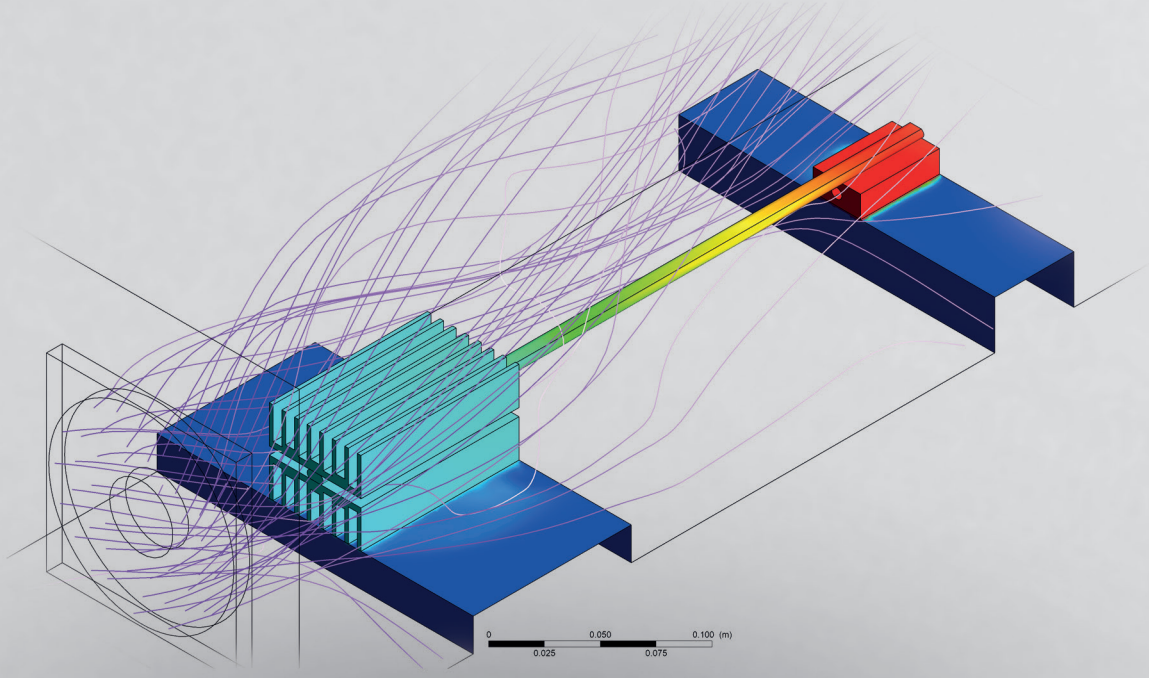
Zurich University
of Applied Sciences

School of Engineering

ICP Institute of Computational Physics

Research Report 2021



CFD simulation illustration of a heat pipe with 100 °C heating temperature and forced air cooling via aluminum cooling fins.

Introduction

Computational Physics & Artificial Intelligence

We are experiencing an extremely active research period in the field of artificial intelligence. Some practical applications are already being used extensively by large corporations, while for small and medium-sized enterprises the benefits of this new technology are not yet clear. The Centre for Artificial Intelligence (https://www.zhaw.ch/cai/) is currently being established at ZHAW. We wish them a successful start and are looking forward to future close collaboration.

What significance does this development have for ICP? What are our projects on this topic? And what could be our contributions in this emerging field in the future? Currently there are two projects at ICP. They are described in detail on pages 29 and 41. In section 5, Evelyne Knapp lays the foundation for further discussions on the merging of computational physics and artificial intelligence. The current state of research is summarized and the questions posed above are organized. At ICP, we are currently expanding partner networks and considering promising applications for industrial partners. All should actively participate in the discussion.

The COVID-19 pandemic has demanded a lot from us and has drastically changed our working environment. I would like to thank everyone for the extraordinary efforts that have been made at ICP. We have found new ways of productive collaboration, even remotely. But we also long to meet again regularly in person. I would like to call on you all to play an active role in shaping this return. In the foreseeable future we will likely need to continue experimenting with hybrid meetings and perhaps with forms of virtual social sharing. Maybe we need to look closely at shortfalls and deficits that have arisen during the time of working from home. Maybe unconventional and spontaneous actions are needed. Let us cultivate a healthy optimism and good human contact. In this sense, a sincere "Welcome Back!" in the hope that we can meet again soon at our Winterthur location.

Andreas Witzig,
Head of Institute ICP

Table of Contents

1 Multiphysics Modeling

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

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

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

Our specialties in this context include the application, extension and development of coupled models using our own finite element software SESES, the fluid dynamics software OpenFoam (open source) and commercially available products such as COMSOL.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1.1 Powder Coating: Simulation-Based Prototype Development of Novel Powder Coating Nozzles

Through the development of an extensive numerical Euler-Lagrangian simulation model, highly efficient nozzle geometries were developed. The simulations were validated on measurement series covering several thousand experiments. The new nozzles which resulted out of the project achieved an increase in coating efficiency by over 15%.

Contributors: G. Boiger, M. Boldrini, V. Lienhard, B. Siyahhan, V. Buff
Partner(s): Wagner International AG
Funding: Innosuisse
Duration: 2017–2020

In the course of this project, an extensive numerical Euler-Lagrangian simulation model for powder coating applications was developed and comprehensively validated. The model couples all relevant physical influencing factors such as electrostatic field strength, air flow, particle size distribution, particle - substrate interaction, particles - particle interaction and gravitation. The solver was validated by several thousand coating experiments and their evaluation. With this new numerical model, a powder coating process can now be quantified in a previously unattainable quality, both quantitatively and qualitatively. This new numerical analysis method has already provided far-reaching insights into the interrelationships between process parameters and coating results.

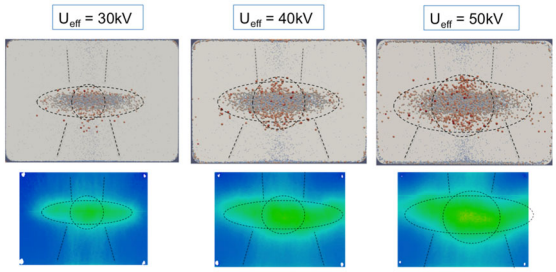


Fig. 1: Simulation results in comparison to measurements on a U-profile substrate. Example for qualitative correspondence of simulated (top) and measured (bottom) coating patterns. Here the front side of an A4-plate substrate was coated at a pistol-substrate-distance D=20cm, while applying an airflow rate Q=3m^3/h and effective voltages U_{eff} of 30kV, 40kV and 50kV respectively. It can be seen that the main qualitative coating-pattern-features, as well as trends of simulations and experiments match well, [1].

Based on these simulation results and extensive measurements, it was possible to design a set of new internal geometries for the nozzle part of the pistol. These new nozzle types, while in a prototype stage, showed the potential to increase process metrics such as homogeneity and coating efficiency. From the set of suggested new geometry types, two were selected by the customer for further investigation. Both selected types showed an increase of the coating efficiency by over 15% for the complete parameter range.
Through further investigation and development on the selected nozzles, the design was improved to achieve a coating efficiency increase of 23-31% for the most commonly used parameter ranges.

Literature:

[1] Boiger, G.; Boldrini, M.; Lienhard, V.; Siyahhan, B.; Khawaja, H.; Moatamedi, M., 2019. 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. DOI: 10.21152/1750-9548.14.1.1
[2] Boiger G., Bercan S.; Lienhard, V.; 2020. Advancing the Validation and Application of a Eulerian-Lagrangian Multiphysics Solver for Coating Processes in Terms of Massive Simultaneous Cloud Computing. Multiphysics 2020. 15th International Conference of Multipysics, Online, 10-11 December 2020. International Society of Multiphysics. ISSN (online) 2409-1669.

1.2 Development of a Tubular Resonator Sensor Platform for Inline Process Fluid Monitoring

Monitoring fluid properties such as viscosity is crucial in many industrial processes. For sanitary processes, cleanability is a crucial factor. A tubular non-intrusive resonant sensor was developed to measure the viscosity in the process line, avoiding any flow obstructions and cleanable in place using industry-standard processes. To develop these sensors, a comprehensive, scalable model was developed to describe the fluid-structure interaction of the fluid with the resonator.

Contributors: D. Brunner, G. Boiger
Partner(s): Rheonics GmbH
Funding: Innosuisse, Rheonics GmbH
Duration: 2018–2021

In this study, a tubular torsional resonator was developed. Its resonance was driven and sensed using electromagnetic transducers.
The operating principle of the sensor is based on the excitation of a torsional mode, and subsequent measurement of the resonant response. The damping and resonance frequency are determined from the response signal. Resonance frequency and damping are then related to the fluid's viscosity.
A comprehensive numerical model of a tubular resonator has been developed and validated. The sensor used for the validation study had an inner diameter of 5.25 mm (1). For most industrial processes, larger tube diameters are required. Therefore, using the previously validated models, a larger version of a functionally similar sensor was built and tested. The larger resonator was based on a 20 mm inner diameter tube, as shown in Figure 1.
The sensor was calibrated, and the calibration verified, using a series of NIST traceable viscosity reference fluids. The sensor measured the fluid's viscosity-density product $\rho\eta$ over a wide range from 1 to 100'000 mPa.s. The measured values of the bandwidth divided by the resonance frequency (Γ/f_0) were in good agreement with the predictions of the numerical model (see Figure 2), showing the utility of the model as a development tool for scaling to larger diameter tubes.

Figure 1: DN20 tubular resonator (left), DN20 tubular resonator operating in an experimental flow loop.

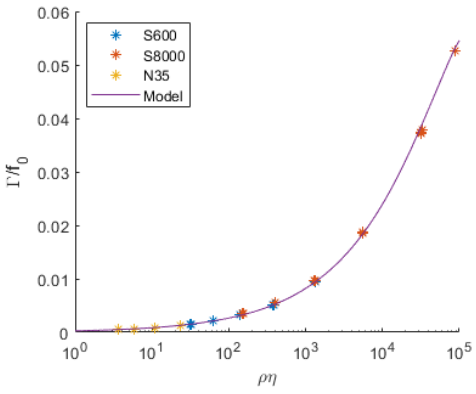


Figure 2: Bandwidth divided by the resonance frequency (Γ/f_0) vs. the viscosity density product $\rho\eta$ for different fluids and the numerical prediction.

Source:

D. Brunner, J. Goodbread, K. Häusler, S. Kumar, G. Boiger, H. Khawaja, Analysis of a Tubular Torsionally Resonating Viscosity-Density Sensor, MDPI Sensors, 2020, 20 (11), 3036. https://doi.org/10.3390/s2011

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 impairs 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.

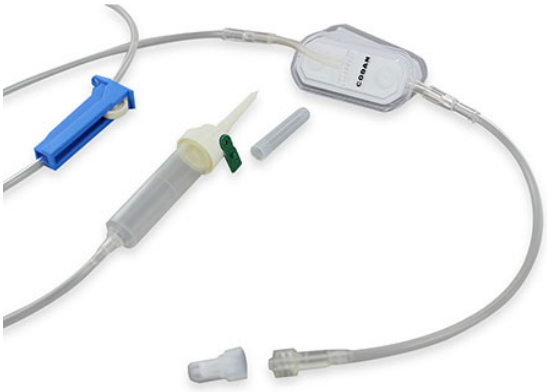


Figure 1: Different components of an infusion system (from left to right: flow controller, drop-counter, filter and tubing).

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 Figure 1) can be better realized and a broader application of the product is enabled.

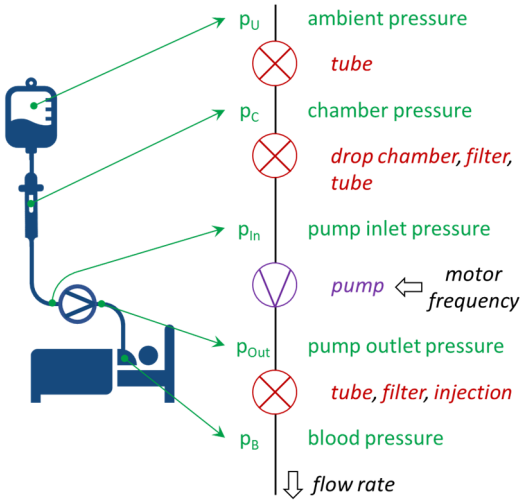


Figure 2: Model of the infusion system with pump and various components.

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 to characterize the pump and the viscoelastic behavior of the peristaltic tube.
Based on the measured data of the individual components and the findings from the characterization of the pump and peristaltic tube, the flow dynamic model of the infusion system is developed (see Figure 2), and is validated by means of specific experiments.

1.4 CFD Modelling of Droplet Impact into Resting Fluid

When transporting a vial filled with liquid, the fluid is exposed to external vibrations from the transport vehicle. These vibrations cause motion and therefore shear stresses and pressure forces in the fluid. When it comes to pharmaceutical fluids, it is essential to understand these shear and pressure conditions because they can lead to the degradation of the drug. In certain conditions, droplets can be formed. The presented work investigates the re-impact of such a droplet into the surface of the fluid and the corresponding shear forces using detailed CFD simulations.

Contributors: M. Hostettler, D. Brunner, G. Boiger
Partner(s): F. Hoffmann-La Roche Ltd. Basel
Funding: F. Hoffmann-La Roche Ltd. Basel
Duration: 2020–2021

During the transportation of liquid drugs, the mechanical stress on the fluid has a major impact on the degradation of the active ingredient of the drug. Former studies investigated the vibration-based formation of wave patterns and wave intensities at the surface of the fluid inside a transport vial. These waves can lead to splashing. The present study focuses on the estimation of the shear stress caused by splashing to gain insight about the relevance of this phenomenon and to determine the most important influence parameters.
Thereby, a falling droplet (see Figure 1), which impacts into a surface of a resting liquid in a cylindrical domain is considered. The impact and immersion of the droplet into the surface generates complex agitation of the fluid and leads to the occurrence of shear stresses. These shear stresses depend on parameters such as falling height, droplet diameter and viscosity of the fluid.

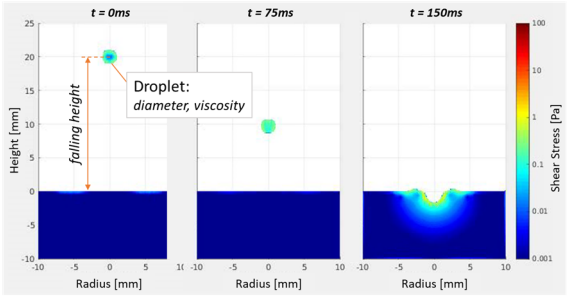


Figure 1: Side view on splashing test-case with falling droplet (top) and resting fluid (bottom) in a cylindrical domain. Time progresses from left to right; color indicates magnitude of azimuthal shear stress average.

Using computational fluid dynamics for a two-phase system, said degrees of freedom were investigated in relation to associated shear conditions. Due to the symmetrical nature of the simulation, the resulting shear stresses in the fluid phase have been averaged in azimuthal direction to gain insight into the spatial region of energy dissipation. Furthermore, based on a statistical evaluation of the occurring shear stress values, a reliability function (see Figure 2) has been calculated to analyze the probability of occurrence of a certain shear load when changing a parameter.

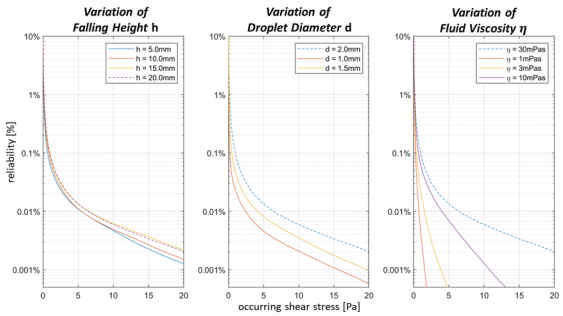


Figure 2: Reliability function (probability of occurrence of a certain shear stress) used to compare the effect from changing one of the parameters. Left: marginal effect when varying the falling height; Middle: medium effect when varying droplet diameter; Right: large effect when varying fluid viscosity.

The study has shown that peak shear stresses due to splashing are much higher (up to 20 times more) than for simple wave motion scenarios.
Further, a significant increase of occurring shear stresses and a decrease of the penetration depth can be seen when increasing the fluids viscosity. The falling height and the droplet diameter have only minor influence on the effects.
An experimental setup has been designed to validate the simulation. The test-case has been realized using water glycerol solutions of varying viscosity in a 6ml vial and methylene blue colored droplets from a needle, positioned above the vial. The droplet impact has been captured on video for qualitative comparison of the resulting penetration depth.

1.5 Development of a Multi-Physics Solver for Powder Coating Processes with Arbitrarily Moving Pistol

In the scope of this study, an existing multi-physics solver [1] to simulate particle, flow and electrostatic interactions for powder coating applications has been extended to incorporate moving coating pistols. Although the existing solver has been validated experimentally [2], the lack of the capability to incorporate motion of a coating pistol prevented it from directly simulating real life industrial applications.

Contributors: B. Siyahhan, G. Boiger
Partner(s): internal
Funding: Internal
Duration: since 2020

Powder coating is an environmentally friendly alternative to conventional liquid paint-based surface finishing methods, especially suited for thin coatings. It is employed in a vast range of industrial applications (automotive, household appliances, etc.). The process involves a powder cloud transported along with an air flow within a coating pistol, where an electrical corona is formed at the tip of a mounted electrode. After passing through the corona, the solid particles are ionized and following their discharge from the pistol, they coat a grounded substrate upon impact. Due to the complex interaction involved amongst the fluid dynamic, electrostatic forces and the motion of individual powder particles, the process is extremely challenging to simulate. Therefore, in the lack of scientific tools, the industry has relied mainly on trial-and-error based methods and practical know-how. To remedy this situation, a multiphysics solver capable of taking into the aforementioned interactions has been developed [1] within the framework of OpenFOAM. The solver firstly resolves the electric field based on the solution of Equation (1):

$$\nabla^2\Psi = -\frac{\rho_c}{\epsilon_0} \quad (1)$$

Where ψ(V) is the electric potential, ρ_c(C/m^3) the charge density ϵ_0(F/m) is the permittivity of free space. Independently, the flow field is also resolved based on the incompressible continuity and the Navier-Stokes Equations (2) and (3) respectively.

$$\nabla \cdot \vec{U} = 0 \quad (2)$$

$$\frac{\partial \vec{U}}{\partial t} + \vec{U} \cdot \nabla\vec{U} = -\nabla p' + \nabla \cdot \nu_{eff}\nabla\vec{U} + \overrightarrow{S_u} \quad (3)$$

Where U(m/s) denotes the fluid velocity, p'(m^2/s^2) the pressure normalized by the fluid density ν_{eff}(m^2/s) the viscosity and S_u(m/s^2) volume source terms. The resolved fields can be used to derive the future trajectory of individual powder particles based on the momentum balance Equation (4).

$$m_p\ddot{x}_p = \rho_p\pi\frac{d_p^3}{6}\ddot{x}_p = F_D + F_{el} + F_g \quad (4)$$

Where m_p(kg) is the mass of the particle and x_p(m) is its position, ρ_p(kg/m^3) its density and d_p(m) its diameter. The force F_D(N) is the flow particle interaction force, F_{el}(N) is the electrostatic force on the particle and F_g(N) is the gravity force. This theoretical basis of the existing solver is complemented by the ability of the coating pistols to move in accordance with any periodic function represented by a Fourier series expressed in Equation (5):

$$f(t) = a_0 + \sum_{n=1}^{\infty} a_n\cos\omega t + \sum_{n=1}^{\infty} b_n\sin\omega t \quad (5)$$

In addition to developing the required motion definition libraries in OpenFOAM, the particle injection model has been updated to accommodate the moving and multiple pistol cases, and the case set-up and special boundary conditions necessary for the interfacing of a moving region of computational cells to stationary ones have been investigated. The modifications mentioned above allow the simulation of practical coating applications in real time as depicted in Figure 1, providing the basis for a scientific tool for a priori process design and optimization for powder coating applications.

