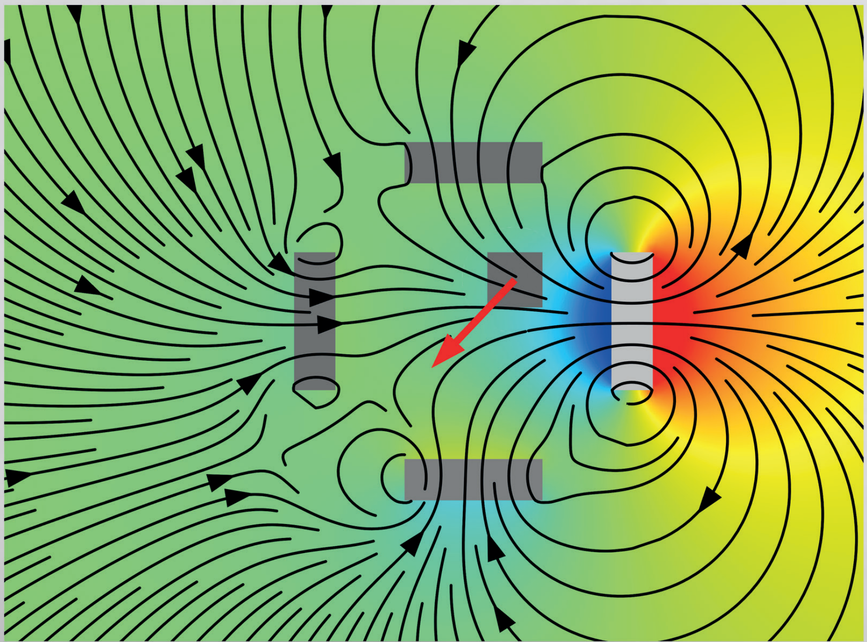
Zurich University
of Applied Sciences

School of
Engineering

ICP Institute of
Computational Physics

# Research Report 2020



The cover picture shows the simulation results of a magnetically controlled free-floating magnet. In the figure the resulting magnetostatic force is represented by a red arrow. The magnetic field lines are drawn in black.

# Introduction

## Be brave! Continue research!

No, this introduction is *not* dedicated to the COVID-19 pandemic! I would just like to take this opportunity to thank the ICP staff. With extraordinary commitment and great flexibility we succeeded in smoothly continuing both, our teaching and R&D responsibilities, despite the state of emergency.

In a time of uncertainty, a demanding and satisfying job gives us stability. At the ICP, we benefit from a good and close exchange and mutual support. Creative minds generate good ideas, but project proposals require teamwork and successful research projects need close collaboration. Interesting research requires good risk management: At the beginning it is uncertain whether intermediate results will be achieved and what the final result will look like. Crazy ideas are simply pursued with courage and creativity. If you then persist until the end of the project, you have a good chance of applying the gained scientific knowledge in practice.

Last year, we were able to initiate a number of new national and international research projects at the ICP, thus maintaining already established collaborations and building up new ones with new partners. We further expanded our relationships with industrial partners and international scientists. In addition to courage, a certain persistence is also required. It can happen that you get distracted, for example by complicated procedures in project management or because doctoral students or top international researchers can sometimes only be employed with an administrative balancing act. But as soon as these hurdles are overcome, the projects receive your full attention again. Then the team spirit in the institute and the common drive for research provide the breeding ground for good results.

As usual, the first part of the research report presents the current research work, structured according to the ICP teams. This is followed by a discussion of spin-off companies. I am particularly pleased to support the formation of a new business venture: David Schaltegger from the ICP and Pascal Vögeli from the INE are founding a new company in the summer of 2020. They use their skills acquired at ZHAW to offer consulting services in the field of environmental services. Congratulations on this courageous step and much success!

The School of Engineering and ZHAW are currently engaged in intensive discussions about know-how transfer and startups, which is why we are devoting a separate chapter in this year's ICP annual report to this topic. Repeatedly, we have been successful in motivating employees to take up this venture. In the last chapter, we report on the institute's culture and the concrete support that promote these activities.

Enjoy reading this report!

Andreas Witzig,
Head of Institute

# 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, a Google search of the neologism “Multiphysics” returns more than 3,640,000 results. The possible range of applications has been widely expanded and numerical methods have become increasingly sophisticated and adapted to exploit available computational resources. Today, detailed physical-chemical models combined with robust numerical solution methods are almost a necessity for the design and optimization of multifunctional technical devices and processes.

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

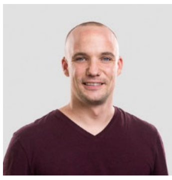
Our extensive experience in numerical analysis, modeling and simulation allows us to successfully apply simulation-based optimization in many fields. We are familiar with a wide range of governing physical equations and find numerical solutions even when the effects are closely interrelated. We also 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


D. Brunner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## 1.1 Experimental Studies on the Copper Refining Process

**Hydrometallurgical raffination or copper electrolysis is the bottleneck of refining copper. Industrial copper electrolysis is still a relatively slow diffusion based process, which can be accelerated by selective use of forced convection. An experimental copper electrolysis facility has been developed in order to replicate and investigate said effects.**

Contributors: V. Buff, M. Boldrini, D. Brunner, D. Lienhard, G. Boiger
Partner(s): Internal
Funding: Internal
Duration: 2017–2021

Copper electrolysis is used to refine blister copper from a purity of around 98.5% up to 99.999%. Therefore, a cathode of pure copper is placed in a bath of electrolyte which consists of copper sulphate, sulphuric acid and some additional agents like glue and alcohol [1]. The anode, usually made of blister copper, is placed parallel to the cathode. During the process a voltage of around 0.3V is applied between the cathode and the anode. As a consequence, the anode is dissolving. The copper ions follow the electric field to the cathode where they deposit. Impurities and more precious metals than copper sink to the ground where they can be collected as anode slime. Lower grade metals stay in the solution. During the process a second kinetic effect based on natural convection appears: The ion transport from anode to cathode changes the copper concentration in the electrolyte. Due to the resulting differences in density, the electrolyte sinks alongside the anode and rises alongside the cathode resulting in a circular flow field.

Industrial application of the copper electrolysis is relatively slow. The kinetics of the ion transport process is based on natural convection and diffusion processes. Therefore, the electrolysis is the bottleneck in the whole copper supply chain. Internal simulation-based pre-studies [2] have shown that the existing electrolytic refining process can be significantly accelerated by well-aimed intervention (forced convection) in the prevailing ion transport mechanisms between the electrode plates. Well-controlled, directed and constructive flow conditions can substantially support the slow, diffusion and natural convection driven ion transport. Up to present, this aspect has been considered only rudimentarily in the design of currently operating copper refining plants.

Figure 1:Commisioning of the copper electrolyis facility at the ICP, January 2020.

To investigate the behaviour of the developed flow devices a test stand that simulates the industrial electrolysis process was built. The process consists of two DC sources which produce the desired electrical voltages and currents. The copper electrolysis takes place in the large tank where anodes and cathodes are placed in parallel [Figure 1]. During electrolysis, the electrolyte is increasingly contaminated and heated. A circulation pump transports the electrolyte from the electrolysis tank to the liberator where the amount of copper in the solution gets reduced. After the liberation, the electrolyte gets conditioned in the conditioner. In the conditioner the acidity is adjusted and, if necessary, base metals which are still dissolved in the electrolyte are precipitated. If required a temperature management system will implemented as well. After the conditioner the electrolyte is returned to the electrolysis tank.

*Source:*
[1] H. Sicius, Kupfergruppe: Elemente der ersten Nebengruppe, 2017.
[2] D. Brunner et al., Model Based Analysis of Forced and Natural Convection Effects in an Electrochemical Cell, 2017.

## 1.2 Investigation of Modal Distortion on Torsional Resonators

**Monitoring fluid properties such as viscosity is crucial in many industrial processes. Using mechanical resonators allows measuring the viscosity in an online manner, which enables a quick response and to maintain a high quality of a chemical or biochemical process. To develop these sensors, accurate models that fully describe the fluid-structure interaction of the fluid with the resonator are needed.**

Contributors: D. Brunner, H. A. Khawaja, G. Boiger
Partner(s): Rheonics GmbH, UiT The Arctic University of Norway
Funding: Innosuisse (CTI)
Duration: 2018–2021

The torsional resonator investigated in this study is a tubular resonator comprised of a tube, permanent magnets and decoupling masses, as schematically shown in figure 1.

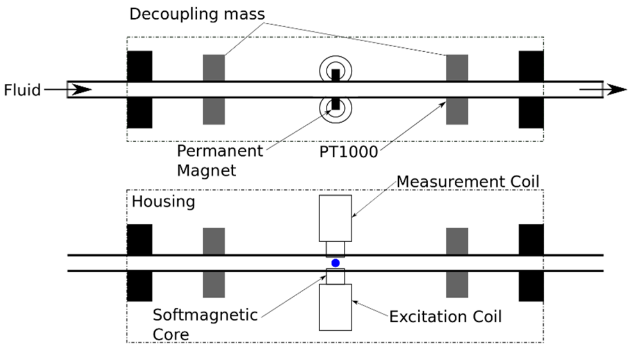



Figure 1: Schematic of the sensor[1]

The working principle of the sensor is based on the excitation of a torsional mode, and the subsequent measurement of the oscillation. Based on the measured signal, the damping and resonance frequency are determined. Resonance frequency and damping can be related to the fluid's viscosity.

An important aspect of the resonator modelling is the interaction of the resonating structure with the fluid. To fully resolve this interaction, the sensor was modelled using a strong fluid-structure interaction model which was solved using LS-DYNA. Thereby, the Navier-Stokes equations as well as the structural equations were solved simultaneously. The benefit of this method is that the distortion of the structural mode can be considered. This effect was neglected in previous models, where the resonator was modelled in the frequency domain using a weak fluid structure interaction.

To investigate the effect of modal distortion, the tubular sensor was modelled with different inertial masses in the centre. The inertial mass represents the permanent magnets and allow to vary the ratio between inertial forces and fluid forces. Thus, with a lower inertial load, the fluid has a larger impact on the mode, which may result in a larger modal distortion.

The results of the simulation indicate, that the fluid slightly deforms the resonating mode. However, the magnitude of this distortion is small, meaning the relative modal distortion with respect to a low viscous fluid $(A - A_{\eta_0})/\max(A)$ is below 0.5 % even for very high fluid viscosities.

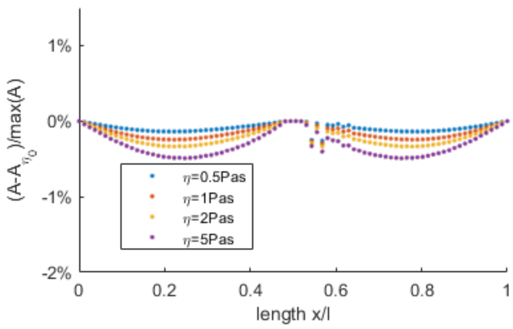



Figure 2: Relative modal distortion caused by different fluid viscosities.

It was shown that strong fluid-structure interaction can be used to model a torsional resonator and consider effects such as modal distortion. However, the effect of the modal distortion is small, and in most cases, including the tubular resonator of this study, it can be neglected.

*Source:*

[1] 14th International Conference of Multiphysics, Dubai, UAE, 14-15 December 2019.

## 1.3 Simulation-Based Calibration of Infusion Systems

**Infusion systems enable the continuous administration of drugs in liquid form. For medical operation it is necessary to maintain an exact volume flow, which is achieved by using peristaltic pumps. However, the calibration of such pumps requires complex measurements, which impair the broad application of such systems. By means of a simulation model, the fluid dynamic behavior of the pump and infusion system shall be modelled in order to enable a more efficient calibration, and to apply different configurations of the product.**

Contributors: M. Hostettler, G. Boiger
Partner(s): Codan Argus AG
Funding: Innosuisse
Duration: 2019–2021

When using medical infusion systems, a high degree of accuracy regarding the amount of injected medication is required. Peristaltic pumps, among others, are used to set a desired volume flow. Since very small volume flows are required, direct volumetric determination of the flow rate is not possible. The flow rate must be determined from the system and pump parameters. For the necessary calibration of the pump, however, individual and extremely extensive measurements are necessary, which considerably limit the efficient use of such devices.


Figure 1: Different components of an infusion system (from left to right: flow controller, drop-counter, filter and tubing).

In the present work, the basic flow behavior in the hose system and peristaltic pump is investigated and a model is developed to make the calibration of such systems more efficient.

With this model, any configuration of the components installed in the infusion system (see Fig. 1) can be better realized and a broader application of the product is enabled.

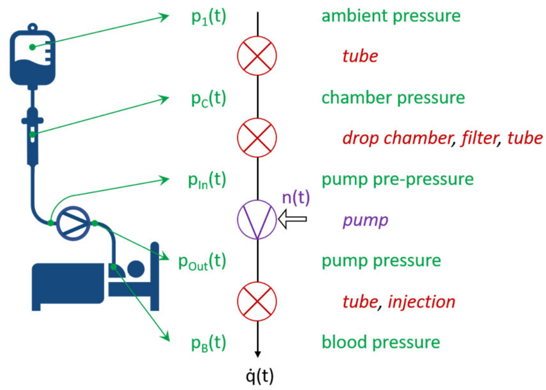



Figure 2: Model of the infusion system with pump and various components.

Within the scope of the project, comprehensive experimental measurements are used to individually characterize the behavior of all flow-carrying components. Various numerical models (from simple one-dimensional methods to detailed CFD simulations including fluid-structure coupling) are investigated and compared with measurements for the characterization of the pump.
Based on the measured data of the individual components and the findings from the pump characterization, the flow dynamic model of the infusion system is developed (see Fig. 2) and is validated by means of specific experiments.

## 1.4 A Multiple Rotating Reference Frame (MRF) Based Spatial Averaging Methodology for Stirred Reactors

**Stirred reactors play an essential role in preparation of chemical mixtures in the pharmaceutical industry. Hence efficient simulation methods to assess the performance of these reactors are of utmost importance in this field. In this study, a MRF based computational fluid dynamics (CFD) methodology is developed for stirred reactor tanks. The underlying idea is to combine a series of steady state MRF flow fields to predict the distribution of a certain chemical species within the tank, avoiding computationally costly transient simulations.**

Contributors: B. Siyahhan, G. Boiger
Partner(s): Novartis Pharma AG
Funding: Direct Funding, Novartis Pharma AG
Duration: 2020

The simulation of stirred reactors is challenging as it requires dynamic mesh regions, where the computational cells rotate along with the impeller, with respect to the rest of the stationary domain. OpenFOAM, an open-source computational fluid dynamics (CFD) simulation library, offers several solvers that can handle such dynamic meshes. However, these solvers are inherently transient in nature. Hence it is computationally very expensive to simulate the whole mixing process since there are stringent conditions on the size of the time steps allowed.

Alternatively, an MRF based method can be used, whereby the body forces due to rotation are introduced for a region surrounding the impeller, while keeping the whole mesh stationary. This allows for fast, steady state simulations to be performed for a fixed configuration of the impeller.

The main idea behind this study is to leverage the computational efficiency of the MRF simulations, by combining a series of them, with the impeller in differing configurations, to derive a spatially averaged flow field. This steady flow field is used subsequently in a transient passive scalar simulation to resolve the concentration of the chemical species in the tank and quantify its residence time.

The first step of the methodology requires meshes to be generated at different impeller configurations. In order to achieve this, a python-based script has been developed, that rotates the input geometry files in STL format by given rotation angles as demonstrated in Figure 1. The generated geometry files are meshed with cfMesh, a highly automatable open source mesher compatible with OpenFOAM.

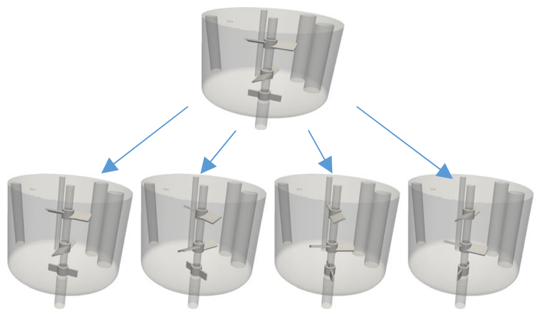


Figure 1: The impeller of the reference geometry if rotated by a given incremental angle.

On the generated meshes, the steady state flow field is simulated. These flow fields are subsequently mapped and averaged on a mesh void of the rotating parts as shown in Figure 2. Then the chemical species concentration is simulated on this averaged field for an improved match to experimental data as in Figure 3.

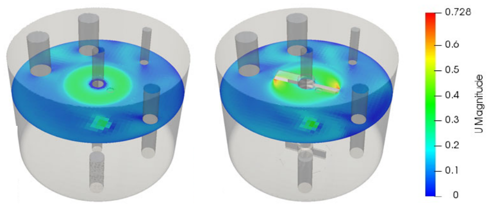



Figure 2: On the left the averaged velocity field in the domain void of the impellers, in comparison to the velocity field from an instance of an MRF solution on the right.

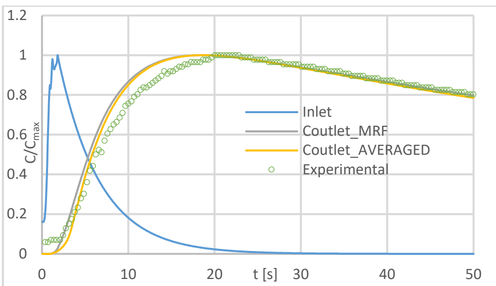



Figure 3: The averaging method Coutlet_AVERAGED, matches the experimental data better than the MRF simulation, Coutlet_MRF, with fixed impeller configuration.

