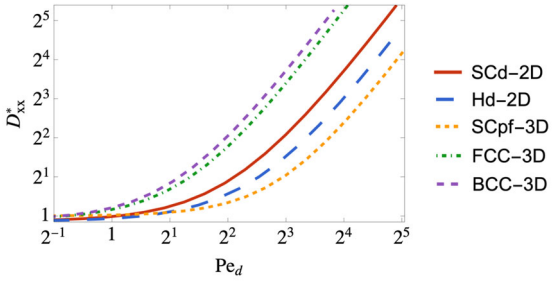

Fig. 2: Total dispersion as a function of the Péclet number for the above unit cell geometries.

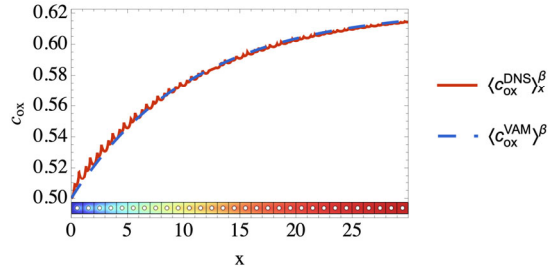

Fig. 3: Comparison oft he evaluated species concentrations of an electroactive substance between DNS and VAM over 30 unit cells (SCd-2D) oft he porous electrode.

Literature:

[1] SONAR project web site: https://www.sonar-redox.eu

[2] GitHub repository: https://github.com/Isomorph-Electrochemical-Cells

2.3 Robust PEMFC membrane electrode assemblies 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/cm² at a cell voltage of 0.65 V, with a platinum loading of 30 g/kW.

Contributors: J. Schumacher, R. Schärer, A. Cucchi
Partner(s): CEA, Chemours, DLR, Heraeus Deutschland GmbH & Co. KG, IMERYS, IRD Fuel Cells
Funding: Horizon Europe (HORIZON-JTI-CLEANH2-2022-03-02)
Duration: 2023–2026

The project aim is to overcome the durability limitations of polymer electrolyte membrane fuel cells (PEMFC) 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 of providing the innovated and improved different sub-components for the catalyst coated membrane (CCM).

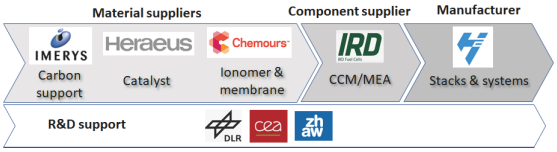

Fig. 1: Main contributions of the PEMTASTIC partners

The workflow has been divided into different objectives: Objective 1 addresses the definition of fuel cell operation protocols and cycling tests for heavy duty application and the proposition of operation strategies for high fuel efficiency. Next, parametrization of degradation models is performed in order to predict MEA lifetime and identify improvements for CCM and its sub-components (Objective 2). Thus, the development of robust catalyst support, membrane and ionomer is conducted for operation at increased temperature (Objective 3 and 4). Successively, catalyst layers and CCMs with increased durability for applications will be identified for use in heavy duty vehicles (Objective 5). Finally, ad-hoc strategies will be defined in order to ensure the dissemination of the project results, its promotion and its exploitation (Objective 6).

The objectives mentioned above are implemented via a specific methodology of collaborations between the partners of the project. Truck mission profiles will be analyzed for defining relevant fuel cell operation protocols. Degradation tests will be carried out in differential cells by use of physical-chemical material characterization. For CCMs, advanced corrosion resistant supports materials will be used in combination with novel catalyst deposition technique. As for the ionomers and membrane, prototype Nafion® ionomers and membranes with high conductivity in dry conditions will be used. A combination of micro- and mesoscale models in 1D and 2D cell scenario will capture the impact of the material parametrizations on performance and durability. The purpose is to assure well defined data for parametrizations of degradation models and select CCM materials which will be used by the industry partners.

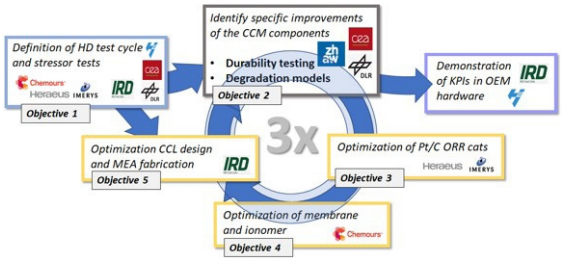

Fig. 2: Workflow methodology of the PEMTASTIC partners

References:

https://cordis.europa.eu/project/id/101101433

2.4 New synthesis concepts for pharmaceutical/fine chemical industry

MiEl is a research and training project funded by the European Union's Marie-Sklodowska-Curie programme. MiEl involves 9 partner organisations and 5 associated partners from 9 different countries, who will recruit 12 PhD students for the project. MiEl will develop a novel synthesis technology for the chemical industries, combining the advantages of electrochemistry, micro process engineering and flow chemistry. The ambitious research objective is to upscale these technologies using integrated cell concepts such as printed circuit board (PCB) technology with integrated process control functionalities, which can be assembled in arrays for the safe, flexible and sustainable synthesis of chemical products. It will allow new synthetic routes for the sustainable chemical industry of the future.

Contributors: J. O. Schumacher, R. P. Schärer
Partner(s): Fraunhofer ICT, University of Amsterdam, Technical University of Denmark, University for Continuing Education Krems, UCT Prague, University Paris Cité, Innoverda, eChemicles, Janssen Pharmaceutica
Funding: European Union: Horizon-MSCA-2021-DN-01-01
Duration: 2023–2026

In the European doctoral network project MiEL 12 doctoral students will develop synthesis technology for the chemical industries of the 21st century by combining the advantages of electrochemistry, micro process engineering and flow-chemistry. In theory, electrochemical technologies offer the highest energy efficiency in production as well as microfluidics offer the highest safety and best process control in chemical processes. A combination of these two technologies seems to be the logical step towards a more reliable, flexible, safe and sustainable chemical industry. Especially for the synthesis of fine chemicals or pharmaceuticals with relatively low output but specific chemistry like fluorination, this route offers some advantages in production.

Three synthesis routes will be investigated:

- two-phase electrosynthesis
- aqueous
- non-aqueous electrolytes

These three reaction paths can be regarded as relevant model processes for the pharmaceutical/fine chemical industry. The ambitious research objective is to upscale these technologies using integrated cell concepts such as printed circuit board technology (PCB technology) with integrated process control, with in-situ optimized yield control.

The cells can be assembled in synthesis arrays for the safe, flexible and sustainable synthesis of chemical products, which can also be used for catalytic screening. This approach will allow to find new synthetic routes for the sustainable chemical industry of the future.

MiEls network is embedded into a modelling community, which develops models on different length scales helping to simulate electrode structures with multi-phase flow of fluids, multi-electron step reactions, and electrochemical flow cells. A tecno-economical investigation provides guidance of all disciplines and ensures that the outcome of the project is to define the economic and ecologic "sweet spot" in applied electrosynthesis.

Fig. 1: Organization of work in the MiEl research project

References:

[1] MiEl project web site: https://project-miel.eu

2.5 Macroscopic Cell Models for Organic Redox Flow Batteries

Redox flow batteries (RFBs) 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. However, identifying well-suited compounds for RFBs is challenging due to the large chemical space available. 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 RFB 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
Partner: ICT (DE), SCAI (DE), DTU (DK), LRCS (FR), KIT (DE), UNSW (AU)
Financing: European Union's Horizon 2020 research and innovation programme
Duration: Jan. 2020 – Dec. 2023

RFBs 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 electro-active 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 non-linear 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 RFB cell as a function of the electric current density as predicted by the RfbScFVM 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].

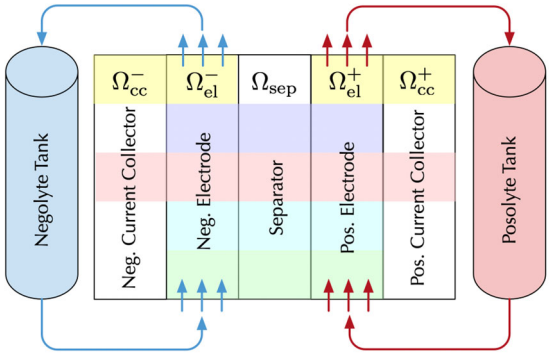

Fig. 1: Simplified model geometry of a flow cell.

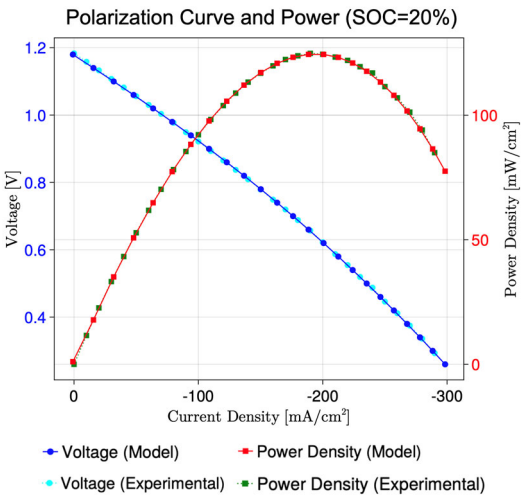

Fig. 2: Cell voltage and power density of a lab sized cell at state of charge 20%.

Literature:

[1] SONAR project web site: https://www.sonar-redox.eu

[2] GitHub repository: https://github.com/Isomorph-Electrochemical-Cells

3 Organic Electronic 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.


M. Auer


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S. Shaji


A. Schiller


M. Torre


W. Tress


O. Zbinden


S. Zeder

3.1 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: Şevki Can Cevher, Gabriela Kissling, Evelyne Knapp, Kurt Pernstich
Partner(s): Fluxim AG
Funding: Swiss National Science Foundation (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 multiphysics 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. The data will be fed into a detailed theoretical model. Common numerical models can then be optimized using our experimental results.

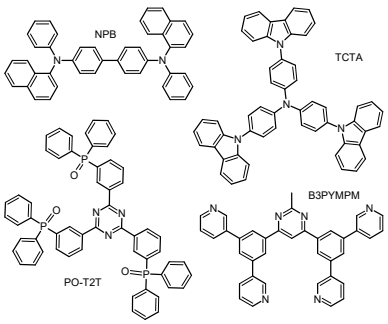


Fig. 1: Molecular structures of four common OLED materials.

We are using electrochemical methods to characterize organic semiconductor materials, consisting of molecules such as the ones shown in Fig. 1. 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 Fig. 2, and correlate well with literature data.

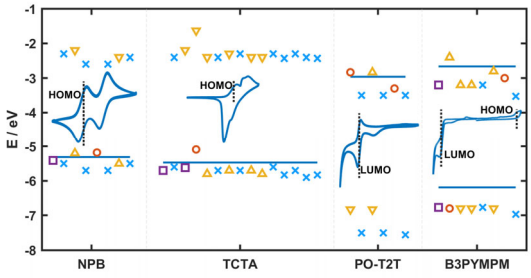


Fig. 2: Exemplary cyclic voltammetry measurements of the various OLED materials and comparison of measured HOMO/LUMO (lines) energies with literature data (markers).

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. Fig. 3 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.

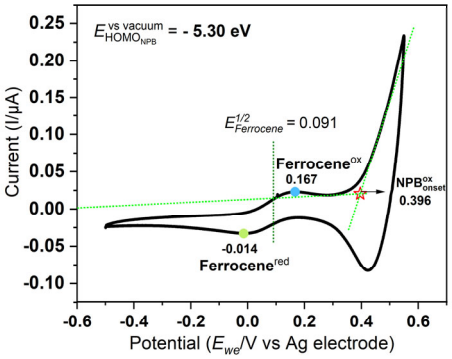


Fig. 3: Cyclic voltammetry measurement of an NPB film.

3.2 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: Kurt P. Pernstich, M. Frioud, A. Bachmann, C. Kirsch, M. Regnat, B. Ruhstaller
Partner(s): 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. Fig.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.

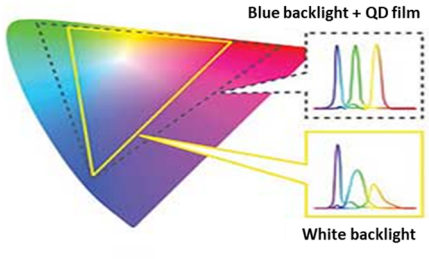


Fig. 1 Color gamut and spectral output of a display using a blue backlight plus QD film or just a white backlight unit. Source: Photonics.com.

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 also in the development of a measuring device for the detailed investigation of QD films and QD-OLEDs. Fig.2 shows the second prototype of this instrument, which allows to measure the edge-degradation of QD films at various temperatures and different environmental conditions such as an inert nitrogen atmosphere or dry/humid air.