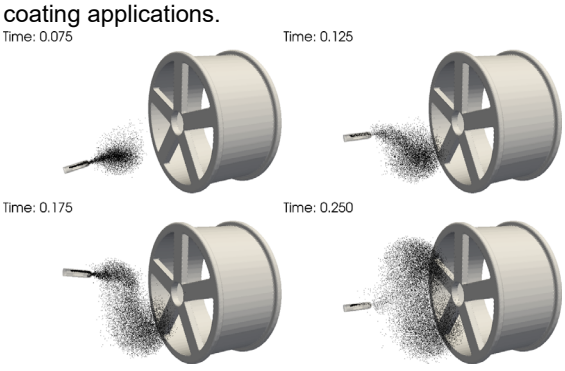


Figure 1: Snapshots from a simulation of a car rim being coated with a pistol with combined translational and rotational motion.

Literature:

[1] Boiger, G., 2016. Eulerian-LaGrangian model of particle laden flows and deposition effects in electro-static fields based on OpenFoam (2016). Int.Journal of Multiphysics; 10(2), pp. 177–194(8); DOI: 10.21152/1750-9548.10.2.177
[2] Siyahhan, Bercan; Boldrini, Marlon; Hauri, Samuel; Reinke, Nils; Boiger, Gernot Kurt, 2018. Procedure for experimental data assessment for numerical solver validation in the context of model-based prediction of powder coating patterns (2019). Int.Journal of Multiphysics. 12(4), pp. 373-392. DOI: 10.21152/1750-9548.12.4.373.

1.6 Thermophoretic Force on Suspended Particles

This project aims to study the potential of the thermophoretic force to collect particles from the atmosphere. For that we performed a computational study of the air flow through a collection chamber, including aerosol particles of diverse size and density and a vertical thermal gradient that will control the particle deposition in the collection region. A fluid dynamics model is built to describe the air flow, and the size dependent drag force of the air on the particle is also considered in full detail. The effect of the particle characteristics (size, thermal conductivity, density), air flux and turbulences on the deposition process is analyzed prior to perform the first tests in the physical device.

Contributors: A. Zubiaga, M. Boldrini, G. Boiger
Partner(s): myLab Elektronic Gmbh
Funding: Innosuisse
Duration: 2019–2020

Ambient air can have a sort of suspended or aerosol particles of different origin and sizes. They can be natural particles like pollen, dust or bacteria and viruses, but they can also have human origin like smog or soot. The sizes can range from a fraction of a millimeter down to a nanometer or below. Particulate matter is transported by the carrier gas until their deposition by buoyancy effects, if their size is large enough. Particles smaller than a micrometer, however, can remain an indefinite time suspended in the air. This increases the adverse effects that they can have on our health. Fine and ultrafine particulate matter can, for instance, enter deep in the lungs and in the cardiovascular system. One obvious way to control and limit their malignant effects is by collection for monitoring or other purposes.

In this project, we studied the potential of the thermophoretic force to collect particles from the atmosphere. We considered first the air flow through the collection chamber. The real geometry was used for the study and special attention was given to the minimization of the adverse effect of turbulences once a steady state flow is reached. Next, the transport of the particles in the air was considered. The particle size dependence of the fluid drag force was carefully taken into account. Finally, the thermophoretic force was introduced by adding an extra force on the particle dependent on a thermal gradient within the fluid. The new force has been shown to strongly enhance the deposition of the suspended particles.

The deposition range, however, depends on the thermal properties of the particles and the particle size is seen to affect it the strongest. Therefore, a non-uniform distribution of the particles within the chamber is predicted, with particles of larger size having larger deposition range. The conclusions of the study will be validated by tests done using the physical device.

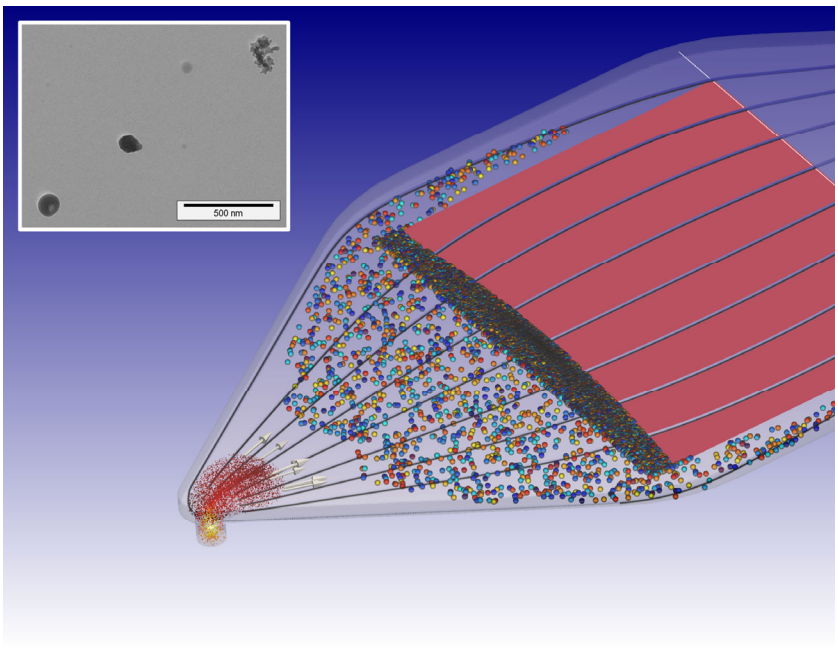


Figure: Computational Fluid Dynamics of a particle collection chamber. The Flow lines show the air flow direction. The point clouds represent the incoming particles' distribution and their velocity. The larger particles in the right represent a typical deposition pattern of the collected particles. The red square represents the collection region where the thermophoretic force is active. A large part of the particles is deposited in the few millimeters after entering the deposition range because of the thermophoretic force. The micrograph in the inset shows a typical size of the collected particles.

1.7 Three-Dimensional Powder Snow Avalanche Modeling

It is generally accepted that snow avalanche modeling can be divided into the flow of the heavy snow-core and the lighter powder-snow-cloud consisting of a mixture of ice-dust and air and that to a first order, the avalanche core is not influenced by the cloud. At SLF, the RAMMS software is available to model the avalanche snow-core by solving a system of hyperbolic equations on a 2D non-flat mountain-terrain. Recently, however, there has been interest in modeling the pressure distribution of the powder-snow-cloud ahead of the avalanche in order to estimate possible damages. Within this project, a 3D modeling of the powder-snow-cloud has been developed coupling to the RAMMS software.

Contributors: G. Sartoris
Partner(s): Dr. P. Bartelt, SLF
Funding: SLF
Duration: 2020

The modeling approach to solve this powder snow avalanche simulation has been chosen as follows. From the RAMMS software, we obtain the ground velocity consisting of a tangential component representing the avalanche slope velocity and a normal component determining the injection of powder snow into air. Air and powder snow are then considered as a 3D unsteady two-phase miscible and incompressible flow and their governing equations are solved with the freely available SESES software. It is assumed that this 3D powder-snow cloud flow does not couple back to the heavy snow-core solved by RAMMS.
Since simulations of the 2D dense core is a pretty fast task compared to 3D simulations of the powder cloud and since this latter has more stringent conditions on the mesh size, for simplicity we assume the 2D mesh is subordinate to the 3D one, i.e. along the mountain-terrain they agree and no space-interpolation is thus required for the setting of BCs. However, due to the simplicity of a time-interpolation, we do not assume both simulations use the same time discretization.
In summary, one first construct a 3D mesh for the powder cloud simulation. The bottom of this mesh which is aligned with the mountain-terrain also defines the 2D mesh for the dense core simulation which is run as first and independent task. This dense core simulation must write at constant time intervals, the velocity values which are used by the 3D powder cloud simulation, here done by running SESES, as time-dependent boundary conditions. For the solution of this time-dependent problem, we use the PISO-method as follow. At each time-step, one solves in a segregated manner for the mass fraction, velocity components and pressure in their linearized form. In practice, except for the pressure, these equations are assembled and solved by applying a Gauss-Seidel smoother and for the pressure, we use a few iterations of an algebraic multigrid solver. This single PISO-step is then repeated upon convergence of the pressure and afterwards one proceeds with the next time-step. An optimized strategy consists in performing just a single global iteration so that the convergence of the pressure must be controlled by an adaptive time-step selection. For the time-integration algorithm, several first, 2nd and third order algorithms are available. For a 2nd order method, an automatic error-based time-step selection is available, but this is generally inferior to a selection based on the CFL condition. We note here that due to missing dynamic terms, the discretized equations are not absolutely stable, hence a time-step limitation is always required. In the selection of the time-step, we are pretty flexible and it is up to the user to combine together adaptive time-step proposal, CFL condition and repetition of the current time-step due to slow convergence or even divergence.

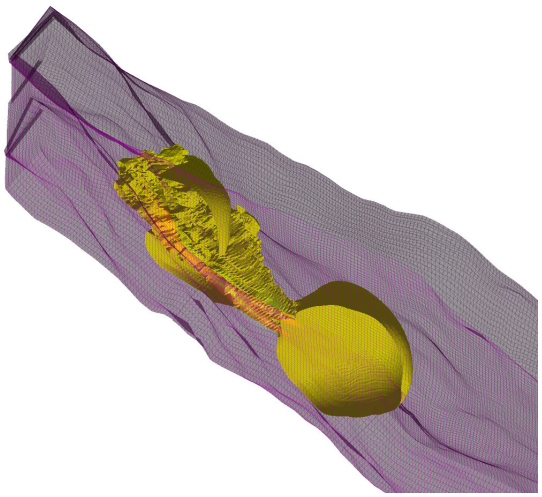


Figure: Simulated avalanche pressure front (view from below).

1.8 3D Pore Microstructures and Computer Simulation: Effective Permeabilities and Capillary Pressure during Drainage in Opalinus Clay

In the present work, model pore structures of Opalinus Clay were used to predict critical material properties related to gas transport. This topic is important, for example, because rocks such as Opalinus Clay are considered as potential host rocks for the disposal of radioactive waste. Thereby, these transport properties are of interest in connection with the production of gas, for example through corrosion of the waste containers, and its subsequent transport through the rock material surrounding the radioactive waste. The produced gas can be transported from the place of formation through the rock by various transport processes (e.g. diffusion, advection, two-phase flow etc.). Here, the focus is on the so-called two-phase transport where the produced gas displaces the water in the pores as a separate phase.

Contributors: L. Keller
Partner(s): Nagra, EURAD
Funding: Nagra, EURAD
Duration: 2020–2023

The 3D reconstruction of the pore space in Opalinus Clay is faced with the difficulty that high-resolution imaging methods reach their limits at the nanometer-sized pores in this material. Until now it has not been possible to image the whole pore space with pore sizes that span two orders of magnitude. Therefore, it has not been possible to predict the transport properties of this material with the help computer simulations that require 3D pore structures as input. Following the concept of self-similarity, a digital pore microstructure was constructed from a real but incomplete pore microstructure.

The constructed pore structure has the same pore size spectrum as measured in the laboratory. Computer simulations were used to predict capillary pressure curves during drainage, which also agree with laboratory data. It is predicted, that two-phase transport properties such as the evolution of effective permeability as well as capillary pressures during drainage depend both on transport directions, which should be considered for Opalinus Clay when assessing its suitability as host rock for nuclear waste. This directional dependence is controlled on the pore scale by a geometric anisotropy in the pore space.

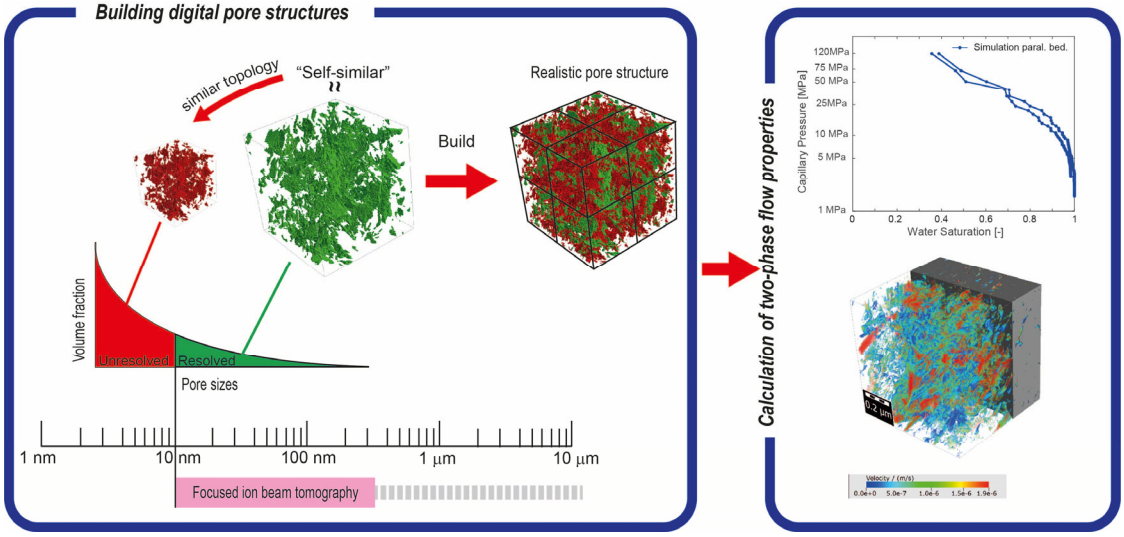


Figure 1: Graphical abstract related to the project.

1.9 Model Based Optimization of MIEC 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 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 MIEC 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 AG
Funding: SFOE
Duration: 2019–2022

For the next generation of solid oxide fuel cells (SOFC), 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 mixed ionic and electronic conductors (MIEC) like doped ceria and perovskite materials. 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.

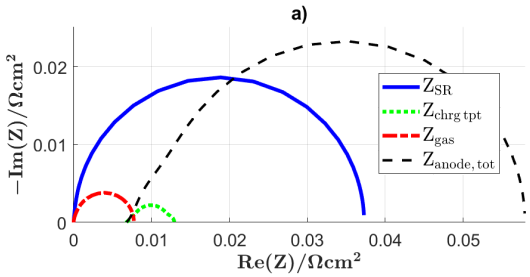


Fig. 1: Deconvolution of the simulated anode EIS-spectra: Z_{SR} = hydrogen oxidation surface reaction impedance, $Z_{chrg\ tpt}$ = charge carrier transport imped., Z_{gas} = gas imped., $Z_{anode,tot}$ = total anode imped.

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. 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 an appropriate interpretation 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.

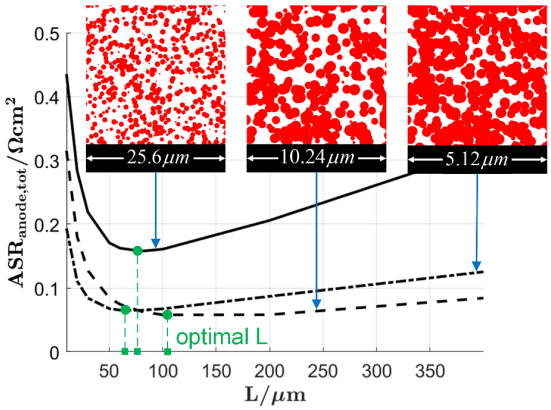


Fig. 2: Area specific resistance (ASR) of CGO-anodes for different microstructures as a function of the anode layer thickness L.

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.

1.10 Massive Simultaneous Cloud Computing (MSCC) for Data Driven Optimization of SOFC Electrodes

Digital Materials Design (DMD) enables a systematic model-based development and optimization of material systems and microstructures. Applying DMD for the development of Solid Oxide Fuel Cell (SOFC) electrodes results in a very large parameter space, which is very time-consuming with conventional computing approaches. The concept of Massive Simultaneous Cloud Computing (MSCC) allows the access of almost unlimited computational resources on demand. This drastic reduction of computation times enables to exploit the full potential of the DMD approach for the development of the next generation of SOFC electrodes.

Contributors: L. Holzer, P. Marmet, T. Hocker, G. Boiger, J. M. Brader, J. G. Grolig, H. Bausinger, A. Mai, M. Fingerle
Partner(s): Hexis AG, Math2Market GmbH, Kaleidosim Technologies AG
Funding: SFOE
Duration: 2019–2022

Digital Materials Design (DMD) is a modern approach for model-based materials optimization. In our DMD approach for optimization of SOFC electrodes, we combine stochastic microstructure modelling (i.e. simulating the effect of fabrication parameters on 3D morphologies), virtual testing of 3D microstructures and a multiphysics electrode model. This approach is capable to cover a very large parameter space, which then provides a good basis for data driven microstructure optimization.

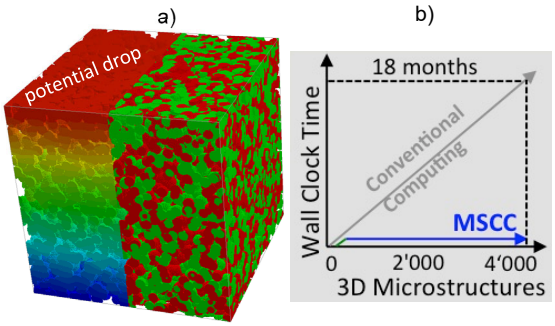


Figure 1: a) Virtual LST/CGO structure of an SOFC anode with computed potential drop, b) comparison of computation time with classical and MSCC approach.

However, very long computing times usually put strong limitations for extensive parameter sweeps. New concepts for Massive Simultaneous Cloud Computing (MSCC) were recently developed in a collaboration of ZHAW, Kaleidosim AG and Math2Market, which gives access to almost unlimited computational resources. Thousands of microstructures can be calculated in parallel. For a parameter study with e.g. 103–104 3D-scenarios as visualized in Fig. 1 b), the computing time for stochastic simulations and associated virtual testing typically takes more than 1 year with a classical approach on a local server. In contrast, with MSCC the computing time is almost independent from the number of parameter combinations and therefore it reduces to only 1–2 days.

