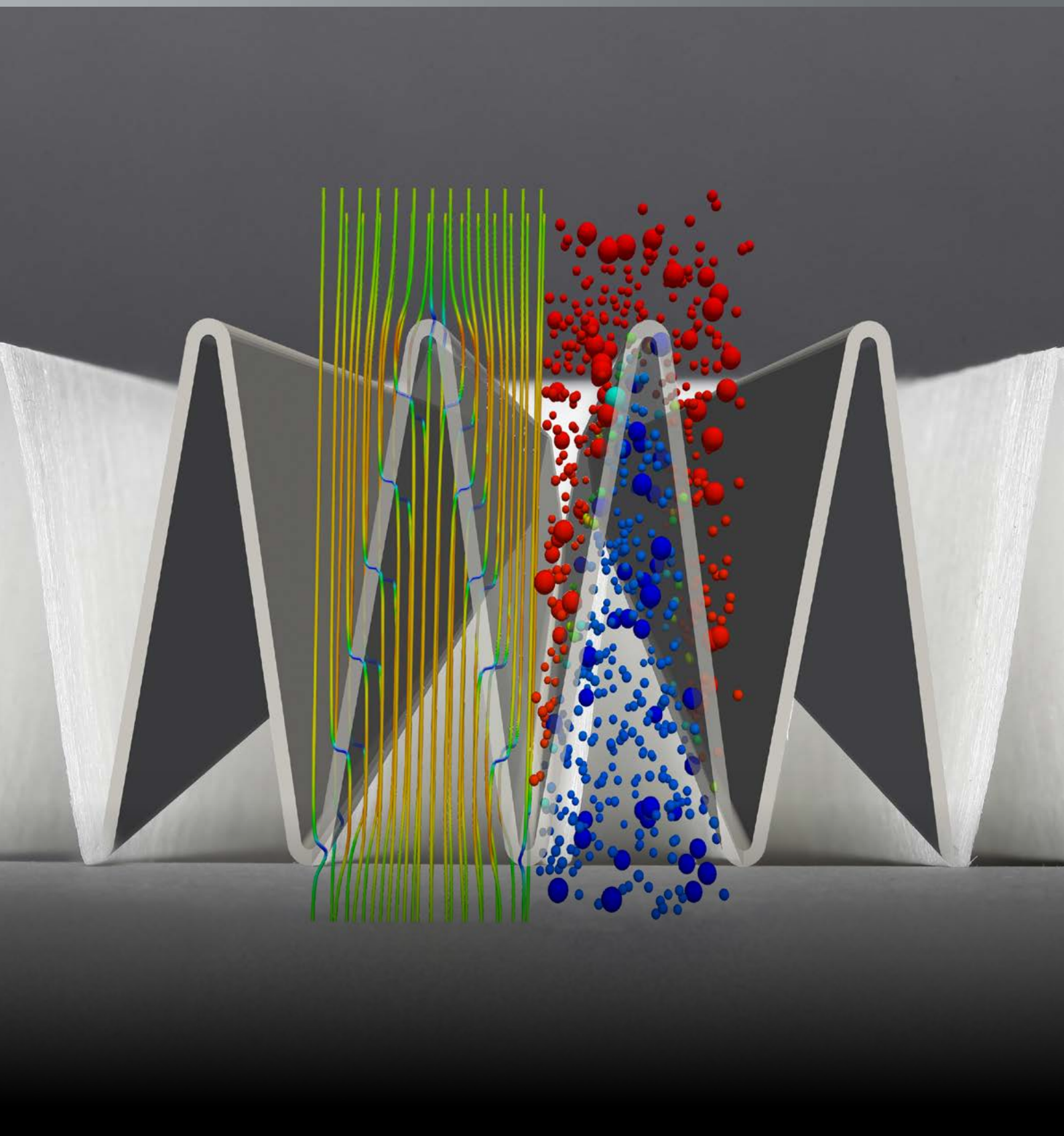
FLOW AND MATERIAL SIMULATION



DR. KONRAD STEINER
HEAD OF DEPARTMENT

MULTI-SCALE SIMULATION AND CUSTOMIZED SOFTWARE FOR INDUSTRIAL APPLICATIONS

Our department, Flow and Material Simulation develops multi-scale methods and software tools for product development and process engineering. One of the typical challenges is to model the interrelated influences of production processes and multi-functional local material properties. Our unique knowhow lies in the development of company-specific software and the supply of specific, industrial use application solutions featuring multi-scale and multi-physics approaches. As indicated by our name, the department is divided into two major areas of expertise. The subject area "Computer-aided material design and microstructure simulation" focuses on simulation-based optimization of the functional properties of porous materials and composites. We experience a high demand for our highly efficient, micro-mechanical simulation methods for material engineering of fiber reinforced composites and technical textiles. Currently, our major research focus is on the design and structural optimization of programmable materials and on modeling the production process by means of additive processes.