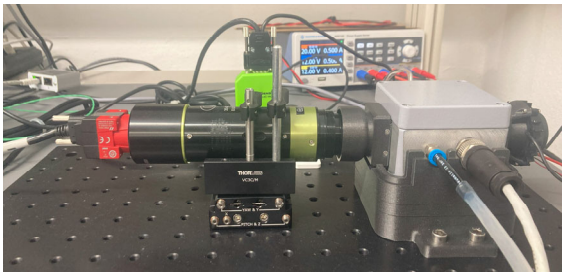


Fig. 2 Second prototype of the thin film degradation tool with the environmental chamber, LED illumination, lens, and camera.

Fig. 3 shows the measured and simulated spectra of a blue backlight unit without (blue) and with red-emitting QD film (red). At present, the prototype implementation of the newly developed optical model that maintains the polarization state is being implemented by our industrial partner Fluxim.

Having a fully developed QD model allows to optimize the QD film and the parameters of the backlight unit respectively the OLED simultaneously to find an optimal combination.

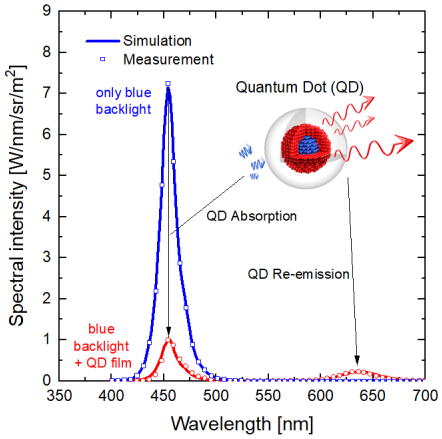


Fig. 3 Simulated (lines) and measured spectra (symbols) of blue backlight without (blue) and with red emitting QD film (red). Inset image illustrates absorption of blue light and re-emission of red light of a quantum dot. Source of inset image: Osram

3.3 Understanding Solar Cells at Nanoscale for Efficient Renewable Energy

Contributors: Amit Kumar Sachan, Hajar Moumine, Nasim Kabir, and Wolfgang Tress
Funding: ERC Starting Grant
Duration: 2020–2025

Photovoltaics (PV) plays the key role for the transition of our energy supply system to a sustainable low-CO_2 economy. Among PV, the perovskite solar cell (PSC) recently has garnered much attention due to its exemplified improvement in the power conversion efficiency (PCE) from ~3% to more than 25% on the lab scale in the timespan of just over a decade. A typical working PSC device (thickness below 1 µm) contains a series of thin material layers (thicknesses from few nanometers to ~ 500 nm), and the photoactive perovskite thin layer, prepared either from solution or thermal evaporation, contains polycrystalline grains (10-400 nm in sizes) and grain boundaries (GBs). Imperfections within grains and on differently oriented grain facets and GBs can lead to localized energy states causing trapping of photogenerated carriers and yielding lower photogenerated potential and efficiency. Therefore, to further improve the efficiency of PSCs to the theoretical limit of ~ 33%, it is warranted to study and understand the phenomenon at the nanoscale dimensions.

In this project, we aim to uncover the opto-electronic phenomena happening at the nano- and microscale within photo-active layer (perovskite) and other essential layers as well as at the heterojunction interfaces of PSCs fabricated in-house in a glovebox environment as well as by collaborators. To achieve the goals, we are exploiting the state-of-the-art atomic force microscopy (AFM) technique where a force-sensitive mechanical probe (up to piconewton sensitivity) is routinely used to scan the material' surface and yields morphological properties at the nanoscale dimensions. High-end derivatives of AFM technique, such as Kelvin probe force microscopy (KPFM) and conductive AFM (cAFM) are being used to understand how the nano and microstructures, including intragrain defects, GBs, and heterojunction interfaces, affect the charge generation, transport, trapping and extraction properties. Probing structural and functional phenomena at the interfaces is more challenging due to their sub-micron dimensions, however we developed a novel methodology for successful and reproducible cross-section fabrication of devices. We intend to monitor *in situ* reversible/irreversible structural changes and electronic and ionic processes in the thin films as well as interfaces w.r.t. the application of different voltage bias and/or light excitation densities and environmental conditions. To achieve in-depth understanding of structural and opto-electronic responses, we perform colocalized studies by combining AFM, KPFM, cAFM techniques with confocal Raman spectroscopy and Photoluminescence spectroscopy. To break the diffraction-limited optical microscopy resolution (usually ~ 400 - 200 nm), we will apply the AFM-based tip-enhanced spectroscopy techniques, which have the potential to offer nanoscale identification (< 50 nm resolution) of chemical compositions and interaction between molecules and resultant opto-electronic processes in a working PSC.

Guided by this invaluable information, we will design and fabricate more stable and higher efficiency PSC devices. In addition, measuring and understanding materials and processes on these scales will help to advance materials science.

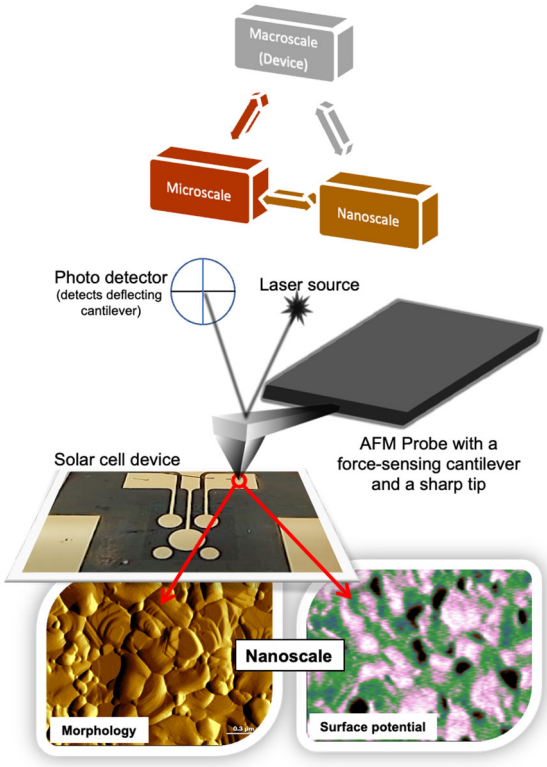


Fig. 1: Schematic of high-resolution investigation of morphological and opto-electronic properties of solar cell devices using atomic force microscopy and its high-end derivative techniques. Shown are few μm^2.

3.4 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 ionic-electronic 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
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.

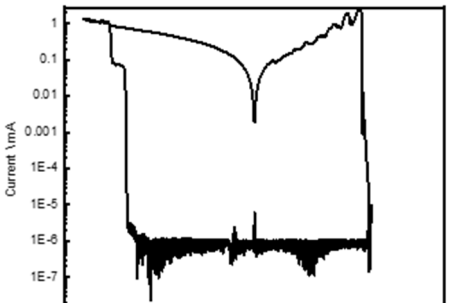


Fig. 1. Current-voltage curve of a resistive switch fabricated in our labs.

3.5 Perovskite Solar Cells & Machine Learning

Perovskite Solar Cells are a type of solar cell 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 assist in improving the efficiency of Perovskite Solar Cells and understand processes of degradation.

Contributors: W. Tress, O. Zbinden
Funding: DIZH
Duration: 2021-2023

The efficiency of perovskite solar cells (PSCs) has almost doubled to more than 25% 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.
In our project, we want to introduce machine learning (ML) to the development chain of PSCs in the lab. 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 experimentalist 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.
Before applying the models, they have to be trained with data. Since sufficient experimental data is not available, we generated synthetic data by device simulations with the software Setfos, developed by an ICP spin-off [2]. 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 current-voltage-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 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 V_{oc}-j_{sc} -*ff* space, where V_{oc} is the voltage at open circuit, j_{sc} the short circuit current-density, and *ff* the fill factor of the jV-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.
We applied our model to reported values in publications and could get plausible results that can be physically explained. However, there are some restrictions where ML can be applied to this problem when it comes to real-world cells: 1. The device under examination must perform similar as our initial models. 2. If the performance is already very close to the modelled maximum, the algorithm cannot find a parameter to be optimized. 3 Device performance should not be heavily limited by more than one parameter.

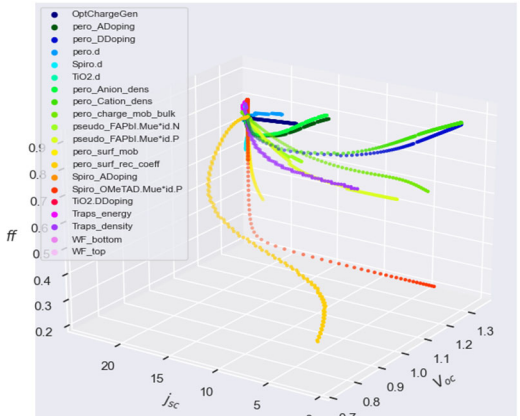


Fig. 1: 3D V_{oc}-J_{sc} -ff plot for the different varied parameters.

Sources:

[1] NREL. Best research-cell efficiency chart plotted by national renewable energy laboratory, USA, 2023.
[2] Fluxim AG. Semiconductor simulator (setfos) https://www.fluxim.com/
[3] Arthur Julien, Jean-Baptiste Puel, and Jean-Francois Guillemoles, Energy & Environmental Science, 16(1):190–200, January 2023

3.6 Multifunctional electro-optical characterization of novel semiconductors

Successful development of novel semiconductor devices such as solar cells and memristors requires highly accurate and reliable analyses. For this purpose, an advanced opto-electronic characterization setup has been built in this project. The setup consists of a unique combination of methods ranging from photoluminescence (spectrum, transient) to electroluminescence to measurements of absorption and spectral response of solar cells. Using a spectrally filtered super-continuum laser source combined with a source-measure-unit, these measurements can be performed with highest sensitivity. Small-area devices can be contacted in a probe station. Beyond variation of the excitation wavelength and intensity, different environments in terms of temperature, humidity and atmosphere can be created. Convenient operation and data acquisition is facilitated by computer control and a high degree of automation.

Contributors: K. Meraji, M. Torre, W. Tress
Partner(s): Nima Taghavinia, Sharif University, Iran
Funding: SNF R'Equip, Leading House South Asia and Iran
Duration: 2022–2023

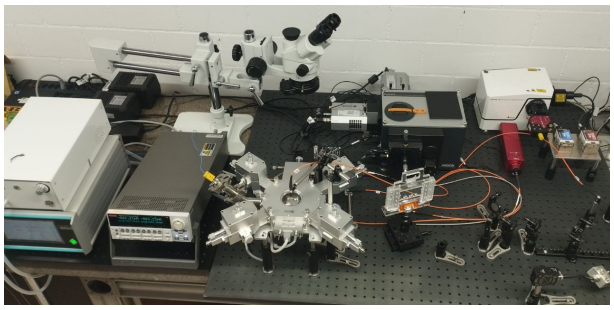


Fig.1: Photograph of the setup

The setup consists of the following components (Fig. 1):

- CCD spectrometer
- TCSPC detector
- CW lasers and super continuum laser with spectral filter
- Probe station with temperature and atmosphere control

It enables various measurements, some of them described here:

Incident photon-to-current efficiency (IPCE): IPCE is defined as the number of free electrons (which are produced by the incident photons) collected from the device to the external circuit of the device per photon incident on it. It is also called spectrally resolved external quantum efficiency, and a standard method in solar-cell research. Compared to standard setups, our setup is highly sensitive and can be used to determine sub-bandgap absorption, e.g. the Urbach tail or further tail states (Fig. 2).

Photoluminescence (PL) and Time-resolved photoluminescence (TRPL): These measurements provide insights on the energy and lifetime of optically generated charge carriers and are thus well suited to determine the band gap and study loss mechanisms due to recombination. Performing these measurements as a function of excitation wavelength, the location of absorption in the layers can be tuned due to wavelength-dependent absorption coefficients. Changing intensity and temperature, radiative and non-radiative recombination channels can be distinguished and characterized.

With the **probe station** we can perform all measurements under different temperatures and nitrogen or other atmospheres (gas, humidity) in order to investigate environmental parameters on efficiency and stability of fabricated devices. Furthermore, micron-scale device such as our memristors can be connected and a transfer stage is available for sample handover without exposure to ambient from the glovebox.

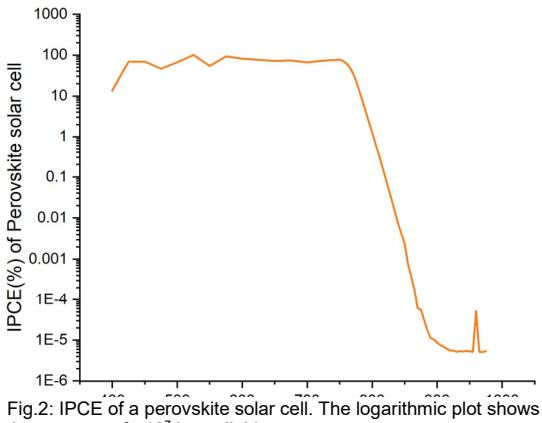


Fig.2: IPCE of a perovskite solar cell. The logarithmic plot shows that a range of >10^7 is available.