## 1.5 CFD Model of Exhaust Emission Pollutants in Tromsø Harbor

**Plumes emissions from industrial activities and chimneys of large boats can carry a number of pollutants to the nearby cities causing a detrimental effect on the life quality and health of local citizens and ecosystems. They are transported by the local wind over habited areas and traces of it will reach the street level, leading to contamination of the air. The main pollutants are waste products of the industrial activity or the combustion processes emitted in gas phase or as particulate matter. Gas phase pollutants diffuse in the surrounding air and they are transported by the wind flow over habited areas. The local level of contamination is difficult to assess without real scale atmospheric simulations. A realistic simulation model should describe the atmospheric conditions (temperature, wind, pressure), the local topography and the characteristics of the emission plume (temperature, combustion by-products, height of chimney).**

Contributors: A. Zubiaga, H. A. Khawaja, G. Boiger
Partner(s): UiT The Arctic University of Norway, Tromsø, Norway
Funding: Internal
Duration: 2019

The main pollutants are waste products of the industrial activity or the combustion processes, mainly carbon monoxide ($CO$), nitrogen and sulfur oxides ($NO_x$, $SO_x$) in gas phase and solid particulate matter.
Carbon dioxide ($CO_2$) is the main by-product in exhaust plumes. Although it does not have any health effect, the fluid-dynamics behavior of $CO_2$ is comparable to and representative of any gas pollutant in the plume. In the present work, we have made a comprehensive study of the effect that $CO_2$ plumes from the harbour of Tromsø (Norway) have in the contamination levels in the city.
We have used computational fluid dynamics modelling of $CO_2$ transport and diffusion in air. OpenFOAM® has been used for the simulation of the gas mixture. The Navier-Stokes equation has been solved including compressibility effects of perfect gases and buoyancy effects. Turbulence effects have been treated using Reynolds Averaged Navier–Stokes (RANS) models. The online platform KALEIDOSIM® has been used to run large parameter studies simultaneously, improving noticeably the work flow.
A high wind speed and chimney height are seen to be the main factor decreasing the pollutant concentration in the surrounding area of the emission plume. On the other hand, the wind direction determine which zones are more affected by the plume emissions. The local orography also has a large effect on the gas flow and can enhance or deplete the deposition of emission gases[1].
The presented results will help to evaluate the impact of pollutants in the everyday life of local citizens.

*Source:*

[1] 14th International Conference of Multiphysics, Dubai, UAE, 14-15 December 2019.

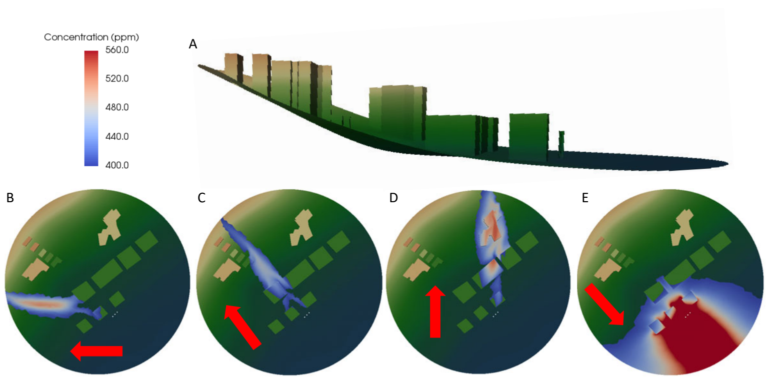



Figure 1: A) The topographic model shows the local orography in Tromso harbor. The top views represent the pollutant concentration at street level for 4 wind directions: B) West, C) North-West, D) North and E) South-East. The pollutant deposition in the sea, E, is enhanced by the lack of orographic obstacles to the wind, as compared to C where the wind blows uphill inland.

## 1.6 Model Based Optimization of CGO-Ni Based SOFC Anodes

**Costs and lifetime are currently the limiting factors for a broader use of Solid Oxide Fuel Cells (SOFC) with natural gas for combined heat and power. Therefore, a systematic optimization of materials and cell-concepts is needed to enable the use of cheaper components and to increase lifetime and efficiency. In our approach we build on digital materials design (DMD), whereby methods for multi-physics simulation, 3D microstructure characterization (tomography data) and electrochemical impedance spectroscopy (EIS) are combined. Based on the DMD approach, the relations between material properties, microstructure, cell-design and performance are established on a quantitative level. This approach helps to define design guidelines for optimized electrodes and accelerates the innovation cycle for future SOFC devices.**

Contributors: P. Marmet, L. Holzer, T. Hocker, J. Brader, J. Grolig, H. Bausinger, A. Mai
Partner(s): Hexis
Funding: Swiss Federal Office of Energy
Duration: 2019–2022

For the next generation of SOFC cells, the requirements of the market call for higher efficiency, longer lifetime and lower system costs. In order to meet these requirements we elaborate on new anode concepts, which are based on doped ceria with nickel combined with cheap ferritic interconnectors. However, complex physico-chemical processes are involved including transport of gas in the pores, transport of ions and electrons in the ceria phase, fuel oxidation reaction on the surface of ceria etc. Hence, there are numerous conflicting requirements, which complicate the development process. Therefore, sophisticated methods including mathematical models as well as experimental methods are needed for a systematic optimization of the system.

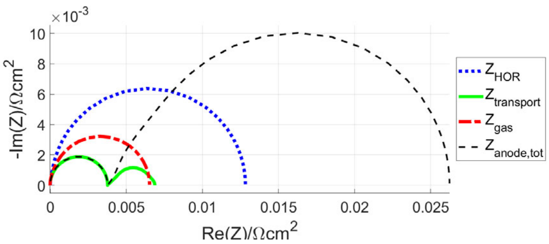



Fig. 1: Deconvolution of the simulated anode EIS-spectra: $Z_{HOR}$ = hydrogen oxidation reaction impedance, $Z_{transport}$ = charge carrier transport imped., $Z_{gas}$ = gas imped., $Z_{anode,tot}$ = total anode imped.

In SOFC research, electrochemical impedance spectroscopy (EIS) is an essential characterization tool, which serves as a basis for materials optimization on the electrode, cell and stack levels. However, overlapping processes in the EIS spectra and lacking knowledge about the detailed physico-chemical processes makes it difficult to interpret the EIS-spectra correctly. Multi-physics simulation models developed at ICP with AC and DC modes, enable the simulation of the EIS-spectra as well as the DC behaviour during the normal cell operation. Therewith, a basic understanding of the complex physico-chemical processes and a deconvolution of the EIS-spectra is achieved. A calibrated simulation model is then used to predict the impact of design adjustments (e.g. material and microstructure variations) on the cell performance. A key point thereby is to include the effects from microstructure appropriately in the model.

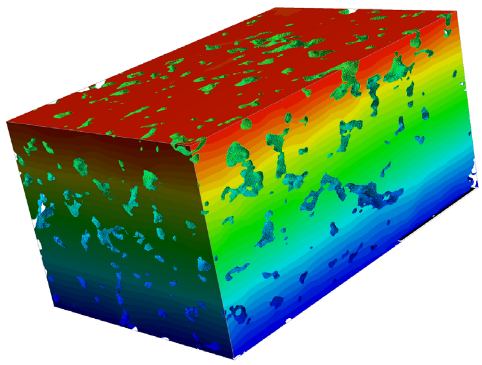


Fig. 2: Potential drop along an anode microstructure to determine the effective conductivity using GeoDict©.

Microstructure analysis based on FIB-tomography enables to quantify morphological characteristics (tortuosity, porosity etc) and the associated transport properties. With the digital materials design (DMD) approach, the effect of microstructure variation on the cell performance can be assessed. By establishing the relation between material properties, microstructure, cell-design and performance, guidelines for a new anode materials design can be deduced. This allows for a faster and more systematic development of new SOFC electrodes.

## 1.7 Development of a New Generation of High-Performance Air Heaters

**The controlled heating of air flows plays a big role in a number of industrial processes. Leister Technologies AG is a world leader in plastic welding and process air equipment that relies on the efficient and reliable supply of heated air. In collaboration with D. Penner's team at ZHAW-IMPE and S. Koll's team at ZHAW-ZPP, this project explores new materials, manufacturing and design routes to develop a new generation of high-performance air heaters for application in future Leister products.**

Contributors: G. Boiger, S. Ehrat, T. Hocker, G. Sartoris, B. Siyahhan
Partner(s): ZHAW IMPE Team D. Penner, ZHAW ZPP Team S. Koll, Leister Technologies AG
Funding: Innosuisse
Duration: 2018–2020

Recent advances in the development of new materials and manufacturing methods provide a large potential for improving the performance of air heating devices at reduced manufacturing costs. However, while the choice of potential heating materials and designs is large, optimizing derived products purely by trial and error would be an impossible task due to the large number of selectable parameters and ambitious performance requirements. Instead, it is much more efficient to employ validated computer models to gain a basic understanding of the physical phenomena taking place and to allow one to run extensive parameter studies for optimization purposes.

In collaboration with our partners ZHAW-IMPE, ZHAW-ZPP and Leister Technologies AG, we develop new heating elements made of electrically conducting ceramics based on our recent patent application WO2019185291A1. The later manufacturing will be based on cost-efficient injection molding. To avoid overheating under higher power inputs, an electro-mechanic-thermo-fluidic hybrid FE/FV-model has been developed and implemented in our in-house simulation software SESES.

The model is made of the actual heating element, the surrounding air flow as well as the housing and consists of about 10 million elements. All materials parameters are temperature-dependent, which is crucial for capturing the thermal behavior of a real heating element. The model calculates the produced heat from the nonhomogeneous electrical current flow through the heater. Heat is then transferred to the surrounding turbulent air flow by forced convection and to the housing by surface-to-surface radiation.

The thermal materials parameters of the model have been calibrated by IR-temperature measurements using a simplified sample geometry. As shown in Figure 1., the agreement between the model and the IR-data is excellent.

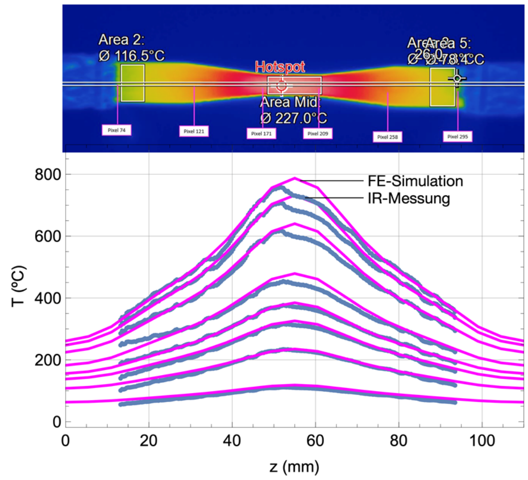



Figure 1: Model calibration based on IR T-measurements of a sample heater at different power levels.

Figure 2 shows the temperature distribution under steady-state operation conditions of a typical heating element. Since the to be heated air flow enters from the back and leaves at the front, there is a huge temperature-increase from back to front of almost 1000 ºC. The observed radial T-differences result from the nonhomogeneous heat production.

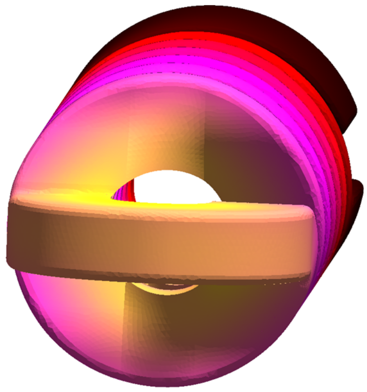


Figure 2: Temperatures of a newly developed air heating element under steady-state operation conditions. Brighter colors indicate higher temperatures. The used SESES FE/FV-model consists of about 10 million elements.

## 1.8 Test Rig for Welding Plastic Samples

**Infrared welding is an established method for joining plastic pipes. The pipes are heated at their end faces by infrared heating until the plastic melts. Then the tubes are pressed together with a defined force and cooled down. Due to the contactless heating of the tubes, the weld seams are of high purity. For this reason, this process is used for example for the production of pipelines in clean rooms in the semiconductor industry. Different heating system solutions are to be evaluated on a test rig on the basis of simple plastic samples with regard to optimum weld seam quality.**

Contributors: N. Jenal, M. Gorbar, S. Spirig, T. Hocker, C. Brändli
Partner(s): ZHAW IMPE Teams C. Brändli und D. Penner, Georg Fischer Piping Systems
Funding: Innosuisse
Duration: 2018–2021

In cooperation with Georg Fischer Piping Systems, a test rig was developed to join cuboid-shaped plastic samples with the infrared welding process. Different heating system concepts can be tested on the test rig with regard to optimum weld seam quality, see figure 1.

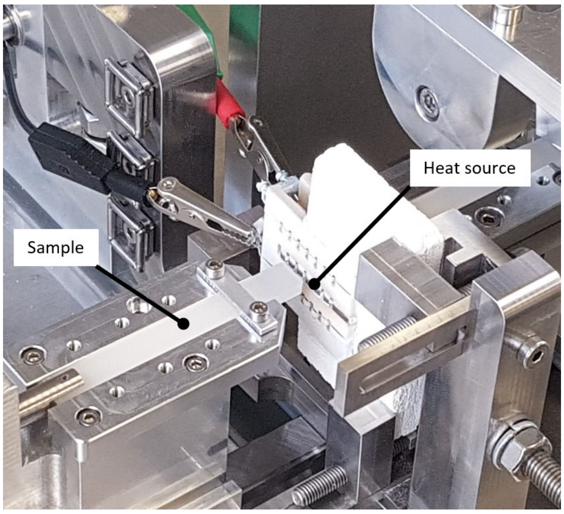



Figure 1: Test rig for welding plastic samples.

A welding process consists of three steps. First, the end faces of the samples are heated until the plastic melts. Second, the samples are pressed together. Afterwards the cooling takes place until the weld seam solidifies. The faces of the samples are not in contact with the heating system during heating. For this reason, the ends are heated primarily by thermal radiation. A new type of heating system should provide a melt front that is as uniform as possible.

The melt front describes the transition between the liquid and solid plastic after the heating process, see figure 2.

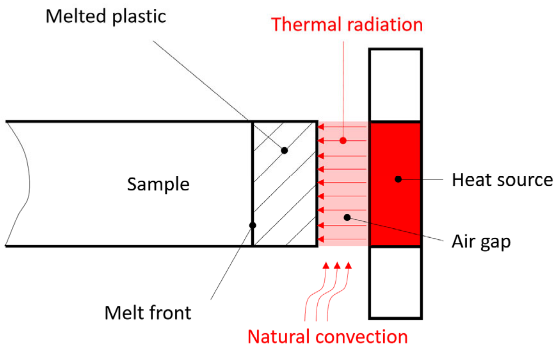



Figure 2: Contactless heating of cuboid-shaped plastic samples.

Microtome section are taken from the welded samples to examine the shape of the melt front under a light microscope, see figure 3. These images are used to evaluate the best heating system and to validate the CFD models. The simulations are used to reproduce the entire welding process.

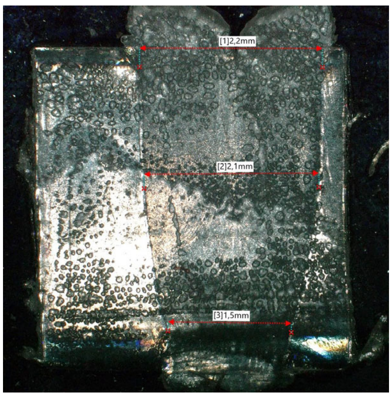


Figure 3: Microtome section under microscope.

## 1.9 Innovative Airborne Wind Power System

**Classical wind power systems are not always an applicable energy solution in regions where winds are not sufficiently strong at the altitude of traditional windmills. On the other hand, at several hundred meters above ground level, winds are stronger and much more consistent. To harvest strong wind power at that elevation, a buoyant gas aerostat is used to lift up an electrical generator. The system hovers in the sky and sends electricity through a cable-tether connection to the earth. A new "Lighter-Than-Air (LTA) wind power turbine" is introduced by Zarawind. The efficiency of this concept comes from the fact that it maintains the airborne system stationary operating at high altitude with an efficient harvesting of the strong wind power. Among many others, this technology is advantageous due to the applicable deployment of the efficient buoyant airborne system in the wide economic areas of the high-altitude strong-winds. In this research project, we characterize the aerodynamics of an innovative blade concept for LTA wind power turbine, we study the influences of the geometry on the performance of the new wind power rotor, we analyze the durability of rotor's materials.**

Contributors: Y. Safa
Partner(s): Zarawind, IMPE Institute of Material and Process Engineering and ZAV Center for Aviatiation
Funding: SFOE, Swiss Federal Office of Energy
Duration: 20018–2020

At several hundred meters above ground level, wind currents are stronger and much more consistent than those close to the ground. To harvest such a strong wind power, Zarawind presents a new concept of a wind power rotor-generator system carried by an aerostat to send electricity through a tether-cable connection to the ground. The efficiency of this concept comes from the facts: first, the system can be maintained at high altitudes independently from wind conditions, second, it ensures a continuous and economic harvesting of the wind power at high performance coefficient. This is based on an innovative vertical counter-rotating rotor the first implemented using flexible blade which operates with passive folding and deployment promoting the aerodynamic performance Fig. 1. Such innovative benefits are satisfied in the designed system at reduced payload installation cost.

Indeed, the omni-directional vertical rotor is built-up through a tensional-integrity (tensegrity) concept. This ensures a reliable toque transmission through rotor stages at reduced-mass components that are bending and shear free. As such, the rotor can maintain a high power performance at controlled payload of the buoyant system.

In the real conditions of wind flow, buoyant aerostat, rotor, and tether cable are exposed to aerodynamic drag forces. This denotes an inevitable inclination of the vertical tethered rotor. Competitive effects between tether-traction, tether-cable load, and aerostat forces govern the curved-shape of the tether Fig. 1. Indeed the tether angle exhibits variation from the aerostat confluence point level to the ground mooring (attachment) point. Investigation of different aerostat models, stated that tether angle could range from zero in "no-wind", until 45 degrees in strong winds depending on aerostat models. However, uncontrolled tether-inclination (or curvature) could affect the rotor performance when the airborne tethered system is blowing down to lower-wind-speed altitudes. To ensure a stationary positioning of the aerostat at higher altitudes, one can suggest to over-design the buoyant volume, this increases however, the installation costs of the system. However, uncontrolled tether-inclination (or curvature) could affect the rotor performance when the airborne tethered system is blowing down to lower wind-speed altitudes. Through an innovative solution, the rotor produces an upward-thrust force Fig. 1, this force counters the tether curvature effects in strong winds. To provide such a service, the rotor is designed like a bionic-inspired concept where blades mimic the birds interaction with winds. The novel "wing-kite blade" is passively deployed to take a kite configuration producing both drag forces (driving rotation) and lift forces. The flexible blade is passively folded in upwind motion to take wing configuration producing lift forces driving rotation and elevation. For a successful implementation of the technology, the rotor should insure a threshold aerodynamic performance. In this project supported by SFOE, Swiss Federal Office of Energy, the research tasks are conducted between three groups from ICP, IMPE and ZAV at ZHAW. This combine numerical simulations, material tests, model constructions, wind tunnel experiments, and engineering design-analysis works.