An example of a relatively small parameter study is shown in Fig. 2, where the composition and porosity of an LST/CGO anode is varied.

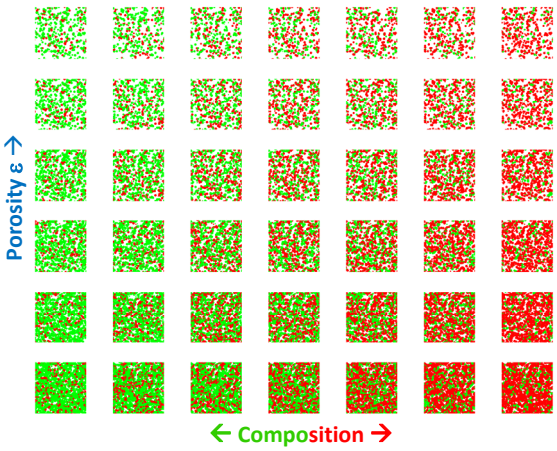


Figure 2: Example of a small parameter study for different porosities and compositions of an LST/CGO anode.

Combined 3D analyses and numerical simulations are used to characterize the virtual microstructures. Subsequently, the resulting effective properties are used as input for an electrode model, which provides the corresponding electrode performances in Fig. 3. The statistical analysis of these results leads to new design guidelines for electrodes with improved properties.

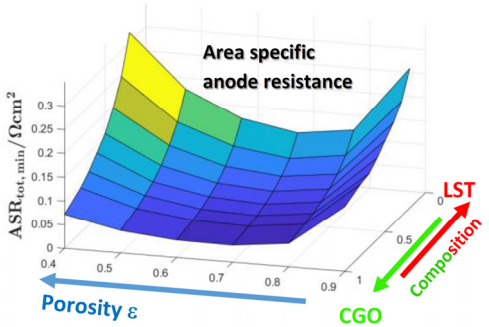


Figure 3: Resulting area specific anode resistance as a function of porosity and composition of an LST/CGO anode.

1.11 Model-Based Development of Ceramic Filters for Masks, Air Purifiers and Air Conditioning Systems

The Covid-19 pandemic showed the importance of appropriate filters to prevent infections and the need of more efficient and sustainable filter solutions. Ceramic filters have some significant advantages regarding their sterilizability and environmental compatibility. Therefore, ceramic filters are developed by an interdisciplinary team from ZHAW with a model-based approach. Thereby, the manufactured multiscale ceramic filter structure is virtually reconstructed. By simulating the pressure loss and filter efficiency of many virtual filter designs, design guidelines for an appropriate fabrication of the ceramic filters can be established.

Contributors: P. Marmet, L. Holzer, R. Kontic, M. Gorbar, D. Penner
Partner(s): Institute of Materials and Process Engineering (IMPE)
Funding: ZHAW
Duration: 2020–2021

In a project funded internally by the School of Engineering at the ZHAW Zurich University of Applied Sciences, a team of researchers is investigating the advantages of custom-made ceramic filters for aerosol filtration and virus removal. Ceramic filters have some significant advantages over standard filters, which are made from polymer fibre fleeces. The microstructure and geometry of the ceramic pore channels can be adjusted over a wide range as desired. Ceramics can be easily sterilised by simple heating, making multiple use and internal regeneration of a filter possible. Ceramics are uncritical in terms of environmental impact and recycling, while the massive use and uncontrolled waste of polymer microfibres represents a significant source of microplastics.
A team composed from researcher from the Institute of Materials and Process Engineering (IMPE) and from the Institute of Computational Physics (ICP) is using state-of-the-art modelling tools to create virtual models of the porous ceramics produced in the laboratory and to investigate the pressure loss, permeability and filtration performance of the materials. Based on microscopy imaging (Fig. 1 a, b) the microstructure is virtually reconstructed using GeoDict software. Thereby, the mesoscale and the microscale structures are captured in two different geometrical models (Fig. 1 b, c). In a first step, the permeability and the filter efficiency statistics of the microscale are determined. Flow- and filtration simulations (Fig. 2 a, b) are then performed on the mesoscale, where the microstructure is modelled as a porous media, calibrated by the permeability and filter efficiency statistics of the microscale simulation. Therewith, the permeability and the filter efficiency statistic can be determined for the complex multiscale structure. The results can then be compared with real measurements on individual ceramic samples.

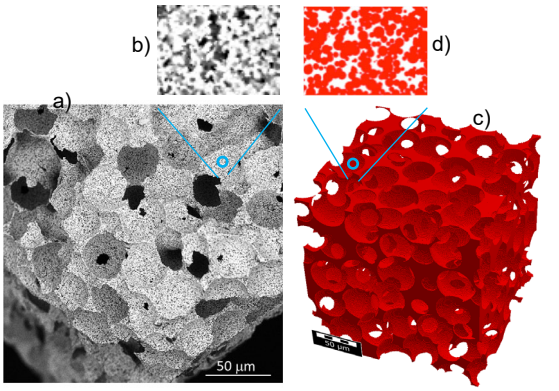


Figure 1: Microscopy image of the ceramic multiscale structure of the mesoscale a) and microscale b). Virtual reconstruction of the mesoscale c) and microscale of the multiscale filter structure using GeoDict.

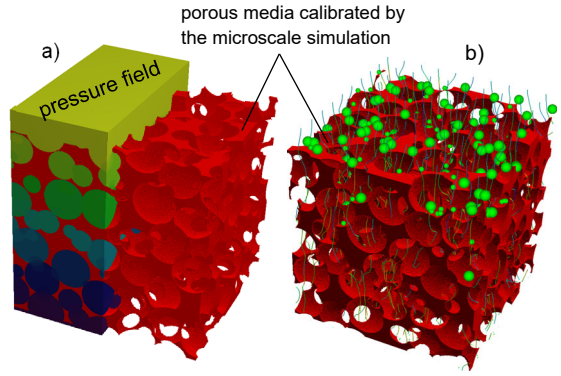


Figure 2: a) Simulation of the pressure drop in order to determine the permeability and b) filtration simulation to determine the filter efficiency using GeoDict. The microscale of the structure is respected by calibrating its permeability and filter efficiency statistics in the porous media of the mesoscale structure.

Once the model has been validated, laws can be derived from hundreds of virtually created structures, which in turn serve ceramic researchers as a design basis for their development. This reduces the number of laboratory tests required to develop optimised filter materials that already take into account the standard requirements for the filter materials as a set framework.

1.12 Efficient Thermal Model for the Precise Prediction of Welding Times for Infrared Welded Plastic Pipes

Infrared welding is an established method for the welding of plastic pipes, characterised by a high purity of the weld seam. In this process, the end faces of the pipes are heated by an infrared heater until a fusion front of a few mm thickness is formed. The tubes are then pressed together and cooled until the weld seam is solidified. To reduce the welding time to a minimum, an efficient thermal model was developed that precisely predicts the temperature curve in the weld seam during the entire welding process and thus provides the optimum time for unclamping the welded pipes.

Contributors: T. Hocker, D. Kempf
Partner(s): ZHAW-IMPE Teams C. Brändli and D. Penner, Georg Fischer Piping Systems
Financing: Innosuisse
Duration: 2018–2021

Models for the thermal simulation of the infrared welding process of plastic pipes are usually implemented in FE or CFD tools. In these models, the pipe ends to be welded, the IR heater and the surrounding air are discretized in 10^5–10^6 elements. For each time step, the energy balance must be solved in each element of both the pipe and the heater, and the mass and momentum balances must also be solved within the ambient air. The resulting simulation times in the range of several hours are too long to be used in the control software of the IR welding machine. For this purpose, a model is needed that simulates the T-progression in the weld seam during the entire welding process in only a few seconds.
Therefore, in cooperation with Georg Fischer Piping Systems, a new model was developed that divides the pipe ends to be welded into only five segments, see Figure 1.

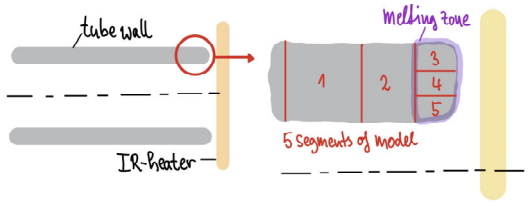


Fig. 1: The model is based on the discretisation of the pipe ends into only five segments.

In each of these five segments, an energy balance is solved which takes into account all heat flows by conduction, natural convection, forced convection and thermal radiation. The phase transitions during melting and subsequent recrystallisation of the tube ends are represented by a model that is calibrated using DSC data.
Figure 2 shows the typical behaviour of the weld temperatures simulated in the model and the corresponding measurement data determined in real welding tests. Details such as the T-plateau during recrystallisation are also correctly predicted.

Figure 3 shows the savings potential for the welding time resulting from the precise prediction of the optimal unclamping time of the welded pipes. The model has now been implemented in Java and is to be used in the future in the GF welding machines.

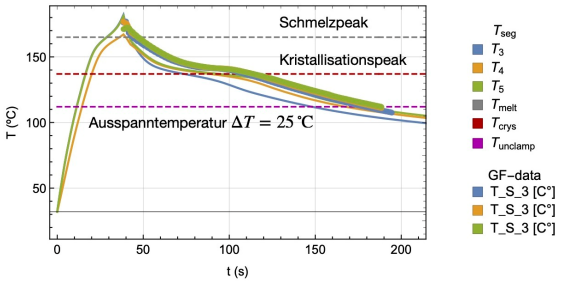


Fig. 2: Validation of the weld temperatures predicted by the model via welding tests with T-sensors placed in the weld seam.

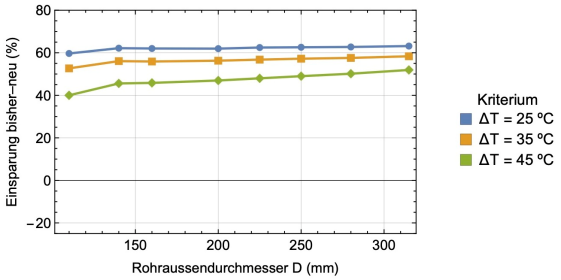


Fig. 3: Shortening of the welding time of plastic pipes when using the newly developed model, which simulates the behaviour of the weld seam temperatures and thus predicts the optimum unclamping time of the welded pipes.

1.13 Development of a New Type of IR Heating Concept for Contactless Welding of Plastic Pipes

If the purity of the weld seams is central when joining plastic pipes to form entire piping systems, infrared welding technology is often used. Here, the pipes are first heated at their end faces by an infrared heater using radiant heat until the plastic melts, and then pressed together. The plastic melts combine, and cooling produces a material bond. The introduction of a new type of IR heating concept is intended to shorten the heating process and thus the entire welding process.

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

The previous heating system consists of a solid plate with a high thermal mass and is characterized by a homogeneous surface temperature. However, this heating technology, which has proven itself over decades, has two decisive disadvantages: the heating is very sluggish, and the large-area heat emission can lead to uneven melting of the tube ends. Therefore, a new IR heating concept was developed in cooperation with GF, with which the heating can be operated dynamically, zone-based and adaptively. The new heater consists of several fine heating wires on a ceramic support, which enable a targeted and economical heating process. This concept was developed using thermal-fluid computer models and verified with the aid of a designated welding test rig, see Fig. 1.

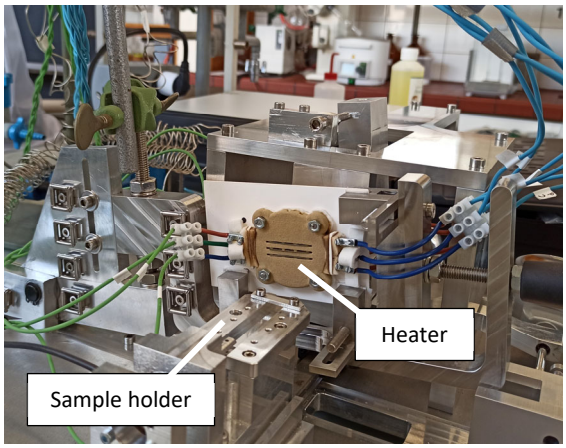


Fig. 1: Test bench for welding plastic samples.

With the new IR heater, it was shown that the used cuboid plastic specimens could be optimally welded. Their melt fronts had a very uniform shape along the wall thickness, see Fig. 2.

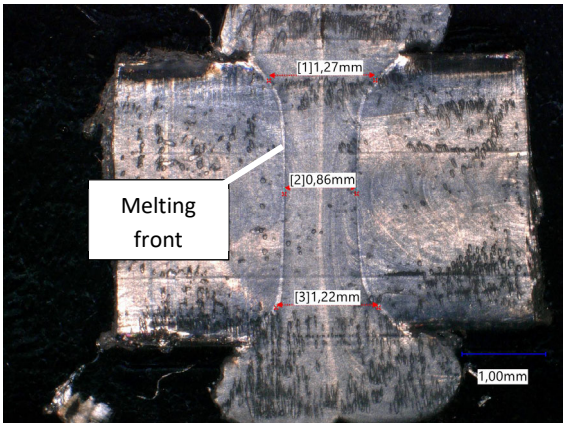


Fig. 2: Microtome section of a weld seam under a light microscope.

However, the step from a small prototype heater to a large prototype heater close to the application represents another hurdle. To get closer to this goal, a combination of theoretical and experimental methods is used. For example, undesirable, inhomogeneous temperature distributions on the heating wire surface due to thermally conductive contact points between the heating wire and the support are optimized via CFD models, see Fig. 3.

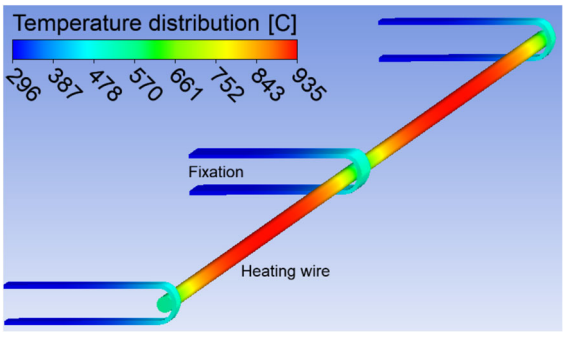


Fig. 3: Temperature distribution on the heating wire surface.

1.14 Effective Thermal Conductivity and CFD Implementation of a Heat Pipe

Due to their construction, heat pipes have a tremendous effective heat conductivity and are now indispensable in electronic devices such as smartphones or laptops. However, they also have great potential for other technical applications. It is therefore essential to know their heat transport properties precisely and to realize an accurate, simple implementation in CFD models.

Contributors: S. Ehrat, T. Hocker
Partner(s): Wöhner GmbH
Funding: Master's Thesis
Duration: 2020–2021

Figure 1 shows the test setup for measuring heat pipes. The heat pipe at the right edge of the picture is heated by a temperature-controlled heating cartridge inside a copper block. At the opposite end of the heat pipe is an aluminium heat sink, which dissipates the heat to the environment. This is done either purely by natural convection and heat radiation or by switching on the fan on the left edge of the picture by means of forced convection. The temperature is logged at eight different points using type K thermocouples, see Figure 1.
In order to ensure the best possible heat transfer between the copper block and the heat pipe as well as between the heat pipe and the cooling fins, all contact surfaces are covered with thermal paste and braced against each other. The temperature sensors are attached to the surface with aluminium adhesive tape. In addition, there is a little thermal paste under the adhesive tape to minimise the influence of air pockets.

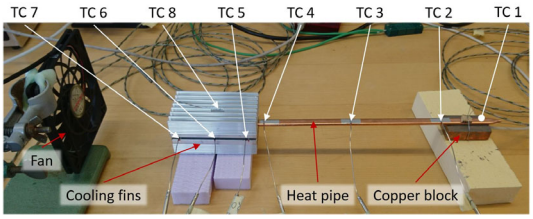


Fig. 1: Test setup for measuring the eff. thermal conductivity of a heat pipe; copper block with heating cartridge (right), heat pipe (centre), cooling fins (left), fan for forced convection (left); designations of the T-measuring points above the diagram.

The CFD implementation of the test setup is realised in ANSYS CFX. To simplify the simulation environment, the heat source is defined as a boundary temperature in the copper block. The heat pipe itself is divided into two areas, a copper shell and an inner space for the working fluid. This division reflects the real structure of a heat pipe and is therefore close to reality.
Figure 2 shows the result of a steady-state simulation with forced convection and a heating temperature of 100°C. The heat pipe exhibits a high temperature over the entire length of the pipe. The heat pipe has a temperature drop of 56°C over the entire length and induces a heat flow of 43.6 watts.

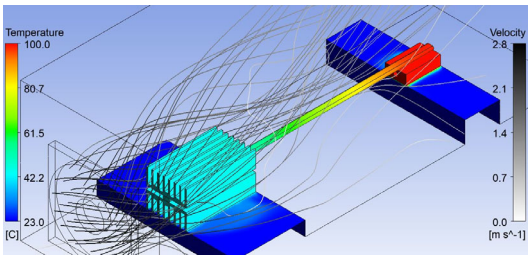


Fig. 2: Representation of the CFD simulation results with 100°C heating temperature and forced convection generated by a PC fan. The surface temperatures are shown in colour and the air flow in black and white.

Figure 3 shows the results of the validation of the CFD model for the operation of the heat pipe with and without fan. The temperatures at the measuring points TC 1 and TC 8 show a good match between measurement and simulation. Therefore, the thermal conductivity used, which is the only fit parameter in the CFD model, can be considered validated. The lower temperature of TC 8 with forced convection indicates a dry-out of the heat pipe in the area of the copper block, which leads to a reduction of the effective thermal conductivity.
When heat is removed by natural convection and radiation, the working fluid inside the heat pipe reaches an effective thermal conductivity of 50'000 W/(m*K). This conductivity is reduced to a value of 4,440 W/(m*K) in the case of forced convection, because the heat pipe reaches its performance limit.

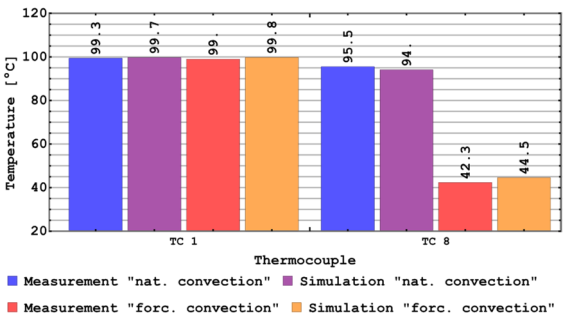


Fig. 3: Validation of the CFD model for 100°C heating temperature and 23°C room temperature with and without fan operation. TC 1 indicates the measuring point on the heater, TC 8 that on the cooling fins.