The subject area "Simulation-aided design of complex flow processes" studies the associated production processes like mixing, dispersing, injecting, filtering, coating, and separating. With the new tool FOAM we simulate the reaction injection molding process of rigid and flexible foam for various applications as well as the foaming of vehicle seats, the insertion of insulation foam or the infiltration of textile reinforcements for composite components.

Another use case is in the field of electro-chemistry where we investigate various aspects of the production and material design of batteries and fuel cells, for example, the filling of the battery cells with electrolyte.

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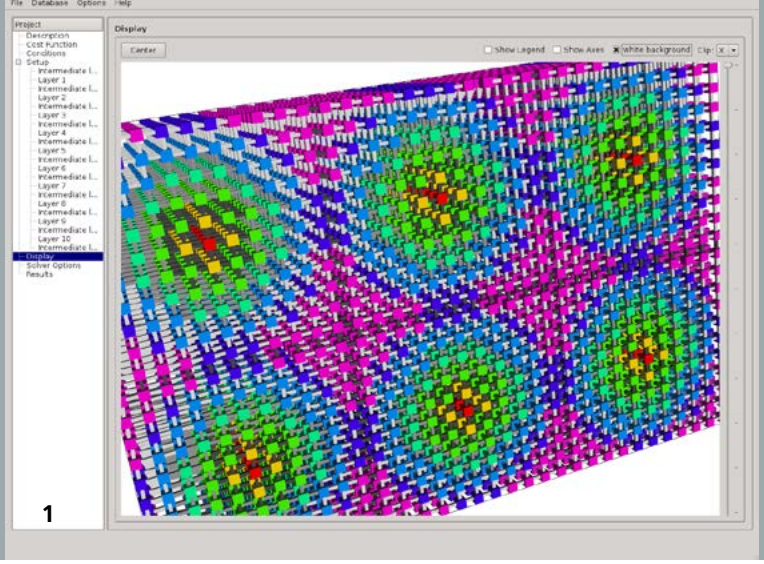
MAIN TOPICS

- Technical textiles and nonwovens
- Virtual material design and microstructure simulation
- Lightweight and insulation materials
- Filtration and separation
- Complex fluid dynamics and multiphase flows
- Electrochemistry and batteries



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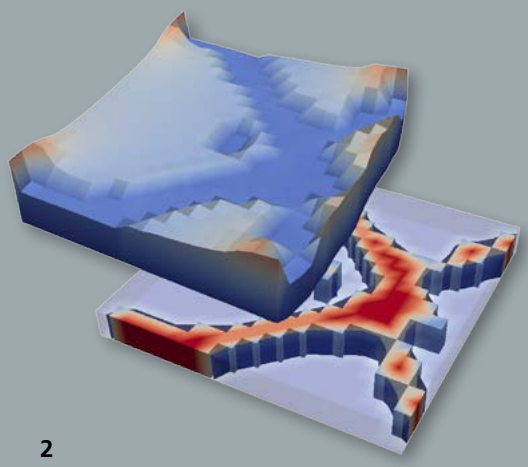


2

PROGRAMMABLE MATERIALS – MECHANICS AND TRANSPORT ON REQUEST

1 *Design study for a metamaterial, constructed from different elementary cells*

2 *Non-linear deformation of a topologically optimized metamaterial*

Giving materials new functionalities? We are finding ways to do that in various projects in the field of "Programmable Materials." What we find is that not only the basic material itself is changed, but also its internal structures.