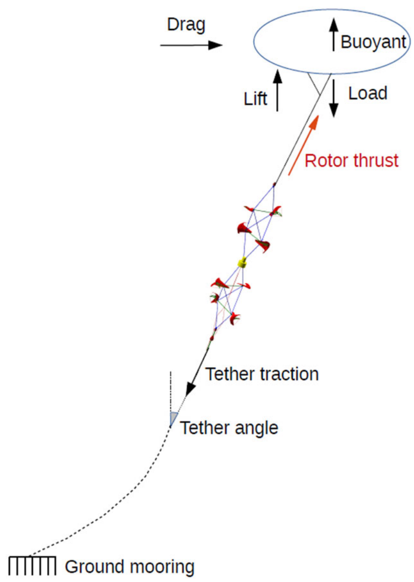



Fig. 1: Mechanism of Zarawind system hovering at high-altitudes. Upward rotor-produced thrust counters inclination.

## 1.10 Development of a Test Stand for Measuring of Thermal Conductivity

**Nowadays, computer simulations of heat and material flows are essential in the development of thermally systems. Crucial for its accuracy are the material parameters used therein. Especially thermal conductivities for the description of heat conduction phenomena are often only roughly known and only at room temperature. Therefore, we are developing a test rig that measures thermal conductivity of solids and composite structures over a large T-range.**

Contributors: S. Ehrat, T. Hocker
Partner(s): ZHAW-IMPE Team D. Penner & Team C. Brändli, Georg Fischer Piping Systems
Funding: Innosuisse
Duration: 2018–2021

Heat conduction phenomena play an important role in our R&D projects. The computer models used to optimize such systems are limited in their validity and accuracy by the thermal conductivities used in the model. The latter usually show a strong temperature dependence and depends on the porosity of microstructure materials. Further uncertainties result from thermal contact resistances between different material layers, which can only be determined by thermal conduction measurements of the entire composite arrangement. For these reasons, we have decided to develop a test rig for determining the thermal conductivity of solids.

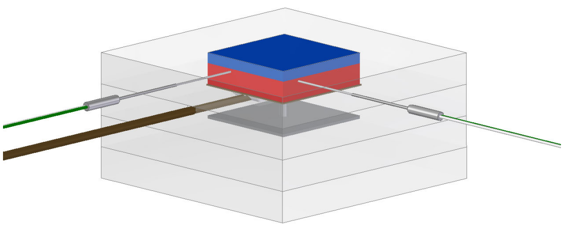


Fig. 1: CAD representation of the test stand with sample material in blue, copper block in red, heating foil in brown, as well as thermocouples (green, white) and first insulation layer (transparent).

Figure 1 shows the simple structure of the planned test bench. The sample (blue) is brought to the desired temperature by means of a heated copper block (red) and kept there. With the measured temperature difference between the top and bottom side of the sample in the stationary state, as well as the known heating power and the sample thickness, the thermal conductivity of the sample can be calculated. The temperatures on the bottom side of the sample are measured by type K thermocouples, while a thermal camera is mounted on the top side for temperature measurement. In order to extract T-values from the thermal images as accurately as possible, the emissivity of the investigated samples must also be determined. An electrical resistance heater is embedded in a MICA foil (brown), which can reach temperatures up to 500 °C.

CFD simulations have been used for the design of the thermal insulation. The optimal solution is a composite arrangement of different insulation materials. The first insulation layer is a nanoporous insulation layer based on silicon dioxide. This insulation is followed by a layer of rock wool and a final XPS insulation board.
Figure 2 shows the stationary temperature distribution of this arrangement. In the centre of the picture the heated copper block and the above placed sample can be seen. These components are surrounded by the nanoporous insulation. This insulation layer is only 3 cm thick, but reduces the temperature by 300-400 °C. The top side is open to the environment and therefore air-cooled. This can be seen in the figure by means of the hot air rises by natural convection.

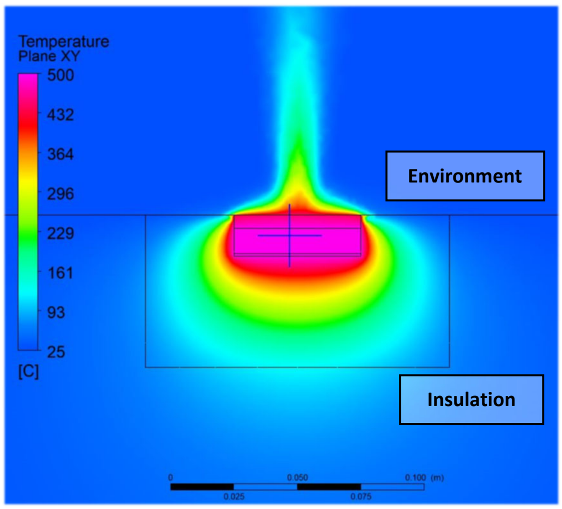



Fig. 2: CFD simulation of the temperature distribution in the test stand. The highest temperatures prevail in the heated copper block (violet). Furthermore, the effect of natural convection in the ambient air above the sample can be seen.

## 1.11 Model-Based Characterization of the Movement of Hot Air Balloons

**The hot-air balloon is the oldest aircraft and still fascinates young and old. This project aims to develop a detailed physical model of a hot-air balloon that describes its movement based on real weather data. The model will later be used in the aviation studies program to promote the understanding of the phenomena occurring during ballooning and as a planning and analysis tool for hot-air balloon pilots. As a prerequisite for "virtual" balloon flights, unknown model parameters must first be determined using literature data and experiments. For the latter, the ambient conditions and the temperature of the balloon envelope were measured during a parallel balloon flight.**

Contributors: J. Stoll, T. Hocker, S. Ehrat
Partner(s): Air Ballonteam Stefan Zeberli GmbH
Duration: 2020

The movement of a hot-air balloon results from its mass and the forces acting on the balloon, i.e. its weight, its buoyancy and the air resistance force, which depends on the winds prevailing at the respective position. The hot air temperature is decisive for the ascent and descent behaviour, which in turn depends on the energy supply via the burner and the heat losses via the balloon envelope. For this reason, during a parallel balloon flight with Lea and Stefan Zeberli, the ambient conditions and the temperature of the balloon envelope at different altitude levels were measured and the fuel consumption estimated.

A thermal imaging camera is used for surface temperature measurement, as it measures large areas. However, measurements with this instrument are complicated because the emissivity of the balloon envelope, the measuring distance, the ambient temperature and the humidity all influence the accuracy of the measurement. Therefore, it is important to take measures to minimize the measurement errors when developing the measurement procedure. For example, a shielding device for the thermal imaging camera has been developed to protect it from radiation from the burner. Furthermore, it must be taken into account that, depending on its position, the proportion of thermal radiation emitted by the balloon and absorbed by the atmosphere must be calculated. Based on this proportion, the temperature of the balloon envelope is then corrected.

Figure 1 shows a typical thermal image taken during a parallel balloon flight at an altitude of 1080 m. It can be seen that the temperature of the balloon envelope increases from bottom to top. Furthermore, it can be seen that the balloon envelope is made of different fabric strips with different emissivities, which lead to significant measurement errors in the thermal image.

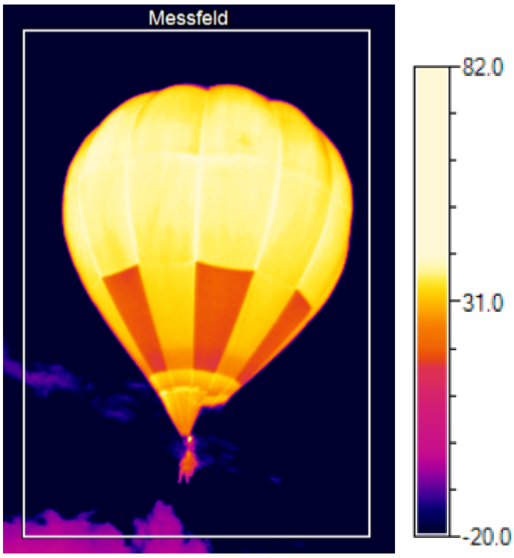



Figure 2 Thermal image of the hot air balloon flight of Lea Zeberli at an altitude of 1080 m, temperature scale in °C.

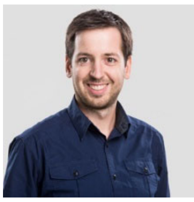
For a complete model, numerous influencing variables of the atmosphere have to be taken into account. Specifically, wind speed, wind direction, temperature, humidity and air pressure have to be considered depending on the respective position. In this regard, extensive research on national and international weather models was carried out to obtain forecast and reanalysis data. It has proved to be difficult to obtain freely accessible weather data with sufficient local resolution. For 2020 it is planned to use the weather data for the validation of the model, for the analysis of real balloon flights and for the planning of future flights.

# 2 Electrochemical Cells and Microstructures

Fuel cells are a prime example of electrochemical cells. They convert fuels such as hydrogen, natural gas or methanol into electrical energy and heat. Fuel cells can be used as a battery replacement in portable electronic devices, for combined production of heat and electricity in households and as electricity source in vehicles. Due to their flat design, fuel cells are easily scalable by connecting them in series to form stacks. Electrical efficiencies over 60% are feasible which is much higher compared to other decentralized electricity generation technologies. Redox flow batteries are considered as a promising energy storage technology. These batteries are highly efficient and they provide an energy storage solution for fluctuating energy from wind mills and photovoltaic cells.

The ICP supports the progress in the research and development of electrochemical cells by multiphysics computer models. In general, modeling helps to better understand the coupling of chemical, thermal, electrical, mechanical and fluidic processes with the goal to detect weaknesses of the system and provide design improvements. Often these models rely on detailed information about the microstructures of the investigated materials. Hence the characterization of gas diffusion layers and electrolyte micro-structures in 2D and 3D is an integral part of our modeling efforts.

In addition to fuel cells, we also do research on novel hydrogen production techniques. For example, we model photo-electro-chemical cells (PECs) which use solar energy to split water and thus produce hydrogen fuel. Most research projects are conducted in collaboration with our strategic partners Hexis AG in Winterthur (SOFC), Paul Scherrer Institut in Villigen (PEFC), EPFL (hydrogen generation) in Lausanne and Universität Ulm (virtual microstructures).


D. Bernhardsgrütter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J. Wlodarczyk

## 2.10 Macro-Homogeneous Models for Organic Redox Flow Batteries

**Redox flow batteries are a promising technology for stationary energy storage. The usage of abundant low-cost organic compounds is an attractive alternative to conventional electrolytes. However, the identification of well-suited organic compounds for redox-flow batteries is challenging due to the large available chemical space. In the European-funded project SONAR a multi-scale modeling and optimization framework is being developed that enables high-throughput screenings of chemical compounds, optimizations of redox flow battery components and overall system design. As part of the multi-scale modeling framework, macro-homogeneous cell models in one and three spatial dimensions are being developed at ICP, allowing for the efficient simulation of important physico-chemical processes within an electrochemical cell.**

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Partner(s): Fraunhofer Institute for Chemical Technology, Fraunhofer Institute for Algorithms and Scientific Computing, Technical University of Denmark, Laboratories de Réactivité et Chimie des Solides, Karlsruhe Institute of Technology, University of New South Wales
Funding: European Commission, Horizon 2020
Duration: 2020–2023

The large chemical space available for organic redox pairs allows for a high adjustability of the chemical properties. One of the key aims of the SONAR project [1] is to identify a set of viable organic compounds for redox flow batteries to accelerate the commercial use of safe and cost-efficient energy storage devices. For this purpose, a multi-scale modeling and simulation framework is being developed within the SONAR project that allows for the mathematical description of organic redox flow batteries from the atomistic up to the micro-grid scale.

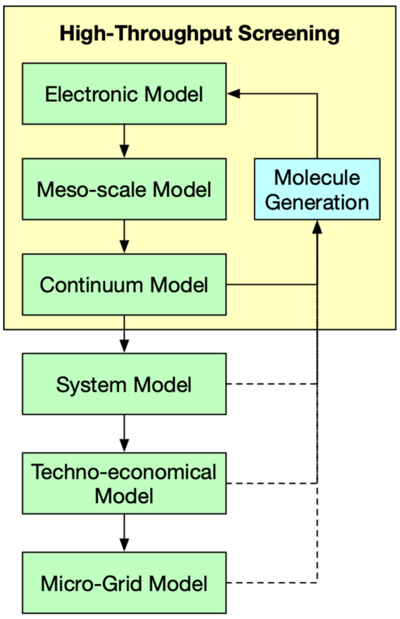


Figure 1: Scale-specific models used in the search for optimal redox pairs and redox flow battery characterization.

The macro-homogeneous, continuum models developed at ICP allow for the simulation of physicochemical effects within a single electrochemical cell. The continuum models describe the driving potentials and fluxes of mass and charge, the electrochemical reactions of the active material in the porous electrodes, as well as the critical transport phenomena within the membrane.

One of the first milestones is the development and publication of a user-friendly, open-source 1D cell model for organic redox flow batteries, which describes the macroscopic field variables, such as mass and charge densities in the through-plane direction of the cell assembly, similar to the open-source fuel cell model [2].

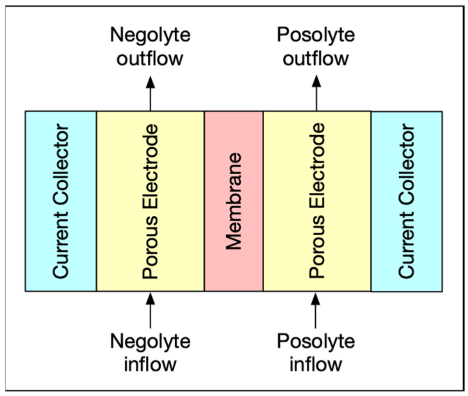


Figure 2: Simplified geometry of a redox flow battery cell.

*Literature:*

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

[2] R. Vetter and J. Schumacher, “Free open reference implementation of a two-phase PEM fuel cell model”, Comput. Phys. Commun., vol. 234, pp. 223–234, Jan. 2019.

## 2.11 DeMaPEM: Development and Marketing of Proton Exchange Membrane Fuel Cells for Transport Applications

**In the project DeMaPEM, we develop and market computational solutions of proton exchange membrane fuel cells for transport applications: a 1-D parameterized model of membrane electrode assembly and a 3-D single cell model. The goal is a faster and more cost-efficient product development in the fuel cell supply chain. Marketing of the models is accomplished via isomorph.ch.**

Contributors: J. O. Schumacher, O. Ilie, R. Herrendörfer
Partner(s): -
Funding: Swiss Federal Office of Energy SFOE
Duration: 2019–2021

In the framework of the Swiss Federal Council's Energy Strategy 2050, the Swiss Federal Assembly has passed a total revision of the energy act, demanding drastically reduced $CO_2$ emissions for private and commercial road vehicles. Our vision is to contribute to reaching this ambitious goal by pushing the advent of fuel cell technology as a competitive and zero-emission electrical power supply. Low-temperature polymer exchange membrane fuel cells (PEMFCs) have the potential to replace fossil fuels by pure hydrogen, thus leading to a substantial decarbonization of the transport sector.

The goal of this project is to allow the ICP to participate in the international value chain of fuel cell powered transport applications. We develop and market computational solutions that are tailored to the needs of companies and research institutes. The focus is put on membrane electrode assemblies (MEAs) and single cell PEMFCs. Our computational solutions in this project, a 1D parameterized MEA model and 3D single cell model (3D-SCM) of a PEMFC, aim for a faster and more cost-efficient product development in the fuel cell supply chain. These solutions are announced on isomorph.ch to make them visible for possible industrial partners.
The 3D-SCM includes gas flow channel plates and a MEA (Figure 1). We aim to improve the macroscopic description of liquid water transport at the interface between gas diffusion layer and gas channels. This is important especially high current densities, where water is produced in the cathode catalyst layer.

The 3D-SCM allows to analyze the water and heat management of the cell, including the temperature distribution (Figure 2) and membrane water content in relation to the gas channels and ribs. With increasing current density, the anode side of the membrane dries out due to the increasing electro-osmotic drag (Figure 3 a-d).

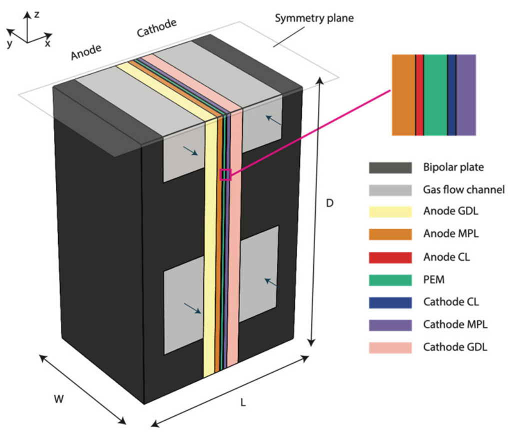


Figure 3: Model setup of the 3D-SCM.

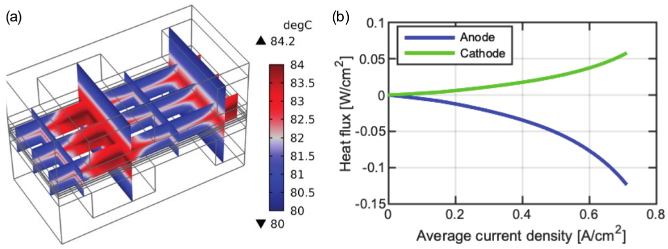


Figure 2 (a): Temperature distribution at 0.025 V cell voltage, (b) heat flux in anode and cathode bipolar plate with increasing current density.