1.15 Simulation of the Envelope Temperature of a Hot Air Balloon

This project aims to develop a detailed physical model of a hot air balloon that describes its motion based on real weather data. In a previous project, the basis for the simulation was developed and a test flight was conducted to generate data to validate the model. In this project, a hot air balloon model will be implemented in Berkeley Madonna to replicate the test flight and compare it to measured envelope temperatures.

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

The physical model of a hot air balloon is implemented in Berkeley Madonna and is based on mass, energy and momentum balances. Through an iterative procedure, the model is extended with balloon-specific features such as parachute, burner control and gas consumption. To solve the balances, input variables are needed. In order to compare the results with the measured variables of the test run, the input variables must match the conditions prevailing during the test. The data concerning the balloon and the loading are provided by Stefan Zeberli. The required weather data are obtained from the NCAR Weather Data Archive. Since the resolution of the weather data is too coarse, a flight in x- and y-direction cannot be reproduced in a reasonable way. Therefore, the focus is on the simulation of the hot air and envelope temperature and the comparison of the measured data.

During the aforementioned test run, the "HB-QZT Homebuilt" hopper was measured. Ambient and envelope temperature as well as relative humidity were recorded at 80m, 600m, 880m and 1100m above ground. In order to obtain data for the comparison, the minimum, maximum and average temperatures are determined from the thermal image over the height of the balloon envelope.

Figure 1 shows the measured as well as the simulated temperatures of the final model plotted over height. It can be easily seen that the envelope temperature depends on the ambient temperature. The model gives good results as the simulated temperature is between the minimum and average temperature and correctly predicts the decrease of the envelope temperature with increasing altitude. A subsequent sensitivity analysis showed that the difference between hot air in the balloon and envelope temperature is 20 K–30 K. The model provides a good basis to predict the temperature decrease with increasing altitude. The model offers a good foundation for investigating how the different parameters are related to each other and react, for example, to changes in environmental influences. These results are equally interesting for the aviation study program as for hot air balloon pilots.

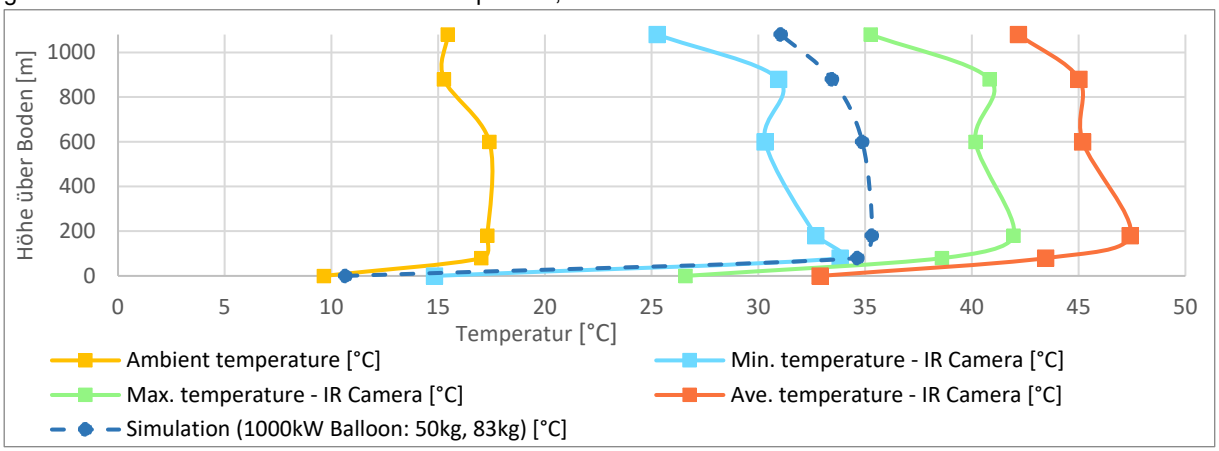


Fig. 1 Comparison of the ambient temperature measured with a temperature sensor in yellow, the minimum/maximum temperature measured with the IR camera in blue and orange respectively, the average value in green and the simulated envelope temperature in dark blue. For the simulation, a burner power of 1'000 kW, a mass of 50 kg and a load of 83 kg is used.

1.16 Lifetime of Gold Contact Components under Adhesive Wear Loading

Adhesive wear problem of gold contact layers affects the service time of crucial components in the electronic circuit of the costly Braille Display instruments. Numerical model is implemented to support automated experimental tests conducted by project partners. The goal is to develop a reliable prediction of mechanical failure and estimated lifetime of Braille display instruments.

Contributors: Y. Safa, U. Mescheder, S. Kipke
Partner(s): Helptech GmbH, Furtwangen University HFU, Germany
Funding: Interreg
Duration: 2019–2021

Innovative solutions are being implemented to improve an independent-life quality of 250 million blinds and vision-impaired persons around the world. Specifically, Braille Display uses a series of raised dots to represent letters and numbers allowing a blind to read a text. A more affordable tool is called Refreshable Braille Display, it allows blinds to interface with their computers. Tactile information is transmitted to blind user by continuously raising and lowering different combinations of pins as he moves the cursor on the screen Fig. 1.

Fig. 1: Braille models developed by German partner Helptech GmbH.

A mechanism of electroactive polymer is used to correctly raise each dot to an updated height, so it can be read. Electro-activation stimulates a compressive stress in a PDMS membrane that raises, by buckling to a specified height. At ICP, we initiated exchange with partners from HFU Furtwangen Germany on a computational prediction of the buckling amplitude of PDMS membrane for given voltage signals Fig. 2.

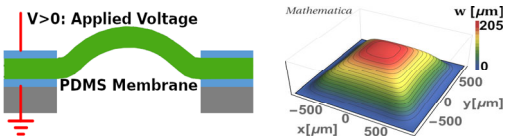
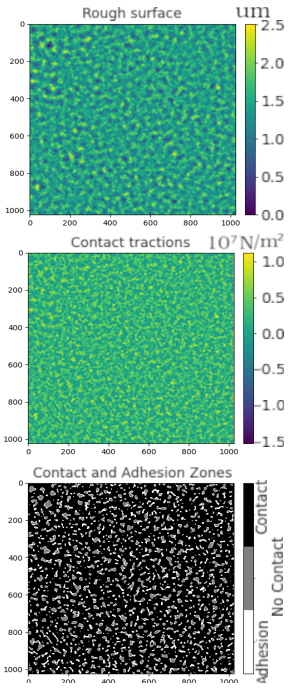


Fig. 2: computational prediction of PDMS buckle under voltage.

Later, in the framework of Interreg project, a wider collaboration has been conducted on the mechanical reliability of Braille button model of the German partner Helptech. A frictional contact occurs between two conductive gold layers between the braille button and an underneath PCB board. When a blind user applies repeatedly an inclined force to the button, an adhesive wear is initiated on the gold surface affecting its functional integrity. Designing a long service life of Braille tool makes it an economic solution for wider blinds community. This requires a reliable predictive capability of adhesive wear gold contact. An automated experimental test has been established at HFU by the group of Prof. Mescheder. The designed system applies repetitive loading using a stepper motor controlled by Arduino. Microscopic visual investigation was performed. Wear on the gold contact surface is produced at a threshold of loading cycles.
Such experiments offer a complementary with computational modeling at ICP ZHAW for a perspective of a model-based button's design. Numerical simulations were conducted considering different parameters such as surface roughness, loading rate, and force inclination from the experimental setup. In a first step, modeling was based on a global approach. An elasto-plastic dynamic friction contact problem is solved on the whole contact surface using an open-source finite element package [1]. A local contact area of high shear-stress was identified. In the second step, a local approach was applied using Boundary Integral Method to solve the adhesive contact problem in aforementioned local area. A random-height rough surface was generated corresponding to measured surface amplitudes. The local contact problem was solved in the Fourier domain of the generated surface spectrum allowing two-order of magnitude faster than traditional FEM [2]. Traction, contact, and adhesive zones, Fig. 3, were obtained in the local contact surface.



Source:

[1] Y. Renard, K. Poulios. GetFEM: https://hal.archives-ouvertes.fr/hal-02532422
[2] Frérot et al.Tamaas: Journal of Open Source Software, 5 (51), 2121, https://doi.org/10.21105/joss.0212

1.17 Enhanced Peridynamics Capability in Mechanical Faillure Prediction

Computational Peridynamics has shown a new capability to predict damage in wide scale of industrial components ranging from mesoscopic devices to large wind turbine. An interesting contribution to the ongoing research is presented by a straightforward and accurate formulation of the stress-strain fields. This enhances Peridynamics applicability in computational fracture mechanics of layered structures like wind power turbine, sensors and actuators.

Contributors: A. S. Fallah, Y. Safa
Partner(s): Brunel University London
Funding: Interreg, SNSF Exchange Programme
Duration: 2018–2020

Damage in layered structures is studied using peridynamics with capability to address the problem adequately for the necessary level of sophistication. Through the use of fracture energy alone the non-local model is capable of capturing intra- and inter-laminar fractures. This has a major impact in design applications where dynamic pulse and impact loads of all natures (accidental, service, etc.) are to be considered. The resulting outcomes may therefore be utilised in design of layered structure like lightweight blades and wings [1].

In the work presented in the report, the non-local stress tensor is derived through implementation of the bond-based formulation of peridynamics that uses an idealised model of interaction between points as bonds. Fig. 1. The method is sufficiently general and can be implemented to study stress states in problems containing stress concentration, singularity, or discontinuities. Two case studies are presented, to study stress concentration around a circular hole in a square plate and conventionally singular stress fields in the vicinity of a sharp crack tip. The peridynamic stress tensor is compared with finite element approximations and available analytical solutions. It is shown that peridynamics is capable of capturing both shear and direct stresses and the results obtained correlate well with those obtained using analytical solutions and finite element approximations. A built-in MATLAB code is developed and used to construct a 2D peridynamic grid and subsequently approximate the solution of the peridynamic equation of motion. The stress tensor is then obtained using the tensorial product of bond force projections for bonds that geometrically pass through the point. To evaluate the accuracy of the predicted stresses near a crack tip, the J-integral value is computed using both a direct contour approximation and the equivalent domain integral method. In the formulation of the contour approximation, bond forces are used directly while the proposed peridynamic stress tensor is used for the domain method. The J-integral values computed are compared with those obtained by the commercial finite element package Abaqus 2018. The comparison provides an indication on the accurate prediction of the state of stress near the crack tip Fig. 2. This accomplishment is shown in the Journal publication [2].

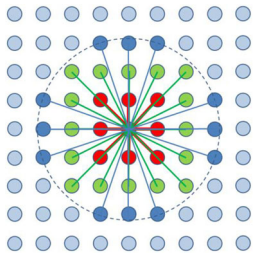


Fig. 1: connectivity in the peridynamic pseudo-lattice (longer bonds are weaker).

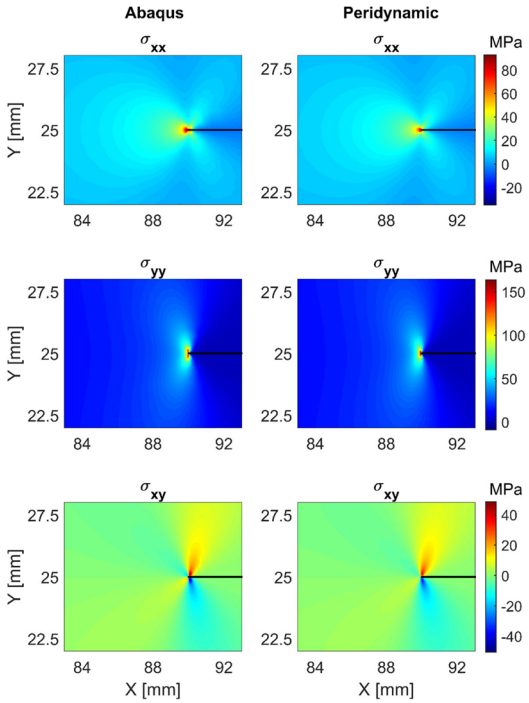


Fig 2: Comparison of the stresses simulated in a plate with a slit crack using Abaqus finite element with those using bond-based peridynamics

Source:

[1] Fallah A. S., Ghajari M., Safa. Y. Computational modelling of dynamic delamination in morphing composite blades and wings. Int. of Multiphysics Volume 13 Number 4 2019
[2] Fallah A. S., Giannakeas I., Mella R., Wenman M., Safa Y., Bahai H. On the computational derivation of bond-based peridynamic stress tensor. Journal of Peridynamics and Nonlocal Modeling 2, 352–378 (2020).

1.18 Coupling XFEM and Peridynamics for Brittle Fracture Simulation – Part I: Feasibility and Effectiveness

In order to make use of computational resources most efficiently and reduce analysis time while retaining accuracy, an efficient algorithm is devised to allow combining peridynamics and XFEM. While both methods are well established, the combination of the two is rather novel and opens the door to investigation of interesting features in multi-scale study of wave propagation and fracture.

Contributors: I. N. Giannakeas, T. K. Papathanasiou, A. S. Fallah, H. Bahai
Partner(s): Brunel University London
Duration: 2016–2019

A peridynamics (PD)–extended finite element method (XFEM) coupling strategy for the simulation of fracture in brittle materials is presented.
To maximise computational efficiency, the nonlocal interactions are restricted to small PD domains in the vicinity of crack tips. The proposed methodology combines the PD patch in the neighbourhood of the crack tip with the XFEM that captures the crack body geometry outside the domain of the localised PD grid. The feasibility and effectiveness of the proposed method on a Mode I crack opening problem are examined.

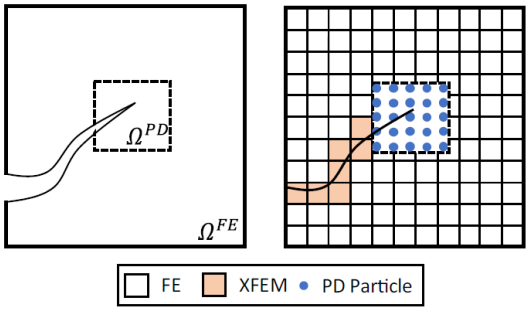


Fig. 1: Schematic of the PD-XFEM coupling.

The method proposed allows for accurate simulation of crack propagation including branching without the need to use extraneous parameters as T-stress.

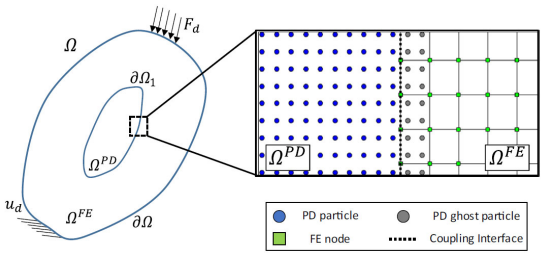


Fig. 2: Introduction of ghost particles and discretization near the coupling interface

Furthermore, through introduction of ghost particles at interface, it is possible to capture wave propagation across the interface with minimum spurious reflection.

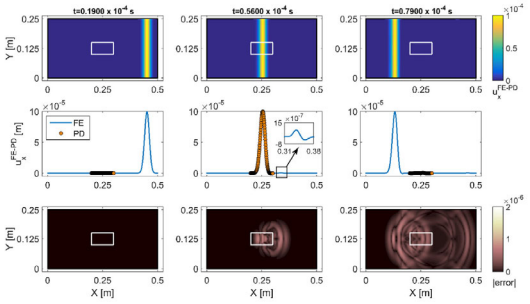


Fig. 3: Pulse propagation in the coupled FE–PD model captured at three-time instants.

As it is observed in a 2D problem the error is less than one percent i.e. merely 1% of the wave is erroneously reflected from the interface between the two domains.
The effectiveness and feasibility of the coupling scheme proposed and implemented is evaluated through a series of examples. Two simple problems are solved first to evaluate the coupling under static and dynamic conditions. Both fracture propagation under static loading and wave propagation due to pulse loading are studied and the efficiency of the method proposed is quantified through a comparison of the computational cost.

Source:

Giannakeas, I. N., Papathanasiou, T. K., Fallah, A. S. and Bahai, H., 2020. Coupling XFEM and peridynamics for brittle fracture simulation—part I: feasibility and effectiveness. Computational Mechanics, 66(1), pp. 103-122.

1.19 Coupling XFEM and Peridynamics for Brittle Fracture Simulation – Part II: Adaptive Relocation Strategy

In order to make use of computational resources most efficiently and reduce analysis cost while maintaining accuracy, the efficient algorithm devised to allow combining peridynamics and XFEM is implemented and used to study problems of solid mechanics. A cost-effective model is thus ensured to be used in investigation of exciting features as multi-scale study of wave propagation and fracture.

Contributors: I. N. Giannakeas, T. K. Papathanasiou, A. S. Fallah, H. Bahai
Partner(s): Brunel University London
Duration: 2016–2019

The peridynamics (PD)–extended finite element method (XFEM) coupling strategy for the simulation of fracture in brittle materials presented in the previous work is implemented through an adaptive relocation strategy. To maximise computational efficiency, the nonlocal interactions are restricted to small PD domains in the vicinity of crack tips and are allowed to expand and contract adaptively throughout the analysis. The adaptive relocation strategy allows for this expansion and contraction of the patch to ensure computational efficiency and accuracy. The feasibility and effectiveness of the proposed method on a Mode I crack opening problem are examined.

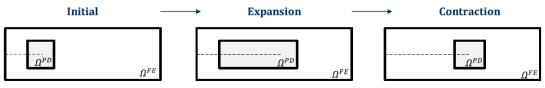


Fig. 1: Schematic illustration of the two-step process for the adaptive relocation of the PD domain.

The method proposed allows for accurate simulation of crack propagation including branching and is demonstrated to render multiple PD subdomains possible.

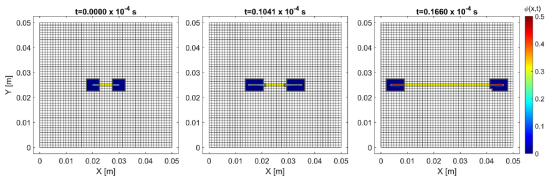


Fig. 2: Adaptive relocation of multiple PD patches for a single crack in the medium.

The segment of a crack in the XFEM subdomain is signified using the level set method which allows jumps in the displacement field across the crack. Limiting the nonlocal area where the PD theory is applied can lead to improvement of the overall computational cost of the solution. The numerical results presented here indicate significant savings in terms of memory requirements and CPU time.

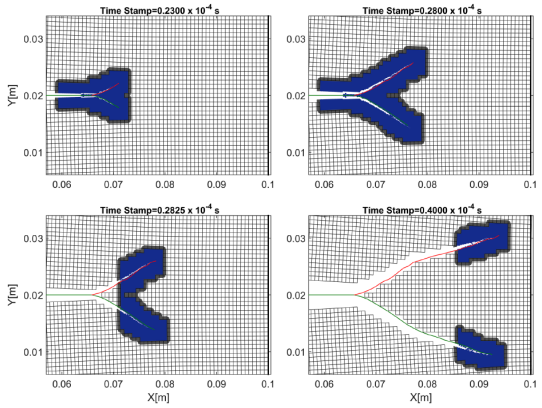


Fig. 3: Branching and relocation strategy.