3.7 Multispectral image analysis and machine learning for PV quality assurance

For the upscaling of perovskite solar cells, the production of homogeneous and defect-free layers is crucial. Therefore, in this project we measure and model screen-printed perovskite solar cells with a novel measurement setup and extract material parameters for a computer model.

Contributors: M. Battaglia, E. Comi, C. Kirsch, E. Knapp, B. Ruhstaller
Partner(s): Fluxim AG, Solaronix AG
Funding: Innosuisse
Duration: 2022-2025

The measurement set-up developed in this project uses various imaging methods such as electroluminescence (EL), photoluminescence (PL) and dark lock-in thermography (DLIT) as well as classical current-voltage characteristics and impedance spectroscopy data to find and to analyze defects on perovskite solar cells. In Fig. 1, solar cells were measured with the new measurement setup.

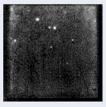
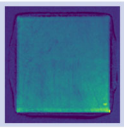
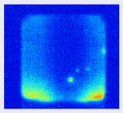
Imaging-Methode	Bild
Visual	
Electroluminescence	
Photoluminescence	
Dark Lock-In Thermography	

Fig. 1: Images of different perovskite solar cells with different imaging methods.

The final goal is to create a model of the component under test as accurate as possible. This allows the cell to be further optimized and enables predictive modelling.
Initially, we focus on the measurements of the solar cells and analyze the defects that occur in the different imaging methods and compare them with each other. For the processing of spatial information, we have developed customized software that enables the comparison of images by cell recognition and superposition of different cells, shown in Fig. 2.

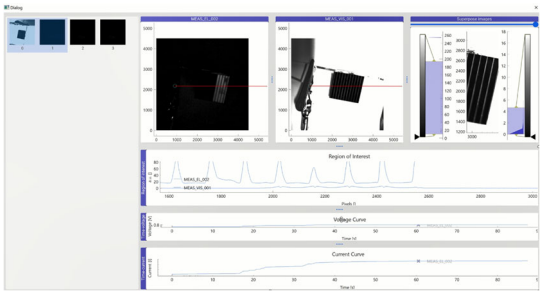


Fig. 2: Visual analysis of the images in the new software

In a next step, a 1D computer model was developed in collaboration with the project partner Fluxed, which reproduces the behavior of the cell manufactured by Solaronix in various experiments.
We then integrate the 1D model into an electro-thermal, large-area finite element model to achieve a spatial resolution as in the images.
The final step is illustrated in Fig. 3, where the material and device parameters for the simulation are extracted from the measurements using various machine learning methods.

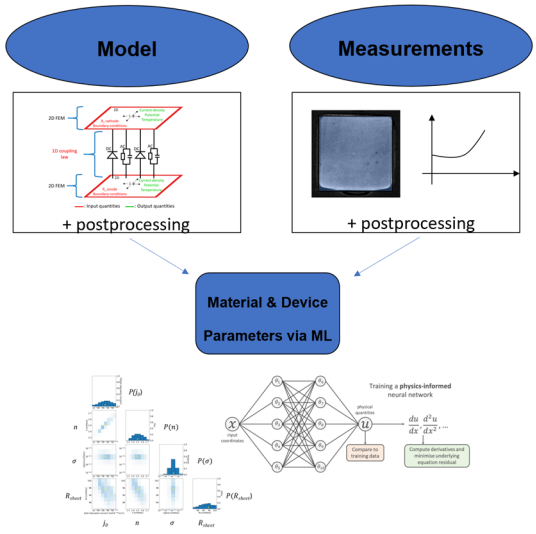


Fig. 3: Extraction of simulation parameters using ML methods.

3.8 Development of a terahertz reflection system

The aim of this project was to develop and validate a terahertz (THz) reflection system, to complement the existing transmission system at ICP. The reflection system will be used to gain additional information on samples that do not transmit enough THz radiation to be measured only with the transmission setup.

Contributors: M. Auer, M. Jazbinsek, U. Puc
Funding: Specialization Project VT2, MSE Photonics
Duration: 2022

THz spectrometry with pulsed waveform, especially time-domain spectroscopy (THz TDS), is a suitable method for material characterization over a wide frequency range. Since the existing transmission setup at ZHAW cannot measure samples which absorb or reflect too much THz radiation, an additional reflection setup was developed, as part of a specialization project in MSE [1]. To use as many existing elements as possible, such as the laser source, modulator, and delay line, flipping mirrors were placed in the existing system. They direct the laser beams to either the transmission or reflection system.

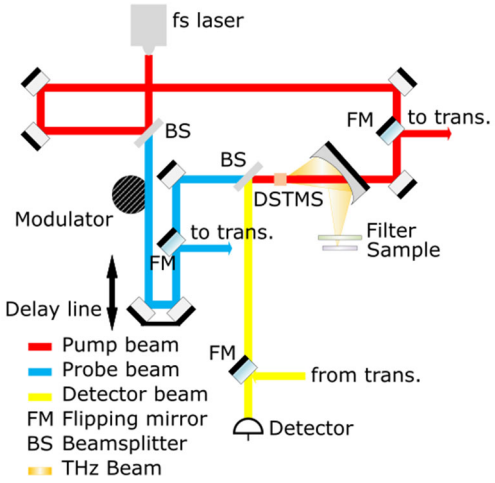


Fig. 1: Scheme of the reflection system.

To validate the reflection system, the signal to noise ratio (SNR) was investigated. The measured SNR is in good agreement with the theoretical values. Furthermore, different samples were measured with the reflection and transmission system, and the thickness and frequency-independent refractive index were compared. The deviation for the measured thickness is below 3%, and for the refractive index is below 1%. The signal change due to the change in position of the flipping mirrors was also investigated. It was found that the signal changes minimally when the mirrors are flipped. However, over longer time periods (3-4 weeks) the signal may change significantly due to factors like temperature change and relative humidity change. This signal change can be corrected, but the reflection system needs to be realigned. The frequency dependent refractive index and absorption coefficient of a Potassium Bromide (KBr) sample were extracted from THz reflection measurements and compared with literature data, showing a good agreement [1]. Since KBr has a high reflection in the lower THz range, and a high transmission in the higher THz range, it was also measured in transmission. The resulting amplitudes of the reflected and transmitted electric field in the frequency domain are shown in fig. 2. These results nicely demonstrate that reflection measurements can efficiently supplement transmission measurements in certain frequency ranges.

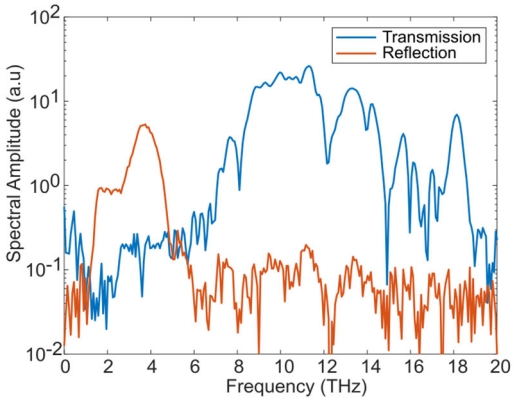


Fig. 2: Measured THz spectrum for the same KBr sample in transmission and reflection system [1].

In summary, we have developed a functional THz reflection system, which uses the same elements as the transmission system wherever possible. The measured results are in good agreement with theory, literature, and equivalent transmission measurements. The flipping mirrors used to switch between the transmission and reflection measurements work as expected, and the long-term signal change can be quickly compensated for by minor optical realignment.

Literature:

[1] M. Auer, “Development of a terahertz reflection system” ZHAW School of Engineering, Specialization Project VT2 MSE, 2022.

3.9 All-organic terahertz photonics

We are developing a terahertz (THz) system based on an all-organic approach to THz generation and detection. We are exploring the system for a variety of applications ranging from fundamental studies of THz-matter interactions to industrially relevant THz spectroscopy and imaging.

Contributors: M. Jazbinsek, U. Puc, M. Auer
Partner(s): Ajou University, South Korea
Funding: SNSF Bilateral programmes
Duration: 2020–2023

Terahertz (THz) sources based on organic electro-optic crystals have become increasingly important during the last years in the field of THz photonics. This is because of their unique possibilities for extremely high THz electric fields, as well as their ultra-broad coverage of the complete THz range from 0.1 THz to beyond 20 THz, needed to match specific fundamental modes of the matter to be investigated or controlled. This makes organic electro-optic crystals on the one hand essential for the emerging field of nonlinear THz photonics [1]. On the other hand, organic crystals offer a unique opportunity for extending THz spectroscopy and THz imaging applications beyond the few-THz limit of most of the presently employed broadband THz sources [2]. However, the modulation of the THz spectrum due to the phonon and vibrational modes presents a fundamental limit for THz photonics based on organic electro-optic crystals, which we want to overcome in this international project [3]. In this collaboration, the Korean side (Ajou University) is designing novel organic molecular crystals with large macroscopic optical nonlinearity and controlled crystal characteristics. The Swiss side (ICP ZHAW) is evaluating theoretically and experimentally the optical and the THz properties of the developed organic molecular crystals and implementing them for broadband THz applications (see Fig. 2). [4,5].

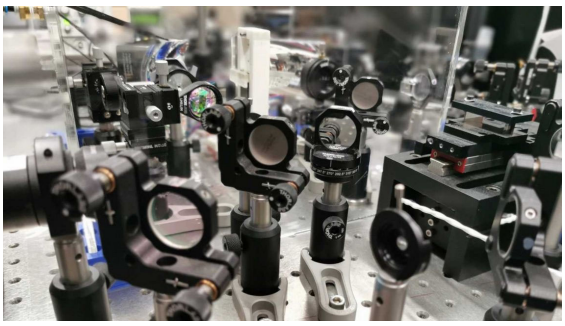


Fig. 1: Custom-built, compact THz spectroscopy setup at ICP employing organic electro-optic crystals for ultra-broadband THz-wave generation and detection.

Using the system (Fig. 1), we are investigating novel organic electro-optic crystals as well as organic charge transport materials interesting for a variety of applications such as e.g., organic solar cells, organic field effect transistors, and organic photodetectors.

Literature:

[1] Kim, Kang, Puc, Jazbinsek, Rotermund, Kwon; Adv. Optical Mater. 9, https://doi.org/10.1002/adom.202101019 (2021).

[2] Puc, Bach, Günter, Zgonik, Jazbinsek; Adv. Photonics Res. 2, https://doi.org/10.1002/adpr.202000098 (2021).

[3] https://data.snf.ch/grants/grant/188194

[4] Yoon, Seok, Puc, Jazbinsek, Kwon et al; Advanced Science 9, https://doi.org/10.1002/advs.202201391 (2022).

[5] Puc, Yang, Kim, Kwon, Jazbinsek, Opt. Mater. Express 13, https://doi.org/10.1364/OME.475427 (2023)

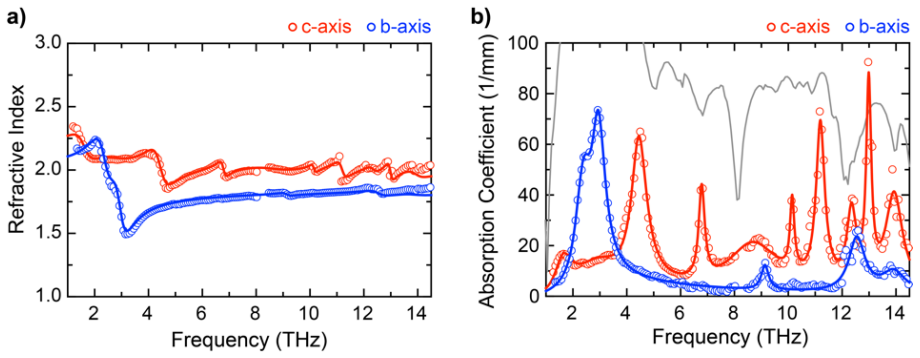


Fig. 2: The measured refractive index a) and the absorption coefficient b) for an organic crystal PMB-4TFS using ultra-broadband THz time-domain spectroscopy at ICP, for the THz field polarization along two crystallographic axes b and c. The peaks correspond to phonon and far-infrared vibrational modes, which are responsible for the dispersion of the real and imaginary parts of the dielectric susceptibility [5].

4 Sensors 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.


D. Bajrami


M. Bonmarin


D. Fehr


Ch. Grossmann


R. Hagen


I. Häusler


D. Paparo


F. Spano


J. Zwicky

4.1 Development of a 3D-Printed Bio-Hybrid Skin Model for Photothermal Therapy Applications

Skin models, particularly optical skin phantoms, are valuable tools for research and development in the field of light interaction with human skin. However, existing optical skin phantoms have limitations in accurately mimicking the complexity of human skin, such as the integration of biological aspects and thermal properties. This research proposes the development of a 3D-printed bio-hybrid skin phantom that combines optical and thermal properties with the embedding of biological cells. The model aims to simulate the effects of photothermal therapy on specific cell populations and investigate the influence of skin structures.