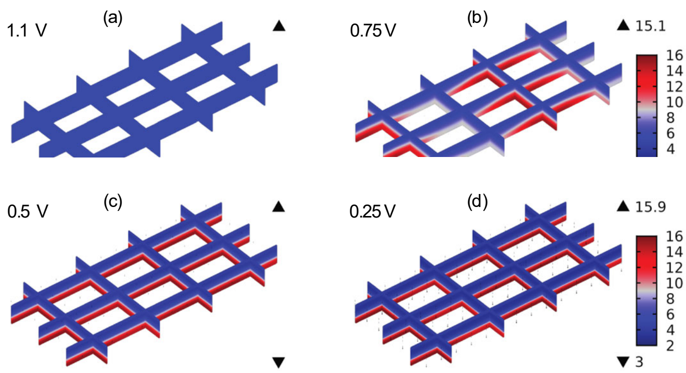


Figure 3: Membrane water content at 4 different cell voltages.

## 2.12 3-D Model of Water and Heat Transport in PEMFCs During Evaporative Cooling and Humidification

**Evaporation in gas diffusion layers with hydrophilic lines have been shown to allow for simultaneous cooling and humidification in proton exchange membrane fuel cells (PEMFCs). The objective of this study is to enhance our understanding of evaporative cooling and humidification using numerical modeling. We investigate the dominant heat and water transport processes and analyse the local sensitivity of the model output to changes in operating conditions and model parameterizations.**

Contributors: R. Herrendörfer, J. O. Schumacher
Partner(s): SCCER Mobility: Swiss energy competence center: Efficient technologies and systems for mobility, Paul Scherrer Institute (PSI)
Funding: Innosuisse
Duration: 2014–2020

Evaporative cooling is a promising concept to optimize the water and heat management in PEMFCs and thereby to reduce costs. It is based on the vaporization of water directly inside the cell to provide simultaneous humidification and cooling. The PSI has developed a concept that is solely based on modifications of the anode gas diffusion layer by locally changing the wettability from hydrophobic to hydrophilic. Experimental work at PSI has demonstrated the usability of this concept [1].
At the ICP, we have developed a 3-D, macro-homogeneous, non-isothermal two-phase model to investigate the dominant heat and water transfer processes during evaporative cooling and humidification in a single-cell PEMFC (Figure 1). We solve for the transport of gas, liquid water, dissolved water, heat, electrons and protons.

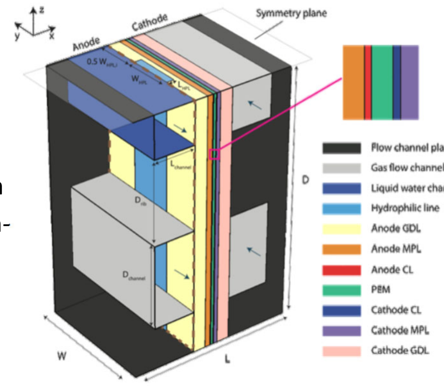


Figure 4: 3-D model setup. Anode flow field with one gas and liquid water channel, respectively, a cathode flow field with two gas channels. The membrane electrode assembly includes the hydrophobic anode gas diffusion layer with one hydrophilic line.

In the reference model, which was adapted to the experimental setup at PSI in terms of operating conditions and properties, most of the water vapour generated along the hydrophilic lines are transported to the outlet of the anode gas flow channel and only a small fraction of water vapour diffuses to cathode side (Figure 2a-b). While most of the evaporation takes place at the interface between gas flow channel and hydrophilic line, a part occurs at the interfaces between the hydrophilic line and hydrophobic GDL (Figure 2b). The water content dissolved in the membrane is the highest on the anode side of the membrane below the hydrophilic line and liquid water channel.

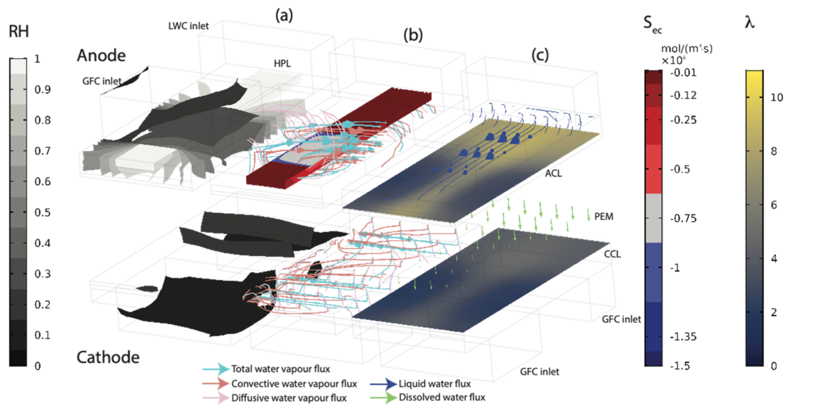


Figure 5: Water management at anode side (top) and cathode side (bottom). **(a)** Relative humidity (RH). **(b)** Evaporation rate and streamlines of water vapour flux. **(c)** Streamlines of liqud water flux and dissolved water flux, water content dissolved in the membrane (λ).

*References:*

[1] Cochet, M., A. Forner-Cuenca, V. Manzi, M. Siegwart, D. Scheuble, and P. Boillat.Fuel Cells 18 (5): 619–26, 2018.

## 2.13 Modelling Capacity Fade in Organic Redox-Flow Batteries: Thermodynamics of Transport in Concentrated Solutions

**Organic redox flow batteries (ORFB) show great promise as a low-cost, sustainable energy storage device, with longer expected lifetime compared to competing storage technologies** [1]**. The aim of this work is to provide a better understanding of the transport processes in ion-exchange membranes, a key component of the batteries regarding lifetime. The ICP collaborates in this regard with the FlowCamp consortium, a research and training project funded by the European Union's Marie-Sklodowska-Curie programme. FlowCamp involves 11 partner organisations from 8 different countries. Research in FlowCamp aims to improve materials for high-performance, low-cost next-generation redox-flow batteries.**

Contributors: G. Mourouga, X. Yang, J. O. Schumacher, T J. Schmidt, C. Iojoiu
Partner(s): ETH Zürich, Univ. Grenoble-Alpes, JenaBatteries
Funding: European Commission, Horizon 2020, Marie Skłodowska-Curie Training Networks
Duration: 2018–2021

One of the organic systems studied within the FlowCamp project is the TEMPO/Paraquat all-organic redox couple [2] developed by the German startup JenaBatteries:

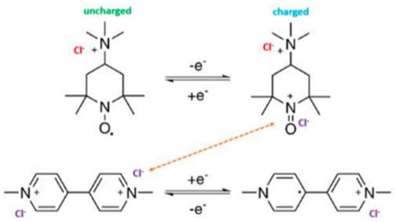


Figure 6. TEMPO (up) and Paraquat (down) oxidation and reduction via chloride exchange.

These molecules yield a fast chloride-coupled electron transfer process, and the absence of precious metal catalysts make this chemistry an interesting candidate for green, low-cost energy storage [2].
A common issue faced by ORFBs, however, is the transfer of both active organic molecules and solvent through the ion-exchange membrane, which separates the positive and negative electrode.

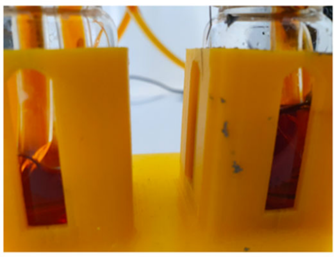

Figure 2: Picture of positive (left) and negative (right) reservoirs after cycling. The height was initially equal.

Understanding the transport processes that lead to active molecule crossover and solvent transfer is an important step towards improving battery lifetime and requires a careful thermodynamic formulation of transport in concentrated solutions.

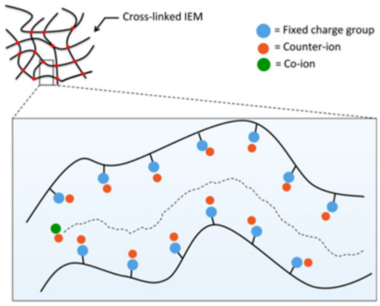


Figure 3: illustration of charge interactions in concentrated solutions and ion-exchange membranes.

The aim of our work in the FlowCamp project is to provide a thermodynamically consistent approach to the simulation of transport in concentrated solutions, including modelling of chemical activity and osmotic processes.
This approach, applied to ion-exchange membranes in flow batteries, is aimed at understanding and predicting capacity fade, an important advance towards further improvement of membrane design and battery lifetime.

[1] X. Wei *et al.*, "Materials and Systems for Organic Redox Flow Batteries: Status and Challenges," *ACS Energy Lett.*, vol. 2, no. 9, pp. 2187–2204, Sep. 2017.
[2] T. Janoschka *et al.*, "An aqueous, polymer-based redox-flow battery using non-corrosive, safe, and low-cost materials," *Nature*, vol. 527, no. 7576, pp. 78–81, Oct. 2015.

## 2.14 Quantifying the Impact of Convective Flow and Microstructure Inside Porous Electrodes on Electrochemical Performance of Flow Batteries

**Rapid transitioning to renewable energy resources carries an urgent need for large-scale energy storage. At present, renewable energy shares cannot exceed a certain threshold for the grid to remain stable. A novel, forthcoming technology for balancing electric power demand and supply by means of reversible electrochemical reactors called flow batteries is currently studied. Understanding of the impact of macroscopic electrolyte flow in porous electrodes on the rate of reactant conversion paves the way to improved electrode microstructure design. The study is a part of the FlowCamp project [1] (a research and training project funded by the European Union's Maria Skłodowska-Curie program) and the SONAR project [2].**

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Partner(s): Fraunhofer ICT (Germany), LRSC Amiens (France), among others
Funding: The European Union, Horizon 2020, Maria Skłodowska-Curie Actions
Duration: 2018–2021

Porous electrodes are widely used in applications such as electrochemical sensors, electroorganic synthesis, or electric power generation. Highly developed surfaces promote an increased current output from a condensed, compact and stackable electrode. The complexity of the porous electrode internal structure poses numerous problems from the theoretical perspective. While the theory of regular flat electrodes is well established, the interplay of uneven surface effects, disturbed transport processes in inhomogeneous media, and superimposed electrolyte flow inside porous electrodes complicates their mathematical analysis. Understanding the impact of convective flow inside the pores on electrochemical performance of porous electrodes is critical for improved design and optimization of operating conditions.

In the FlowCamp and Sonar projects, the aforementioned issues are addressed in a systematic study by means of numerical models on par with experimental model validation. In the first phase of the investigation, a simple 3D pore-fibre geometry was constructed in micrometre-scale (Figure 1) consisting of 3 crossing fibres, whose geometric area can be precisely calculated. Next, a macroscopic electrolyte flow was superimposed in the cell by solving the Stokes equation. On the very surface of the conductive fibres, a reaction term was defined as a boundary condition. It emulates a simple reduction reaction, Ox → Red, at given rate defined by a first-order rate law. The conversion rate is determined by a reaction constant $k_1$. The result of the simulation, showing product concentration distribution, is depicted in Figure 1. The rate constant can be easily varied to study the average surface concentration of the reactant (Ox), which is shown in Figure 2. Later on, the reaction term will be fitted with electron transfer to simulate electrochemical charge transfer (Ox + $e^-$ → Red). By varying the periodic cell geometry, inhomogeneity can be artificially introduced and its impact on the electrode performance can be quantified.

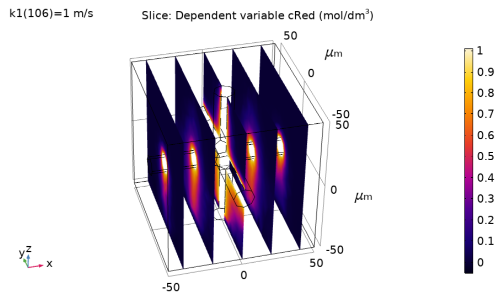


Figure 1. Distribution of reaction product (reduced species) in the pore voids in the simplified pore geometry model.

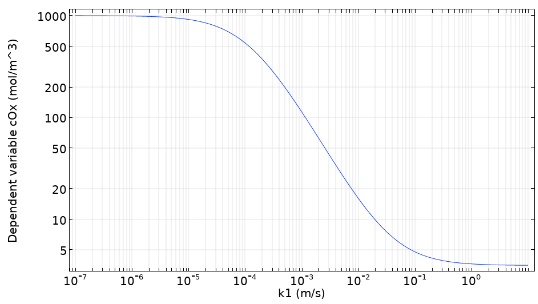


Figure 2. Simulated oxidized species mean surface concentration as a function of heterogeneous reaction rate constant in a simplified pore geometry (average superficial inlet velocity of 1 mm/s).

[1] Project website: https://www.flowcamp-project.eu/
[2] Project website: https://www.sonar-redox.eu/

# 3 Organic Electronics and Photovoltaics

Organic semiconductors have received great attention since 1987 when organic light-emitting devices were invented by leading scientists at Kodak USA. After more than 30 years of R&D and commercialization efforts world-wide, we are now witnessing a wide range of OLED displays in consumer products ranging from mobile phones to 77-inch TVs.

The particular advantages of OLEDs are their thin construction, large viewing angle, color gamut and high energy conversion efficiency. OLEDs consist of a sequence of thin organic semiconductor layers placed in-between two metallic electrodes. Organic semiconductors have equally gained attention as strong light absorber and charge transport materials in organic solar cells, with which flexible PV modules can be built. In recent years, organic semiconductors have also been key to the ground-breaking hybrid organic-inorganic perovskite solar cell technology, which is the hottest emerging photovoltaics technology and shows great potential for LED applications, too. Further into the invisible range of electromagnetic waves, terahertz photonics is a growing technological field for non-invasive diagnostics applications.

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


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## 3.10 AI-Assisted Thermal and Electrical Characterization of Large-Area PV Modules

**In order to detect defects in solar panels during manufacturing, we apply experimental characterization as well as modelling and simulation of photovoltaic cells. Machine learning and traditional methods are used and compared to estimate model parameters.**

Contributors: E. Comi, C. Kirsch, E. Knapp, B. Ruhstaller
Partner(s): Fluxim AG
Funding: Innosuisse
Duration: 2019–2020

In the AIPV project, the ICP collaborates with Fluxim AG that provides simulation software and measurement hardware for industry and academia. One of the commercially available software is Laoss which is used for simulations of large-area solar cells and OLEDs where the top and bottom electrodes are reduced to 2D domains and coupled with a local IV curve. During the course of the project, the software has been extended from DC to AC mode and the coupling is completed by local impedance data such as conductance and capacitance. The model consists of an electrical and thermal part and allows for the prediction of the potential and temperature distribution in the electrodes. Joule heating in the device and the electrodes causes the device to heat up and affects the temperature-dependent material parameters which can in return lead to an increase in Joule heating. In the AC mode Laoss calculates the impedance of large-area devices. The impedance of cells is also measured experimentally. The measurements are then fitted with simulation and material and cell parameters can be extracted. This step is performed with traditional parameter extraction methods e.g. the Levenberg-Marquardt algorithm. Additionally, we also train a machine model (1d convolutional neural network) with simulation data that were previously generated by randomly varying the material and cell parameters. We then feed the measurements to the machine model to predict the underlying material parameter set of the measurements. In Fig. 1 the three steps of building the machine model are illustrated. The extracted parameters of the machine model are analyzed and compared with the results from the traditional parameter extraction method.

In a second phase of the project, thermal images are also investigated in a similar manner as the impedance data with the aid of machine learning.

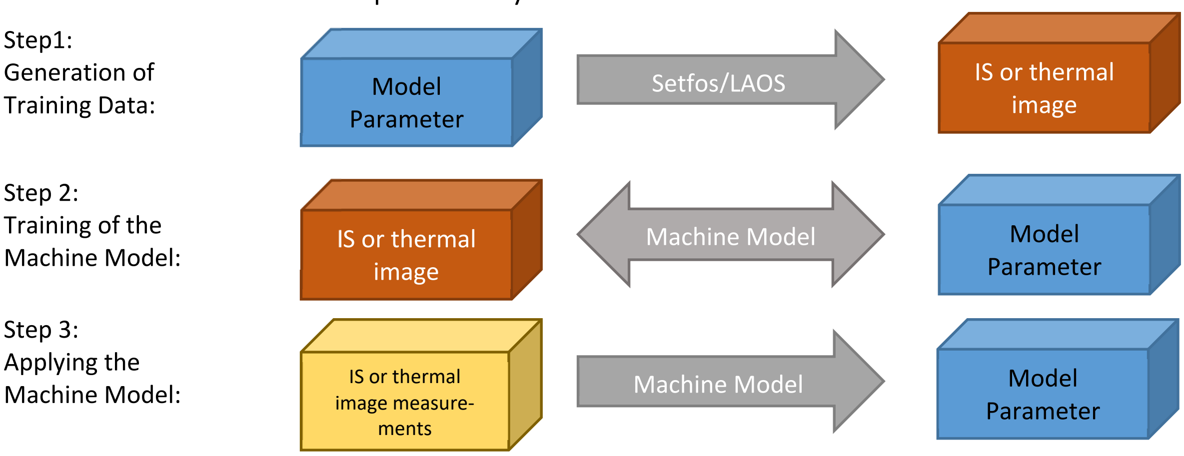


Fig. 1: Visualization of the three steps to build a machine model. Step 1: training data is generated by feeding model parameters to a simulation software that calculates impedance spectra or thermal images. Step 2: The training data is used to establish a link between the impedance spectra or thermal images and the model parameters. Step 3: Measurements of impedance spectra or thermal images are fed to the machine model that provides the underlying model parameter.