The effectiveness and feasibility of the coupling scheme proposed is evaluated through a series of examples. The expansion/contraction procedure allows to first capture the crack pattern and then relocate as required, with the ability of splitting in case the initial crack branches. Furthermore, in static problems where the final crack length is unknown, the expansion step can be repeated as many times as necessary until convergence is achieved.

Source:

Giannakeas, I. N., Papathanasiou, T. K., Fallah, A. S. and Bahai, H., 2020. Coupling XFEM and peridynamics for brittle fracture simulation—part I: feasibility and effectiveness. Computational Mechanics, 66(1), pp.103-122.
Giannakeas, I. N., Papathanasiou, T. K., Fallah, A. S. and Bahai, H., 2020. Coupling XFEM and Peridynamics for brittle fracture simulation: part II—adaptive relocation strategy. Computational Mechanics, 66(3), pp. 683-705.

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 microstructures 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 in Lausanne (hydrogen generation) and Universität Ulm (virtual microstructures).


D. Bernhardsgrütter


R. Herrendörfer


G. Mourouga


R. Schärer


J. Schumacher


J. Wlodarczyk

2.1 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 are being developed at ICP, allowing for the efficient simulation of important physicochemical processes within an electrochemical cell.

Contributors: R. P. Schärer, G. Mourouga, J. Wlodarczyk, J. O. Schumacher
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 primary goals of the SONAR project [1] is the identification 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.

The 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.

Our 0-D U-I-SoC model allows the prediction of the cell performance with respect to the state of charge (SoC) of the battery and the electric current density. The model takes into account the crucial activation and concentration overpotentials at the electrode surface, as well as the electro-osmotic effect leading to volume changes due to the transfer of solvent between the half-cells. Thanks to the dimensional reduction, the model can be evaluated in real-time. The model serves as a solid basis for the development of more comprehensive macroscopic cell models.

Figure 1 shows a contour plot of the cell voltage and power density as a function of the state of charge and current density as predicted by the 0-D U-I-SoC model. Preliminary validation studies with the MV/TMATEMPO system show promising agreement between the model and polarization experiments. A first version of the model, which is under active development, has already been published as open-source software [2].

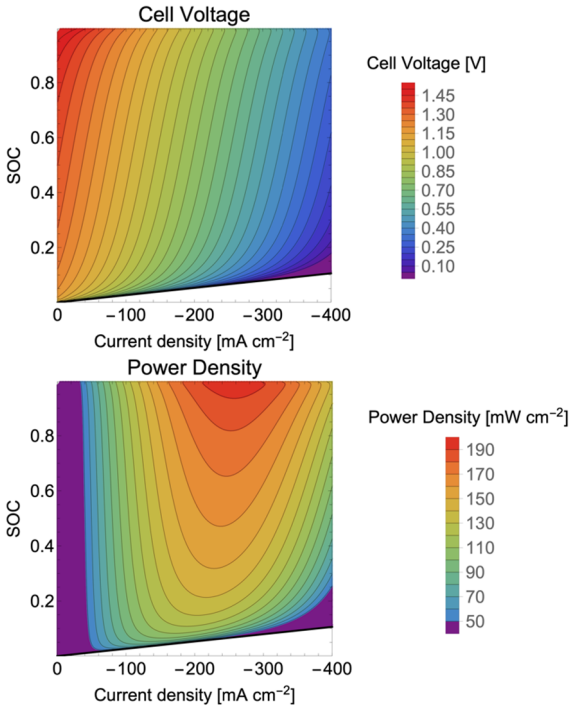


Figure 1: Predicted cell voltage (above) and power density (below) of an electrochemical cell using the 0-D U-I-SoC model.

Literature:

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

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

In this project, we develop computational solutions of proton exchange membrane fuel cells (PEMFCs) for transport applications. To prepare the marketing of models and simulation services we have created a web page with customer-oriented product descriptions. Furthermore, we are working on a business plan.

Contributors: R. Herrendörfer, J. O. Schumacher
Partner(s): Paul Scherrer Institute (PSI)
Funding: SFOE
Duration: 2019–2021

Proton 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 participate in the international value chain of fuel cell powered transport applications. We prepare to market computational solutions that are tailored to the needs of companies and research institutes with a focus on membrane electrode assemblies (MEAs) and single cell PEMFCs.

In collaboration with the Paul Scherrer Institute, we have developed a model for simulating evaporation inside a gas diffusion layer (GDL) in contact with a gas flow channel (GFC) (Figure 1). In our 2-D isotropic and isothermal along-the-channel model (Figure 1b), evaporation is limited by convection in the GFC at low gas velocities and mainly by through-plane diffusion inside the GDL at high gas velocities (Figure 3), which is demonstrated by normalizing the results for different temperatures and carrier gas types (Figure 2). Non-isothermal effects are shown to become important for high evaporation rates at high temperatures, gas velocities and diffusion coefficients. Comparison to the 3-D model shows that the contribution of evaporation below the rib cannot be neglected.

To further improve our models, we have implemented a new boundary description of liquid water flux at the interface between a gas diffusion layer and gas flow channel in a time-dependent 1-D model including droplet formation, growth and detachment.

To prepare the marketing of models and simulation services we have created a web page with customer-oriented product descriptions. The web page addresses partners from industry and academia. We are currently working on a first version of a business plan. To further increase the visibility of our products, we have provided access to our open-source 1-D master MEA model via a Github software repository (https://github.com/Isomorph-Electrochemical-Cells/PEMFC-1DMMM).

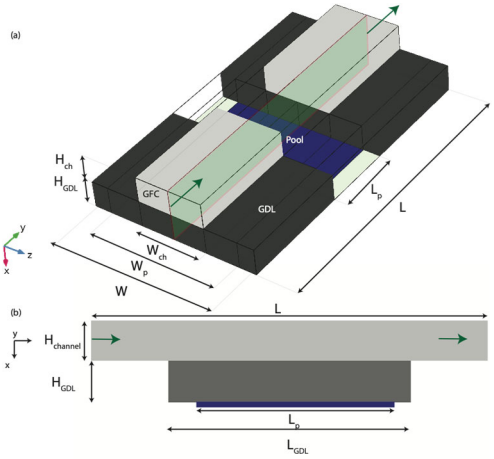


Figure 1: Setup of (a) 3-D and (b) 2-D model of evaporation in a GDL in contact with a gas flow channel.

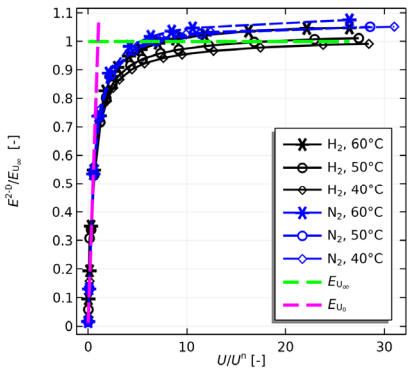


Figure 2: Normalized evaporation rates as a function of normalized gas velocities. Normalization is based on convective and diffusive transport limitations at low and high gas velocities, respectively.

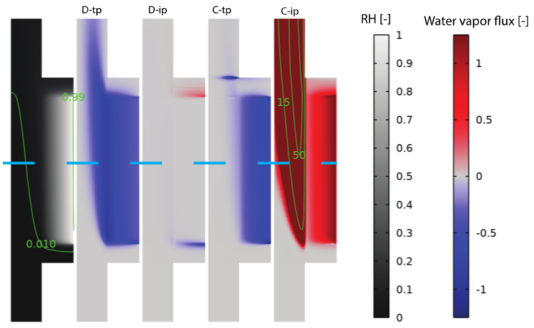


Figure 3: 2-D model results at high U/U^n: relative humidity RH (left) and diffusive (D) and convective (C) through-plane (tp) and in-plane (ip) normalized water vapor flux.

2.3 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 analyze the local sensitivity of the simulation results to changes in operating conditions and model parameterizations.

Contributors: R. Herrendörfer, J. O. Schumacher
Partner(s): SCCER 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 [1-2].

At the ICP, we have developed a 3-D, macro-homogeneous, non-isothermal two-phase model to investigate the dominant heat and water transport processes during evaporative cooling and humidification (Figure 1). We solve for the transport equations of gas, liquid water, dissolved water, heat, electrons and protons.

In our reference model of a test cell, which was adapted to the experimental setup at PSI in terms of operating conditions and material properties [1], evaporation takes place in the hydrophilic line of the GDL primarily in contact with the gas flow and, to a smaller degree, in contact with the hydrophobic part of the GDL (Figure 2b). Most of the generated water vapor is transported to the outlet of the anode gas flow channel and only a small fraction of water vapor diffuses to cathode side (Figure 2a-b). 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 2c). Furthermore, the role of the water evaporation transfer coefficient is evaluated with respect to water vapor transport limitations.

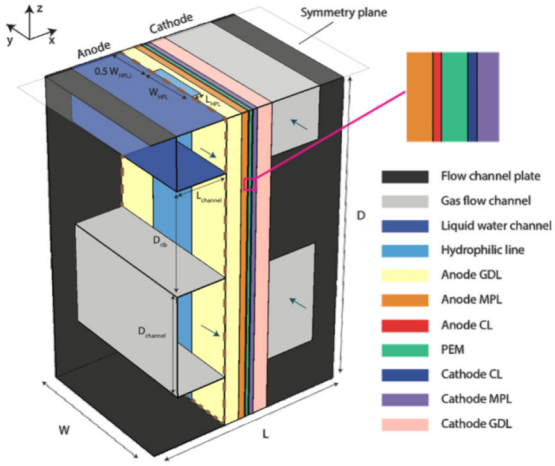


Figure 1: 3-D model setup. Anode flow field with one gas and liquid water channel, respectively, a cathode flow field with two gas channels. The membrane electrode assembly includes the hydrophobic anode gas diffusion layer with one hydrophilic line.

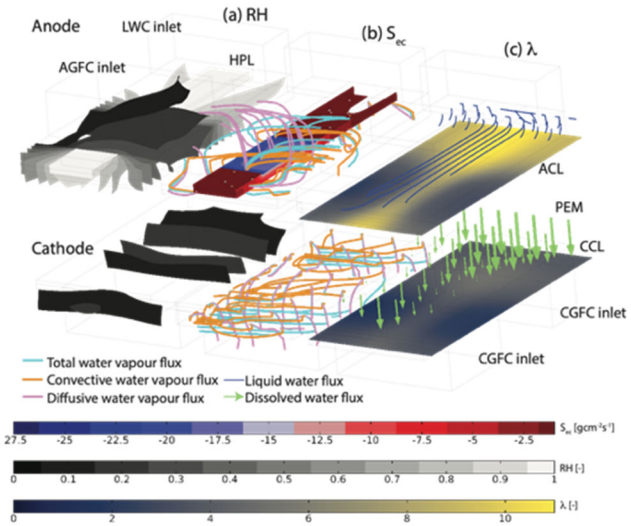


Figure 2: Water management at anode side (top) and cathode side (bottom). **(a)** Relative humidity (RH). **(b)** Evaporation rate and streamlines of water vapor flux. **(c)** Streamlines of liquid water flux and dissolved water flux, water content dissolved in the membrane (λ).

References:

[1] Cochet, M., A. Forner-Cuenca, V. Manzi, M. Siegwart, D. Scheuble, and P. Boillat. Fuel Cells 18 (5): 619–26, 2018
[2] Cochet, M., A. Forner-Cuenca, V. Manzi, M. Siegwart, D. Scheuble, and P. Boillat. JEC, 67 (8): 084518, 2020

2.4 A New Thermodynamical Framework for Improved Aqueous Flow Battery Modelling

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 thermodynamics of aqueous electrolytes, in order to predict more accurately the performance and lifetime of these batteries. The ICP collaborates in this regard with the FlowCamp consortium, a research and training project funded by the European Union's Marie Sklodowska-Curie funding 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, R. P. Schärer, E. Baudrin, J. O. Schumacher, T. J. Schmidt
Partner(s): ETH Zurich, Univ. Grenoble-Alpes, JenaBatteries GmbH, Univ. Picardie
Funding: European Commission, Horizon 2020, Marie Skłodowska-Curie Training Networks
Duration: 2018–2021

The limitation of many flow battery models stems from the use of species concentrations for voltage or transport predictions. Formulating a battery model based on species concentrations implies making the dilute solution hypothesis, where the electrolyte would remain in a hypothetical ideal state and species would mix without interactions:

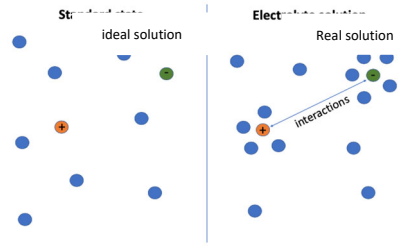


Figure 1: Ideal solution (left): interactions are neglected / Real solution (right): electrostatic and short-range interactions affect electrolyte properties.

Interactions are captured by correcting concentrations with an activity coefficient γ, which is solute-dependent and needs to be measured experimentally. The interactions affecting the freezing point of the solution, it is possible to calculate the activity coefficient γ by measuring the freezing point as a function of composition.

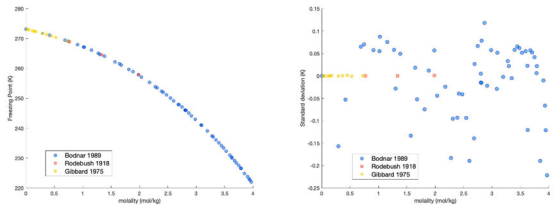


Figure 2: Freezing point of Calcium dichloride as a function of composition and standard deviation from least-square regression.

Activity coefficients also affect the osmotic transfer of water across the ion-exchange membrane during battery operation.

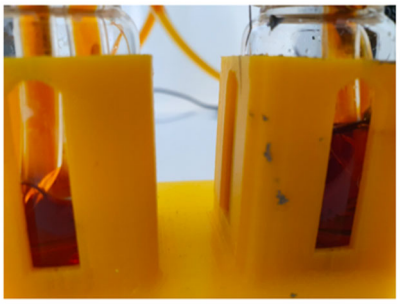


Figure 3: Picture of positive (left) and negative (right) reservoirs after cycling. The height was initially equal.

Through the Nernst law, it is also possible to make more accurate cell voltage predictions when parameterizing calculations with activities rather than concentrations.
The aim of our work in the FlowCamp project is to provide a thermodynamically consistent approach to the simulation of aqueous redox-flow batteries, including operating conditions, transport processes and thermal management.

[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.

2.5 Microscale Modelling Study of Coupling Mass Transport with Convective Flow in Porous Electrodes for the Application in Redox 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 Marie Skłodowska-Curie program) and the SONAR project [2].

Contributors: J. K. Włodarczyk, G. Mourouga, R. P. Schärer, J. O. Schumacher
Partner(s): Fraunhofer ICT (Germany), LRSC Amiens (France), among others
Funding: EU, Horizon 2020, Marie Skłodowska-Curie Actions
Duration: 2018–2021

Electrochemical flow cells for energy storage such as redox flow batteries, operate at high current densities to meet the specific charge-discharge characteristics. In order to increase the allowable current density limit during cell cycling, the use of porous electrodes with high specific surface area is required. 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 [1] and SONAR [2] projects, we addressed the aforementioned issues in a systematic study by means of numerical models. At the current stage we aimed at a possibly simplest representation of a porous cell by means of periodic electrode element (Figure 1). It consists of an electrode matrix (solid phase) indicated in white and void, where the liquid electrolyte is flowing. On the left- and right-hand sides of this cell, we implemented a periodic boundary condition for fluid velocity and on the top and bottom edges, a symmetry boundary condition. We assumed a no-slip boundary condition on the matrix walls. By changing the radii of the fibres, we were able to alter the electrode porosity. For given pressure differentials across the cell (flow from the left to the right) we solved for the Navier-Stokes equations for laminar flow, probed the volumetric flow rate and thus we were able to calculate the permeability K of the material. We then normalized K in order to compare this model to a study published by Yazdchi et al. [3] which is presented in Figure 2. With a good agreement in the laminar flow regime (low pressure differentials) we now intend to couple the convective flow with chemical species transport and electrochemical reaction to gain a better view on the reactant distribution problem on the pore-size scale, which is one of the limiting factors in flow batteries operation.

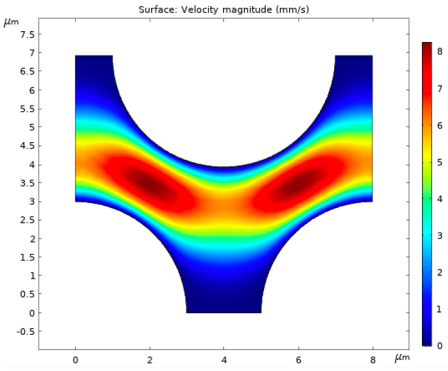


Figure 1. Geometry of the proposed periodic cell used to study combined macroscopic flow and mass transport phenomena (liquid velocity magnitude contours are superimposed). White semi-circles are the cross-section of periodic electrode matrix (fibres).

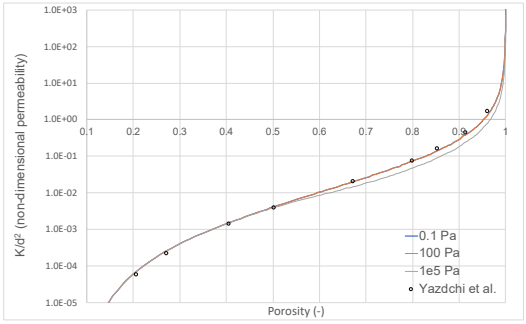


Figure 2. Validation of the model using a study of Yazdchi et al. [3] as a benchmark.

[1] Project website: https://www.flowcamp-project.eu/
[2] Project website: https://www.sonar-redox.eu/
[3] K. Yazdchi, S. Srivastava, and S. Luding, "Microstructural effects on the permeability of periodic fibrous porous media," International Journal of Multiphase Flow, vol. 37, no. 8, pp. 956–966, Oct. 2011, doi: 10.1016/j.ijmultiphaseflow.2011.05.003.

3 Organic Electronics and Photovoltaics

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

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

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


M. Auer


M. Battaglia

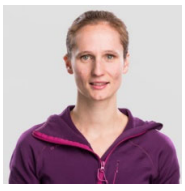

E. Comi


F. Ebadi Garjan


M. Jazbinsek


C. Kirsch


G. Kissling


E. Knapp


K. Pernstich


U. Puc


M. Regnat


B. Ruhstaller


A. Schiller


W. Tress


S. Züfle

3.1 Silicon Solar Cell Parameter Estimation by a Convolutional Neural Network Trained on Simulated Data

Simulations support the optimization process of solar cells by predicting important cell performance metrics. For this purpose, we trained a convolutional neural network (CNN) with simulated electroluminescence (EL) images and then validated the predicted parameters with an EL measurement of a silicon solar cell with an intentionally induced defect.