Contributors: D. Bajrami, M. Bonmarin, R. Rossi (EMPA), F. Spano, K. Wei (EMPA)
Partner(s): EMPA
Duration: 2022–2026

Skin models or skin phantoms are synthetic or natural constructs used to mimic the structure and function of human skin. Optical skin phantoms have gained attention as valuable tools for simulating light interaction with human skin in research and development [1]. However, existing optical skin phantoms have limitations in accurately replicating the complexity of real human skin, particularly in terms of incorporating biological aspects and simulating the application of photothermal therapies.

The objective of this research project is to address these limitations by developing a 3D-printed bio-hybrid skin phantom capable of replicating the optical and thermal properties of human skin. This innovative model will be created through a combination of an optical and thermal skin model, along with the integration of biological cells. By incorporating biological cells, the bio-hybrid skin phantom will allow for the simulation of photothermal therapy effects on specific cell populations. Moreover, it will facilitate the optimization of treatment parameters to achieve maximum efficacy and safety.

Another aspect of the study involves investigating the influence of skin structures such as skin thickness and color on photothermal therapy [2]. Understanding how these factors impact treatment outcomes can enhance the development of personalized approaches and improve the effectiveness of photothermal therapies. Furthermore, the knowledge gained from this research can have broader applications beyond photothermal therapy. It can contribute to advancements in tissue engineering, hair transplant science, and soft robotics by providing valuable insights into skin biology and its interactions with various technologies.

The utilization of 3D printing technology in creating the bio-hybrid skin phantom is a significant advancement in the field [3]. This technology enables the fabrication of intricate structures and has a profound impact on the testing, investigation, and development of photothermal therapies. By combining the advantages of 3D printing with the incorporation of biological cells, this research project aims to create a more realistic optical skin model that better represents human skin.

In conclusion, the research project strives to develop a sophisticated bio-hybrid skin phantom by integrating biological cells and considering skin structures. The 3D-printed model holds immense potential in providing valuable insights into photothermal therapy and other optical treatments. Its impact extends to the fields of skin biology, treatment device development, and imaging technologies, ultimately contributing to advancements in healthcare and well-being.

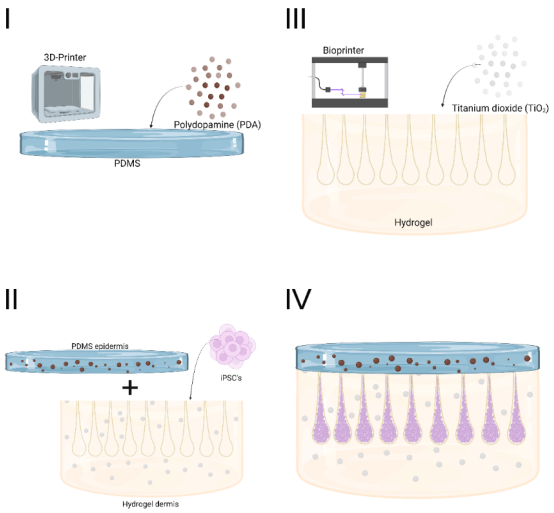


Fig. 1: Bio-hybrid model (I) Creation of epidermal layer (II) Creation of dermal layer (III) Cell seeding and culturing (IV) Finished bio-hybrid structure

Source:

[1] B. W. Pogue and M. S. Patterson, "Review of tissue simulating phantoms for optical spectroscopy, imaging and dosimetry,"
[2] M. W. Sjoding, R. P. Dickson, T. J. Iwashyna, S. E. Gay, and T. S. Valley, "Racial Bias in Pulse Oximetry Measurement," (in eng), *N Engl J Med.*
[3] W. Yim *et al.*, "3D-Bioprinted Phantom with Human Skin Phototypes for Biomedical Optics," *Advanced Materials.*

4.2 Development of a thermotherapy device for the treatment of cutaneous leishmaniasis

Cutaneous leishmaniasis is a disease endemically affecting several low-income countries. Aside medication, current treatments are based on heat therapy: the lesion is heated up to 50° to kill the responsible parasite. Unfortunately, current devices available on the market are still too expensive and out of reach for the affected countries. In this project our goal was to design and build a low-cost version of such a thermotherapy device.

Contributors: A. Bachmann, R. Hagen, D. Fehr, F. Spano, M. Bonmarin, I. Häusler and D. Paparo
Partner(s): Drugs for Neglected Diseases Initiative DND*i* and Gebert Rüf Foundation
Funding: Direct funding & student projects
Duration: 2020-2023

Commercial thermotherapy devices use radiofrequency heating to allow reaching a temperature of 50°C for several seconds (usually around 30 seconds). They contain two separate parts: a handheld electrode to be applied on the skin lesion and a base controlling the handset. The device should be safe, portable and battery operated. Besides it should be robust to be easily transported to remote places.
Based on these requirements, the Sensors and Measuring Systems developed a new thermotherapy device. The device consists of a handset that is connected to a main unit (fig. 1). The temperature is controlled via a non-contact sensor that measures the surface temperature between the electrodes (Fig. 2).

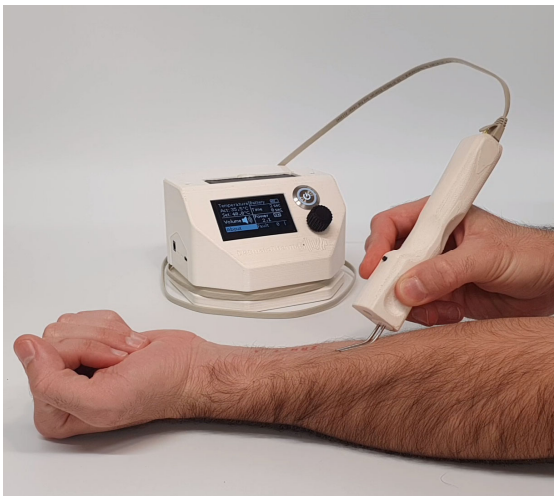


Fig. 2: Picture of the device in use with electrodes and a start button. All parts have been 3D printed in house.

Each component has been carefully selected to keep production cost as low as possible without compromising performances. The radio-frequency modulator has been designed to increase efficiency and battery life.

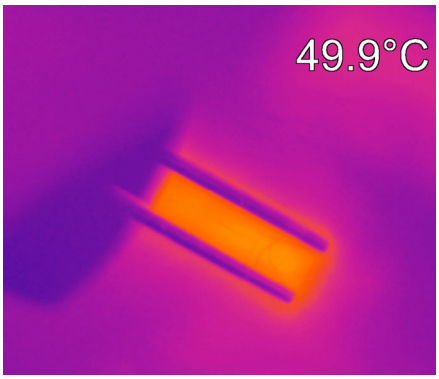


Fig. 1: Infrared camera caption during application. Temperature is measured on the skin surface between the two electrodes.

Basic validation tests on porcine skin and live human arms have been performed (fig. 3). The device has been delivered to DND*i* for further testing. The Project has received startup funding from the Gebert Rüf foundation and is being further developed into a startup under the name DermatoTherma.

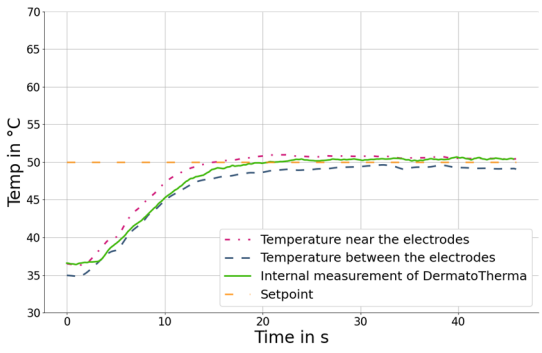


Fig. 3*:* Temperature course increases steadily to target temperature of 50°C without any overshoot, leading to higher patient safety during application.

4.3 A new thermography-based method to quantify sweat glands activity in vivo

The quantitative investigation of sweat glands is relevant for the diagnostic or follow-up of various diseases. Current methods are mostly based on absorbent that are put in contact with the skin but do not allow the monitoring of individual sweat glands or the dynamics. We proposed a new technology based on passive thermal imaging and capable of monitoring several sweat glands in parallel, quantifying time-dependent sweat rate.

Contributors: V. Vescoli, T. Werhmüller, A. Schmid, R. Hagen, D. Fehr, F. Spano, M. Bonmarin, A. Drexelius (UC Cincinnati), J. Heikenfeld (UC Cincinnati)
Partner(s): Novel Device Lab, UC Cincinnati
Funding: Student projects
Duration: 2020-2023

An IR camera is used to monitor the skin surface temperature (see fig. 1). Sweat glands appear as dark/cold spot on the IR images (see fig. 2).

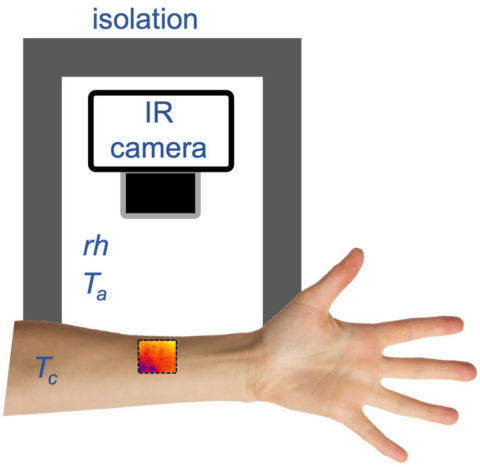


Fig. 1: Experimental setup. An IR camera monitor the skin surface.

Using mathematical modelling, the temperature difference between the sweat glands and the skin as well as the ambient humidity and temperature can be used to retrieve a sweat rate (see fig. 2).

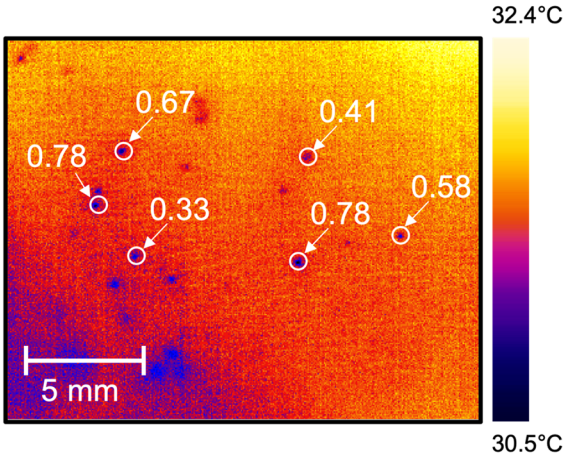


Fig. 2: Sweat glands are easily visible as dark spot. Thanks to mathematical modelling the temperature difference is converted in sweat rate (in nL/min).

Another advantage of the method is that it allows to follow sweat glands dynamics (see fig. 3).

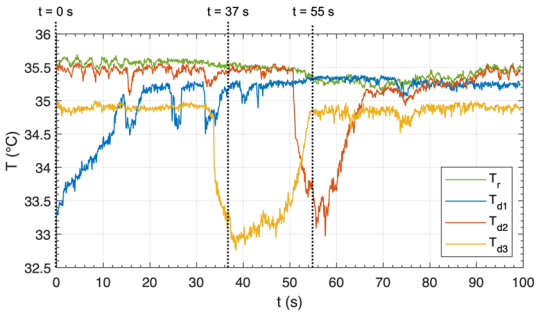


Fig. 3: Dynamic of 3 sweat glands together with a reference over 100 seconds.

Thanks to several student projects, a first prototype has been built and will be tested in several clinical and non-clinical study in Switzerland and Germany.

Source:

A. Drexelius, D. Fehr, V. Vescoli, J. Heikenfeld and M. Bonmarin, "A simple non-contact optical method to quantify in-vivo sweat gland activity and pulsation," in IEEE Transactions on Biomedical Engineering, doi: 10.1109/TBME.2022.3151938.

4.4 Design and Development of Artificial Skin Models for Tactile Sensing Applications

Contributors: F. Spano, D. Fehr, M. Bonmarin, J. Blunschi, R. Sassenburg
Duration: 2019–2023

Despite the forthcoming arrival of entirely cell-based skin models, the development of the artificial skin models is still progressing and relevant. Indeed, the cell-based skin models are far from reproducing the human skin properties and the needs of the community. In particular, there is still a need for reproducible and stable artificial skin models mimicking different properties of the human skin. Moreover, and fortunately, due to new regulations and ethical issues, animal testing is not anymore tolerated. So, the design and development of artificial skin models simulating various properties of the human skin, as for example, the mechanical, thermic, sweating and tactile properties of the human skin are considered [1-2].