New manufacturing methods make it possible to specifically produce structures in the micrometer range. These methods include for example, additive processes like 3D-printing. An engineer uses these methods not only to design the outer shape, but also to target the internal microstructures to give certain properties to a component. In cooperation with other Fraunhofer Institutes, we go one step further and define multiple states for such microstructures and apply external stimuli to switch between them.

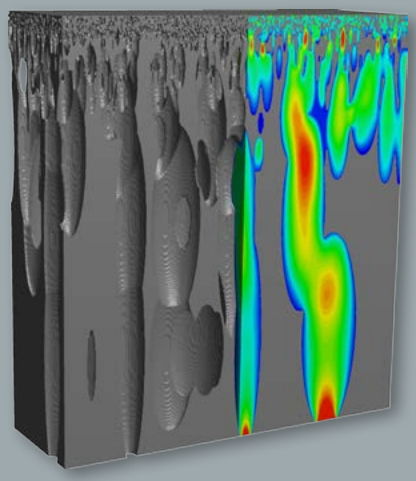
Programmable mechanics and a tool kit full of structural possibilities

At Fraunhofer Cluster of Excellence "Programmable Materials", we develop mathematical procedures for optimizing structures and provide support to engineers in designing production processes and choosing the appropriate microstructures. Working with the Fraunhofer Institute for Mechanics of Materials, IWM, we develop the microstructures for 3D-printing, which can change the internal stiffness or the surface shape as desired when subjected to external mechanical stress. Specifically, we have achieved extraordinary mechanical effects that do not exist in the naturally occurring material.

For example, the so-called pentamode mechanical meta-materials are solid structures that behave like liquids. These materials consist of three-dimensional arrays of cubic cells. Each cell exhibits a non-linear mechanical behavior and multiple stable states. Such cells are developed, printed, and tested at Fraunhofer IWM.

Algorithms for very special cells

There are many different ways to shape these cells. One type is known as auxetic cellular material that expands orthogonally when under tension, that is, it becomes thinner when compressed and thicker when stretched. Many more options are created when thousands of these unit cells are arranged into an array. We develop an algorithm that computes a possible selection and arrangement of the cells on request. We developed a graphical user interface for the design of programmable materials made from these unit cells – similar to the CAD software used in architecture. In the long term, these computed structures will be output for immediate use as input to 3D-printers.



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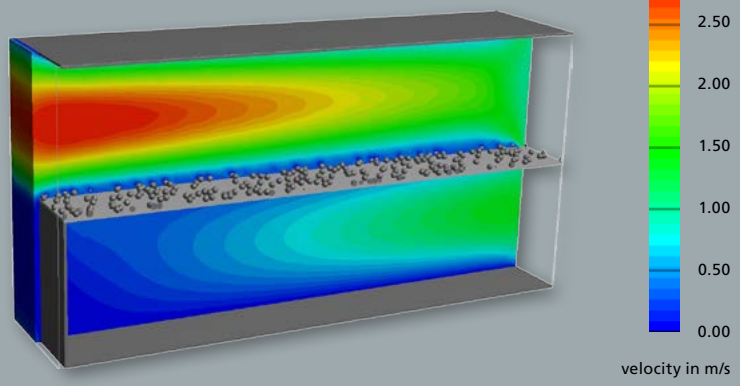

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Programmable transport: Clean filters with smart materials

Together with the Fraunhofer Institute for Applied Polymer Research IAP, we are developing filter membranes. In this case, the focus is on the use of programmable materials that can change their properties as a result of external stimuli, in particular, in the area of effective filter cleaning.

These membranes are made from thermally activated shape memory polymers, with or without a porous structure, that can change form at the time of cleaning and make the process more effective. Shape memory polymers are polymers that seem able to "remember" their previous form. The project also studies membranes with additional surface structuring for applications with cross-flow filtration. Such structuring can delay the fouling process during the filtration phase, for example, by keeping away bacteria from the membrane. Another kind is the chemo-selective membranes, where permeability can change depending on the presence of certain chemicals. This effect is used to block pollutants. In all cases, we assist project partners with simulations to support their development efforts.