Contributors: M. Battaglia, E. Comi, E. Knapp, B. Ruhstaller
Partner(s): Fluxim AG
Funding: Innosuisse
Duration: 2019–2021

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 in which the top and bottom electrodes are reduced to 2D domains and coupled with a local IV curve.
In this project, we want to find out whether manual fitting of cell parameters can be replaced by machine learning. For this purpose, we trained a CNN with a training set of 150’000 EL images, which were simulated in Laoss. The successful training of neural networks requires a large amount of data. For this reason, synthetic data from simulations are ideally suited for this purpose, as they can be generated in large quantities including extensive parameter variations. With the simulated training data, however, it must be ensured that the properties of a real measured cell are carefully modelled to ensure the transferability of the CNN for an accurate prediction of the cell parameters. The simulated cell consisted of a shunt, an active area and several well conducting metal fingers. The desired parameters from these three subdomains (internal resistance, sheet resistance and dark saturation current) were randomized for the training of the CNN.
Figure 1 a) shows the EL measurement of a shunted silicon cell and the simulated EL image is depicted in Figure 1 b). The measured EL image was then used to estimate the cell parameters of the three subdomains. The cell was subsequently resimulated with the extracted parameters and compared to the measurement. This is shown in Figure 1 c) using a horizontal cross-section in the region of the shunt, comparing the junction voltage. These results show that it is possible to extract the cell parameters with a CNN trained with synthetic image data.

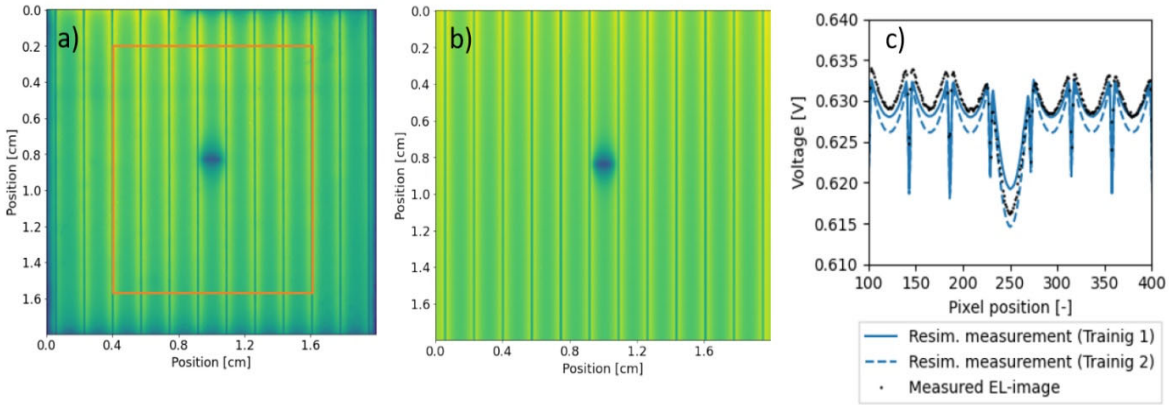


Figure 1: Measured (a) and with Laoss simulated (b) EL image of a silicon solar cell with an intentionally induced shunt and metal fingers (vertical lines). A horizontal cross-section of the resulting junction voltage, when the device is resimulated with the parameters extracted from the CNN, trained with two different training sets is shown in c).

3.2 Experimental Validation of an Electro-Thermal Small-Signal Model for Large-Area Perovskite Solar Cells

To improve defect detection in perovskite solar cells, we apply an oscillating small-signal voltage to the devices and measure the temperature response with an infrared camera. A comparison with simulations helps to determine the origin of the defects and allows to quantify them.

Contributors: E. Comi, E. Knapp, B. Ruhstaller
Partner(s): Fluxim AG, Empa, Solaronix S.A.
Funding: Master's Thesis, Innosuisse
Duration: 2020–2021

Perovskite thin-film solar cells have attracted a lot of attention in recent years due to rapidly increasing efficiencies. The upscaling of this technology from small laboratory cells to large-area devices without compromising efficiency and stability, however, is still a challenge to be solved for successful commercialization.
Printing perovskite modules entirely by screen printing is an important step towards industrialisation, which is why we are carrying out an electro-thermal analysis of screen-printed carbon-based hole transporter-free perovskite dual cells with various interconnection widths. For this purpose, we used the FEM (Finite Element Method) software Laoss that supports the upscaling process from small- to large-area devices by solving for the potential and temperature distribution in 2D top and bottom electrode domains, which are coupled by a vertical 1D coupling law. In this master's thesis we presented electrical and thermal DC and AC simulations of dual cells and a reference cell without an interconnection and compared the simulation results with measurements.

The software can not only perform electrical and thermal steady-state simulations but also determine the influence of non-ideal electrodes in the frequency domain. Therefore, we also introduced the small-signal dark lock-in thermography (SS-DLIT) method to measure and simulate electro-thermal effects in perovskite solar cells in the dark with high accuracy thanks to the use of a small, periodic voltage modulation at a chosen offset voltage. This adapted DLIT method can be simulated with the thermal AC module in Laoss and allows the investigation and quantification of various defects, such as shunts or the interconnection quality of perovskite solar cell modules.
Figure 1 shows the amplitude of a SS-DLIT simulation of a perovskite dual cell with built-in shunts on the left. The SS-DLIT measurement is shown for comparison in right the image.

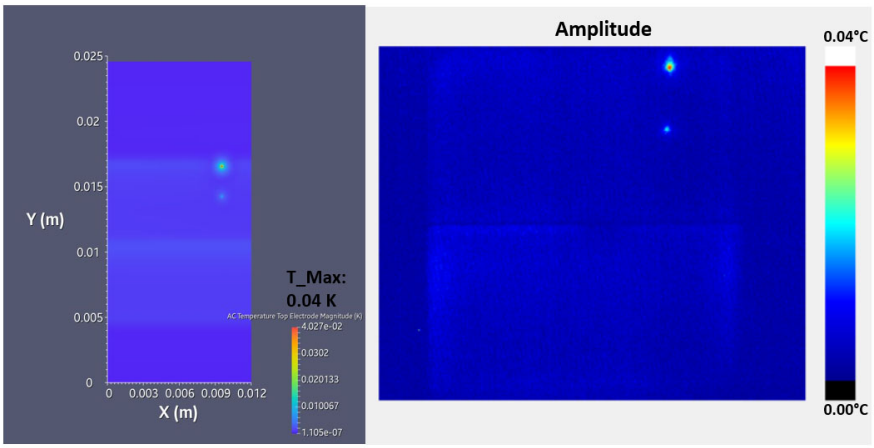


Figure 1: Simulated SS-DLIT amplitude image of a perovskite dual cell showing a temperature increase at the shunts and the interconnection. The SS-DLIT amplitude measurement is shown on the right, displaying two hot spots in the upper cell as well, which cause losses during operation.

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

In this Swiss-German collaboration the 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, will be investigated. 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, S. Züfle, B. Ruhstaller
Partner(s): Prof. Wolfgang Brütting, Universität Augsburg
Funding: SNSF / DFG
Duration: 2020–2023

In this project we study 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 the established 1D drift-diffusion approach [1] and combine it with a novel 3D Master equation model [2] as well as compare it with 0D analytical formulas.
Figure 1 shows exciton and charge transfer processes that can occur, in both, organic light-emitting diodes (OLEDs) and organic solar cells.

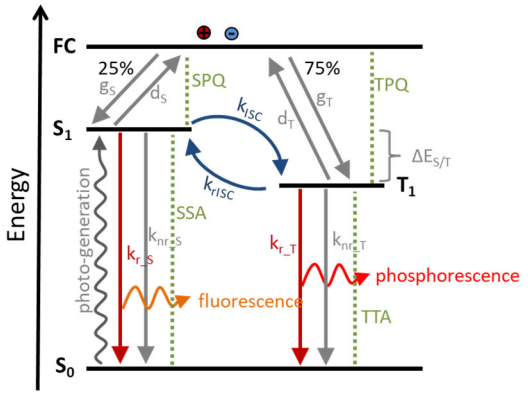


Figure 1: General exciton and charge transfer processes. FC denotes the free carriers, S1 the singlet, T1 the triplet exciton, and S0 the ground state.

In a first part of this project we are using advanced simulations to better understand the influence of different exciton quenching processes, such as triplet-polaron quenching (TPQ) and triplet-triplet annihilation (TTA), on the efficiency of an OLED device for different emitter concentrations.
Figure 2 shows the excited states lifetime τ* data (directly proportional to the efficiency of an OLED) of a green phosphorescent OLED stack with an emitter concentration of 2% and 16%. From fitting of the data with 0D analytical formulas the underlying exciton quenching mechanism for the reduction of the excited states lifetime at increasing current densities is either TPQ or TTA.

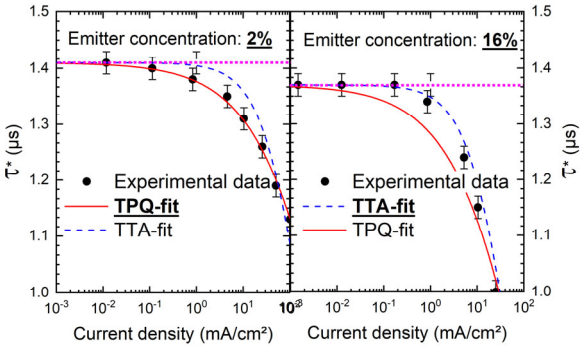


Figure 2: Excited states lifetime data for increasing current densities of an OLED with an emitter concentration of 2% (left) and 16% (right). Fit to experimental data clearly shows that the decrease at higher currents is better described by TPQ for the case with 2%, and by TTA for the case with 16%.

With the combination of 3D Master equation and 1D drift-diffusion approach it should be possible to set up an electro-optical model that is able to reproduce both cases with one set of parameters and thus allows us to understand the exciton processes in this OLED better.
In the end it should be possible to predict the optimum emitter concentration for the highest efficiency and the lowest efficiency roll-off at high current densities.

References:

[1] Simulation software Setfos, www.fluxim.com/setfos-intro (April 2021)
[2] Zeder et al. „Coupled 3D Master Equation and 1D Drift-Diffusion Approach for Advanced OLED Modeling“. *Journal of the Society for Information Display* 28, Nr. 5 (2020): 440–49. https://doi.org/10.1002/jsid.903

3.4 New Tools for Characterizing Quantum-Dot Displays

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

Contributors: K. P. Pernstich, C. Kirsch, B. Ruhstaller
Partner(s): Fluxim AG
Funding: Innosuisse
Duration: 2021–2024

In newer LCD screens, the backlight no longer consists of a light source that emits white light, e.g. a white LED, but of a combination of a blue LED and a quantum dot (QD) film. The QD film absorbs the blue light and emits it in one of the other primary colors, i.e. red or green, resulting in a more brilliant color reproduction.

In addition to LCD screens, organic light-emitting diodes (OLEDs) have also established themselves as a market-ready technology. Among certain other advantages, OLED screens offer better image quality than LCDs. Recent developments now seek to leverage the advantages of both technologies and use QD films together with blue OLEDs as a new technology. Figure 1 illustrates this new trend in the display industry.

To benefit from this new technology, Korean and Swiss partner organizations have joined forces in this international Innosuisse project. The Swiss partner company Fluxim is expanding its products in the areas of measuring instruments and simulation software. The Korean partner company is developing a process to encapsulate the quantum dots and thus make them more durable. At the Institute of Computational Physics, we are involved in the further development of a model to calculate the propagation of light as a function of its polarization direction and also in the development of a measuring device for the detailed investigation of QD films and QD OLED films. The academic partners in Korea are working on the fabrication and optimization of blue OLEDs and on an inkjet printing process to selectively deposit the QD films over individual OLEDs. Figure 2 shows the structure of such an OLED pixel with QD layer.

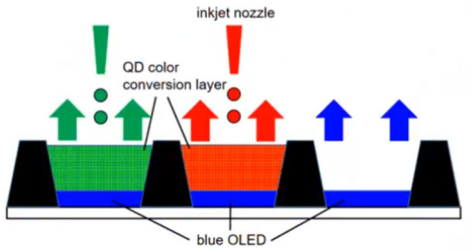


Fig. 2: Schematic representation of an OLED pixel with a QD film..

The project has only recently begun and the first QD films are already on their way to Switzerland to be characterized by us.

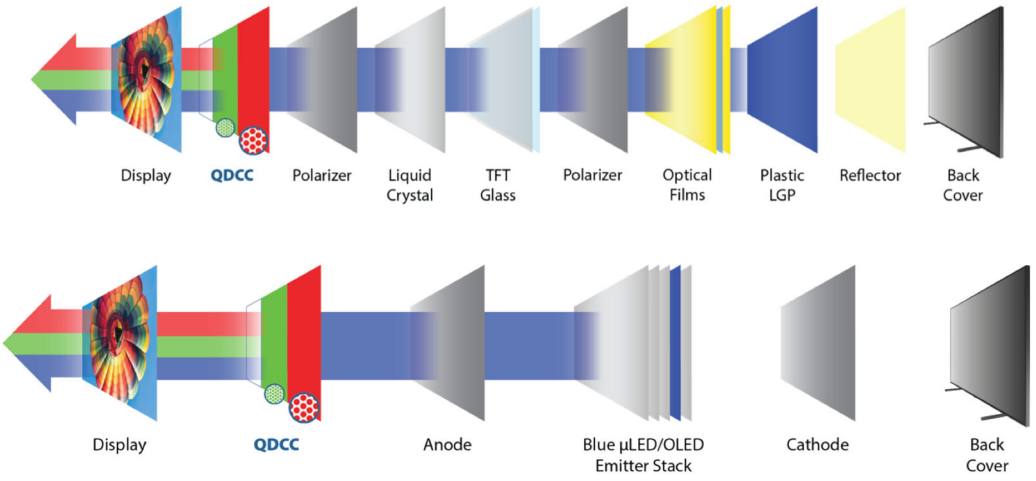


Fig. 1: QD film in an LCD screen (top) and in an OLED screen (bottom). Source: Nanosys Inc..

3.5 Investigating Charge Transport in Organic Semiconductors with Electrochemical Methods and Modelling

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

Contributors: G. Kissling, E. Knapp, K. Pernstich
Partner(s): Fluxim AG
Funding: 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.

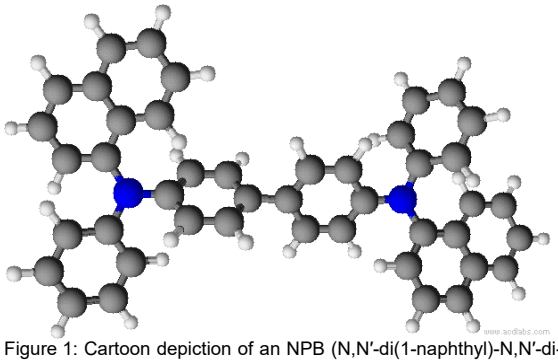


Figure 1: Cartoon depiction of an NPB (N,N′-di(1-naphthyl)-N,N′-diphenyl-(1,1′-biphenyl)-4,4′-diamine) molecule which is used for OLED fabrication.

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 1**. 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 2a and b show electrochemical measurements obtained on NPB thin films. **Figure 2a** shows a typical cyclic voltammogram. The signal at 0.8 V originates from the valence band of the organic semiconductor. The smaller signal at around 0.1 V can be associated with the reverse reaction. The inset, **Figure 2b,** shows electrochemical impedance spectra that were measured at the potentials indicated by the colored symbols in **Figure 2a**. The impedance spectra help us understand the electrochemical behavior of the thin film semiconductors in more detail.

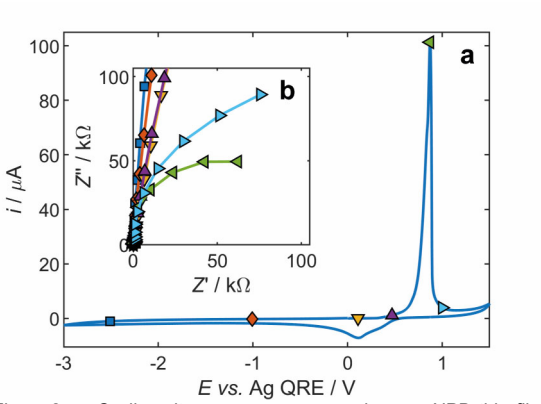


Figure 2: **a**: Cyclic voltammogram measured on an NPB thin film. The impedance spectra shown in **b** were obtained at different potentials marked by symbols in **a**.

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.

3.6 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.

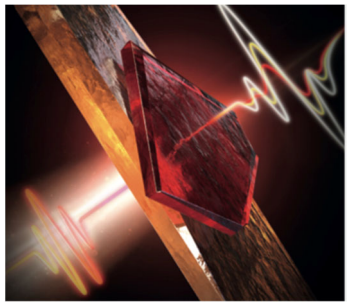


Fig 1.: In this project, organic electro-optic crystals and their combinations are used for ultra-broadband THz-wave generation. Illustration: DOI: 10.1002/adfm.201707195

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).

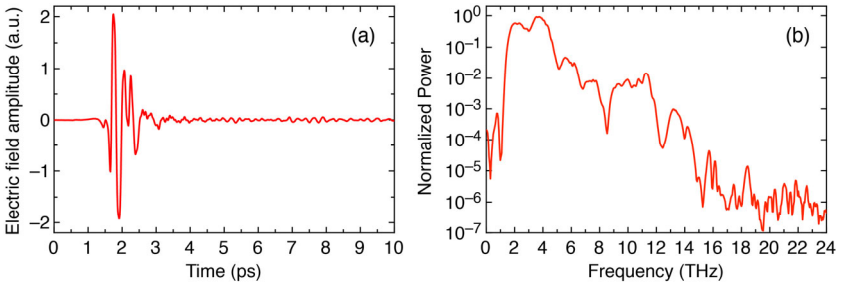


Fig 2.: THz time-domain signal (a) and the corresponding power spectrum (b) of the THz setup based on organic crystals: The aim of this project is to reduce the modulation of the signal seen in (b) to achieve a flat spectral response over the whole frequency range.

3.7 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: U. Puc, V. Michel, M. Jazbinsek
Partner(s): Rainbow Photonics AG
Funding: Innosuisse, Master's Thesis
Duration: 2019–2021

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 developed ultra-broadband THz time-domain spectrometer shows 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. [1] 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.