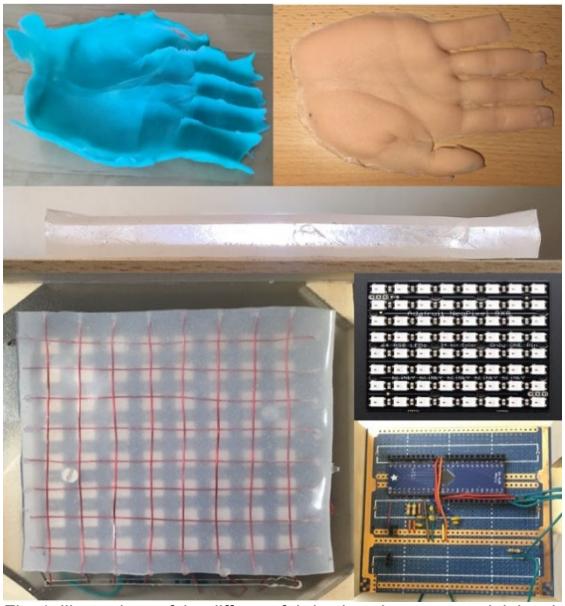


Fig. 1: Illustrations of the different fabrication phases: material development and real palm replica; Multi-layered skin model with the capacitive-sensing grid and the LED matrix, controlled by the prototyped electronics.

The artificial skin models are generally constituted by a multi-layered combination of materials mimicking the real human skin and its different layers (stratum corneum, epidermis, dermis and sub dermis). The materials used to simulate the physical properties of the real human skin are various [3], often silicon-based materials such as polydimethylsiloxane or gelatinous materials [4]. They are selected in function of the properties to simulate. Concerning the fabrication processes, we are using classical deposition techniques such as drop casting and bar coating for example. Additionally, we are implementing new technologies such as 3D bioprinting for example.

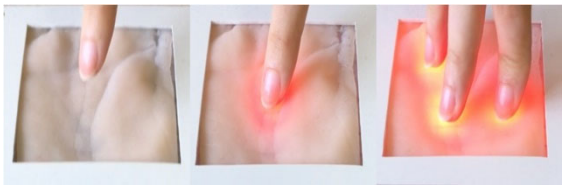


Fig. 2: Illustrations of the tactile capabilities of the artificial skin model implementing the real human texture and mechanical properties in addition to the change of colours in function of the applied force and the multipoint capacitive sensitivity.

In this particular Bachelors' project, we focus on the design and fabrication of an artificial tactile skin, a skin model combining the mechanical properties of the human skin and its texture, and in addition a capacitive sensing device combined with a LED matrix (fig. 1) indicating the multipoint localization and the applied forces by simple changes in colours as illustrated in fig. 2).
Attention was provided on the fabrication and replication of a real human palm. The mechanical properties were obtained by generating a multi-layered material made of several silicon-based polymers layer by layer (Dragon skin FX Pro and Ecoflex). Moreover, a replica of a real human palm was realized reproducing precisely the hand texture increasing the feeling to interact with a real human hand. Separately, a flexible capacitive sensor was designed and fabricated by implementing a grid of wires embedded in a polymeric matrix. In a successive step, a LED matrix was connected to the capacitive grid and programmed. The tactile skin is able to react to multipoint touch and indicate the variation of applied pressure by change of colours. Such skin models can be envisaged for providing an interface for robots to interact in a world surrounded by humans, or simply for interactive devices for communication in smart cities.

Literature:

[1] M. Guan et al., Development of a sweating thermal skin simulant for heat transfer evaluation of clothed human body under radiant heat hazard, *Applied Thermal Engineering* 166, 114642 (2020).
[2] L. Zhai et al., Development of a multi-layered skin simulant for burn injury evaluation of protective fabrics exposed to radiant heat, *Fire and Materials* 43 (2), 144-152 (2019).
[3] A. K. Dabrowska et al., Materials used to simulate physical properties of the human skin, *Skin Research and Technology* 2016; 22: 3-14.
[4] A. Dabrowska et al., A water-responsive, gelatine-based human skin model, *Tribology International* 113 (2017) 316-322

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.

D. Kempf

M. Schmid

F. Schranz

C. Tello

A. Witzig

5.1 Quantify energy-saving measures with building simulations

When implementing energy-saving measures it is a challenge to predict its effectiveness. Physics-based dynamical simulation would be a good means for facility management to optimize HVAC systems and to guarantee indoor comfort. However, setting up a simulation with today's commercial simulation tools is often too elaborate. We propose a methodology that uses 3D plans, generates vertical 2D cuts and runs a simulation. By using existing databases and computational resources the new approach has the potential to simplify energy analysis.

Contributors: Andreas Witzig, Camilo Tello, Franziska Schranz, Johannes Bruderer
Partner(s): Leicom AG, IPP-ZHAW, IFM-ZHAW, InES-ZHAW
Funding: Innosuisse
Duration: 2021-2023

Until today, building information modeling (BIM) has not been able to hold its promise to support and enhance the energy performance of buildings. Many attempts have been made to integrate thermal simulation into the BIM workflow. This work proposes to start from a 3D BIM plan, cut it vertically and apply a finite-element discretization for the building structure. The simulation relies on physical material parameters. The approach has the potential to reduce the effort for manually translating from BIM to the simulation model. It applies 2D numerical simulation of the concrete structure. In addition to the heat flow in the solid structures, radiation between the walls is properly accounted for resulting in proper surface temperatures. Air flow in the rooms is approximated by a lumped element model with a small number of dynamical nodes per room as shown in fig. 1.

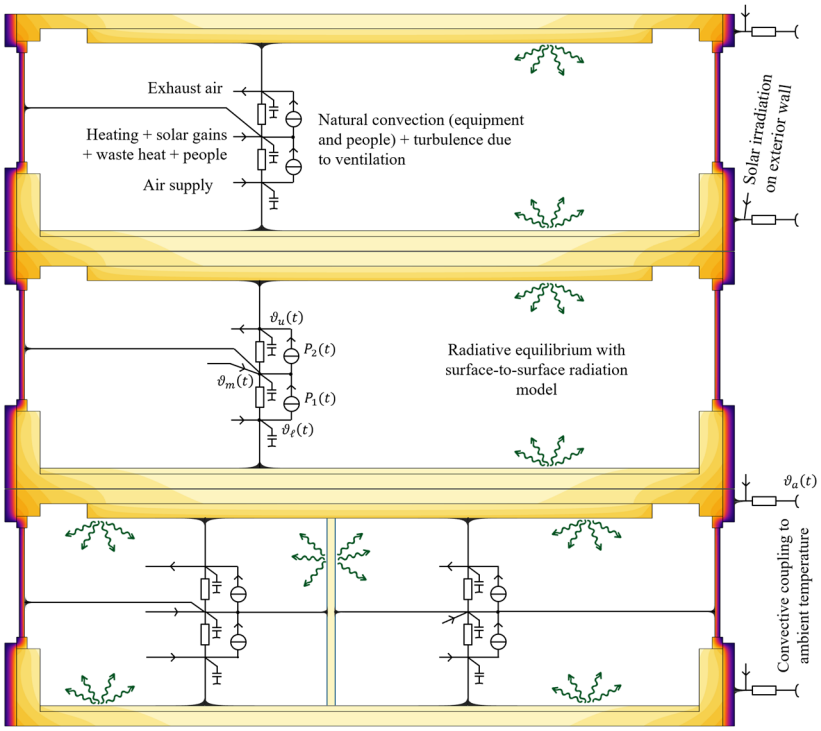


Fig. 1: Simulation domain for the analysis of energy-savings measures implemented in the control strategy of the heating system. Passive solar gains and dynamic energy storage in the concrete structure are fully accounted for while a lumped element model is applied for the stratification in the air domains.

Analyzing the thermal behavior of the buildings aims at quantifying energy savings measures. The finite element simulation fully accounts for energy storage and heat loss through thermal bridges. The dynamic model also contains the control algorithm for the HVAC system and predicts the net primary energy consumption for heating and cooling of the building for any time period. Variants of energy saving measures can be compared and evaluated on a yearly basis with the use of a stochastic model for the outside weather conditions and the user behavior. Besides the physical parameters which are interesting for engineers, the results also contain a cost analysis that is relevant for the owner or manager of the building. The simulation model has been validated to measurements as shown in fig. 2.

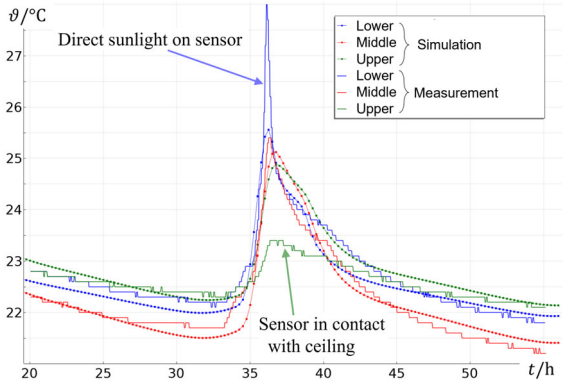


Fig. 2: Good agreement between measurement and simulation has been found in the validation of the simulations.

5.2 Model validation of 3D thermal simulation of buildings

With the advent of full 3D architectural plans and the strong need to optimize the thermal efficiency of buildings, physics-based dynamical simulation has a high potential to gain more attention in the construction industry. This work performs a validation study with reference to the ASHRAE [1] standard, which is a well-known reference for full featured analysis of buildings.

Contributors: Andreas Witzig, Camilo Tello, Franziska Schranz, Johannes Bruderer
Partner(s): Leicom AG, IPP-ZHAW, IFM-ZHAW, InES-ZHAW
Funding: Innosuisse
Duration: 2021-2023

In this work the thermal behavior of buildings is analyzed by means of a full 3D model for the concrete structure in combination with face-to-face radiation between the walls and a lumped element model for the air domains. Boundary conditions include passive solar gains, the outside temperature and thermal load from the usage of the building. The physical parameters used in the thermal conduction and storage in solids are well-known since they are fundamental material parameters. The main parameters of the lumped element components can also be derived from physics, such as the heat transfer between different air layers, or the storage capacity of the air volumes.
The ASHRAE [1] standard proposes a special structure for validation purposes, namely a small building with windows facing south and a heated area on the north side. The 3D simulations with Comsol Multiphysics [2] are compared to IDA ICE [3], a tool that is well-established for buildings simulation.

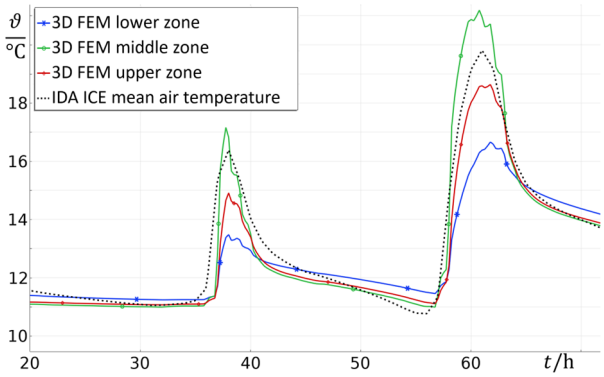


Fig. 2: good agreement between the Comsol simulation (colored lines) and the IDA ICE simulation (dotted line) has been found in the validation of the simulations.

References:

[1] ASHRAE standard 140, case 960, https://www.ashrae.org
[2] Comsol Multiphysics, https://www.comsol.com
[3] IDA ICE, https://www.equa.se/ida-ice

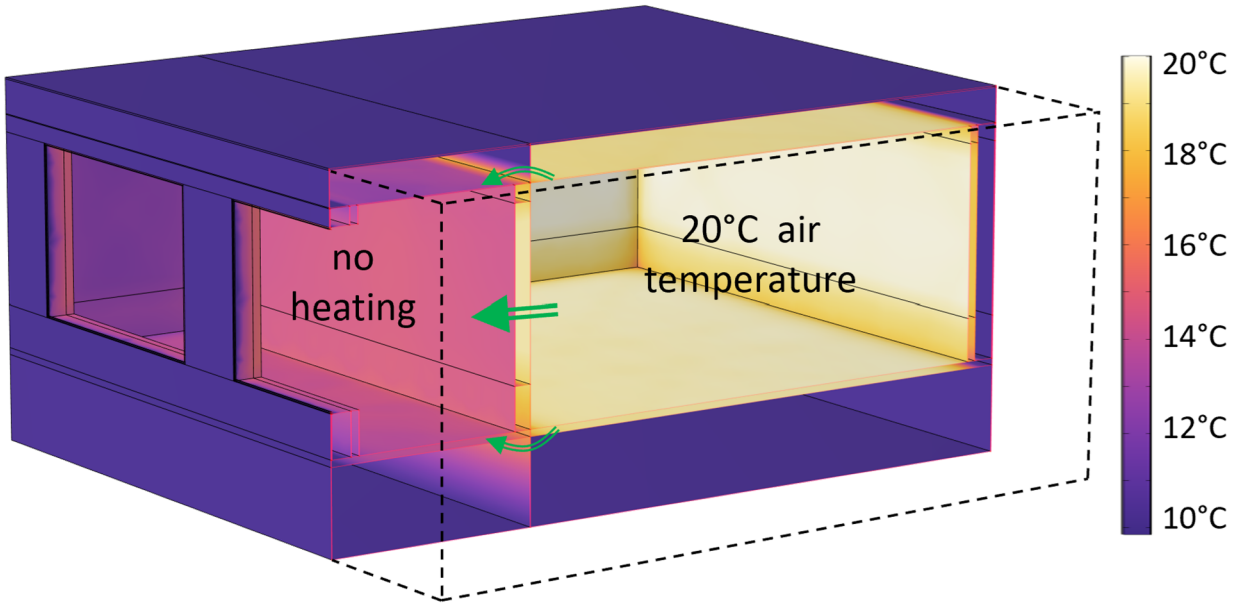


Fig. 1: Comsol-Simulation result for the ASHRAE standard 140, case 960. The picture shows wall temperatures at night when heat is flowing from the heated area in the north towards the unheated space in the south (green arrows). During daytime, the sun is shining through the windows and the room in the south is heating up due to passive solar gains. The example is well suited to test the capability of simulation tools to cope with temperature dynamics and heat storage in the concrete. The Comsol simulations require 16 GB of main memory and 1h CPU time for a simulation of two days.