Adaptive filtration using membrane structure

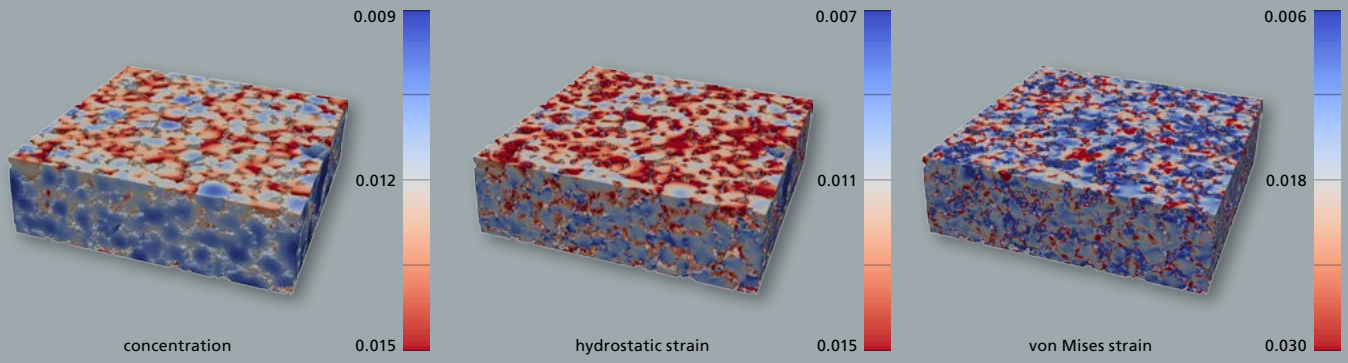
The "Programmable Materials in Science and Engineering (ProMiSE)" project is a collaborative project with other Fraunhofer Institutes, with a research focus on new programmable materials, specifically, "programmable porosity."

As possible trigger mechanisms, we are exploring piezoelectrical and thermo-mechanical effects. The aim is to achieve a deformation of the pore geometry on the micro-scale and, in this way, change the material porosity. This ability can be used in adaptive filtration, for example, in water treatment or chemical processes.

The modeling and simulation of the piezoelectrical effects poses a challenge. These methods describe the changes in electrical polarization and show the presence of electrical current in solids under conditions of elastic deformation. The expansion and orientation of the polymer must be mechanically modeled on a continuum scale. We then compare the effects of differently structured pore geometries. Project partner Fraunhofer Institute for Applied Optics and Precision Engineering IOF, produced the necessary membrane geometries using laser irradiation. The required adaptive filtration is achieved through deliberate deformation.

1 *Flux through a virtual microstructure*

2 *Transversal filtration through a membran with surface structure*



1

BATTERY SIMULATION TOOL BEST – NEW EFFICIENT SOLVERS AND INTEGRATION IN GeoDict

1 *Lithium Ion concentration (mol/cm³), hydrostatic strain, and von Mises strain simulated with BESTmicroFFT for a realistic, stochastic electrode structure (structure generation: Inst. of Stochastics, Univ. Ulm)*

Electric mobility places a high demand on the energy storage systems – mainly lithium-ion batteries. Computer simulations can help in evaluating the performance of new battery cells, in understanding the microscopic reasons for the observed behaviour, and in optimizing the design. Several years ago, ITWM started the development of BEST (Battery and Electrochemistry Simulation Tool), which is continuously updated in public and private industrial projects.