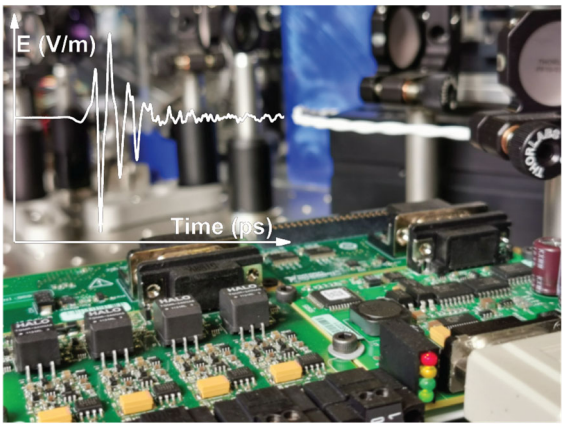


Fig 1: The developed time-domain THz spectroscopy system is based on measuring the electric field with a sub-picosecond resolution. THz electric fields with frequency components up to 20 THz have been generated and detected. This is possible due to integration and optimization of photonics and electronics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

Literature:

[1] Puc, U.; Bach, T.; Günter, P.; Zgonik, M.; Jazbinsek, M., 2021. Ultra-Broadband and High-Dynamic-Range THz Time- Domain Spectroscopy System Based on Organic Crystal Emitter and Detector in Transmission and Reflection Geometry. Advanced Photonics Research 2, 2000098, DOI: 10.1002/adpr.202000098.

4 Sensors and Measuring Systems

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

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

Our core competence is the development of new sensors and measurement methods in biomedical engineering. In particular, we are experienced in skin science and technology: artificial skin models, computer simulations, development of new sensors, etc.

We benefit from the state-of-the-art infrastructure of the Optoelectronic Research Laboratory (OLAB) that allows the development of demanding prototypes.


A. Bachmann


M. Bonmarin


D. Fehr


D. Kempf


R. Hagen


M. Schmid


F. Spano


S. Weber


A. Witzig

4.1 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: M. Bonmarin
Partner(s): Adolphe Merkle Institute of the University of Fribourg
Funding: Innosuisse, Foundations
Duration: since 2012

Nanoparticles are tiny particles which size range from 1 to 100nm (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. 1: 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

4.2 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.

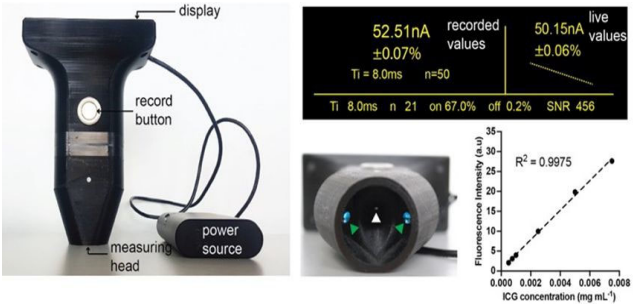


Fig. 1: Left: Autarkic hand tool with battery. Top right: Display. Middle: Measurement opening. Bottom right: Measured value versus actual marker concentration.

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 shrunk 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.

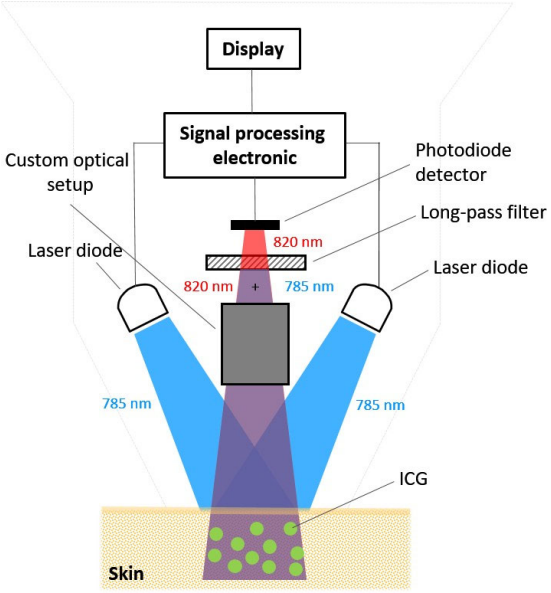


Fig. 2: Optical and electronic components of the handheld device.

Literature:

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

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

Contributors: F. Spano, D. Fehr, M. Bonmarin, J. Blunschi, R. Sassenburg.
Duration: 2019–2021

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].

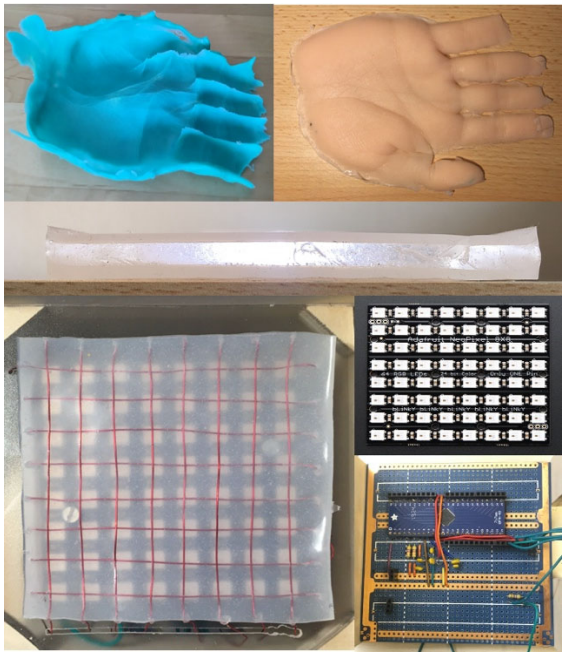


Fig. 1: Illustrations of the different fabrication phases: material development and real palm replica; Multi-layered skin model with the capacitive-sensing grid and the LED matrix, controlled by the prototyped electronics.

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.

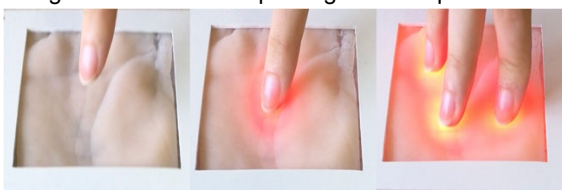


Fig. 2: Illustrations of the tactile capabilities of the artificial skin model implementing the real human texture and mechanical properties in addition to the change of colours in function of the applied force and the multipoint capacitive sensitivity.

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.

4.4 Measurement Technology for Decentralized Energy Systems

The ICP Thermolab has been continuously expanded in recent years and now offers comprehensive analysis options for building energy systems. One of the specialties of the ICP Termolab is that the measurement technology is usually supported by simulations. In addition, in many cases it is worthwhile to systematically store the data in a cloud application – often referred to as a "digital twin". This can be useful for further processing of the data and, for example, enable remote access for maintenance work or the application of digitally supported analysis methods.

Contributors: A. Witzig, T. Hocker, D. Kempf, S. Ehrat
Partner(s): Naef Energietechnik AG, Mivune AG, GreenTEG AG
Funding: Innosuisse
Duration: 2020–2022

The ICP Thermolab covers a large variety of of temperature sensors and general thermal analysis equipment. In addition, the laboratory has now been extended with systems for measuring heat flow in pipelines or heat transport in walls and windows. Furthermore, comprehensive investigation facilities for determining the moisture content in air and in building materials have been established.

While in the past mainly industrial applications were addressed, the focus has now been widened and also covers building energy systems. In close cooperation with practitioners, current research questions cover the optimization of control strategies, the development and improvement of products, and the comprehensive analysis of the building physics in specific construction projects.

Measurements with modern sensor technology are by nature a hardware topic. In the context of the digital twin, a connection to the Internet and suitable data processing is another prerequisite in order to provide a useful application. Finally – and this is a specialty of the ICP Thermolab – a direct link is created to the simulation of physical processes. In most cases, several coupled physical effects must be understood and taken into account in the measurement setup. For example, the heat transfer coefficient (often called U-value in the building sector) depends on the moisture content of the building materials. Consequently, in addition to the heat transport and heat storage capacity of the walls, the water content and moisture transport are also of interest in a detailed investigation. Oftentimes, the system boundaries are also at issue: In most cases, the immediate surroundings of the sensor system have to be included in the analysis. The temporal course also plays a significant role: what effect does it have if the sun shines on the outer wall during a U-value measurement? How can the concrete structure of a building be used to optimize comfort and reduce primary energy consumption? How can underfloor heating contribute to the regeneration of geothermal probes?

The combination between measurement technology and physics simulation often requires a model reduction on the side of numerical analysis. Thus, the amount of data and the complexity of the measurement system can be reduced.

Fig. 1: Measuring system for determining the heat transfer coefficient (U-value). The installation was carried out for test purposes on the "TK" building on the campus of the School of Engineering of ZHAW. The figure shows a temperature measurement on the outer wall. It is important to note that wall surface temperature and air temperature are recorded separately.

Fig. 2: On the inside of the wall, in the heated zone of the building, surface temperature and air temperature are also measured. In addition, the heat flow and air humidity are recorded. The data is transmitted wirelessly to a server via a base station and processed in a cloud application.

Fig. 3: The ultrasonic flowmeter determines the velocity of heating water in a pipe, without having to cut any it open. Together with two temperature measuring points, it is then possible to determine the heat flow transported from one part of the system to another.

4.5 Artificial Intelligence (AI) Heat Pump Controller

Many buildings are now heated with heat pumps, often in combination with a geothermal heat probe. The heat pump extracts heat from the ground at a low temperature level to always ensure comfortable room temperature. Even more important than with fossil heating systems is the design of the heating system and the correct commissioning. This work has the goal to shown how a neural network can be trained by means of simulations in such a way that no parameter settings in the heat pump controller must be adjusted during commissioning. During the training phase, the AI heat pump controller has learned many different scenarios with different buildings, variable weather, and stochastic user behavior. As a result, the heat pump is operated in an energy-optimized manner without having to know the building during installation.

Contributors: L. Joos, S. Pfyffer, A. Witzig, D. Kempf, V. Ziebart (IAMP), N. Schmid (IAMP)
Partner(s): Institut für Angewandte Mathematik und Physik (IAMP)
Funding: Innosuisse / Bachelor's Thesis
Duration: 2020–2021

In the Energy Strategy 2050 of the Swiss government, the use of ambient heat will play an important role for heating. The heat pumps used for this purpose should be operated with the highest possible proportion of renewable electricity from hydropower, wind farms and photovoltaic systems. The corresponding control units should optimize energy and costs and guarantee indoor comfort at all times. To do this, they also use the storage masses of the buildings and react to weather conditions and changes in user behavior. In traditional controllers, some parameters such as the heating curve of the building or the size of a locally available photovoltaic system must be set correctly. This is done during commissioning of the heat pump or during a later check by a service technician.

Within the framework of several student projects, an AI heat pump controller was developed that optimally controls the system components based on training with simulation data. The aim of the research work is that an AI heat pump controller achieves the same good performance (cost and energy optimization) as traditional controllers, but with significantly less effort during installation and commissioning.

To ensure that the AI heat pump controller continuously guides the system hydraulics to the optimum operating point, it is trained with a dynamic system before delivery. In several study projects, the simulation software Polysun and the "OpenAI Gym" platform were used for the training phase.

As shown in the figure to the right, a neural network consisting of two layers with 16 neurons each is used in [1]. Reinforcement learning is used to optimize the corresponding coefficients of the neural network on the basis of a large number of simulations. A cost function is defined which penalizes the careless use of energy and the undercutting of the set temperature in the building.

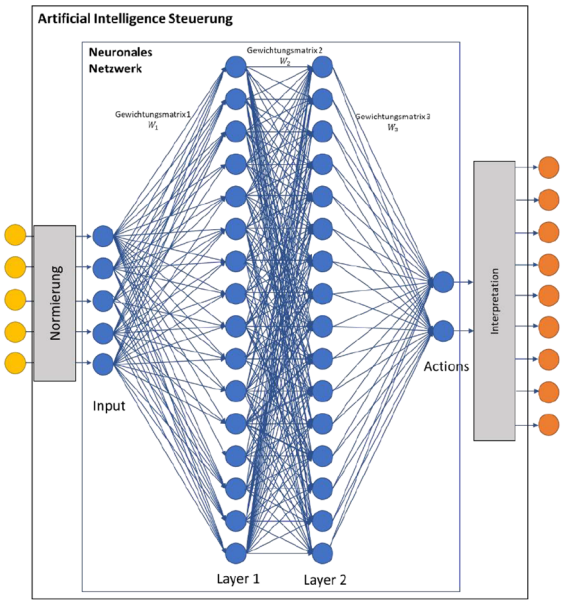


Figure: Neural network used in [1]. Input datapoints (signals from sensors) are symbolized with yellow circles, output data (signals to actors) are shown by orange circles.

References:

[1] Laurenz Joos, Selina Pfyffer, Reinforcement Learning für Wärmepumpensysteme mit PV, Betreuer: A. Witzig, V. Ziebart, Bachelorarbeit in Energie- & Umwelttechnik.

5 Computational Physics and Artificial Intelligence

Artificial intelligence (AI) algorithms and methods are already being used with great success in numerous commercial fields. Some of these new applications affect our everyday lives and our data is used every day by large corporations. While the use of personal data as a basis for training is a matter of social and ethical discourse, AI algorithms are an interesting field of research from a technical-scientific point of view, which is currently experiencing a pronounced surge in innovation and on its part also enables many innovations in other fields.

At ICP, we are interested in applications that combine computational physics and artificial intelligence. Specifically, we are interested in machine learning (ML) and its combination with numerics. Our core competence continues to be in physical models, which describe natural or technological phenomena, usually through differential equations, and which are derived from physical laws. It is a great opportunity at this stage to combine this knowledge with the emerging field of machine learning. In the following, we present the possible areas of application and show what contributions we can make.

Physical simulation for the generation of synthetic data

Physical simulations are used to provide the necessary training data for the ML algorithms during the learning phase. Classical numerical methods are used, and the challenge is to find the right questions and to translate the results into useful applications. Often, the neural networks are trained with simulated data and then applied to unseen real data.

Currently there are two projects at ICP. They are described in detail on pages 29 and 41 of this research report. Briefly:

Supporting solar cell analysis with neural networks: For this purpose, a neural network is trained with simulated image data. The simulations are based on a multi-physical finite element model, which is evaluated thousands of times for the training step.

Optimal control of a heat pump: A simulation comprising of several hundred years of operation is used to train a neural network in a heat pump control system. The neural network is thus trained to run the pump using as little electricity as possible, to effectively compensate for the stochastic fluctuations of the weather, and to provide a comfortable indoor climate at all times.

Our expertise in dealing with industrial projects and our entrepreneurial mindset allow us to build bridges in this field and make machine learning accessible to companies that, until now, have not had access to this new analysis method.

Physically informed neural networks

The goal when merging the disciplines of physics simulation and machine learning is to integrate the laws of physics into ML algorithms. Either as constraints or, for example, also into the structure of the neural networks. In the process, a huge new field of research is emerging and currently more open questions are posed than answered [1]. The community is moving away from the premise that data-driven models should be found with a minimal prior knowledge and a large amount of training data. Rather, an attempt is made to integrate domain knowledge acquired over centuries into the algorithms. This combination leads to explainable data-driven models that rely on less data than classical machine learning.

Scientific Machine Learning

The aim of scientific machine learning is to use structured scientific models (differential equations) together with unstructured data-driven machine learning models in order to accelerate the simulations; to better approximate machine learning to true physical systems; and to maintain the robustness and explainability of the mechanistic dynamic models.

A holistic approach focuses entirely on the application when formulating the initial problem and leaves the choice of method open at the beginning. Thereby, well-known optimization methods like the balancing calculation are available as an option, as well as learning with synthetic training data or with data-driven models, which are close to the differential equations of physics. Methods for inverse problems and automatic model finding are also available. First applications of scientific machine learning come from the fields of sustainable energy production, sensor technology, consumer electronics and medical technology. Concrete optimization steps are supported by machine learning. Applied research and development will thus be accelerated, especially in areas where pure physics-based models reach their limits of practical applicability. The particular challenge of scientific machine learning is how to efficiently and effectively integrate knowledge from physical modeling into the machine learning concept.

Evelyne Knapp and Andreas Witzig

References:

M. Raissi et. al., Physics-informed neural networks: *A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, Journal of Computational Physics, Vol. 378, Pages 686-707, Feb 2019. https://www.sciencedirect.com/science/article/pii/S0021999118307125

Appendix

A.1 Student Projects

S. AEBERSOLD, W. WONG, *Bildverarbeitung von Fluidbewegungen im Pharmabereich mittels KI*, Betreuer: B. Boiger, M. Hostettler, D. Brunner, Projektpartner: F. Hoffmann-La Roche AG, Bachelorarbeit in Informatik.

B. BASSO, *Inline-Gewichtsbestimmung von Tabletten mittels Mikrowellensensor*, Betreuer: D. Fehr, M. Bonmarin, F. Spano, Projektpartner: Krämer AG, Bachelorarbeit in Maschinentechnik.

B. BÖSCH, *Development of an Optical Electronic Skin for Pressure Sensing Applications,* Betreuer: F. Spano, D. Fehr, M. Bonmarin, Projektpartner: EMPA Sankt Gallen, Bachelorarbeit in Energie- und Umwelttechnik.

S. BREITER, J. G. WENGER, *Entwicklung einer Softwarekomponente zur automatischen Erkennung rassistischer oder beleidigender Userkommentare*, Betreuer: M. Roos, P. von Däniken, Projektpartner: we.publish, Bachelorarbeit in Informatik.

R. BRUNNER, S. KELLER, *Entwicklung einer Inline-Viskositäts-Regelung*, Betreuer: M. Bonmarin, F. Spano, D. Fehr, Projektarbeit in Energietechnik.

J. BÜRGIN, *Repair Process Turbine Rear Frame*, Betreuer: S. Koll (ZHAW-ZPP), T. Hocker, Projektpartner: SR Technics Switzerland AG, Bachelorarbeit Maschinentechnik.

M. CAPRAK, R. FÜEG, *Entwicklung eines mechatronischen Systems zur Positionierung und Trennung von Permanentmagneten*, Betreuer: G. Boiger, V. Lienhard, V. Buff, Bachelorarbeit in Maschinentechnik.

E. COMI, *Experimental Validation of an Electrothermal Small-Signal Model for Large-Area Perovskite Solar Cells*, Betreuerin: E. Knapp, Projektpartner: Fluxim AG, Masterarbeit Masterstudiengang.

D. DUDLI, N. SCHELLENBERG, *Design und Simulation einer Wasserentkeimungsanlage mit UV-LEDs*, Betreuer: K. Pernstich, V. Lienhard, Bachelorarbeit in Energie- und Umwelttechnik.

L. EGLI, G. VINZI, *Automatisierte Bildverarbeitung von Fluidbewegungen im Pharmabereich*, Betreuer: G. Boiger, M. Hostettler, D. Brunner, Projektpartner: F. Hoffmann-La Roche AG, Bachelorarbeit in Systemtechnik.

I. ERNI, O. LENGWEILER, *IR-Schweissen*, Betreuer: T. Hocker, W. Siegl (ZHAW-IEFE), Projektpartner: Georg Fischer Piping Systems, Bachelorarbeit Maschinentechnik.