5.3 Saving energy through optimal energy management in office buildings

Large office buildings have a proven potential for energy optimization. The joint project with Leicom AG and the ZHAW shows how the digital twin can be used to save energy. Specifically, the information from room temperature sensors and the status in the energy center will be used to optimize heating, ventilation, and cooling. The aim is to always ensure indoor comfort and to save energy.

Mitwirkende: Andreas Witzig, Camilo Tello, Johannes Bruderer, Franziska Schranz
Partner: Leicom AG, ZHAW: InES, ZPP, IFM
Finanzierung: Innosuisse
Dauer: 2021–2023

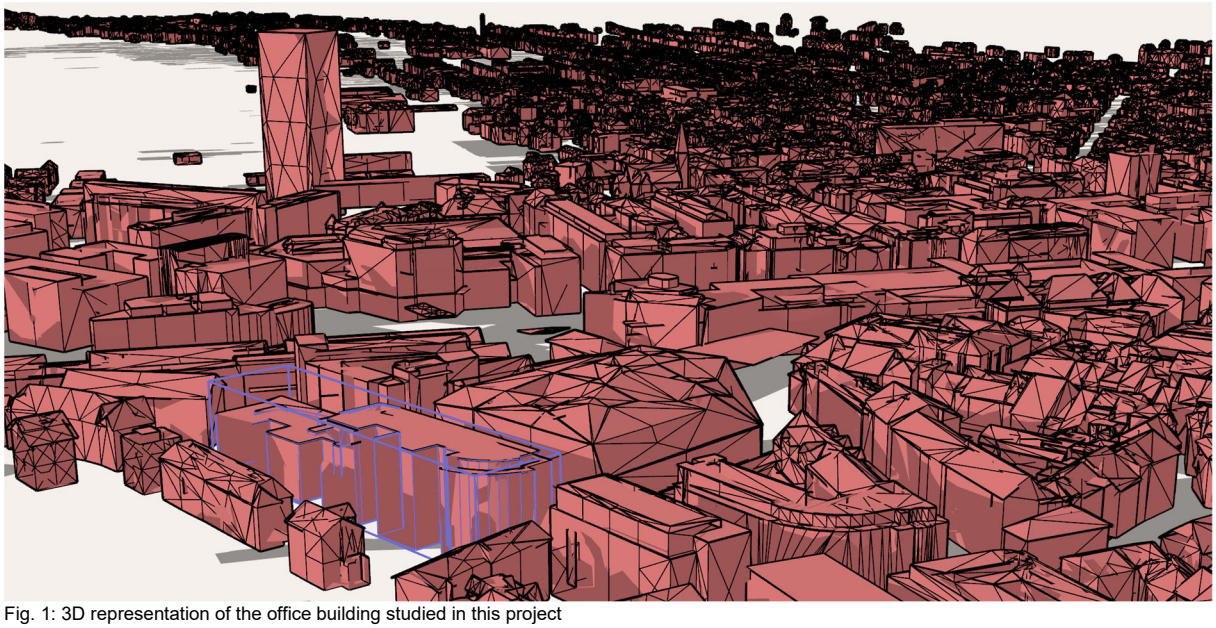


Fig. 1: 3D representation of the office building studied in this project

The variety of publicly available information is constantly increasing. In the present project, a 3D building dataset is used to efficiently set up a digital twin. Based on sensor data, an intelligent monitoring of the indoor climate and the HVAC system is developed. The algorithm runs on a server and uses configuration data in the installation process and real-time measurement data during operation as input. The proposed method is robust in the sense that it can handle incomplete data both during setup and during operation. Missing data is filled in by applying a full-scale building simulation and optimized using weather data and statistical user behavior.
In the current research project, two models are established that are hierarchically dependent on each other: a computationally intensive model simulates the indoor environment in detail, and a compact model runs during operation as an integral part of the digital twin.

The project bridges the gap between Internet of Things (IoT) technology and the requirements of facility management, which must receive added value from the digital twin in day-to-day operations. With its Eliona platform, industry partner Leicom AG is already a driving force in digitalization in the building sector

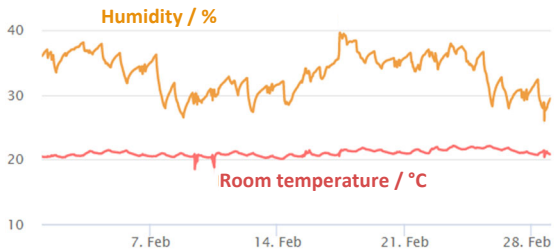


Fig. 2: IoT-Data in the dashboard of the Eliona platform. In addition to the current display of the relevant comfort parameters, the time history is also displayed.

Quellenangabe:
www.leicom.ch/smart-building/
www.swisstopo.admin.ch/de/geodata/landscape/buildings3d3.html

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

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

Contributors: M. Battaglia, E. Comi, M. Bonmarin, E. Knapp
Partner: FHNW, Considerate AG, BSF Swissphoto
Financing: 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 multiper-spective 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.

The ICP is responsible for the scientific monitoring of the data acquisition with the infrared measuring technique and tries to improve the evaluation and correction of the data by means of known and new approaches. In addition, in the next phase of the project, it will contribute its know-how in building simulation in order to be able to make statements on the annual consumption of the respective objects from the point measurement of the outside temperatures of the building envelope.

Figure 1 shows a schematic of the currently used data processing pipeline. Due to their increased thermal inertia and the time of flight in Grenchen in the evening of a sunny day, flat roofs had to be removed from the data set. Likewise, metal roofs detected by roof material classification were omitted due to their property as mirrors in the infrared range. A heat transmission value was then estimated from the averaged roof temperature of a main class area using a simple thermal model of the roof.

The test flight in winter 2023 was carried out using the system developed specifically for the project, which in addition to vertical images of the roofs also includes oblique cameras for recording the facades. In a next step, the potential of such a multi-perspectival system will be analyzed and the evaluation will be further developed.

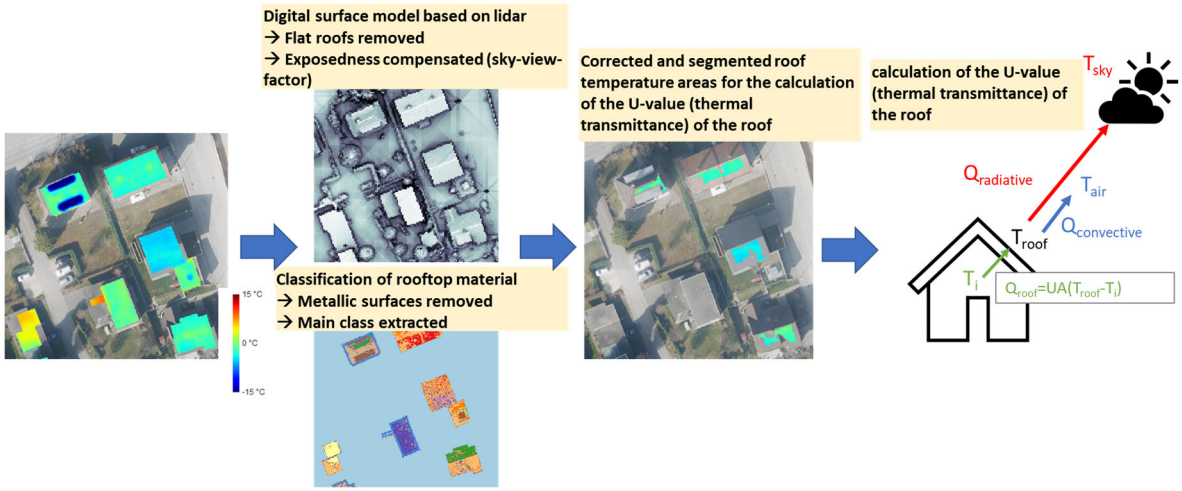


Fig. 1: Data processing starting from the corrected roof temperature from the infrared measurement. A heat transmittance value is estimated from the appropriate roof areas.

5.5 POLYSUN Multi-Objective Optimization and Machine Learning

Planers use the software Polysun to design energy systems in buildings and find the best solution with regards to economic and sustainability targets. Today, designing optimal energy systems with Polysun is time consuming. System variants have to be manually defined, simulated and compared. The project goal is to shift the focus from selling a simulation tool towards offering genuine optimization services that use massively parallel computations in the cloud.

Contributors: Mattia Battaglia, Johannes Bruderer, Franziska Schranz, Andreas Witzig
Partner: Vela Solaris AG
Financing: Innosuisse
Duration: 2023-2025

Energy systems for buildings and districts are designed to harvest solar energy and environmental heat and to guarantee indoor comfort. The seizing of the components and the setup of the energy management systems (EMS) are currently still a challenging task. Generally, the environmental benefits have to be maximized with a strong awareness of costs. With many parameters to choose from and a poorly defined optimization target, most systems currently have a great potential for improvement, even if they have just been installed. As an estimation, several experts see the potential with regards to system optimization and cost reduction to figure between 20% to 50%. Typical design questions with regards to optimization are:

- What is the minimal size of system components (e.g. size of energy storage, installed capacity of heat pump, number of PV modules) which still reliably covers energy demand?
- How robust is a chosen energy system with regards to a variety of weather data, especially in systems with only renewable sources for heating/cooling?
- What energy management system (EMS) set-up combines the heat pump in a cost-efficient way with the PV production?

The simulation software Polysun developed by Vela Solaris allows its users today to dynamically simulate energy systems including all commercially available technologies for heating, cooling, and electricity.

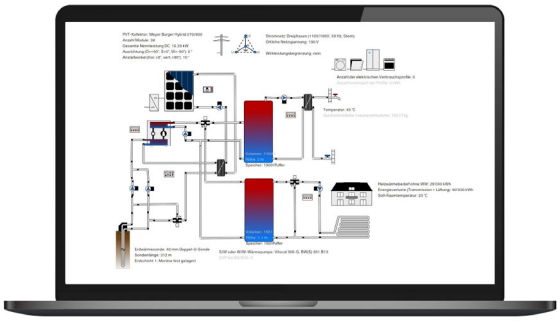


Fig. 1 Representation of a solar heat pump system in Polysun.

It is a general claim that simulation empowers users to design robust and efficient energy systems. Sector coupling, energy storage and the use of various renewable energy sources is strongly supported by the software. In today's solution with the Polysun desktop application, users design the optimal systems by trial and error. This means that the dimensioning and the control logic of an EMS is iteratively improved by comparing different manually defined options. An example of a system layout in the user interface of Polysun is shown in Figure 1.

The Innosuisse project “POLYSUN Multi-Objective Optimization and Machine Learning” seeks to enhance the system optimization process by deploying Polysun in the cloud. The vision is to enable the customers to optimize their energy system by providing an intuitive way to set up the massively parallel simulations and an interactive dashboard that visualizes the results of ensemble simulations and parametric runs. An additional goal of the project is to deliver optimization as a digital service to Polysun customers. It is envisioned to advance the current state of building energy system optimization by combining the already advanced calculation core of Polysun with well-established multi-objective optimization algorithms such as Genetic Algorithms or Particle Swarm Optimization.

Finally, building on the foundation of the newly developed environment for stochastic ensemble simulation and the ability to run large numbers of simulations in parallel on the cloud, the opportunities of optimizing an EMS in Polysun based on traditional rule-based control as well as novel machine learning algorithms will be evaluated.

5.6 Sound Transmission Analysis of Carbon Prestressed Concrete Structures with reduced Carbon Footprint

Carbon Prestressed Concrete (CPC) has the potential to significantly reduce the carbon footprint in the construction sector by providing similar static properties with a considerably reduced mass. However, the reduction of the used amount of material has the drawback of worse acoustic insulation properties compared to conventional concrete structures. Thus, the acoustic properties of the novel CPC elements are modelled and optimized in this project using coupled acoustic-structure Multiphysics simulations.