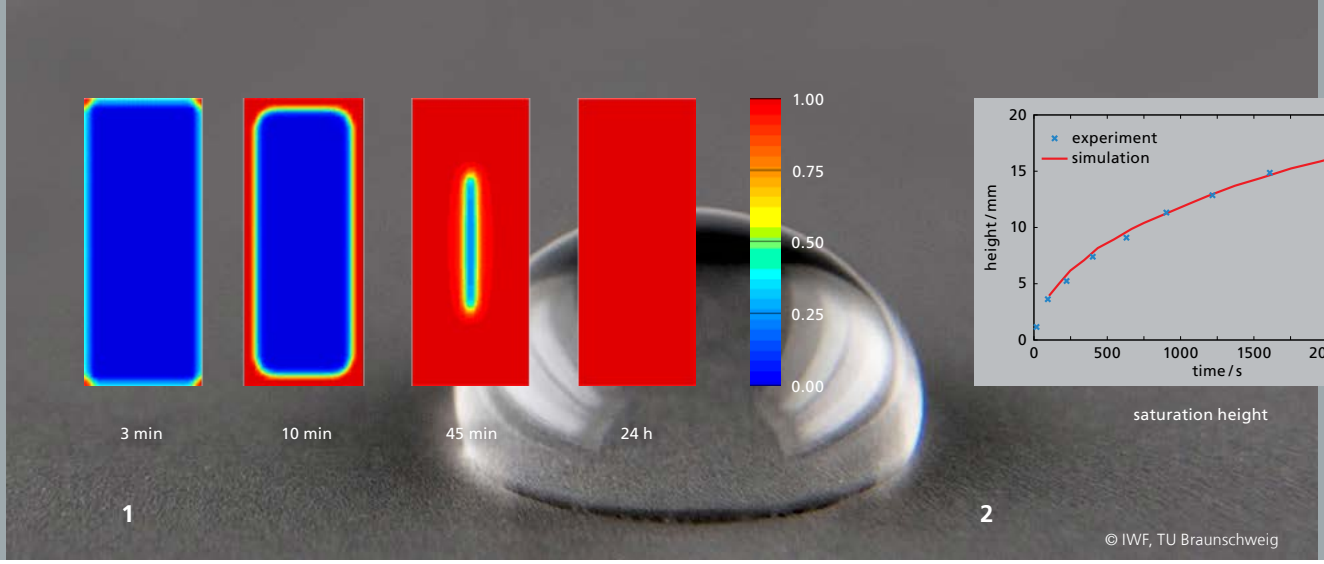
Interesting problems range from design issues at the macroscopic battery cell scale (BESTmeso) to the effects of the microscopic design of electrodes (BESTmicro) on the electric, thermal, and mechanical characteristics of the cell. Two different software components are used to account for these multiscale aspects: BESTmeso and BESTmicro.

BESTmicroFFT reduces computing and storage costs

Simulations that account for the three dimensional microstructure of electrodes are very expensive because of the fine spatial discretization required. BESTmicro can sometimes take several days of computing time on common work stations. In many standard cases, the recently developed BESTmicroFFT software-module provides the remedy. Similar to ITWM's mechanical solver FeelMath, the new solver is also based on a Fourier method (FFT) and requires significantly less computing and storage effort for simulations. The user can now decide between the two micro-solvers depending on the current requirements.

BatteryDict as new GeoDict component

The BESTmicro and BESTmicroFFT solvers are fully compatible with the structure generators in the GeoDict software from Math2Market (M2M). In the area of battery simulation, we began collaborating with M2M last year on the joint development of the new GeoDict module BatteryDict. The new module is now commercially available in the GeoDict2018 release and offers BESTmicroFFT-based battery simulation in a fully integrated GeoDict workflow. The GeoDict2019 version has been expanded to provide for electrodes made from different active materials (electrode blends) and additional material classes (conductive additives).



MODELING THE PRODUCTION PROCESS OF LITHIUM-ION BATTERIES

Scientists at twelve German universities and research institutes are working in the competence cluster for battery cell production (the ProZell Cluster) for the purpose of studying and improving the production process of battery cells and assessing various influences on cell properties and product development costs. Their work will provide the scientific basis for the sustainable development of a globally competitive battery cell production industry in Germany. We are involved in the project Cell-Fi which aims at improving the electrolyte filling process.

1 *Electrolyte saturation within electrode plane at different times during the wetting process*

2 *Comparison of liquid rise in porous electrode in simulation and experiment Exp. data: IWF, TU Braunschweig)*

Cell-Fi: Modeling electrolyte filling of battery cells

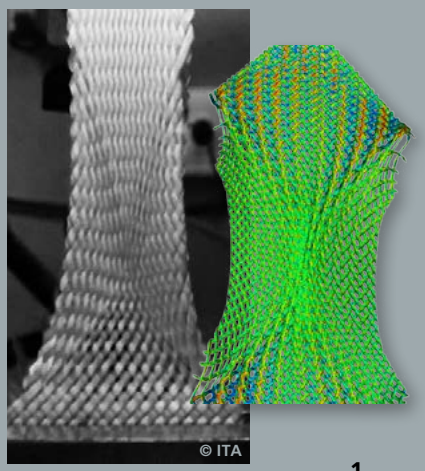
The topic of the project Cell-Fi is the acceleration of electrolyte uptake through optimized filling and wetting processes: After the assembly of the cells, billions of pores of the battery components – at most only a few micrometers in diameter – are filled with an electrolyte solution. The process takes several hours because the solution penetrates via the cell's small side faces into the pore volume only driven by capillary forces. Furthermore, it is difficult to assess the time required to ensure a uniform wetting.