## 3.11 Dynamics of Charge Transfer States in Organic Semiconductor Devices: A Combined Experimental and Simulation-Based Approach (CTDyn)

**This new Swiss-German collaboration investigates charge transfer states (CT excitons) that play a crucial role in the understanding and further improvement of the efficiency of organic electronic devices such as OLEDs and organic solar cells. We choose an approach that combines optical and electronic measurements with numerical simulations, and will improve the underlying physical models and numerical methods.**

Contributors: M. Regnat, C. Kirsch, S. Züfle, B. Ruhstaller
Partner(s): Prof. W. Brütting, Universität Augsburg
Funding: SNF/DFG
Duration: 2020–2023

Organic light-emitting devices (OLEDs) are a disruptive flat panel display technology rivalling with established LCD technology. OLEDs have reached a very high maturity level for applications in mobile devices and large TV panels. Hereby a major increase of the luminance yield has been realized by an improved understanding and control of the exciton physics in organic materials in the last decades. This involved moving from fluorescent to phosphorescent dyes, to host-guest systems and recently to thermally activated delayed fluorescence (TADF) systems where 100% internal quantum efficiency can be realized. Especially in TADF devices important material parameters are determined using temperature-dependent (mostly optical) measurements. Furthermore, with increased driving currents additional excitonic processes occur that can lead to (reversible or irreversible) performance loss. While these processes are well-known today, a complete model including all relevant physics for charges and excitons and describing a full set of experiments is still a big challenge.

The project CTDyn studies the dynamics of excitons and interplay between different exciton species as well as between excitons and charge carriers, both in the bulk of individual layers (intra-molecular) and at interfaces of multilayer organic semiconductor devices (inter-molecular). We will extend our established 1D drift-diffusion approach and combine it with a novel 3D Master equation model as well as compare it with 0D analytical formulas.

This requires the preparation of clean model systems to isolate the underlying processes by dedicated experiments on the one hand; on the other hand the model needs to be extended to capture the enhanced complexity of these systems.

The physics of exciton processes can be studied in both OLED and solar cell configurations. In fact, due to basic thermodynamics and reciprocity many of the findings from OLEDs may be transferred to solar cells and vice versa. For example, we plan to measure the open-circuit voltage of OLEDs (suns-Voc experiment) or the luminance of solar cells. With regards to simulation we aim for a comprehensive and universal model covering all processes and which can be employed for both OLEDs and solar cells.

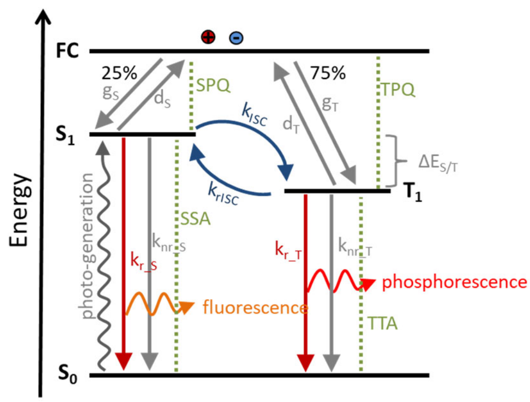


Figure 1: General exciton and charge transfer processes. FC denotes the free carriers, S1 the singlet and T1 the triplet exciton, and S0 the ground state. The TADF process is linked to the krISC rate.

## 3.12 Investigating Charge Transport in Organic Semiconductors with Electro-Chemical 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: G. Kissling, E. Knapp, K. Pernstich
Partner(s): Fluxim
Funding: Swiss National Science Foundation (SNSF)
Duration: 2020–2022

Nowadays organic semiconductors are widely used in display and lighting applications (OLED TVs and light panels) and also 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 (theoretical) 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.

We are using electrochemical methods to characterize organic semiconductors, such as NPB (N,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine), shown in **Figure 1c**. NPB will either be studied as a molecule in solution or as a thin film adsorbed onto a substrate. The stability and the semiconductor properties (such as the positions of the valence and conduction band and of defect states) of the material will be investigated.

**Figure 1a and b** show preliminary electrochemical data simulated for NPB in solution obtained using COMSOL Multiphysics® software [1]. The red part of the trace in Fig. 1a was simulated using experimentally determined parameters from the literature [2]. The blue part and the electrochemical impedance spectra in Fig. 1b are based on an educated guess and will be confirmed or rejected by our own experimental results over the coming year.

This project may lead to an improved understanding of the current state of the art by providing inputs that lead to the development of more accurate models for organic semiconductor materials characterization. In collaboration with our industrial partners the research may also lead to the development of a commercial product.

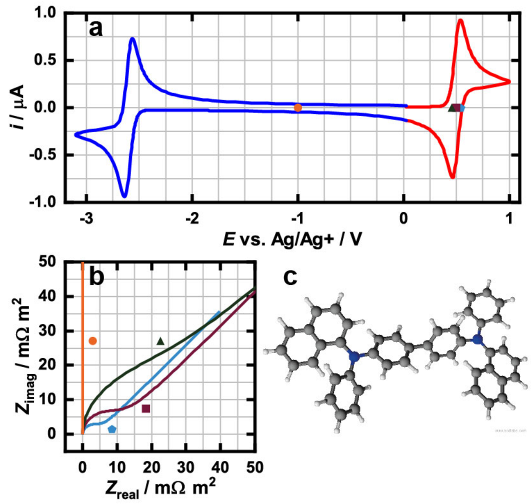


Fig. 1: **a** First Simulated cyclic voltammograms for NPB in solution. The red data were simulated using experimental results from the literature [2]. The blue data are based on an educated guess. The electrochemical impedance spectra in **b** were simulated for the potentials indicated in **a**. The spectra were simulated for potentials of -1 V (orange circle), 0.46 V (dark green triangle), 0.5 V (purple square) and 0.54 V (blue pentagon). **c** cartoon representation of an NPB molecule.

*Literature:*

[1] COMSOL Multiphysics® v. 5.5. www.comsol.com. COMSOL AB, Stockholm, Sweden.
[2] J.-E. Park, S. Song and I.-S. Shin, Int. J. Electrochem. Sci., 2016, 11, 5891–5899.

## 3.13 Investigation of the Efficiency and the Lifetime in OLEDs

**In the research project TripLED, promising OLEDs fabricated by Professor Jang-Joo Kim's group from Seoul National University were investigated. Using different, partly newly developed, characterization methods in combination with electro-optical 1D simulations, improvements in efficiency and lifetime could be predicted.**

Contributors: M. Regnat, K. Pernstich, B. Ruhstaller
Partner(s): Prof. Jang-Joo Kim Gruppe von der Seoul National University, Südkorea
Funding: SNF
Duration: 2016–2019

Organic light-emitting diodes (OLEDs) can be nowadays found in displays of mobile phones, televisions and lamps for illumination. Current research is being conducted on the next generation of OLEDs using thermally activated delayed fluorescence (TADF) in order to achieve increases in efficiency with sufficient lifetime.

In a first step of this project, such TADF OLEDs have been investigated using different characterization methods with the Paios measurement system [1] and electro-optical 1D simulations with Setfos [2]. As a key result, different routes to enhance the efficiency in these OLEDs by up to 400 % (at 1000 cd/m2) could be demonstrated, as shown schematically in figure 1 [3].

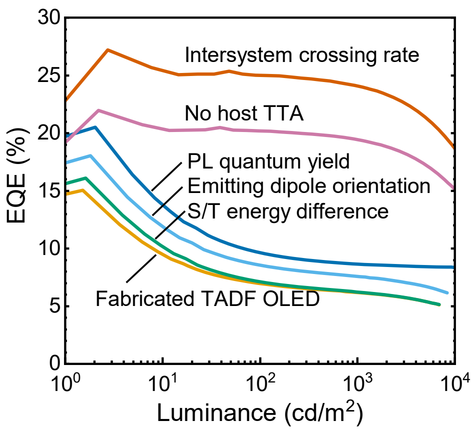


Figure 1: Possible routes to enhance the external quantum efficiency (EQE) of the investigated TADF OLEDs.

In a further step, the lifetime of highly efficient TADF OLEDs was investigated. For this purpose, they were operated under constant current and characterized at regular intervals. Based on these measurements, a quantitative electro-optical model was developed to describe the degradation over the lifetime. The decrease of the current-voltage characteristics in the investigated period was mainly due to the increase of traps in the hole transport layers of these TADF OLEDs (see figure 2).

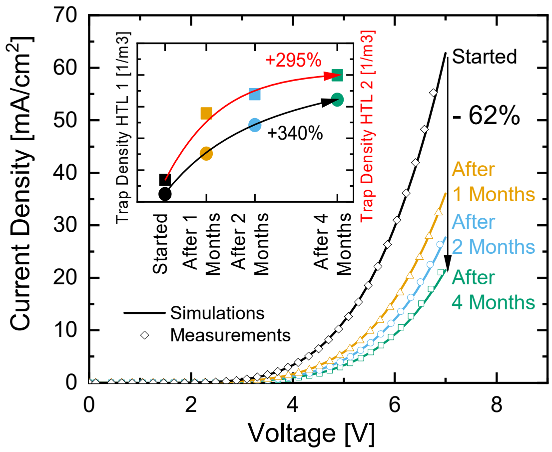


Figure 2: Measured and simulated current-voltage curves of the fresh and degraded TADF OLEDs. The inset shows the increase of the trap densities in the hole transporting layers during the investigated period.

In this project we have demonstrated that the combination of different characterization methods with electro-optical 1D simulations can be a valuable tool for increasing the efficiency and the lifetime of OLEDs.

*References:*

[1] Setfos 5.0, https://www.fluxim.com/setfos-intro/.
[2] Paios, CS 4.2, https://www.fluxim.com/paios.
[3] Regnat, Markus, et al, Advanced Electronic Materials (2019): https://doi.org/10.1002/aelm.201900804

## 3.14 All-Organic Gap-Free Terahertz Photonics

**The goal of this project is to develop an all-organic and gap-free broadband terahertz (THz) generation and detection approach that will be highly valuable for a variety of applications ranging from fundamental studies of THz-light-matter interactions to industrially-relevant THz spectroscopy and imaging.**

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

Terahertz sources based on organic electro-optic crystals have become increasingly important during the last years for THz photonics. This is because of their unique possibilities to combine extremely high THz electric fields needed for studying light-matter interactions, 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 and controlled. This makes organic electro-optic crystals on the one hand essential for the emerging field of nonlinear THz photonics. 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. [1] However, these materials themselves possess intrinsic molecular phonon and vibrational modes in the THz range, which leads to unwanted modulation including complete gaps in the generated THz spectrum. This modulation presents a fundamental limit for linear and nonlinear THz photonics based on organic electro-optic crystals, which we want to overcome in this project for gap-free THz photonics applications.

In this interdisciplinary international project collaboration, the Korean side (Ajou University) is designing and synthesizing novel organic molecular crystals with large macroscopic optical nonlinearity and controlled crystal characteristics by various crystal-engineering approaches. The Swiss side (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.

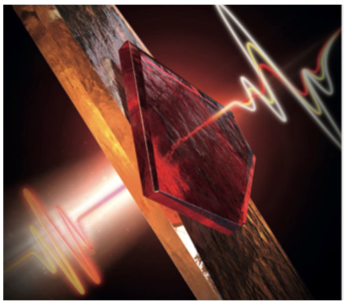

Fig 1: In this project, organic electro-optic crystals and their combinations are used for ultra-broadband THz-wave generation. Illustration: Ajou University Universität [DOI: 10.1002/adfm.201707195].

Finally, profiting from the advantages offered by the newly developed all-organic gap-free THz photonics approach, we will investigate various novel organic transporting materials interesting for a variety of applications such as organic solar cells, organic field effect transistors, as well as organic photodetectors and gas-sensing applications.

*Literature:*

[1] Jazbinsek, M.; Puc, U.; Abina, A.; Zidansek, A., 2019. Organic crystals for THz photonics. Applied Sciences. 9(5/882). Invited review paper.

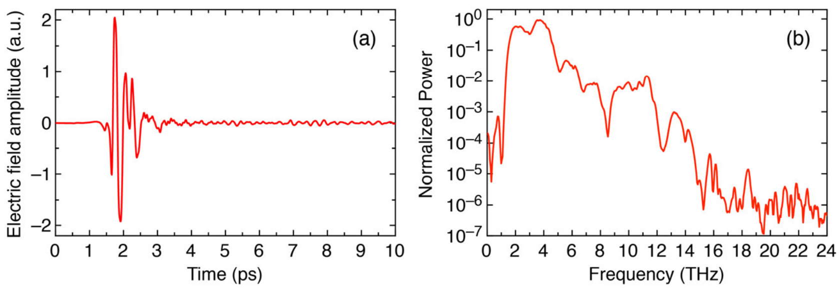


Fig 2: THz time-domain signal (a) and the corresponding power spectrum (b) of the THz setup based on organic crystals: The aim of this project is to reduce the modulation of the signal seen in (b) to achieve a flat spectral response over the whole frequency range.

## 3.15 Hardware-Software Integration and Validation of a Compact THz System

**At ICP we are developing a new compact instrument for terahertz (THz) non-destructive material testing and characterization. The new system is used for THz spectroscopic measurements, THz imaging and THz thickness measurements with an ultra-broadband spectral range beyond 15 THz.**

Contributors: V. Michel, U. Puc, T. Bach, M. Jazbinsek
Partner(s): Rainbow Photonics AG
Funding: Master thesis, Innosuisse
Duration: 2019–2020

Terahertz (THz) photonics is a fast-growing field with very promising applications in non-destructive material testing, imaging and material identification/spectroscopy. During the last two decades, many different approaches to generate THz waves for both research and industrial applications have been suggested. Presently, most commercial and laboratory THz time-domain spectroscopy systems record spectra up to few THz only. The experimental system developed at ICP in collaboration with the company Rainbow Photonics AG, however, can measure frequencies up to 20 THz, as it benefits of the combination of organic crystals (DSTMS) and a compact telecom femtosecond laser used for generation and detection. Moreover, the system is designed to facilitate the implementation of an optical-pump THz-probe option without losing any functionalities of the basic time-domain spectrometer.

The scope of this thesis has been the validation of the frequencies, linearity and sample parameter extraction of the ultra-broadband THz time-domain spectrometer.

The results have shown an excellent linearity of both generation and detection of the THz time-domain spectrometer, which is a prerequisite for a reliable sample parameter extraction, including the thickness and the complex refractive index. The measured frequencies of narrow water absorption lines are in excellent agreement with absorption spectrum according to literature, thus successfully validating the DSTMS-based spectrometer over the full 20 THz bandwidth with an accuracy of 2.7 GHz. Thickness measurements of samples in reflection geometry have shown a remarkable accuracy, enabling the measurement of samples thinner than 50 µm with a relative error of 1%, therefore opening new possibilities for the presented methods. Simultaneous refractive index and thickness measurement of about 0.5 mm thick germanium wafers with an accuracy of 0.1% have been demonstrated in transmission geometry. The conductivity changes of a germanium sample when optically excited in the newly developed optical-pump THz-probe system are clearly observed as the THz transmission changes by more than 50% in the low THz frequency range.

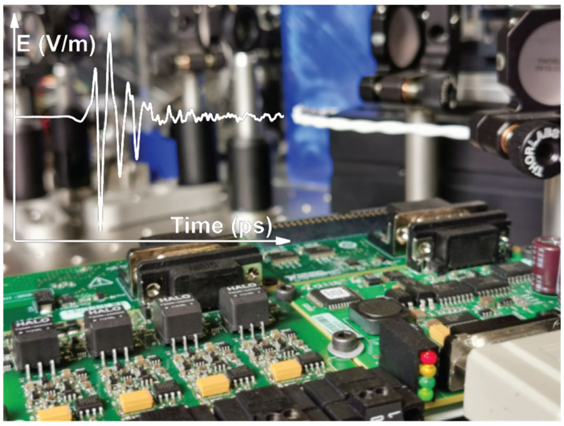


Fig 1: The developed time-domain THz spectroscopy system is based on measuring the electric field with a sub-picosecond resolution. THz electric fields with frequency components up to 20 THz have been generated and detected. This is possible due to integration and optimization of photonics and electronics components and data acquisition software.

The performed work demonstrates advanced capabilities of the compact THz time-domain spectroscopy system implemented as a bench setup at the ZHAW with potential further improvements in detection electronics optimisation in order to minimise the laser noise influences and considerably improve the systems signal-to-noise ratio. In addition, further development of data extraction algorithms will allow for better accuracy in thickness and material parameter extraction, which is interesting for various research and industrial applications.

# 4 Sensor and Measuring Systems

Our team of talented ZHAW engineers and scientists has been applying for more than nine 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.


A. Bachmann


M. Bonmarin


D. Fehr


D. Kempf


V. Metry


D. Schaltegger


M. Schmid


F. Spano


S. Weber


A. Witzig

## 4.10 Detecting Nanoparticles in Complex Environments

**Nanoparticles are everywhere from Medtech products to cosmetics or food and therefore it is important to have tools to monitor them *in situ*. Current methods to detect and characterize nanoparticles are limited to specific environments (liquids for example) or required extensive and expensive sample preparation. For this reason, we are developing in collaboration with the Adolphe Merkle Institute of the University of Fribourg new thermography-based methods to detect stimuli-responsive nanoparticles in complex environments.**

Contributors: Mathias Bonmarin
Partner(s): Adolphe Merkle Institute of the University of Fribourg
Funding: Multiple funding (Innosuisse, Foundations)
Duration: 2012 – Ongoing

Nanoparticles are tiny particles which size range from 1 to 100 nm (to give an order of comparison the thickness of a sheet of paper is roughly 100’000 nm). Nanoparticles are nowadays used in many products like composite or medical devices but also in cosmetics or food. Regulation is increasing for the use of nanoparticle especially in Europe. Therefore, it is of a particular importance to have accurate tools to detect them. Several methods are available to detect and characterize nanoparticles, but they often demonstrate limitations in term of the medium in which the particles can be investigated or the preparation of the sample and associated costs. Many nanoparticles are stimuli-responsive meaning that they have the ability to produce heat when stimulated (by light or alternating magnetic field). The resulting infrared radiation his can easily be captured by a thermal camera. Using this principle, we developed together with the Adolphe Merkle Institute in Fribourg a new method to characterize nanoparticles in complex environments like cells culture, tissue or composite materials with very high accuracy. We developed several instruments for magnetic nanoparticles like SPIONs or plasmonic particles like gold. The technology has been protected (2 patents) and the startup company NanoLockin GmbH based in Fribourg is commercializing the research results.

We are convinced that thermography is a promising method to investigate stimuli-responsive nanoparticles and we are still investigating the potential of the technique for many applications in the field of nanoscience.

Fig. 7: Picture of the Calorsito VIS-NIR device developed by the company NanoLockin GmbH, a spin-off from the Adolphe Merkle Institute and the ZHAW Institute of Computational Physics.