Contributors: J. Pfammatter, D. Schweizer, P. Marmet, A. Witzig
Partner(s): School of Architecture, Design and Civil Engineering, ZHAW, Centre for Building Technologies and Processes
Funding: Innosuisse
Duration: 2022–2024

Reducing greenhouse gas emissions becomes more and more important for all industry sectors. Depending on the specific composition, the production of one ton of cement leads to almost as much emitted CO_2. Carbon Prestressed Concrete (CPC) technology uses carbon fibers infused in concrete structures to increase their mechanical strength. Thus, CPC plates reduce structure weights significantly compared to conventional reinforced concrete. However, the sound transmission loss of a structure directly depends on its mass. Thus, the reduced mass of the CPC plates leads to an inherently worse acoustic insulation compared to conventional concrete elements. As a consequence, the CPC plates need to be design appropriately in order to fulfill the legal requirements for the sound transmission loss (STL) defined in the corresponding norm. In order to accelerate the development process and to limit the needed experimental studies to a minimum, the sound transmission is modelled using coupled acoustic-structure Multiphysics simulations based on the finite element method (FEM). Thereby, three-dimensional full-wave acoustics simulations considering physics coupling between mechanical structures and the surrounding air are implemented in the Comsol Multiphysics software package. The model is formulated in the frequency domain and a diffuse field excitation is used to model the noise in a broad frequency range. An example of the resulting acoustic pressure field for such a simulation is shown in Fig. 1 for the novel CPC element. Performing such simulations for the whole relevant frequency range results in a sound transmission loss (STL) spectrum, as reported in Fig. 2 deduced from simulation results for a common concrete structure. All the relevant physical phenomena like the stiffness of the structure (dominant for lower frequencies), the eigenfrequency of the concrete structure (observable as a pronounced dip of the STL spectrum at the first eigenfrequency) and the mass law (dominant for higher frequencies) are considered. Such simulated STL spectra allow for a direct comparison with the specification defined in the corresponding norm. Hence, the application of this Multiphysics simulation tool supports the efficient and cost-effective development of novel CPC structures, which fulfill all the requirements to be successfully introduced in the construction industry.

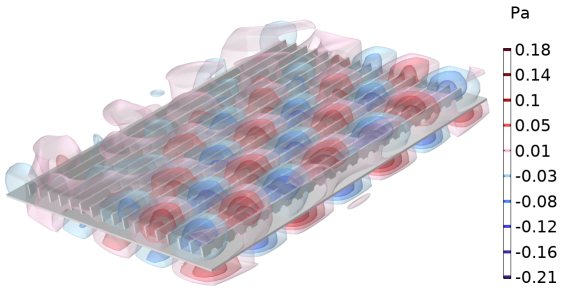


Fig. 1: 3D sound transmission analysis of the novel concrete structures using Comsol Multiphysics: Isosurfaces of the acoustic pressure at a frequency of 180 Hz.

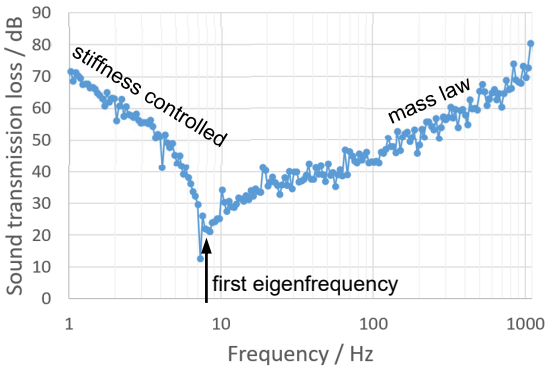


Fig. 2: Example of a simulated sound transmission loss (STL) spectrum for a conventional concrete element using Comsol Multiphysics.

6 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 Lab

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 Lab

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 (copper electrolysis)

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 electroplating methods). The plant is fully electrically controlled, has an advanced interface, a self-cleaning system and appropriate aeration/deaeration systems.

Soft Materials Lab

We have a fully equipped laboratory with 2 chemical fume hoods where we can work safely with various soft materials (such as polymers, hydrogels, etc.). Examples of available equipment: 3D bio-printer (liquid printing), bar coater, ultrasonic cleaner, centrifuge, magnetic stirrers, hotplates, pH-meter, etc. With these devices we can develop sophisticated prototypes for biomedical applications.

Thermal Design Lab

Physicochemical computer models are valuable tools for the development of new functional materials and industrial processes. However, their reliability and practical usefulness depend heavily on the substance data used. In addition, extensive calibrations and validations are usually necessary before they can be used. With the Thermal Design Lab, we are pursuing the goal of generating the most precise possible inputs for our computer models using temperature and heat flow measurement technology in combination with thermal material data determination. Currently, the Thermal Design Lab includes a wide range of contact temperature sensors and thermal imaging cameras with different spectral ranges. Furthermore, we use various methods to determine the thermal conductivity of liquids and solids.

Preservation and expansion of laboratory infrastructure, offer for joint use

The interaction of laboratory activities and simulation is an important unique selling point of the ICP with a proven benefit for both research projects and teaching. For years, we have been investing in the expansion of existing laboratories or in the construction of new measuring equipment. The joint use of laboratory infrastructure is a frequent starting point for in-depth collaboration with other institutes or with industrial partners. We are therefore happy to grant interested researchers access to our measurement technology and accept corresponding enquiries at any time.

Appendix

A.1 Student Projects

M. Auer, *Development of a terahertz reflection system*, mentor: M. Jazbinsek, Specialisation project 2 in the Master's programme.

M. Auer, *Ultra-broadband terahertz optical characteristics of perovskite energy materials*, mentor: M. Jazbinsek, Master's thesis.

L. Baptista Giesbrecht, M. Wüest, *Investigation of the Fluorescence and Photobleaching Properties of Bilirubin*, mentor: F. Spano, M. Bonmarin, D. Fehr, project partner: SpectraPad GmbH, Bachelor's in Systems Engineering.

B. Bender, Y. Meier, *Long high-precision opto-mechanical delay line for spectroscopy applications*, merntors: M. Jazbinsek, U. Puc, Bachelor's in Mechanical Engineering.

R. Bertschinger, L. Meier, *Web-community basierte Datenbank zum Austausch von Materialdaten für die OLED-Entwicklung*, mentor: B. Ruhstaller, B. Seeliger, project partner: Fluxim AG, Bachelor's in Computer Science.

A. Bosshart, R. Hefti, *Real-time emulation of electrically interfaced mechanical resonators*, mentor: F. Spano, M. Bonmarin, D. Fehr, project partner: Rheonics AG, Bachelor's in Electrical Engineering.

S. Delbari, *Introduction to & Computational Performance Analysis of CoatSim: A Simulation Software for Powder Coating Applications*, mentor: G. Boiger, Specialisation project 2 in the Master's programme.

S. Delbari, *Modelling of coating thickness distribution and its application*, mentor: G. Boiger, Master's thesis.

R. Hagen, Time-resolved fluorescence measurement, mentor: M. Bonmarin, Specialisation project 1 in the Master's programme.

I. Häusler, D. Paparo, *Development of a New Thermotherapy Device for the Treatment of Cutaneous Leishmaniasis*, mentor: F. Spano, M. Bonmarin, D. Fehr, project partner: DNDi Drug for Neglected Diseases initiative, Bachelor's in System Engineering.

J. Hirsbrunner, M. Zoller, *Development of a point of care device - Electronic and Software Implementation of a Volume Sensor*, mentor: F. Spano, M. Bonmarin, D. Fehr, Bachelor's in Electrical Engineering.

S. Pfyffer, *Simulation SeasonCell*, mentor: A. Witzig, Specialisation project 2 in the Master's programme.

J. Michel Rivero, *Automated test system for Cloud-based Computational Fluid Dynamics (CFD) simulations*, mentor: G. Boiger, Specialisation project 2 in the Master's programme.

J. Michel Rivero, *Cluster emulation using massive simultaneous cloud computing*, mentor: G. Boiger, Master's thesis.

A. Nuredini, *Berechnung der Leistungsaufnahme von OLED Bildschirmen / Calculation of OLED Display Power Consumption*, mentor: C. Kirsch, R. Ruhstaller, project partner: Fluxim AG, Bachelor's in Energy and Environmental Engineering.

P. Preisig, J. Zwicky, *Development of an Optoelectronics Sensor*, mentor: F. Spano, M. Bonmarin, D. Fehr, Projektpartner: Versantis AG, Bachelor's in Systems Engineering.

A. Schmid, T. Wehrmüller, *Transdermal Bilirubin Measurement - Electronic and Software Development*, mentor: F. Spano, M. Bonmarin, D. Fehr, project partner: SpectralPad GmbH, Bachelor's in Electrical Engineering.

M. Yassin, *Regulatory requirements to manufacture medical devices in a University-lab setting*, mentor: M. BONMARIN, Specialisation project 1 in the Master's programme.

M. Yassin, *Evaluation of the impact of X-ray and gamma irradiation on material interaction / stickiness - between CoCr implants and product packaging material*, mentor: M. BONMARIN, Master's thesis.

R. Wirth, *Multi-Spectral Image Analysis for Quality Control of Perovskite Solar Cells*, mentor: E. Knapp, Specialisation project 1 in the Master's programme.

R. Wirth, *Cell Boundary Definition and Mapping of local resistance and dark saturation current of PSC*, mentor: E. Knapp, Specialisation project 2 in the Master's programme.

A.2 Scientific Publications

U. Aeberhard, S. J. Zeder, and B. Ruhstaller, „Impact of photon recycling on the light extraction from metal halide perovskite light emitting diodes“, *Optical and Quantum Electronics*, Vol. 54, Nr. 10, S. 617, 2022, doi: 10.1007/s11082-022-03791-9.

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M. Bonmarin, S. Läuchli, and A. Navarini, „Augmented and virtual reality in dermatology: where do we stand and what comes next?“, *Dermato*, Vol. 2, Nr. 1, S. 1–7, 2022, doi: 10.3390/dermato2010001.

Z. Chen, W. Tress *et al.*, „A transparent electrode based on solution-processed ZnO for organic optoelectronic devices“, *Nature Communications*, Vol. 13, Nr. 1, S. 4387, 2022, doi: 10.1038/s41467-022-32010-y.

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A. Fakharuddin, W. Tress *et al.*, „Perovskite light-emitting diodes“, *Nature Electronics*, 2022, doi: 10.1038/s41928-022-00745-7.

V. N. Gorshkov, O. V. Bereznykov, G. K. Boiger, P. Sareh, and A. S. Fallah, „Acoustic metamaterials with controllable bandgap gates based on magnetorheological elastomers“, *International Journal of Mechanical Sciences*, Vol. 238, Nr. 107829, 2022, doi: 10.1016/j.ijmecsci.2022.107829.

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C. Jiang, W. Tress *et al.*, „Double layer composite electrode strategy for efficient perovskite solar cells with excellent reverse-bias stability“, *Nano-Micro Letters*, Vol. 15, Nr. 1, S. 12, 2022, doi: 10.1007/s40820-022-00985-4.

L. M. Keller, „The hydromechanical behavior of opalinus clay fractures : combining roughness measurements with computer simulations“, *Frontiers in Earth Science*, Vol. 10, Nr. 945377, 2022, doi: 10.3389/feart.2022.945377.

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A.3 Book Chapers

A. Witzig, „Einzelprojekt ‚Wellen‘“, in *Seamless Learning*, Wiesbaden: Springer, 2022, p. 93–121. doi: 10.1007/978-3-658-34698-0_4.

C. Pickhardt, H. U. Fuchs, E. Dumont, K. Hügel, and A. Witzig, „Modellieren, Visualisieren und die Simulation dynamischer Systeme als Seamless Learning : ein Beitrag zu diesem Prozess aus der Praxis am Beispiel eines Mathematikmoduls“, in *Seamless Learning*, Wiesbaden: Springer, 2022, p. 35–63. doi: 10.1007/978-3-658-34698-0_2.

W. Tress, „Physics of perovskite solar cells : efficiency, open-circuit voltage, and recombination“, in *Perovskite Photovoltaics and Optoelectronics: From Fundamentals to Advanced Applications*, Weinheim: Wiley, 2022, p. 127–172. doi: 10.1002/9783527826391.ch5.

V. N. Gorshkov, V. V. Tereshchuk, O. V. Bereznykov, G. K. Boiger, and A. S. Fallah, „Self-ordering in the dynamics of forming periodic 1D-structures controlled by external irradiation“, in *Prime Archives in Nanotechnology*, Hyderabad: Vide Leaf, 2022. doi: 10.21256/zhaw-26032.

A.4 Conferences and Workshops

G. K. Boiger, *Keynote Address ICM22: Multiphysics simulation of particle clouds in coating: the long journey from modelling to validated industrial application,* International Conference of Multiphysics, Oslo, Norway, 15-16 December 2022.

G. K. Boiger, B. Siyahhan, D. Sharman, A. Cabrero, *A Multiphysics-simulation-based study of process-parameter-impact in key-performance-attributes of the power coating of u-profiles,* International Conference of Multiphysics, Oslo, Norway, 15-16 December 2022.