Until now, the process of electrolyte filling has hardly been scientifically investigated. A great potential exists for companies to achieve higher throughput in production and to save costs if the relationships between process parameters and wetting speed and quality are better understood.

Calculating on micrometer scale and macroscopic scale

Our task in this project is the development of simulation methods that describe the capillary-driven flow within the different porous layers of the cell. This involves several different length scales: The pore morphology at the micro-scale, together with the physical surface characteristics of the materials involved, influences the capillary forces responsible for the wetting speed. We calculate the required input parameters from the micro-scale using the GeoDict simulation software from Math2Market.

On a macroscopic scale, the main influences affecting how the liquid distributes within the cell are the cell dimensions and the positioning of the surfaces through which the electrolyte enters the cell. Here, we use our ITWM software platform CoRheoS. Together, the GeoDict and CoRheoS tools let us predict the wetting times for various cell geometries, pore distributions, and material properties.



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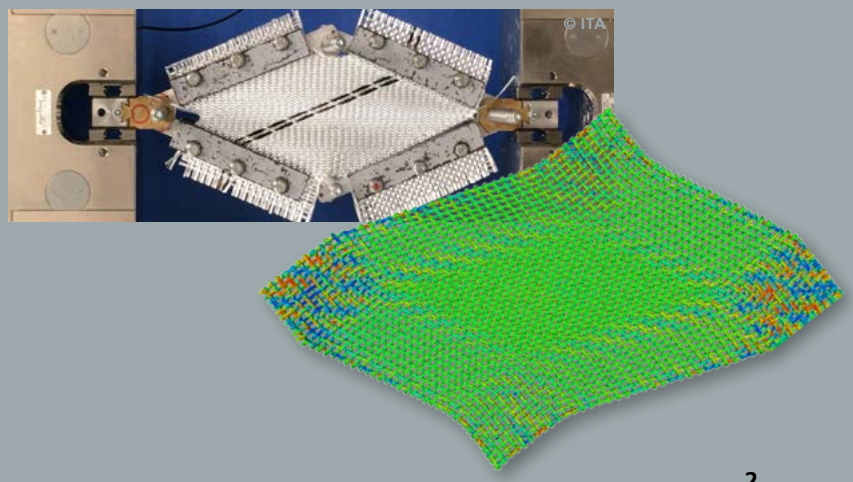


2

OPTIMIZING THE DRAPING PROCESS FOR FRP COMPONENTS MADE FROM HIGH PERFORMANCE TEXTILES

1 *Critical shear angle experiment performed by ITA and simulation of wrinkling*

2 *45°-tension test of a woven fabric with fixed frame performed by ITA and corresponding simulation*

As part of the AIF Project OptiDrape we are developing a draping catalog for small and medium-sized enterprises (SMEs) in cooperation with the Institute for Textile Technology (ITA) and the Institute for Management Cybernetics (IfU), Aachen.

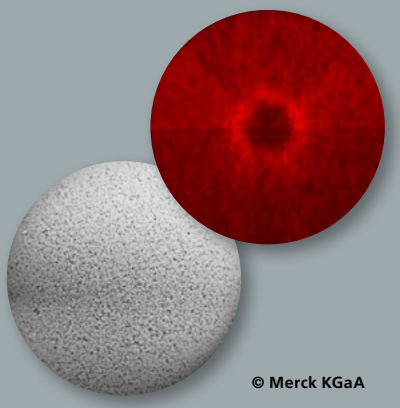
The potential of components made from fiber reinforced polymers (FRP) is highly dependent on the type of reinforcing textiles used and their drapability (ductility). The draping quality is evaluated on the basis of defects and wrinkles in the textile after preforming. Preforming refers to the process for producing a dry reinforcement structure. The potential of the anisotropic material is enormous for lightweight construction and can be specifically exploited only if the textile fibers are present locally in the required orientation. The draping process takes place during the production of complex geometries by experienced specialists. From a technical and economic point of view, the process lacks standards and objective criteria and requires optimization.