*References:*

[1] Journal of Physical Chemistry C, 124(2):1575-1584 (2020)

[2] Particle & Particle Systems Characterization Journal, 36:1900224 (2019).

[3] Journal of Physical Chemistry C, 121(48):27164-27175 (2017).

[4] Journal of Magnetism and Magnetic Materials, 427:206-2011 (2017).

[5] Nanoscale Journal, 8(27):13321-13332 (2016).

[6] www.nanolockin.com

## 4.11 Portable Device for Early Diagnosis of Lymphedema

Contributors: D. Fehr, A. Bachmann, M. Bonmarin
Funding: Innosuisse
Duration: 2018–2020

The probability of developing lymphedema until the end of life is about 30% after breast cancer treatment – and this is only one of the possible risk factors. Millions of people are therefore at increased risk of developing lymphedema. In this disease, the function of the lymphatic system is permanently disturbed, causing e.g. irreversible swelling of the arms if appropriate treatment is not initiated in time. This slows down the swelling or even stops it completely. Early diagnosis of the disease is therefore crucial. Nevertheless, there is currently no standardized, widely available method that allows regular and reliable monitoring of people with an increased risk.

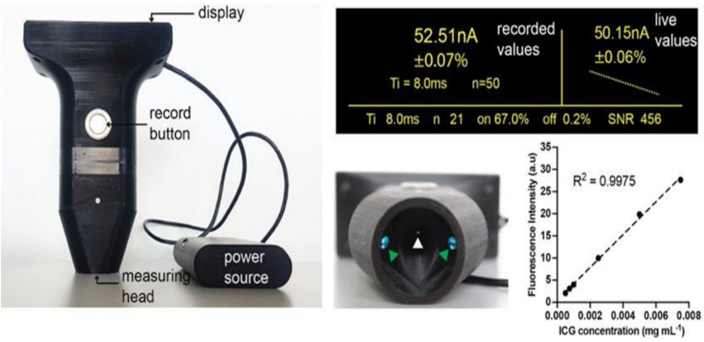


Fig. 1: Left: Autarkic hand tool with battery. Top right: Display. Middle: Measurement opening. Bottom right: Measured value versus actual marker concentration.

In this work, a suitable method for the early diagnosis of lymphedema is being developed in collaboration with the Institute of Pharmaceutical Sciences at ETH Zurich. It consists of a fluorescent marker, which is injected into the skin of the patient, and a simple medical measuring device, which can determine the clearance rate of the marker by means of the fluorescence intensity. If the rate of clearance is reduced, there is a suspicion of developing lymphedema. Ideally, patients will be able to use this method to monitor their lymphatic system independently and regularly – and therefore be able to consult a specialist at an early stage. In various preliminary projects, a suitable fluorescent marker and a first portable measuring device with optical sensor technology for quantifying the fluorescence signal were developed. For this purpose, the existing optics (Fig. 2) were supplemented by a self-sufficient control electronics and operating element and installed in a compact housing (Fig. 1). With this hand-held device, the method could already be validated in various pre-clinical experiments. Currently, it is further investigated in a clinical study in cooperation with the University Hospital Zurich.

Moreover, the measuring device has been revised and realized as a wearable sensor, i.e. the previous handheld device could be shrinked to the size of a sports wristwatch. For this purpose, the optics were redeveloped from scratch, because the existing approach is not suited for further miniaturization. First tests are very promising. While conserving the sensitivity, the optics could be reduced considerably. At the same time, a suitable smartphone app was implemented. It provides the user interface to the wearable sensor and displays the recorded measurements.

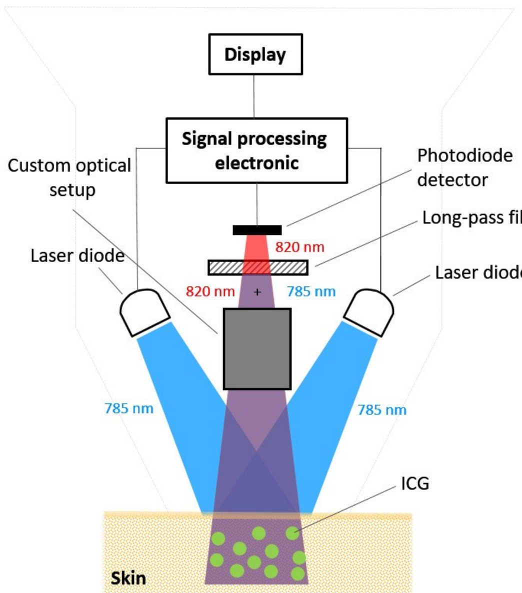


Fig. 2: Optical and electronic components of the handheld device.

*Literature:*

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

## 4.12 Design and Development of Artificial Skin Models for Tactile Sensing Applications

Contributors: F. Spano, D. Fehr, M. Bonmarin, J. Blunschi, R. Sassenburg
Duration: 2019–2020

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].

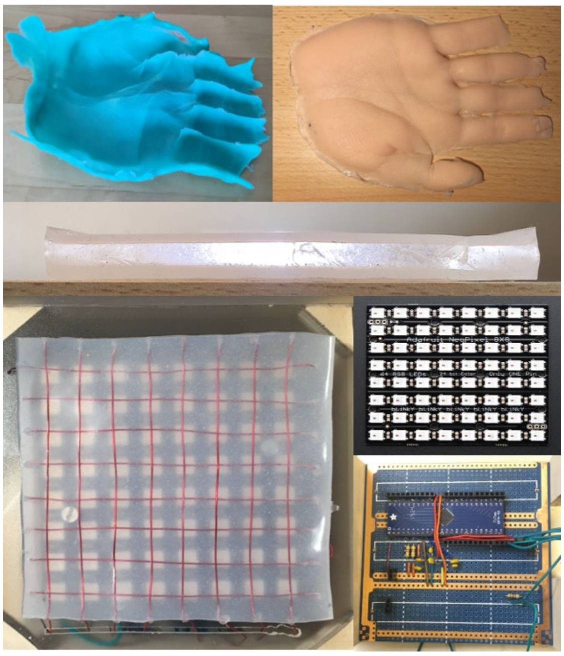

Fig. 1: Illustrations of the different fabrication phases: material development and real palm replica; Multi-layered skin model with the capacitive-sensing grid and the LED matrix, controlled by the prototyped electronics.

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.

## 4.13 Viscosity Control Technologies for the Controlled Application of Coating Materials

**The control electronics and its associated DSP algorithms, which are used to run viscosity sensors, were adapted to a novel inline sensor technology. Next, a flow loop system was developed and set up to test the inline sensors under controlled conditions and to perform a complete characterization of the sensors. Once the flow-loop is extended by an automated thinner dosing, it becomes a fully automatic viscosity control system, which guarantees a constantly high coating quality and thus enables the user to make substantial savings in material, plant and working time.**

Contributors: D. Fehr, U. Vögeli, A. Bariska, S. Hauri, N. Reinke
Partner(s): Rheonics GmbH
Funding: CTI
Duration: 2016–2019

An control unit based on a DSP (Digital Signal Processor) was developed to evaluate the sensor signals of a new type of inline viscometer. The starting point was an electronic system from a previous project and its associated software. The analog front end and the algorithms were adapted to the new inline viscosity sensors.

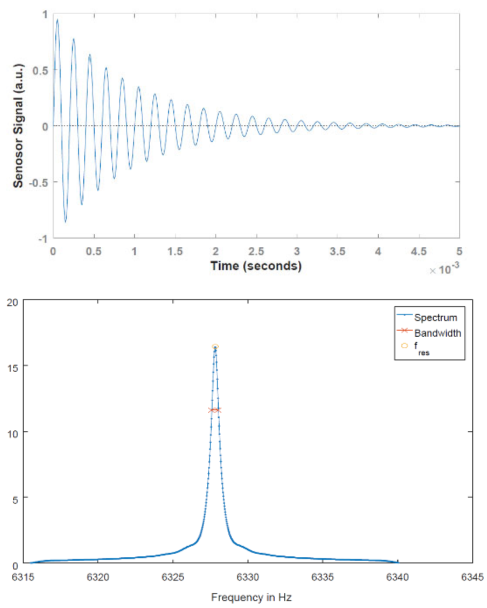


Figure 1: Characteristic decaying oscillation of a mechanical resonator for viscosity determination (top) and the associated spectrum from which the viscosity of the fluid can be deduced by determining the center frequency and bandwidth (bottom)).

The underlying measuring principle can be described as follows: The electronics causes the mechanical resonator submerged in fluid to oscillate. The resonator's resonant frequency and damping depend on the density and viscosity of the fluid. Figure 1 shows a typical oscillation waveform of the sensor, i.e. an exponentially decaying oscillation.

The DSP electronics determines the resonant frequency and damping based on the spectrum of the decay waveform, which is showed in in Figure 1, too.

Parallel to the control electronics, a test system (flow loop) has been designed and implemented (Figure 2). It resembles a typical wet coating process: Conveying of coating material and thinner, a mixer, circulation with the inline viscosity sensor and a tap that simulates the application of the coating material. With the flow loop and the control electronics described above, the viscosity sensors can be tested and characterized under typical operating conditions. Furthermore, the system enables the development of an inline viscosity control system in which thinners are automatically mixed with the coating materials. With this technology a constant viscosity can be guaranteed in industrial coating plants.

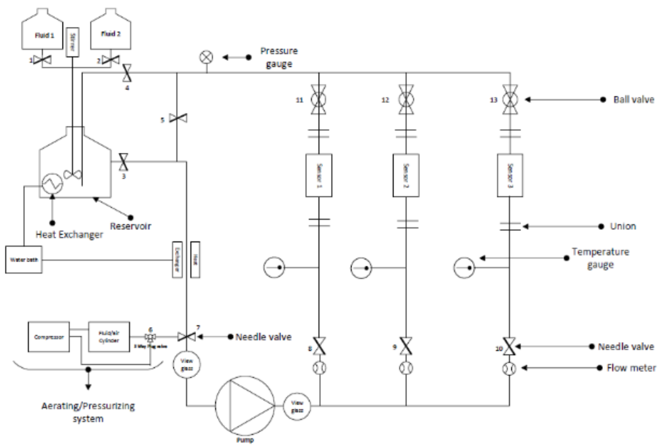


Figure 1: Flow-loop test system.

## 4.14 Artificial-Intelligence Heat Pump Controller

**We are investigating a heat pump control system based on a reinforcement learning algorithm. The application case is small to medium sized systems and our solution is suitable for mass use. Normally, no detailed system optimization is done in these systems. In contrast, the Artificial-Intelligence heat pump controller can react to variations in external conditions and user behavior and continuously optimize the system at no additional cost and without installation effort.**

Contributors: A. Witzig, S. Weber, D. Kempf
Partner(s): V. Ziebart (IAMP), N. Schmid (IAMP), M. Bätschmann (Firma BS2 AG)
Funding: Innosuisse
Duration: 2019–2020

Heat pumps are increasingly displacing oil and gas heating systems. Replacement of fossil fuels is an important pillar of the Energy Strategy 2050 and the global efforts to reduce CO2 emissions. In combination with geothermal probes, heat pumps also have the potential to make a significant contribution to balancing the stochastic energy production of the new renewable energies. They already offer – with suitable design and control – a financially interesting possibility for the owners to directly use locally produced solar energy.

The industrial partner BS2 offers heat pumps the segment of medium-sized systems with ground proves and integrates them into the "2SOL" system, see figure. The novel controller proposed in this study can ideally combine the different energy sources and sinks as well as the energy storage. It keeps the system in an optimal state in case of changing external conditions and variations in user behavior.

In the past, there have already been various attempts to control the heat pump using artificial intelligence. However, the learning sequences for machine learning are usually too short to achieve satisfactory results. In the present work it is shown how a reinforcement learning algorithm can be trained by means of simulations to enable the heat pump controller to adapt to different situations, for example building dynamics, weather influences and user behavior.

The methodology used is simple enough for mass market introduction, it does not require a fast and stable internet connection and no additional sensors must be introduced.

Adjustments to the planning and sales process are not necessary, and no sensitive operating data is generated. The processes during commissioning are simplified thus reducing project complexity and risks. As soon as the heat pump is switched on, it automatically determines the optimum operating point, both for heating operation and, if necessary, for cooling the building in summer. It has the capability of regenerating borehole and therefore prevents the soil from cooling down more and more.

In summary, the system is promising because it simplifies installation, reduces operating costs and increases comfort.

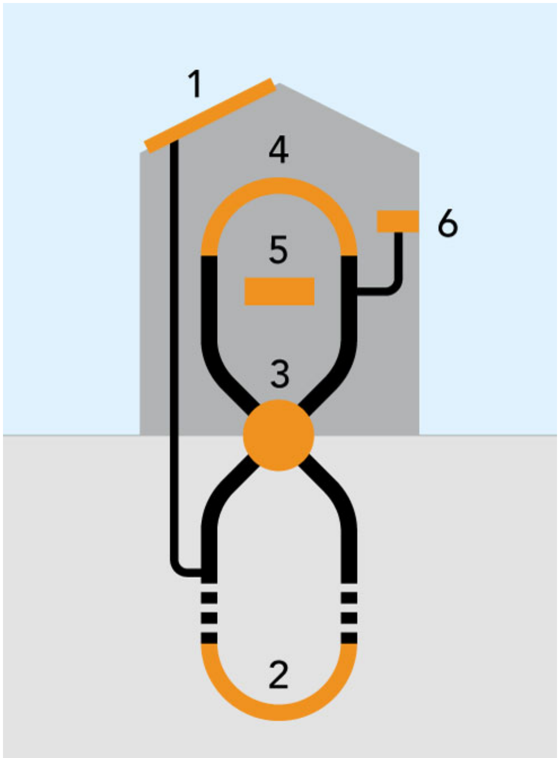


Figure. «2Sol»-system, as in http://www.2sol.ch/: 1. Hybrid photovoltaic and thermal collector , 2. earth probe, 3. heat pump, 4. heat distribution, 5. controller, 6. ventilation with heat recovery.

## 4.15 Climatic Ceiling Thermal Storage Allows Reduction in Façade Insulation

**Tough climate protection requirements in the building sector are often achieved without energy optimization of the heating system. A missed opportunity! The omission is paid for with excessive facade insulation and potential overheating problems in summer. In a validation project, an innovative system was investigated in which an intelligent heat pump system is used for heating and cooling. By activating the concrete ceilings and using them as a storage medium, the system also benefits from fluctuations in electricity prices, as is expected in the future.**

Contributors: A. Witzig, S. Weber
Partner(s): A. Bühler (Klimatop GmbH, Germany)
Funding: Direct
Duration: 2019–2020

Modern concepts for the refurbishment of old buildings aim to ensure that a refurbished building produces more energy than it consumes over the year. A tried and tested approach called "Energiesprong" pursues an innovative and scalable concept that also includes the heat pump heating system [1]. Moderate facade insulation is a cost-optimized solution that is particularly attractive for refurbishment and could play an important role in the German government's climate protection program 2030.

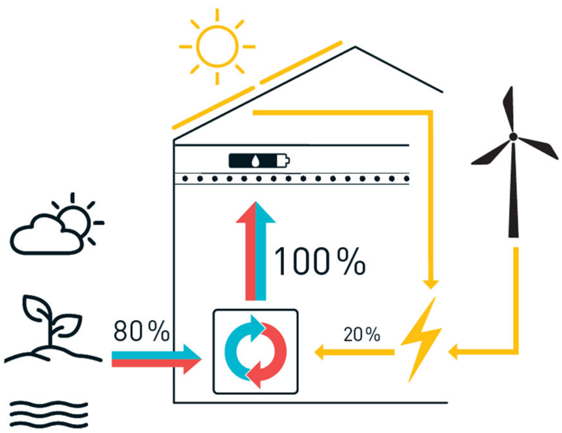


Fig. Heat storage in the climate ceiling and the intelligently controlled heat pump heating system allow a high proportion of renewable energy to be used for heating and air-conditioning of buildings. This makes the system suitable for cost-effective renovation of large buildings and districts. In a long-term perspective, when the ratio of fluctuating energy sources increases, the storage ceilings can also contribute to the stabilization of the power grids.

In order to be able to offer the so-called "serial refurbishment" at a reasonable price, several companies join forces, optimize their internal processes and use the latest digital technologies. In this way they are renewing urban space on a grand scale. Sector coupling - i.e. the interlinking of heat, electricity and mobility - as well as urban planning and social considerations play an important role in this process.

In order to test the planned intelligent system technology and to validate its suitability for widespread use under a wide range of conditions, the proposed heating and cooling system was examined in this project using simulations. The components used must be suitable for mass production and have to be cost-optimized. The planning tools must be digital and support the cooperation between the actors. The future-oriented overall concept also allows the combination of very many units, so that a positive effect for the stability of the power supply can be achieved together in the European network. For this purpose, the concrete ceilings of all buildings are used as a thermal mass and managed as a large energy storage medium.

*Literature:*

[1] «Energiesprong» Energy concept, www.energiesprong.org, currently with projects in the Netherlands, England, France and Germany.

[2] Raum-K network https://raum-k.eu/wp-content/uploads/2020/01/Brosch%C3%BCre_RaumK_Panasonic_200107.pdf

## 4.7 Room Temperature Sensors in the Digital Twin

**In this bachelor thesis the influence of the position of a temperature sensor on the heating control was investigated. This is important in order to optimize energy consumption and comfort in indoor rooms. To address this question, newly implemented functionality in the simulation tool IDA ICE from EQUA AB was used.**

Student: Sara Willi
Category: Bachelor's thesis
Mentoring: A. Witzig, S. Weber
Handed in: 2020

Temperature sensors in heating systems often measure a combination of air temperature and radiation. In digital planning, the control of thermal comfort in buildings is therefore a demanding task. In this work, indoor climate is investigated by means of detailed physical simulation. The temperature measured by sensors and information relevant for the control are brought together.