E. Comi *et al.*, „Electro-thermal model for lock-in infrared imaging of defects in perovskite solar cells“, at the 8th World Conference on Photovoltaic Energy Conversion, Milan, Italy, 26-30 September 2022, in EU PVSEC Proceedings. WIP, 2022, p. 241–246. doi: 10.4229/WCPEC-82022-2BO.8.3.

R. Hagen, D. Fehr, F. Spano, D. Brambilla, and M. Bonmarin, „Portable multi-wavelength fluorescence measurement device“, at the XVII IEEE International Symposium on Medical Measurements and Applications, Messina, Italy, 22-24 June 2022, in 2022 IEEE International Symposium on Medical Measurements and Applications (MeMeA). IEEE, 2022. doi: 10.1109/MeMeA54994.2022.9856591.

M. Hostettler, S. Stingelin, F. De Lorenzi, R.M. Füchslin, C. Jacomet, S. Koll, D. Wilhelm, G. K. Boiger, *Modelling of a peristaltic pumps for viscoelastic tube material properties under consideration of fatigue effects*, International Conference of Multiphysics, Oslo, Norway, 15-16 December 2022.

M. Mahdi, F. Ebadi Garjan, W. Tress, *Performance boosting polymeric finish layer for perovskite solar cells*, 8th International Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP), Winterthur, Switzerland, 7-9 September 2022.

P. Marmet, *Optimization of MIEC-based SOFC anodes by digital microstructure design (DMD),* 18th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies (ModVal), Hohenkammer, Germany, 14-16 March 2022.

J. Noack, E. Baudrin, R. Fornari, A.A. Alejandro, D. Gerlach, G. Xinjie, J. Hamaekers, A. Maas, Ch. Menictas, G. Mourouga, H. Nirschl, N. Roznyatovskaya, R.P. Schärer, J. Schumacher, P. de Silva, M. Skyllas-Kazacos, J. Wlodarczyk, *Modelling and simulation for the search for new active materials for redox flow batteries: results of the international project Sonar*, 241st ECS Meeting, Vancouver, Canada, 29 May - 2 June 2022.

A. Schubiger, D. van Oerle, G. K. Boiger, *Development of a fast cloud-based simulation workflow for the complete aerodynamic evaluation of aircraft*, International Conference of Multiphysics, Oslo, Norway, 15-16 December 2022.

B. Siyahhan, G. K. Boiger, *The modelling of substrate surface interactions in a Eulerian-Langrangian Multiphysics solver and its impact on powder coating pattern prediction*, International Conference of Multiphysics, Oslo, Norway, 15-16 December 2022.

B. Siyahhan, G. K. Boiger, *coatSim: a simulation based digital solution for optimization of production processes for particle-laden flows,* 9th World Congress on Particle Technology (WCPT), Madrid, Spain, 18-22 September 2022.

M. A. Torre Cachafeiro, K. K. Naresh, G. Feng, W. Tress, *Simulating the transient luminescence of perovskite light-emitting diodes under pulsed operation,* 8th International Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP), Winterthur, Switzerland, 7-9 September 2022.

W. Tress, *Mixed ionic electronic conductivity in metal halide perovskite and its effects on solar cells,* ATHENA Intensive Course in Metal Halide Perovskites: From Materials to Applications, online, 7-10 November 2022.

W. Tress, *Device physics of perovskite solar cells*, International Conference on Photovoltaic Science and Technologies (PVCON), Hatay, Turkey, 5-7 July 2022.

W. Tress*, Mixed conductivity in organic and hybrid materials,* Gordon Research Seminar “Electronic Processes in Organic Materials", Lucca, Italy, 25-26 June 2022.

A.5 Teaching

D. Bernhardsgrütter, *Analysis 2 für Data Science und Informatik*, lecture and practice, FS23, Bachelor of Science.

D. Bernhardsgrütter, *Lineare Algebra 2 für Systemtechnik*, lecture, FS23, Bachelor of Science.

D. Bernhardsgrütter, *Analysis 1 für Data Science und Informatik*, lecture and practice, HS22, Bachelor of Science.

D. Bernhardsgrütter, *Lineare Algebra 1 für Systemtechnik*, lecture, HS22, Bachelor of Science.

M. Battaglia, *Physik Engines für Informatik*, lecture, FS23, Bachelor of Science.

G. Boiger, *TSM Two Phase Flow / Heat- and Mass Transfer*, FS23, Master of Science in Engineering.

G. Boiger, *TSM Advanced Thermodynamics*, HS22, Master of Science in Engineering.

G. Boiger, *EVA OpenFoam I - Thermo-Fluid-Dynamic Model Development using OpenFoam*, HS22, Master of Science in Engineering.

M. Bonmarin, *Höhere Mathematik 2 für Informatiker*, lecture and practice, FS23, Bachelor of Science.

M. Bonmarin, *Physik 2 für Systemtechnik*, lecture and practice, FS23, Bachelor of Science.

M. Bonmarin, Thermal Devices in Medicine, lecture and practice, FS23, Bachelor of Science.

M. Bonmarin, *Höhere Mathematik für Informatiker 1*, lecture and practice, HS22, Bachelor of Science.

M. Bonmarin, *Physik 1 für Systemtechnik*, lecture and practice, HS22, Bachelor of Science.

M. Bonmarin, *TSM Medical Market Access*, HS22, Master of Science in Engineering.

D. Fehr, *Grundlagen der Elektrotechnik und Digitaltechnik für Informatik*, practice, HS22, Bachelor of Science.

D. Fehr, *Physikalische Grundlagen der Sensorik*, lecture and practice, HS22, Bachelor of Science.

D. Fehr, *Thermal Devices in Medicine*, lecture and practice, FS23, Bachelor of Science.

T. Hocker, *Aviation Projects 2 für Aviatik*, practice, FS23, Bachelor of Science.

T. Hocker, *Physik 2 für Aviatik*, lecture and practice, FS23, Bachelor of Science.

T. Hocker, *Thermische Energiesysteme*, lecture, FS23, Bachelor of Science.

T. Hocker, *Aviation Projects 1 für Aviatik*, practice, HS22, Bachelor of Science.

T. Hocker, *Physik 1 für Aviatik*, lecture and practice, HS22, Bachelor of Science.

M. Jazbinsek, *Physik 2 für Maschinentechnik und Energie- und Umwelttechnik*, lecture and practice, FS23, Bachelor of Science.

M. Jazbinsek, *Physik 1 für Maschinentechnik und Energie- und Umwelttechnik*, lecture and practice, HS22, Bachelor of Science.

C. Kirsch, *Analysis 2 für Systemtechnik*, lecture and practice, FS23, Bachelor of Science.

C. Kirsch, *Numerik für Elektrotechnik*, lecture and practice, FS23, Bachelor of Science.

C. Kirsch, *Analysis 1 für Systemtechnik*, lecture and practice HS22, Bachelor of Science.

C. Kirsch, *Analysis 3 für Elektrotechnik*, lecture and practice, HS22, Bachelor of Science.

K. Pernstich, *Grundlagenprojekt 2 für Verkehrssysteme*, practice, FS23, Bachelor of Science.

K. Pernstich, *Physik 2 für Aviatik und Verkehrssysteme*, lecture and practice, FS23, Bachelor of Science.

K. Pernstich, *Grundlagenprojekt 1 für Verkehrssysteme*, practice, HS22, Bachelor of Science.

K. Pernstich, *Physik 1 für Aviatik und Verkehrssysteme*, lecture and practice, HS22, Bachelor of Science.

M. Roos, *Höhere Mathematik 2 für Informatiker*, lecture and practice, FS23, Bachelor of Science.

M. Roos, *Numerik für Elektrotechnik und Systemtechnik*, lecture and practice, FS23, Bachelor of Science.

M. Roos, *Höhere Mathematik für Informatiker 1*, lecture and practice, HS22, Bachelor of Science.

M. Roos, *Scientific Computing für Informatik*, lecture and practice, HS22, Bachelor of Science.

B. Ruhstaller, *Advanced Thin Films*, FS23, Master of Science in Engineering

B. Ruhstaller, *Applied Photonics*, HS22, Master of Science in Engineering.

B. Ruhstaller, *EVA Introductory Optics for Photonics*, HS22, Master of Science in Engineering.

M. Schmid, *Analysis 2 für Data Science und Wirtschaftsingenieurwesen*, lecture and practice, FS23, Bachelor of Science.

M. Schmid, *Lineare Algebra 2 für Systemtechnik*, lecture, FS23, Bachelor of Science.

M. Schmid, *Analysis 1 für Data Science und Wirtschaftsingenieurwesen*, lecture and practice, HS22, Bachelor of Science.

M. Schmid, *Analysis 3 für Systemtechnik*, lecture and practice, HS22, Bachelor of Science.

M. Schmid, *Lineare Algebra 1 für Systemtechnik*, lecture, HS22, Bachelor of Science.

A. Schubiger, *Grundlagen der Elektrotechnik*, practice, HS22, Bachelor of Science.

J. Schumacher, *Lineare Algebra 2 für Systemtechnik*, lecture, FS23, Bachelor of Science.

J. Schumacher, *Multiphysics Modelling and Simulation*, FS23, Master of Science in Engineering.

J. Schumacher, *Wasser-Wind-Sektorkopplung-Solare Treibstoffe*, lecture, FS23, Bachelor of Science.

J. Schumacher, *Lineare Algebra 1 für Systemtechnik*, lecture, HS22, Bachelor of Science.

W. Tress, *Physik 2 für Energie- und Umwelttechnik, lecture and practice*, FS23, Bachelor of Science.

W. Tress, *Physik 1 für Maschinentechnik und Energie- und Umwelttechnik*, lecture and practice, HS22, Bachelor of Science.

W. Tress, *Physics on Micro and Nano Scale*, HS22, Master of Science.

A. Witzig, *Physik 3 für Systemtechnik*, lecture and practice, FS23, Bachelor of Science.

A. Witzig, *Physik Engines für Informatik*, lecture, FS23, Bachelor of Science.

A. Witzig, *Wasser-Wind-Sektorkopplung-Solare Treibstoffe*, lecture, FS23, Bachelor of Science.

A. Witzig, *Physik 3 für Verkehrssysteme*, lecture and practice, HS22, Bachelor of Science.

A.6 ICP-Spin-off Companies

NM
Numerical
Modelling GmbH

www.nmtec.ch

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

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 packages Setfos and Laoss, as well as the measurement platform Paios, Phelos and Litos. The combination of simulation software with measurement data allows for the determination of material and device parameters. The 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.

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. The company will be founded in the summer of 2023.

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.zarawind.com

Zarawind is a startup based in Winterthur, Switzerland, which is involved in the development of a wind energy turbine suspended in the air. The goal of the company is to develop renewable energy sources that are still unused today. Zarawind's technology aims to produce renewable and cost-effective electricity from high altitude, strong and consistent wind power. This can be achieved by a rotor that is lifted to several hundred meters above ground by an aerostat. Wind power is a strong, constantly available energy source. The Zarawind concept ensures continuous operation and prevents noise problems, flickering light reflections and bird collisions. It is also suitable for off-grid regions and produces electricity at low cost.

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 ICP Team

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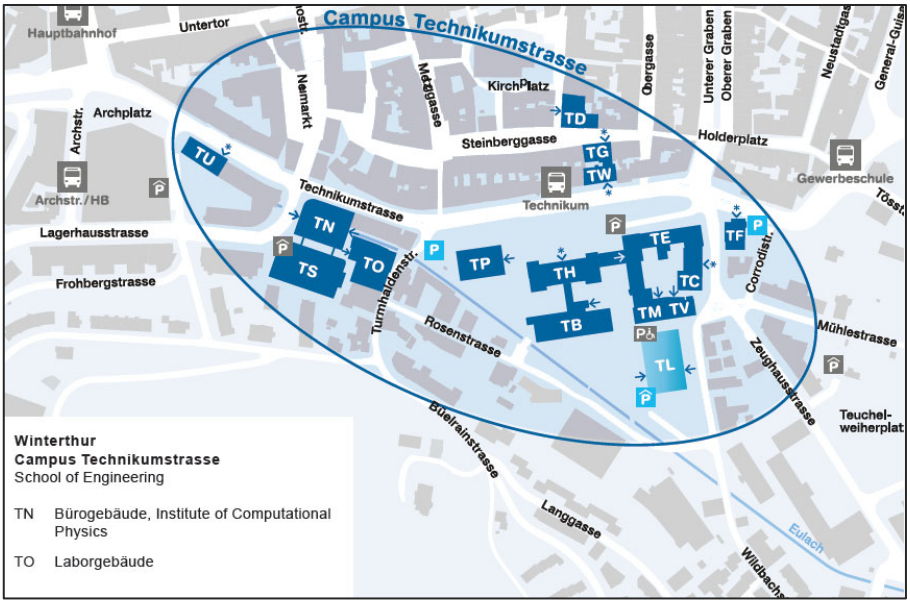

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