Improve quality and shorten times

The aim of the OptiDrape project is to improve the quality of the preforms for FRP components and to shorten the development time. We classify the different mats and weaves in terms of draping properties according to the type of bond as well as by the roving material and cross-sections. A roving is a bundle, strand, or multi-filament yarn made from parallel filaments. Also, a textile-specific shear angle is given. This indicates the point at which the textile starts to wrinkle. We selected a total of 16 carbon and glass fiber textiles with different cross sections and bond types as well as various offsets. ITA conducted a number of experiments and determined the effective tensile, shearing, and bending properties and shear angles. In parallel, we also used our FEM software to simulate and validate these properties. In contrast to experimentation, simulation at the roving level enables a virtual material design with precision detail. Among other things, the roving cross sections as well as the materials and distances of the bonds can be more efficiently varied; and, the experiment catalog was significantly expanded.

Model for a wide range of uses

The project used comprehensive mathematical analysis to develop a predictive model that calculates the critical shear angle. It relies on previously defined roving materials and dimensions, the type of bond, as well as experimentally determined contact point data. Additional model parameters include the offset of the bond as well as the distances. The resulting model not only allows companies to set up a very broad catalog, but also to continuously vary all of the design parameters for any application and requirement in the interests of optimizing the design.



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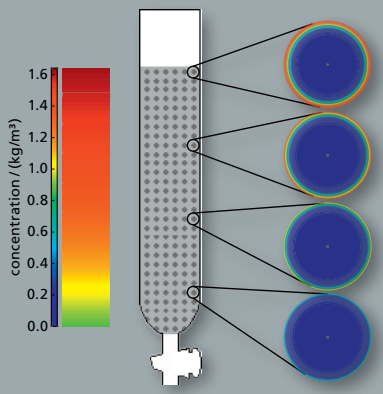

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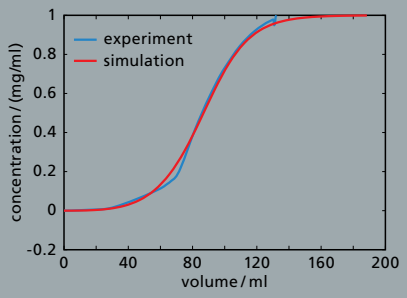

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MODELLING AND SIMULATION OF CHROMATOGRAPHY WITH SPHERICAL BEADS

In the BMBF joint research project AMSCHA, we develop models for the simulation of separation processes of protein and cell suspensions. The abbreviation stands for "Analysis, modelling and simulation of chromatographic purification processes". In collaboration with researchers from the Technical University Kaiserslautern and the University of Applied Sciences Darmstadt, the processes are investigated on different length scales. The chemical and pharmaceutical company Merck KGaA and the manufacturer of optical microscopes Leica Microsystems support the research project as industrial partners.

The separation of target substances from a suspension is an important and often undervalued step in the manufacturing of agents in the pharmaceutical industry, although one cannot imagine laboratory and industrial work without chromatography as a separation process. One well-established form is column chromatography. The efficiency and the throughput of these columns strongly depend on the process conditions and the used chromatographic media.

Model, simulate and optimize protein purification

In one part of the project, we consider the separation of protein suspensions using chromatographic purification. The goal is to extract one target protein from a mixture. This is done with the help of spherical, microporous beads (pearls). In column chromatography, a cylindrical tube – the separating column – is packed with the stationary phase – the beads – and is flowed through by a protein suspension. In this connection, part of the proteins is deposited within the beads.

The industry partner Merck conducts for this application several experiments in the laboratory. To reproduce the processes in the simulation, we determine suitable model parameters based on static and dynamic measurements of the binding capacities (protein concentration). Additionally, Merck visualizes the concentration profiles in the static experiments using confocal laser scanning microscopy.