L. GEERTSEN, F. TOUZIMSKY, *Innovative Tactile skin: Improvement of an Electronic Skin with Touch Sensitivity*, Betreuer: F. Spano, D. Fehr, M. Bonmarin, Projektpartner: intern, Bachelorarbeit in Elektrotechnik.

A. HABLÜTZEL, *Entwicklung einer Kühlvorrichtung für automatisiertes WIG-Schweissen von metallischen Rohrverbindungen*, Betreuer: T. Hocker, S. Koll (ZHAW-ZPP), Projektpartner: Wolfram Industrie GmbH, Vertiefungsarbeit Masterstudiengang.

S. JACCARD, *Simulation of the Joining Process for Resistance Welding of Tungsten Carbide with Steel,* Betreuer: P. Marmet, T. Hocker, Projektpartner: Scintilla AG (Bosch Schweiz), Vertiefungsarbeit Masterstudiengang.

L. JOOS, S. PFYFFER, *Reinforcement Learning für Wärmepumpensysteme mit PV*, Betreuer: A. Witzig, V. Ziebart, Bachelorarbeit in Energie- & Umwelttechnik.

N. JENAL, *Modell-basierte Optimierung eines neuen Infrarot-Heizungskonzepts zum kontaktlosen Schweissen von Kunststoffrohren*, Betreuer: C. Brändli (ZHAW-IMPE), T. Hocker, Projektpartner: Georg Fischer Piping Systems, Masterarbeit Masterstudiengang.

S. KELLER, *Viscosity-Control Demonstrator*, Betreuer: D. Fehr, M. Bonmarin, F. Spano, Projektpartner: Rheonics GmbH, Bachelorarbeit in Elektrotechnik.

J. KRAUSE, P. RAMA, *Optimierung einer kontaktlosen Infrarot-Heizmethode für das Schweissen von PVC-Rohren*, Betreuer: T. Hocker, Projektpartner: Georg Fischer Piping Systems, Bachelorarbeit in Maschinentechnik.

D. LEUENBERGER, *Gamification der Übungen mit der e-Exercises App*, Betreuer: K. Pernstich, W. Eich, Projektpartner: intern, Bachelorarbeit in Informatik.

F. LEUPPI, N. STALDER, *Energiesimulation im BIM-Kontext*, Betreuer: A. Witzig, Projektpartner: Abstract AG, Bachelorarbeit in Energie- und Umwelttechnik.

C. MALNATI, *Simulating the Electrical Properties of the Human Skin for the Development of Hydration Sensors*, Betreuer: D. Fehr, M. Bonmarin, Projektpartner: intern, Masterarbeit Masterstudiengang.

C. REINHART, P. SIEGRIST, *Entwicklung Implementierung eines Holzgasanalysesystems*, Betreuer: G. Boiger, V. Buff, Projektpartner: intern, Bachelorarbeit in Systemtechnik.

C. RUPPERT, *Calcium Imaging Signal Exaction Using Deep Neuronal Networks*, Betreuer: M. Bonmarin, Projektpartner: B: Grewe UZH/ETH, Vertiefungsarbeit Masterstudiengang.

J. STOLL, *Entwicklung und Implementierung eines Heissluftballonmodells in Berkeley Madonna und erste Vergleiche mit Messdaten*, Betreuer: T. Hocker, Projektpartner: Air Ballonteam Stefan Zeberli GmbH, Vertiefungsarbeit Masterstudiengang.

V. VESCOLI, *Thermal Imaging of Sweat Glands*, Betreuer: M. Bonmarin, F. Spano, D. Fehr, Projektarbeit in Systemtechnik.

V. VESCOLI, *Investigating Sweat Glands Activity with Thermal Imaging*, Betreuer: M. Bonmarin, D. Fehr, F. Spano, Projektpartner: UC Cincinnati, Bachelorarbeit in Systemtechnik.

L. VISSER, *Entwicklung und Implementierung eines Kalibrations.- und Prüfverfahrens für Gasanalysesensoren*, Betreuer: G. Boiger, V. Buff, Projektpartner: intern, Bachelorarbeit in Energie- und Umwelttechnik.

D. WYSS, *Mathematical models and numerical simulation of solid-liquid separation in decanter centrifuges*, Betreuer: K. Kirsch, T. Hocker, Projektpartner: T. Hühn (ZHAW-ILGI), Masterarbeit Masterstudiengang.

A.2 Scientific Publications

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, S. MALIK, G. HUSSAIN, H. KHAWAJA, J. ROEMER, G. K. BOIGER; M. MOATAMEDI, *Multiphysics study of infrared thermography (IRT) applications*, Int. Journal of Multiphysics, 14(3), pp. 249-272, 2020, DOI: 10.21152/1750-9548.14.3.249.

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S. BABITY, A. K. POLOMSKA, F. COUTURE, M. BONMARIN, D. FEHR, M. DETMAR, D. BRAMBILLA, *Rational design of a fluorescent microneedle tattoo for minimally invasive monitoring of lymphatic function*, Journal of Controlled Release, 327, pp. 350-359, 2020, DOI: 10.1016/j.jconrel.2020.08.017.

G. K. BOIGER, V. BUFF, D. SHARMAN, M. BOLDRINI, V. LIENHARD, D. DREW, *Simulation-based investigation of tar formation in after-treatment systems for biomass gasification*, Biomass Conversion and Biorefinery, 11(1), pp. 39-56, 2020, DOI: 10.1007/s13399-020-00915-7.

G. K. 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*, Int.Journal of Multiphysics, 14(1), pp. 1-15, 2020, DOI: 10.21152/1750-9548.14.1.1.

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, pp. 9631-9641, 2020.

T. O. BUCHMANN, K. RAILTON, J. EDMUND; M. JAZBINSEK, B. ZHOU, J.-H. SEOK, O.-P. KWON, F. ROTERMUND, P. JEPSEN, *High-power few-cycle THz generation at MHz repetition rates in an organic crystal*, APL Photonics, 5(10), p. 106103, 2020, DOI: 10.1063/5.0022762.

Z. CHEN, J. WANG, H. JIN, J. YANG, Q. BAO, Z. MA, W. TRESS, Z. TANG, *An underestimated photoactive area in organic solar cells based on a ZnO interlayer*, J. Mater. Chem. C, 2021, DOI: 10.1039/D1TC00745A.

I. N. GIANNAKEAS, T. K PAPATHANASIOU, A. SOLEIMAN FALLAH, H. BAHAI, *Coupling XFEM and peridynamics for brittle fracture simulation—part II : adaptive relocation strategy*, Computational Mechanics, 66(3), pp. 683-705, 2020, DOI: 10.1007/s00466-020-01872-8.

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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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G. BOIGER, H. KHAWAJA, M. MOATAMEDI, *Validation: Experimental and semi-analytical validation (in the context of Large (non-)spherical particle modelling for fluid filtration applications)*, Multiphysics Modelling of Fluid-Particulate Systems, Elsevier Academic Press London, 2020.

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A.4 Conferences and Workshops

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.

G. K. BOIGER, B. SIYAHHAN, V. LIENHARD, *Advancing the validation and application of a Eulerian-Lagrangian multiphysics solver for coating processes in terms of massive simultaneous cloud computing*. In: Multiphysics 2020, International Conference of Multiphysics, Online, 11-12 December 2020, International Society of Multiphysics, p. 38, 2020,

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G. K. BOIGER, V. LIENHARD, V. BUFF, B. SIYAHHAN, *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. K. BOIGER, V. LIENHARD, V. BUFF, B. SIYAHHAN, *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. K. BOIGER, 2020. FEA/FV workshop, *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. BRUNNER, J. GOODBREAD, K. HÄUSLER, S. KUMAR, H. KHAWAJA, G. K. BOIGER, *Modelling a viscosity-density sensor based on small amplitude torsional vibrations*, In: Multiphysics 2020, International Conference of Multiphysics, Online, 11-12 December 2020, International Society of Multiphysics. p. 23. https://static1.squarespace.com/static/5c9f89c101232c1d41297d67/t/5fd1bf288185f4776a0d1807/1607581490712/MULTIPHYSICS+2020+-+Abstracts.pdf.

R. HERRENDÖRFER, M. COCHET, P. BOILLAT, J. SCHUMACHER, *3-D simulation of heat and water transport in PEFCs during evaporative cooling and humidification*, In: 17th Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies, Online Conference, 20-22 April 2021.

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M. HOSTETTLER, D. BRUNNER, F. ROSENTHAL, M: CLEMENS, E. KOEPF, G. K. BOIGER, *Analysis of falling droplets into resting liquid and resulting shear stresses*, In: Multiphysics 2020, International Conference of Multiphysics, Online, 11-12 December 2020, International Society of Multiphysics. p. 50. https://static1.squarespace.com/static/5c9f89c101232c1d41297d67/t/5fd1bf288185f4776a0d1807/1607581490712/MULTIPHYSICS+2020+-+Abstracts.pdf.

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.

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

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.

B. SIYAHHAN, G. K. BOIGER, *A dynamic Eulerian-Lagrangian solver for the optimization of powder coating processes*. In: Multiphysics 2020, International Conference of Multiphysics, Online, 11-12 December 2020. International Society of Multiphysics, p. 40. 2020, https://static1.squarespace.com/static/5c9f89c101232c1d41297d67/t/5fd1bf288185f4776a0d1807/1607581490712/MULTIPHYSICS+2020+-+Abstracts.pdf.

W. TRESS, Z. WANG, F. EBADI GARJAN, 2020, *Understanding transient optoelectronic measurements and operation of perovskite solar cells*, In: 7th International Conference on Simulation of Organic Electronics and Photovoltaics (SimOEP), online, 31 August - 2 September 2020.

A.5 Teaching

T. BERGMANN, T. HOCKER, *Thermische Energiesysteme für Maschinentechnik und Energie- und Umwelttechnik*, Vorlesung, FS21, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Analysis 1 für Aviatik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Lineare Algebra 1 für Elektrotechnik und Systemtechnik*, Vorlesung, HS20, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Analysis 2 für Aviatik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

D. BERNHARDSGRÜTTER, *Lineare Algebra 2 für Elektrotechnik und Systemtechnik*, Vorlesung, FS21, Bachelor of Science.

G. BOIGER, *Mathematik: Numerik 2 für Informatik*, Vorlesung, HS20, Bachelor of Science.

G. BOIGER, *TSM Advanced Thermodynamics*, HS20, Master of Science in Engineering.

G. BOIGER, *EVA OpenFoam I - Thermo-Fluid-Dynamic Model Development using OpenFoam*, HS20, Master of Science in Engineering.

G. BOIGER, *Fluid- und Thermodynamik 1 für Maschinentechnik und Energie- und Umwelttechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

G. BOIGER, *TSM Two Phase Flow / Heat- and Mass Transfer*, FS21, Master of Science in Engineering.

G. BOIGER, *EVA OpenFoam II - Thermo-Fluid-Dynamic Model Development using OpenFoam*, FS21, Master of Science in Engineering.

M. BONMARIN, *Höhere Mathematik für Informatiker 1*, Vorlesung und Praktikum, HS20, Bachelor of Science.

M. BONMARIN, *Physik 1 für Systemtechnik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

M. BONMARIN, *Ausgewählte Kapitel in der Medizintechnik für Elektrotechnik und Systemtechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

M. BONMARIN, *Höhere Mathematik II für Informatiker*, Vorlesung und Praktikum, FS21, Bachelor of Science.

M. BONMARIN, *Physik 2 für Systemtechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

D. FEHR, *Grundlagen der Elektrotechnik und Digitaltechnik für Informatik*, Praktikum, HS20, Bachelor of Science.

T. HOCKER, *Aviation Projects 1 für Aviatik*, Praktikum, HS20, Bachelor of Science.

T. HOCKER, *Physik 1 für Aviatik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

T. HOCKER, *Aviation Projects 2 für Aviatik*, Praktikum, FS21, Bachelor of Science.

T. HOCKER, *Physik 2 für Aviatik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

M. JAZBINSEK, *Physik 1 für Energie- und Umwelttechnik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

M. JAZBINSEK, *Physik 2 für Maschinentechnik und Energie- und Umwelttechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

C. KIRSCH, *Analysis 1 für Elektrotechnik und Systemtechnik*, Vorlesung und Praktikum HS20, Bachelor of Science.

C. KIRSCH, *Analysis 3 für Elektrotechnik und Systemtechnik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

C. KIRSCH, *Analysis 2 für Elektrotechnik und Systemtechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

C. KIRSCH, *Numerik für Elektrotechnik und Systemtechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

E. KNAPP, *Numerik für Aviatik und Verkehrssysteme*, Vorlesung und Praktikum, HS21, Bachelor of Science.

V. LIENHARD, *Grundlagen der Elektrotechnik und Digitaltechnik für Informatik*, Praktikum, HS20, Bachelor of Science.

V. LIENHARD, *Physik für Maschinentechnik 3*, Praktikum, FS20, Bachelor of Science.

P. MARMET, *Analysis 1 für Informatik und Wirtschaftsingenieurwesen*, Vorlesung und Praktikum, HS20, Bachelor of Science.

P. MARMET, *Analysis 2 für Informatik und Wirtschaftsingenieurwesen*, Vorlesung und Praktikum, FS21, Bachelor of Science.

K. PERNSTICH, *Grundlagenprojekt 1 für Verkehrssysteme*, Praktikum, HS20, Bachelor of Science.

K. PERNSTICH, *Physik 1 für Verkehrssysteme*, Vorlesung und Praktikum, HS20, Bachelor of Science.

K. PERNSTICH, *Grundlagenprojekt 2 für Verkehrssysteme*, Praktikum, FS21, Bachelor of Science.

K. PERNSTICH, *Physik 2 für Verkehrssysteme*, Vorlesung und Praktikum, FS21, Bachelor of Science.

M. ROOS, *Höhere Mathematik für Informatiker 1*, Vorlesung und Praktikum, HS20, Bachelor of Science.

M. ROOS, *Mathematik: Numerik 2 für Informatik*, Vorlesung, HS20, Bachelor of Science.

M. ROOS, *Scientific Computing für Elektrotechnik und Informatik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

M. ROOS, *Höhere Mathematik II für Informatiker*, Vorlesung und Praktikum, FS21, Bachelor of Science.

M. ROOS, *Numerik für Systemtechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

M. ROOS, *FTP_Tensors*, FS21, Master of Science in Engineering.

B. RUHSTALLER, *Physik 1 für Verkehrssysteme*, Praktikum, HS20, Bachelor of Science.

B. RUHSTALLER, *Applied Photonics*, HS20, Master of Science in Engineering.

B. RUHSTALLER, *Advanced Thin Films*, FS21, Master of Science in Engineering.

M. SCHMID, *Analysis 3 für Elektrotechnik*, Vorlesung und Praktikum, HS20, Bachelor of Science.

M. SCHMID, *Lineare Algebra 1 für Elektrotechnik und Systemtechnik*, Vorlesung, HS20, Bachelor of Science.

M. SCHMID, *Lineare Algebra 2 für Elektrotechnik und Systemtechnik*, Vorlesung, FS21, Bachelor of Science.

J. SCHUMACHER, *Lineare Algebra 1 für Elektrotechnik und Systemtechnik*, Vorlesung, HS20, Bachelor of Science.

J. SCHUMACHER, *Synthetische Treibstoffe*, FS21, Bachelor of Science.

J. SCHUMACHER, *Lineare Algebra 2 für Elektrotechnik und Systemtechnik*, Vorlesung, FS21, Bachelor of Science.

J. SCHUMACHER, *Synthetische Treibstoffe für Maschinentechnik und Energie- und Umwelttechnik*, Vorlesung, FS21, Bachelor of Science.

J. SCHUMACHER, *Numerical Simulation of Solar Cells*, FS21, Universität Freiburg im Breisgau, Master of Science in Engineering.

J. SCHUMACHER, *Multiphysics Modeling and Simulation*, FS21, Swiss course of studies: Master of Science in Engineering.

W. TRESS, *Physik 1 für Aviatik, Maschinentechnik und Verkehrssysteme*, Vorlesung und Praktikum, HS20, Bachelor of Science.

W. TRESS, *Physik 2 für Aviatik und Maschinentechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

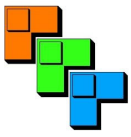
A. WITZIG, *Physik 3 für Verkehrssysteme*, Vorlesung und Praktikum, HS20, Bachelor of Science.

A. WITZIG, *Physik Engines für Informatik*, Vorlesung, FS21, Bachelor of Science.

A. WITZIG, *Physik 3 für Systemtechnik*, Vorlesung und Praktikum, FS21, Bachelor of Science.

A. WITZIG, *Solarthermie für Maschinentechnik und Energie- und Umwelttechnik*, Vorlesung, FS21, Bachelor of Science.

A.6 ICP Spin-Off Companies



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

www.fluxim.com

Fluxim is a provider of device simulation software and measurement hardware to the display, lighting and photovoltaics community worldwide. Our principal activity is the development and the marketing of the simulation software packages Setfos and Laoss, as well as the measurement platform Paios, Phelos and Litos. The combination of simulation software with measurement data allows for the determination of material and device parameters. The R&D tools are used worldwide in industrial and academic research labs for the development of devices and semiconducting materials with improved performance as well as the study of device physics.

www.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.

www.nanolockin.com

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

www.zarawind.com

Zarawind is a 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.

www.reorbis.ch

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

A.6 ICP Team

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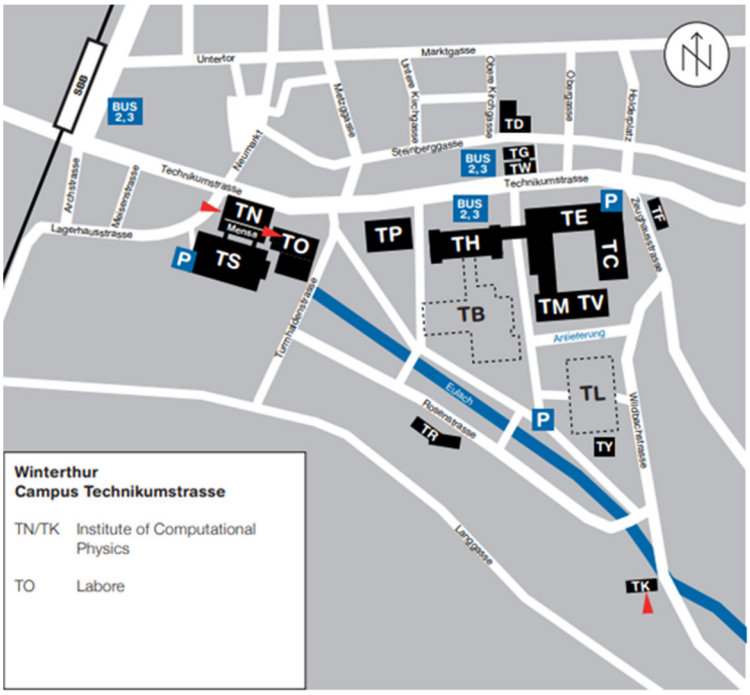

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