Furthermore, the findings are to be incorporated into building planning and operation. For this purpose it may be useful to create a digital twin of the building. This digital twin, which is a numerical representation of a real object, contains models with which physical processes can be represented. For example, the temperature distribution in a room due to a ventilation system can be graphically displayed and the control technology can be improved. The theoretical basics of this topic were already established over 20 years ago. It was shown that the position of the temperature sensor can have a significant influence on the energy consumption. [1], [2]. In planning and especially in digital design, however, these correlations are still rarely used today. Simplified models often assume a homogeneously mixed air temperature, which is not suitable to optimize the positioning of temperature sensors.

The aim of this work is to process the knowledge in a form useful for the construction industry and to use the processes and tools that are available to a broad user group today. For this purpose, several newly implemented software features of IDA ICE have been used to assess their suitability for mapping thermal comfort and energy consumption in the digital twin.

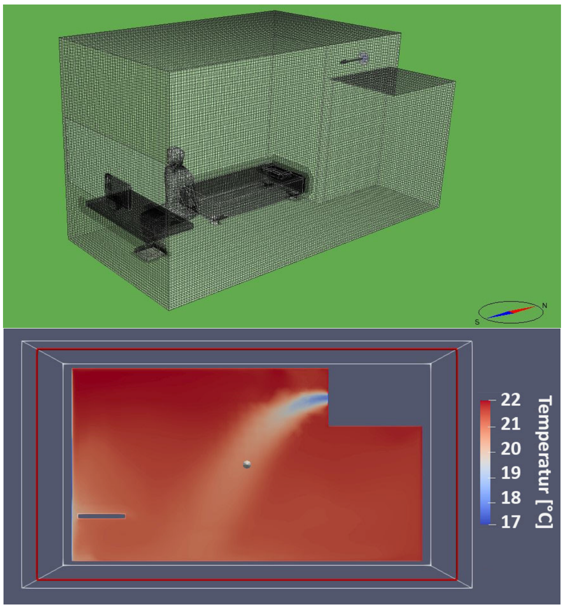


Figure. Temperature distribution in a hotel room with ventilation. Above: Grid, below: Temperature distribution in vertical cross-section. IDA ICE offers both a 3D solution with finite volumes (using OpenFoam) and a numerically efficient layer model with embedded air flows and plumes [3].

*Literature:*

[1] B. Magnum und J. Hill, «Thermal Analysis, Human Comfort, Indoor Environments», National Bureau of Standards (U.S.), Washington, D. C., 1977.

[2] P. Riederer, D. Marchio, J. Visier, A. Husaunndee und R. Lahrech, «Room thermal modelling adapted to the test of HVAC control systems,» Elsevier, Building and Environment, ISSN: 0360-1323, 2002

[3] L. Eriksson, G. Grozmann, P. Grozmann, P. Sahlin, M. Vorre and L. Årenius, «CFD-free, Efficient, Micro Indoor Climate Prediction in Buildings, IBPSA Proceedings, UK, 2012

# 5 Startup Culture at the ICP

Over the years, several spin-off companies have been established at the ICP. They do not yet carry the newly created ZHAW spin-off logo, but the ZHAW Transfer Office confirmed that the university does support the subsequent assignment of the label. This already describes an initial characteristic of ICP spin-offs: they did not come about through a "top-down" initiative but were created "bottom-up" as a by-product of successful and application-oriented research projects. We believe that it is no coincidence that our institute attracts and supports potential company founders, and we recognize a positive impact on the research projects: Spin-off companies are often good research partners and sometimes effective door openers for EU projects.

ZHAW has also recognized the potential of spin-off companies. This year's Department Day at the School of Engineering was dedicated to this topic: Two keynotes [1,2] presented experiences from other universities, and the knowledge gained from these lectures was further explored in small discussion groups. The event was successful in sensitizing the management to the importance of spin-off companies. I am personally connected to this topic, since I myself dared to take the step 15 years ago and gave up my secure employment in a research institute. Together with a small team I placed the results of a research project as a product on the market.

In addition to the technical implementation, the transfer of ideas into a startup company requires the successful financing and introduction of the products to the market. However, at the ICP we do not have a strong background in finance or marketing. The candidates bring these skills with them or obtain them in events that are directly addressed to the founders. What we can offer at the ICP corresponds to what Eliav Haskal summarized in his presentation with the following keywords [1]:

*Creativity + Innovation + Risk Culture + Empowerment*

*Creativity and Innovation*

These are the natural strengths of an engineering school. Projects start with creative ideas, and real innovation occurs when projects are being developed and researchers stay on until someone benefits from the research results. Creativity and innovation are also well represented in teaching at our school, especially in the project track, in some internships and of course in the project and bachelor theses.

*Risk Culture and Empowerment*

A conscious handling of chances and risks is an additional factor in the promotion of entrepreneurial thinking. Something may also go wrong. Even during a project or bachelor thesis, learning from mistakes is more important than reproducing a hidden sample solution. Empowerment goes a little further and characterizes the decision-making structures that promote entrepreneurial spirit. Those who are allowed to participate in decision making and realize that their opinion is worth something, train their independent thinking. This is not always just fun, because you are also held accountable. But researchers that think like entrepreneurs can develop best when their thinking is rewarded.

Support in the startup process is important, especially for young founders. This is not only about knowledge transfer, but also about innovative researchers recognizing their development possibilities and potential. This requires role models and a relaxed atmosphere. A culture of creative coffee breaks will certainly help.

A fair amount of funding is available for institutional startup support. In most cases, founders therefore have an extensive selection of consultants and in some situations need to be careful that the various coaching processes do not have negative effects and become a "waste of time".

Nobody is against spin-offs, but there are organizational forms that weaken entrepreneurship and other structures that strengthen it. In an environment in which everyone prefers to take precautions rather than take responsibility, startup companies rarely emerge. Exaggerated administrative processes inhibit the entrepreneurial spirit (but may motivate taking the step into independence). Those who appreciate the security of well-described processes may prefer to stay on the side of university research.

Not every successful innovation finds its implementation through a startup company. Especially in classical projects at universities of applied sciences, the industry partner implements the research results. Both incremental improvements and groundbreaking innovations can often be implemented more easily in a functioning business. If existing customers can be successfully addressed, the barriers to entry for a new product are many times lower than for the market entry of a newcomer.

An interesting result from the discussions at the School of Engineering: The inspiration that emanates from the spin-off idea can be used as a motivating and activating element in teaching. If it is possible to put the learning objectives into the narrative of a company foundation, this has a positive effect on the cooperation among the students and ultimately on the learning success. Expectations must be set realistically: A spin-off idea is rarely born from the lecture exercise of a module in the bachelor's program. But to support innovative thinking, the spin-off idea is valuable.

The following pages describe the companies that have been created at the ICP. Not all of them survived, but all of them tried and with all of them we made common projects. Of course, it is a disappointment when a company does not make it. It is important that investors and founders also count on this possibility. And as a university partner it is just as important to think about this eventuality. In such a situation, in well-established partnerships the core know-how can often live on and be used in further research activities.

Several of our current research topics have the potential for commercial exploitation. In addition, a good team of founders is needed, because sometimes innovation and implementation strength in the free market are not united in one person, so that a startup can only fly with a good team constellation. There are several other contact points within ZHAW [3] and we are happy to use our personal networks. We look forward to seeing it happen again in the future and to continuing to support innovative students or employees in taking the step towards independence.

Andreas Witzig, Head of ICP

*References:*

[1] Eliav Haskal, *Wie kann man eine Innovations- und Entrepreneurship-Kultur innerhalb einer Forschungsorganisation entwickeln?* Invited talk at the Department Day of the School of Engineering, 17.1.2020, Winterthur

[2] Patrick Link, *Smart-up – Ideen erfolgreich umsetzen.* Invited talk at the Department Day of the School of Engineering, 17.1.2020, Winterthur

[3] Entrepreneurship@ZHAW, Runway Incubator, Startup Challenge

## *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.

FLUXiM

www.fluxim.com

Fluxim is a provider of device simulation software and measurement hardware to the display, lighting and photovoltaics community worldwide. Our principal activity is the development and the marketing of the simulation software 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.

coatmaster

www.coatmaster.ch

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

DERMOLOCKIN

Dermolockin GmbH has developed a method to support dermatological examinations based on active thermography. An important field of application was the diagnosis of skin cancer. Unfortunately, the company had to close down its business in 2019. Due to the close cooperation between the ICP and the spin-off company, essential parts of the know-how can still be used for research.

Nano Lockin

www.nanolockin.com

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

opus néoi

www.skinobi.com

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

ZARAWIND

ZARAWIND More than green power

www.zarawind.com

Zarawind is a ZHAW spin-off 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.

Re

www.reorbis.com

Reorbis GmbH, based in Winterthur, Switzerland, aims to provide services for the manufacturing industry in the form of life cycle analysis (LCA). In the aluminium industry there is great interest in LCA due to a new standard (Aluminium 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 aluminium.

# Appendix

## A.1 Student Projects

J. Albert, K. Sadriu, *Digitalisierung der Lehre mittels Gamification-App*. Betreuer. K. P. Pernstich, W. Eich.

A. Bachmann, *A wireless measurement collection system for LymphMeter*. Betreuer: M. Bonmarin, D. Fehr, Partner: ETH Zürich - Institut für Pharmazeutische Wissenschaften, Vertiefungsarbeit 1.

D. P. Baumann, L. H. Balz, *Auslegung und Bau einer automatischen Holzschnitzelzuführung für ein Holzvergasungssystem*. Betreuer: G. Boiger, A. Fassbind, M. Boldrini, Firmenpartner: Aberta Nova S.A.

D. P. Bee, J. Giger, *Development of an active thermal imaging-based hand held device for dermatological applications*. Betreuer: M. Bonmarin, L. Holzer, Firmenpartner: Fotofinder GmbH, Bachelorarbeit Systemtechnik.

J. Blunschi, R. Sassenburg, *Creating Cell-free Artificial Skin in the Laboratory*. Betreuer: M. Bonmarin, F. Spano, D. Fehr, Firmenpartner: none, Projektarbeit Systemtechnik.

J. Blunschi, R. Sassenburg, *Artificial Tactile Skin: Flexible Pressure Sensitive Skin models*. Betreuer: F. Spano, D. Fehr, M. Bonmarin, Bachelorarbeit Systemtechnik.

E. Comi, *Large-area AC characterization of PV cells*. Betreuer: E. Knapp, B. Ruhstaller, Firmenpartner: Fluxim AG.

E. Comi, *Large-area solar cell model validation*. Betreuer: E. Knapp, B. Ruhstaller, Firmenpartner: Fluxim AG.

I. Erni, O. Lengweiler, *Konstruktion und Realisierung einer Schmelzfront-Messeinrichtung für IR-Schweissen von Kunststoffrohren*, Betreuer: T. Hocker, S. Koll, Projektpartner: Georg Fischer Piping Systems, Projektarbeit Maschinentechnik.

D. B. Felder, F. R. Hörnlimann, *Steuerung und Regelung einer automatischen Holzschnitzelzuführung für ein Holzvergasungssystem*. Betreuer: G. Boiger, A. Fassbind, M. Boldrini Firmenpartner: Aberta Nova S.A.

R. Hagen, D. Wyder, *Thermal Imaging Microscopy of Brown-Fat Cells*. Betreuer: M. Bonmarin, Firmenpartner: none, Projektarbeit Systemtechnik.

R. Hagen, *Development of a multi-wavelengths hand-held fluorescence measurement device*, Betreuer: D. Fehr, M. Bonmarin, F. Spano, Bachelorarbeit Systemtechnik.

C. Haldner, A. Widmer, *Weiterentwicklung und Implementierung einer Pumpensteuerung zur Levelstabilisierung des Haupttankes einer experimentellen Kupferelektrolyseanlage*. Betreuer: G. Boiger, M. Boldrini, Firmenpartner: intern.

N. Jenal, *Entwicklung eines Prüfstands für das kontaktlose Schweissen von Kunststoffproben*, Betreuer: C. Brändli, T. Hocker, Projektpartner: Georg Fischer Piping Systems, Vertiefungsarbeit Masterstudiengang.

N. Jenal, *CFD-Simulationen und Prüfstandschweissungen zur Entwicklung einer Heizung für GFPS-Schweissmaschinen*, Betreuer: C. Brändli, T. Hocker, Projektpartner: Georg Fischer Piping Systems, Vertiefungsarbeit Masterstudiengang.

M. Kaufmann, C. Blättler, *Physik spielend lernen mittels Gamification-App*. Betreuer: K. P. Pernstich, W. Eich.

K. Künzli, *Development of Innovative Sweat Sensors,* M. Bonmarin, F. Spano, D. Fehr, Bachelorarbeit Systemtechnik.

C. Malnati, *Real-time simulation of mechanical resonator*. Betreuer: M. Bonmarin, D. Fehr, Firmenpartner: Rheonics GmbH, Vertiefungsarbeit 1.

C. Malnati, *3D Reconstruction of thermal images*, Betreuer: M. Bonmarin, Vertifeungsarbeit MSE.

V. Michel, *Development of a broadband pump-probe terahertz spectrometer*. Betreuer: U. Puc, M. Jazbinsek, Firmenpartner: Rainbow Photonics AG, Vertiefungsarbeit Masterstudiengang.

V. Michel, *Hardware-software integration and validation of a compact, time-resolved, optical-pump terahertz-probe spectroscopy system*. Betreuer: U. Puc, M. Jazbinsek, Firmenpartner: Rainbow Photonics AG, Masterarbeit Masterstudiengang.

A. Morandi, *Development of a PCB board for signal acquisition and system control*. Betreuer: U. Puc, M. Jazbinsek, Firmenpartner: Rainbow Photonics AG, Projektarbeit Elektrotechnik.

A. Morandi, *Low noise detection and acquisition electronics for a terahertz spectrometer*. Betreuer: U. Puc, M. Jazbinsek, Firmenpartner: Rainbow Photonics AG, Bachelorarbeit Elektrotechnik.

L. Ruckstuhl, *Optimizing the thermal behavior of the Medyria flow sensor using experimental methods and CFD-simulations*, Betreuer: T. Hocker, Projektpartner: Medyria AG, Masterarbeit Masterstudiengang.

D. Schoch, M. Wernli, *Automatisierte Interpolation von Strömungssimulationen*. Betreuer: G. Boiger, A. Zubiaga, Firmenpartner: intern.

J. Scholer, R. M. Ortiz, *Aerodynamische Optimierung eines Rennfahrzeuges mittels CFD-Simulation und Anwendung automatisierter Simulationen*. Betreuer: G. Boiger, M. Boldrini, B. Siyahhan, Firmenpartner: Sauber AG.

S. Spirig, *Thermisch-fluidische Simulation des Aufwärmprozesses von Kunststoffrohren mit der Infrarotschweissmaschine IR-315 A*, Betreuer: T. Hocker, Projektpartner: Georg Fischer Piping Systems, Masterarbeit Masterstudiengang.

J. Stoll, *Experimentelle und theoretische Charakterisierung der Bewegung von Heissluftballons*, Betreuer: T. Hocker, Projektpartner: Air Ballonteam Stefan Zeberli GmbH, Vertiefungsarbeit Masterstudiengang.

T. Studer, M. Tanner, *Klimakammer*. Betreuer: G. Boiger, M. Boldrini, Firmenpartner: intern.

N. Wegmann, *Konzeptentwicklung einer Klimakammer.* Betreuer: G. Boiger, M. Boldrini, Firmenpartner: intern.

S. Weidmann, *Frequency Domain 2D + 1D FEM Simulation of Solar Cells*. Masterarbeit ETHZ, September 2019. Betreuer: B. Ruhstaller, R. Hiptmair, C. Kirsch, R. Hiestand, Firmenpartner: Fluxim AG.

S. Wieser, T. Gasser, *Integration eines geeigneten Heizelementes in den formgebenden Bereich des Verpackungsmaterials einer horizontalen Schlauchbeutelmaschine als Vorheizung*. Betreuer: G. Boiger, D. Brunner, Firmenpartner: Syntegon Packaging Systems AG.

S. Wieser, T. Gasser, *Prototyp eines Schwingungsisolators für Schweizer Pharmaindustrie*. Betreuer: G. Boiger, D. Brunner, Firmenpartner: intern.

D. Wyss, *Modeling the separation of solid-liquid dispersion in decanter centrifuges*, Betreuer: T. Hocker, T. Hühn, Projektpartner: Oro De Cacao, Vertiefungsarbeit Masterstudiengang.

S. Zeder, *Hybrid Master Equation Model for Exciton Dynamics in OLEDs*. Masterarbeit ETHZ, April 2019. Betreuer: B. Ruhstaller, C. Kirsch, R. Hiptmair, Firmenpartner: Fluxim AG.

## A.2 Scientific Publications

U. AEBERHARD, S. ALTAZIN, L. STEPANOVA, A. STOUS, B. BLÜLLE, C. KIRSCH, E. KNAPP, B. RUHSTALLER, *Numerical Optimization of Organic and Hybrid Multijunction Solar Cells*. Proc. IEEE 46th Photovoltaic Specialists Conference (PVSC), 2019; pp. 0105–0111. DOI: 10.1109/PVSC40753.2019.8980824.

U. AEBERHARD, M. NEUKOM, A. SCHILLER, S. ZÜFLE, S. JENATSCH, B. BLÜLLE, S. ALTAZIN, L. STEPANOVA, E. KNAPP, C. KIRSCH, B. RUHSTALLER, *Computational device optimization and parameter extraction for perovskite-based solar cells*. Proc. SPIE 11275, Physics, Simulation, and Photonic Engineering of Photovoltaic Devices, IX, 2020; 112750B. DOI: 10.1117/12.2545507.

Z. ANDLEEB, C. STRAND, S. MALIK, G. HUSSEIN, H. KHAWAJA; G. BOIGER, M. MOATAMEDI, 2020. *Multiphysics Analysis of CFRP Charpy Tests by varying Temperatures* (2020). Int.Journal of Multiphysics. 14(2), pp. 143-160. DOI: 10.21152/1750-9548.14.2.143.

D. BERNHARDSGRÜTTER, M. SCHMID, *Modeling of Intensity-Modulated Photocurrent/Photovoltage Spectroscopy: Effect of Mobile Ions on the Dynamic Response of Perovskite Solar Cells*. J. Phys. Chem. C 123 (50), 30077-30087, 2019.