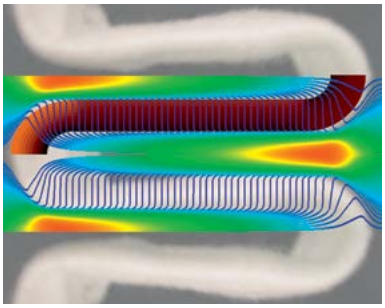
1 *Microscopy image of a chromatography bead. Confocal laser scanning microscopy image of a labeled bead. The dye intensity is indicating the loading (lightest red strongest loading).*

2 *Overview on the simulation of a chromatography column (dynamic process conditions; left: concentration profile in the column, right: the loading of single beads at different positions in the column*

3 *Comparison of the simulated protein breakthrough curve with experimental data*

NEWS

AWARD FOR DISSERTATION ON THE SIMULATION OF CAKE AND DEPTH FILTRATIONS



In November 2018, Dr. Sebastian Osterroth took third place in the ICT Dissertation Award presented by Fraunhofer Information and Communication Technology Group. The jury presents the award to outstanding dissertations originating at the Fraunhofer Institutes that deal with innovative developments and technologies in the computer sciences, mathematics, or related fields.

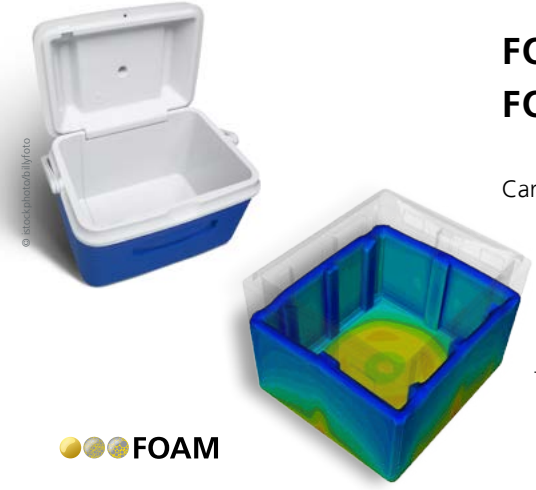
Osterroth's dissertation deals with mathematical modeling and simulation of cake filters and depth filtration. The filter cake functions as a supplemental filter medium, with increasing thickness. This study provides a major contribution towards the optimal design of filter elements.

NEW TEST DEVICE FOR POROUS MEDIA

Departmental lab is home to a new air permeability test apparatus. We are now able to determine the permeability of a wide spectrum of porous materials (for example, nonwoven fabrics, weaves, knits, crochets, foams) because of the device's large measuring range.

In future combination with the existing DMTA (dynamic-mechanic-thermal analysis) test unit, material characterizations with flow and structural mechanics will be possible from a single source. In particular, it enables us to investigate the relationships between mechanical deformation and the associated changes in flow resistance.

FOAM: RELIABLE SIMULATION OF POLYURETHANE FOAM



Car seats, mattresses, and insulation materials mainly consist of polyurethane (PU) foams. The foaming process of the liquid polymer emulsion is complex. In cooperation with colleagues at the Department of Lightweight Structures and Polymer Engineering at Chemnitz University of Technology, our department has developed software to simulate the foaming behavior and reliably characterize the material. FOAM also works for composites where plastic foams are injected into textile structures.

Front, left to right: Dr. Olga Lykhachova, Jan Lammel, Inga Shklyar, Ruturaj Deshpande, Dr.-Ing. Sarah Staub, Pavel Gavrilenko, Alexander Leichner, Dr. Olena Sivak, Dr. Xingxing Zhang, Dr.-Ing. Tobias Hofmann, Christine Roth, Dr. Larysa Khilkova, Pavel Toktaliev, Dr. Sebastian Osterroth, Dr. Dariusz Niedziela, Dr. Konrad Steiner, Jonathan Köbler, Dr. David Neusius, Dr. Ralf Kirsch, Dr. Stefan Rief, Dr. Heiko Andrä, Dr. Aivars Zemitis, Dr. Matthias Kabel, Prof. Dr. Oleg Iliev, Dr. Stephan Kramer, Stephan Wackerle, Riccardo Falconi, Dominik Gilberg, Dr. Torben Prill, Dr. Jochen Zausch, Thomas Palmer, Dr. Hannes Grimm-Strele, Michael Hauck