G. BOIGER, M. BOLDRINI, V. LIENHARD, B. SIYAHHAN, H. KHAWAJA, M. MOATAMEDI, *Multiphysics Eulerian-Lagrangian Electrostatic Particle Spray- And Deposition Model for OpenFoam® and KaleidoSim® Cloud-Platform* (2020). Int.Journal of Multiphysics. 14(1), pp. 1-15, 2019. DOI: 10.21152/1750-9548.14.1.1.

G. BOIGER, V. BUFF, A. ZUBIAGA, A. FASSBIND, P. CAELS, 2019. *Investigating tar formation at low pressures in wood gasification systems, applying a novel thermo-chemical simulation model*. In: Proceedings of the 5$^{th}$Int.Conference of Polygeneration Strategies 2019. 5$^{th}$Int.Conference of Polygeneration Strategies 2019 (ICPS19), Vienna, Austria, 18-20 November 2019.

D. BRAGA, S. JENATSCH, L. PENNINCK, R. HIESTAND, M. DIETHELM, S. ALTAZIN, C. KIRSCH, B. RUHSTALLER, *Modeling Electrical and Optical Cross-Talk between Adjacent Pixels in Organic Light-Emitting Diode Displays*. SID Symposium Digest of Technical Papers 50 (1), 2019; pp. 953–956. DOI: 10.1002/sdtp.13083.

D. BRUNNER, J. GOODBREAD, K. HÄUSLER, S. KUMAR, G. K. BOIGER, H. A. KHAWAJA, *Analysis of a tubular torsionally resonating viscosity–density sensor*. Sensors. 20(11), pp. 3036, 2020. DOI: 10.21256/zhaw-20176.

T. O. BUCHMANN, E. J. R. KELLEHER, K. J. KALTENECKER, B. B. ZHOU, S. H. LEE, O. P. KWON, M. JAZBINSEK, F. ROTERMUND, P. U. JEPSEN, *MHz-repetition-rate, sub-mW, multi-octave THz wave generation in HMQ-TMS.* Opt. Express 28, 9631, 2020.

M. DIETHELM, A. SCHILLER, M. KAWECKI, A. DEVIŽIS, B. BLÜLLE, S. JENATSCH, E. KNAPP, Q. Grossmann, B. Ruhstaller, F. Nüesch, R. Hany, *The Dynamic Emission Zone in Sandwich Polymer Light-Emitting Electrochemical Cells.* Adv. Func. Mat., 2019.

M. DIETHELM, Q. GROSSMANN, A. SCHILLER, E. KNAPP, S. JENATSCH, M. KAWECKI, F. NÜESCH, R. HANY, *Optimized Electrolyte Loading and Active Film Thickness for Sandwich Polymer Light-Emitting Electrochemical Cells*. Advanced Optical Materials 7 (3), 1801278, 2019.

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## A.3 Book Chapters

G. Boiger, H. Khawaja, M. Moatamedi, *Introduction: Large, (non-)spherical particle modelling in the context of fluid filtration applications.* Multiphysics Modelling of Fluid-Particulate Systems, Elsevier Academic Press London, 2020.

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## A.4 Conferences and Workshops

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T. Bach, U. Puc, V. Michel, C. Medrano, P. Gunter, M. Jazbinsek, *Terahertz time-domain spectroscopy up to 20 THz based on organic electro-optic crystals*. 44th International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz). Paris, France, 01-06 September 2019.

T. Bach, U. Puc, V. Michel, M. Jazbinsek, P. Günter, C. Medrano, *Ultra-broadband terahertz time-domain spectroscopy in a compact system with DSTMS organic crystals*. SPIE Photonics West - Conference 11279 «Terahertz, RF, Millimeter, and Submillimeter-Wave Technology and Applications XIII», San Francisco, USA, 1-6 February 2020.

B. Blülle, S. Altazin, B. Frouin, L. Stepanova, S. Jenatsch, B. Ruhstaller, *Light conversion and scattering properties of QD films for display applications: Angle-resolved optical spectroscopy and numerical simulation*. SID Symposium Digest of Technical Papers 50, 407-410, San Jose, USA (2019).

G. Boiger, 2019. *Invited talk on Modeling particle clouds in coating applications: The long road from qualitative modeling to fully validated industrial applicability*. Invited talk, AlGhurair University, Dubai, UAE, September 12th, 2019. https://www.facebook.com/AguDubai/; https://agu.ac.ae

G. Boiger, V. Buff, A. Zubiaga, A. Fassbind, P. Caels, 2019. *Investigating tar formation at low pressures in wood gasification systems, applying a novel thermo-chemical simulation model*. ICPS19. 5$^{th}$ International Conference on Polygeneration Strategies, Vienna, Austria, 18-20 November 2019.

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G. Boiger, V. Lienhard, V. Buff, B. Siyahhan, 2020. *On establishing and applying a system dynamic modeling method in the context of investigating tar formation within wood gasification systems*. Invited talk, NIC National Institute of Chemistry, Ljubljana, Slovenja, January 16th, 2020.

G. Boiger, V. Lienhard, V. Buff, B. Siyahhan, 2020. *Development and Validation of a Eulerian-Lagrangian modelt o predict particle motion and deposition in electrostatic fields*. Invited talk, NIC National Institute of Chemistry, Ljubljana, Slovenja, January 16th, 2020.

G. Boiger, 2020. FEA/FV workshop 2020: *Using OpenFoam in finite volume analysis*. Invited talk, Al-Ghurair University, Dubai, UAE, February 9th-13th, 2020. https://agu.ac.ae/news-events/fea-workshop-2020/; https://agu.ac.ae

D. Braga, S Jenatsch, L. Penninck, R. Hiestand, M. Diethelm, S. Altazin, C. Kirsch, B. Ruhstaller, *Modeling Electrical and Optical Cross-Talk between Adjacent Pixels in Organic Light-Emitting Diode Displays*. SID Symposium Digest of Technical Papers 50, 31-34, San Jose, USA (2019).

D. Brunner, J. Goodbeard, S. Kumar, H. Khawaja, G. Boiger, 2019. *Investigation of modal distortion and temporal effects in torsional resonators*. Multiphysics 2019. 14th International Conference of Multipysics, Dubai, UAE, 14-15 December 2019. International Society of Multiphysics. ISSN (online) 2409-1669.

R. Herrendörfer, J. O. Schumacher, *Advanced characterization of polymer electrolyte fuel cells using a two-phase time-dependent model*. 16th symposium on modeling and experimental validation of electrochemical energy technologies (ModVal 2019), Braunschweig, Germany. Available from: https://doi.org/10.21256/zhaw-2790.

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S. JENATSCH, S. ZÜFLE, P.-A. WILL, B. BLÜLLE, M. NEUKOM, D. BRAGA, S. LENK, S. REINEKE, B. RUHSTALLER, *Quantitative Analysis of Charge Transport in Single-Carrier Devices and OLEDs Combining DC and AC Data*. San Jose, USA (2019).

B. J. KANG, W. T. KIM, S. H. LEE, M. JAZBINSEK, O. P. KWON, F. ROTERMUND, *Recent progress on highly nonlinear organic crystals for efficient broadband THz wave generation*. SPIE Photonics West - Conference 11264 «Nonlinear Frequency Generation and Conversion: Materials and Devices XIX», San Francisco, USA, 1-6 February 2020.

W. T. KIM, M. H. SHIN, S. I. KIM, S. H. LEE, I. C. YU, M. JAZBINSEK, W. YOON, H. YUN, D. KIM, O. P. KWON, F. ROTERMUND, *New design strategy of organic nonlinear crystals via suppression of phonon vibrational modes for gap-free broadband THz generation*. SPIE Photonics West - Conference 11264 «Nonlinear Frequency Generation and Conversion: Materials and Devices XIX», San Francisco, USA, 1-6 February 2020.

C. KIRSCH, AI for Engineering Summer School 2019, Toronto, Canada.

V. LIENHARD, M. BOLDRINI, G. BOIGER, 2020. *Simulation based investigation of an electrostatic method for deflecting charged particle clouds*. Invited talk, NIC National Institute of Chemistry, Ljubljana, Slovenja, January 16th, 2020.

S. MADSEN, A. ZUBIAGA, H. KHAWAJA, G. BOIGER, 2019. CFD *Modelling of Pollutant Transport from a Docked Marine Vessel* [Poster]. In: Proceedings of 14th Int. Conference of Multipysics 2019, 14th International Conference of Multipysics (Multiphysics 2019), Dubai, UAE, 14-15 December 2019. International Society of Multiphysics. ISSN (online) 2409-1669.

G. MOUROUGA, C. SANSONE, F. ALLOIN, C. IOJOIU, J. O. SCHUMACHER, *A multicomponent diffusion model for organic redox flow battery membranes*. 16th symposium on modeling and experimental validation of electrochemical energy technologies (ModVal 2019), Braunschweig, Germany. Available from: https://doi.org/10.21256/zhaw-2792.

G. MOUROUGA, C. SANSONE, F. ALLOIN, C. IOJOIU, J. O. SCHUMACHER, *A multicomponent diffusion model for organic redox flow battery membranes.* International Flow Battery Forum (IFBF 2019), Lyon, France.

K. P. PERNSTICH, *Game-based Learning für MINT-Fächer mit e-Exercises*. E-Learning Café, ZHAW Wädenswil, Switzerland, May 2019.

K. P. PERNSTICH, *Gamification der Physikübungen mit tguishiny/e-Exercise*. Digital Learning Day, ZHAW-IDP Retreat, Winterthur, Switzerland, June 2019.

K. P. PERNSTICH, *Eine App zur Gamification der Übungen in MINT-Fächern*. Bürgenstock-Konferenz der Schweizer Fachhochschulen und Pädagogischen Hochschulen, Lucerne, Switzerland, 10-11 January 2020.

U. PUC, T. BACH, C. MEDRANO, M. ZGONIK, M. JAZBINSEK, *Compact and ultra-broadband terahertz spectrometer based on organic DSTMS crystals*. SPIE Photonics West - Conference 10917 «Terahertz, RF, Millimeter, and Submillimeter-Wave Technology and Applications XII», San Francisco, USA, 2-7 February 2019.

U. PUC, T. BACH, V. MICHEL, M. ZGONIK, C. MEDRANO, M. JAZBINSEK, *DSTMS-based ultrabroadband terahertz time-domain spectroscopy*. Conference on Lasers and Electro-Optics Europe & European Quantum Electronics Conference (CLEO/Europe-EQEC). Munich, Germany, 23-27 June 2019.

J. O. SCHUMACHER, R. VETTER, *Experimental parameter uncertainty in PEM fuel cell modeling.* 8th International Conference on Fundamentals and Development of Fuel Cells (2019), Nantes, France. doi: https://digitalcollection.zhaw.ch/handle/11475/15710.

J. WLODARCZYK, B. CANTU, P. FISCHER, M. KÜTTINGER, J. O. SCHUMACHER, *An enhanced 1-D model of a hydrogen-bromine flow battery.* 16th symposium on modeling and experimental validation of electrochemical energy technologies (ModVal 2019), Braunschweig, Germany. Available from: https://doi.org/10.21256/zhaw-2791.

J. WLODARCZYK, M. KÜTTINGER, P. FISCHER, J. O. SCHUMACHER, *Open-circuit potential prediction and its applications in modeling and simulation of hydrogen-bromine redox flow batteries.* International Flow Battery Forum (IFBF 2019), Lyon, France.

A. ZUBIAGA, D. BRUNNER, F. SAGER, M. CLEMENS, E. KOEPF, G. BOIGER, 2019. *Evaluation of Faraday instabilities in small vessels*. 7th ESI OpenFOAM Conference 2019, Berlin, Germany, 16-17 October 2019.

A. ZUBIAGA, H. KHAWAJA, G. BOIGER, 2019. *Simulation of contamination by exhaust emissions from docked marine vessels*. Multiphysics 2019. 14th International Conference of Multipysics, Dubai, UAE, 14-15 December 2019. International Society of Multiphysics. ISSN (online) 2409-1669.

## A.5 Teaching

T. BERGMANN, T. HOCKER, *Thermische Energiesysteme, FS19*, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Lineare Algebra 1, HS19*, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Analysis 1, HS19*, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Lineare Algebra 2, FS20*, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Analysis 2, FS20*, Bachelor of Science.

G. BOIGER, *Numerische Mathematik für IT 1, V+P, FS19*, Bachelor of Science.

G. BOIGER, *Numerische Mathematik für IT 1, V+P, FS20*, Bachelor of Science.

G. BOIGER, *Numerische Mathematik für IT 2, V+P, HS19*, Bachelor of Science.

G. BOIGER, *Fluid und Thermodynamik 1, V+P, FS19*, Bachelor of Science.

G. BOIGER, *Fluid und Thermodynamik 1, V+P, FS20*, Bachelor of Science.

G. BOIGER, *TSM Advanced Thermodynamics, V+P, HS19*, Master of Science in Engineering.

G. BOIGER, *TSM Two Phase Flow, V+P, FS19*, Master of Science in Engineering.

G. BOIGER, *TSM Two Phase Flow, V+P, FS20*, Master of Science in Engineering.

G. BOIGER, *EVA Thermofluiddynamik Modellentwicklung mittels OpenFoam® 1, V+P, HS19*, Master of Science in Engineering.

G. BOIGER, *EVA Thermofluiddynamik Modellentwicklung mittels OpenFoam® 2, V+P, FS19*, Master of Science in Engineering.

M. BONMARIN, *Physik I, HS19*, Bachelor of Science.

M. BONMARIN, *Physik II, FS20*, Bachelor of Science.

M. BONMARIN, *ATMT, FS20*, Bachelor of Science.

D. FEHR, *Mathematik: Analysis 2 für IT, FS19*, Bachelor of Science.

D. FEHR, *Analysis 1*, *HS19*, Bachelor of Science.

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T. HOCKER, *Systemphysik für Aviatik 1 – Praktikum, HS19*, Bachelor of Science.

T. HOCKER, *Systemphysik für Aviatik 2 – Plenum und Praktikum, FS19*, Bachelor of Science.

T. HOCKER, *Fluid- und Thermodynamik 3 – Vorlesung, HS19*, Bachelor of Science.

M. JAZBINSEK, *Physik für Energie und Umwelttechnik 1 – Vorlesung und Praktikum, FS19*, Bachelor of Science.

M. JAZBINSEK, *Physik für Energie und Umwelttechnik 2 – Vorlesung und Praktikum, HS19*, Bachelor of Science.

M. JAZBINSEK, *Physik 2 für MT und EU – Vorlesung und Praktikum, FS20*, Bachelor of Science.

C. KIRSCH, *MANIT2 – Mathematik: Analysis 2, FS19*, Bachelor of Science.

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C. KIRSCH, *MND1 – Mathematik: Numerik und Differenzialgleichungen 1, HS19*, Bachelor of Science.

C. KIRSCH, *MAE4 – Mathematik: Analysis für Ingenieure 4, FS20*, Bachelor of Science.

C. KIRSCH, *MND2 – Mathematik: Numerik und Differenzialgleichungen 2, FS20*, Bachelor of Science.

E. KNAPP, *Numerik für Energie- und Umwelttechnik, HS19*, Bachelor of Science.

K. P. PERNSTICH, *Physik- und Systemwissenschaften für Verkehrssysteme 2, FS19*, Bachelor of Science.

K. P. PERNSTICH, *Physik 1, HS19*, Bachelor of Science.

K. P. PERNSTICH, *Physik 1 Praktikum, HS19*, Bachelor of Science.

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K. P. PERNSTICH, *Grundlagenprojekt 1, HS19*, Bachelor of Science.

K. P. PERNSTICH, *Grundlagenprojekt 2, FS20*, Bachelor of Science.

B. RUHSTALLER, *Physik- und Systemwissenschaften für Verkehrssysteme 2, FS 2019,* Bachelor of Science.

J. O. SCHUMACHER, *Numerische Mathematik: NMIT1 und NMIT2, FS19, HS19, FS20*, Bachelor of Science.

J. O. SCHUMACHER, *Numerical Simulation of Solar Cells, FS19, FS20*, Master Studiengang *Solar Energy Engineering*, Universität Freiburg im Breisgau.

J. O. SCHUMACHER, *Multiphysics Modeling and Simulation*, *HS19*, Swiss course of studies: Master of Science in Engineering.

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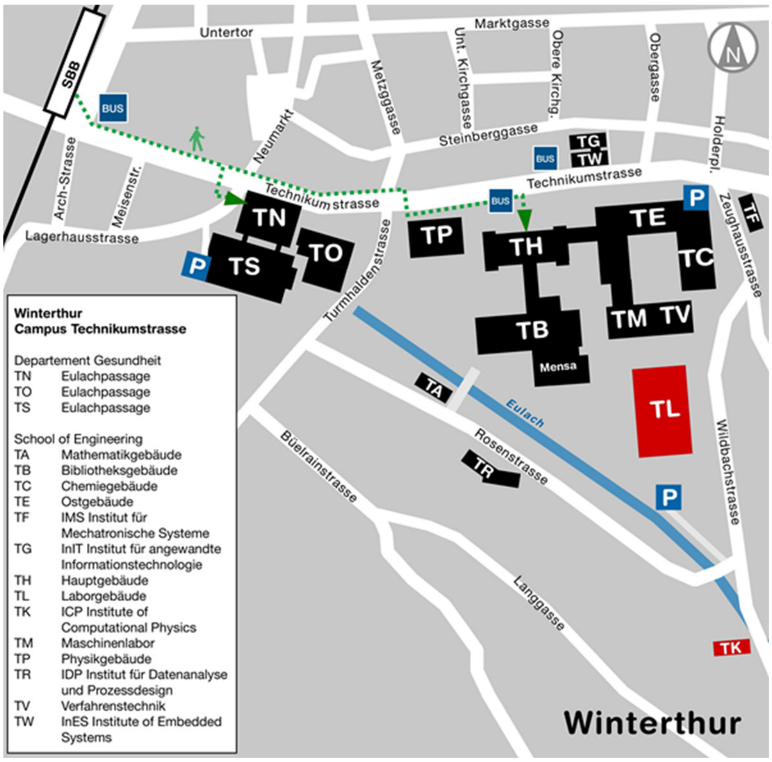


TK Building

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