FLOW AND MATERIAL SIMULATION

A device for dynamic-mechanical thermo-analysis (DMTA) provides the precise in-house characterization of material parameters necessary for the micro structure simulation of porous media and composites. Measurements can be taken in a wide range of temperatures and humidity using nitrogen cooling and humidity generators. Ultimately, the device is used to validate simulation results.

DR. KONRAD STEINER
HEAD OF DEPARTMENT

The Flow and Material Simulation department develops multiscale methods and software tools for the product development and the corresponding process layout. The simulation challenge of the mutual influences of manufacturing processes and restrictions with the multifunctional, local material properties of complete composites under dynamic strain is typical. The strength of the department lies in the development, enabling and specific use of multi-scale and multi-physics methods and customer-specific software solutions suitable for industrial application. The department cuts into two larger fields of competence: By means of "computer-assisted material design and microstructure simulation" it is possible to simulate and optimize numerically the functional characteristics of porous materials and composite materials. There is a strong demand for our highly efficient, micromechanical methods for the material design of fibre reinforced composites and technical textiles. The "simulation-assisted design of complex flow processes" works on the corresponding manufacturing processes such as mixing, dispersing, injection, filtration, coating and segregation. Focusses of the industrial application are processes of filtration and segregation and the product design of filter systems or of other process machines. The projects of application in the area of electrochemistry concern diverse aspects for the design of material of battery cells or fuel cells as well as for their production e.g. the filling of battery cells.
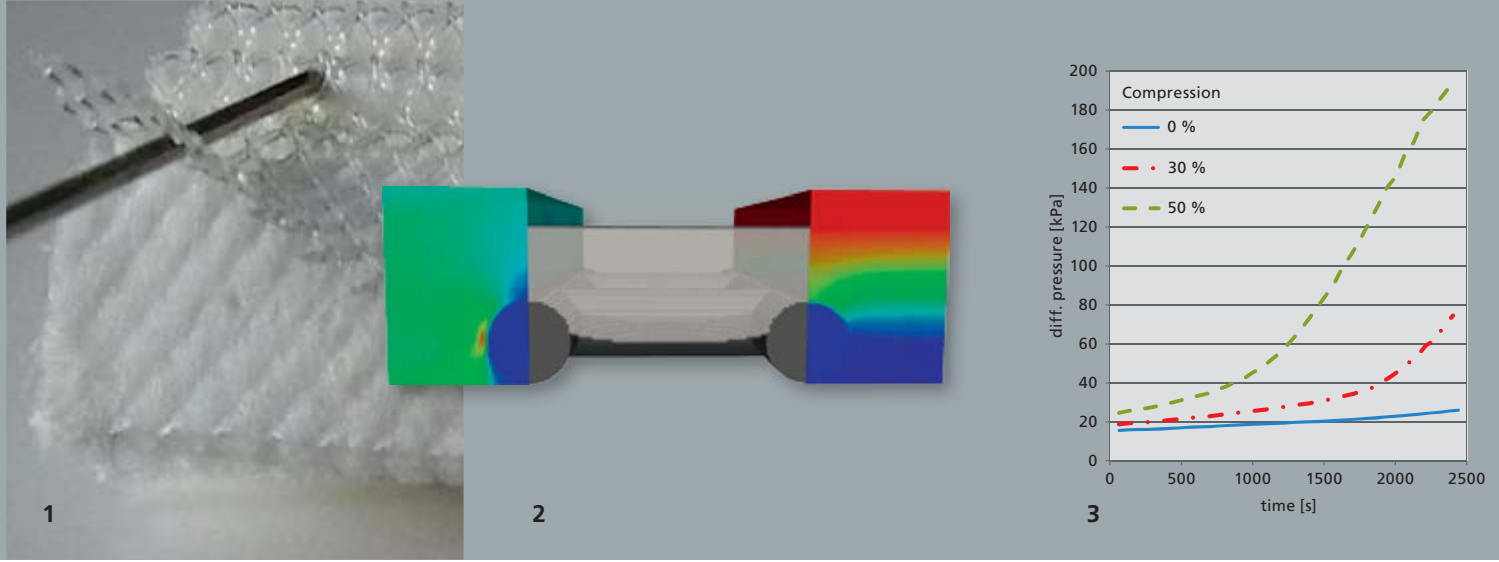
MAIN TOPICS

- Virtual Material Design and Microstructure Simulation

- Complex Fluid Dynamics and Multiphase Flows

- Technical Textiles and Nonwovens

- Lightweight and Insulation Materials

- Filtration and Separation

- Electrochemistry and Batteries

Kontakt
konrad.steiner@itwm.fraunhofer.de
www.itwm.fraunhofer.de/en/sms

1 2 3

MODELING AND SIMULATION FOR THE OPTIMIZA-TION OF MULTI-LAYERED FILTERED FILTER MEDIA

1 *Imprints of the supporting mesh in the filter material due to the pleating procedure*

2 *Simulation of the compaction of the filter material and the corresponding effects. Left: Flow speed, Center: Shape of the nonwoven, right: Pressure distribution in the flow*

3 *Time evolution of the differential pressure caused by the loading of the filter material for different mechanical compression levels*

Specialized simulation tools have proven to be very useful for the innovation and optimization of filter media and filter element designs. In order to produce reliable and predictive results, material parameters such as the fiber volume fraction (porosity), flow resistance (permeability) and mechanical properties are of paramount importance.

The design of filter materials with high dirt holding capacity and filtration efficiency, while featuring a low pressure loss, is a challenging task. Therefore, homogenous filter media usually cannot fulfill all these requirements. In many cases, the filter medium consists of several layers, combining filtering nonwovens with supporting meshes in order to provide mechanical stability even for high volumetric flow rates. During manufacturing of the multilayered medium (e. g. pleating), mechanical compression leads to imprints of the mesh in the softer nonwoven layers, causing tremendous local compaction of the materials, leading to corresponding changes in flow resistance filtration properties. A purely empirical approach to identify suitable material combinations, optimal layer thicknesses and manufacturing process is extremely time-consuming and costly.

The goal of the project "Virtual workbench for the optimization of filter media" (ViWOFiM) is the development of models and algorithms that are able to accelerate the design phase for such filter materials. This is based on the coupling of the software packages FeelMath and FiltEST, developed at the Department of Flow and Material Simulation. Using known mechanical properties of the starting materials and prescribing a compression for the multilayered medium, FeelMath computes the local deformations in the individual components. The obtained local material compactions are translated to a permeability distribution by utilizing suitable models. This is used by the flow simulation module of the software FiltEST for the computation of velocity and pressure distribution in the medium, such that an effective flow resistance of the compressed multi-layered medium. In a similar way, the local filtration properties can be deduced from the corresponding compressions. Subsequent simulation of filtration processes allow for the computation of an effective filter efficiency of the multi-layered structure after the processing.

1
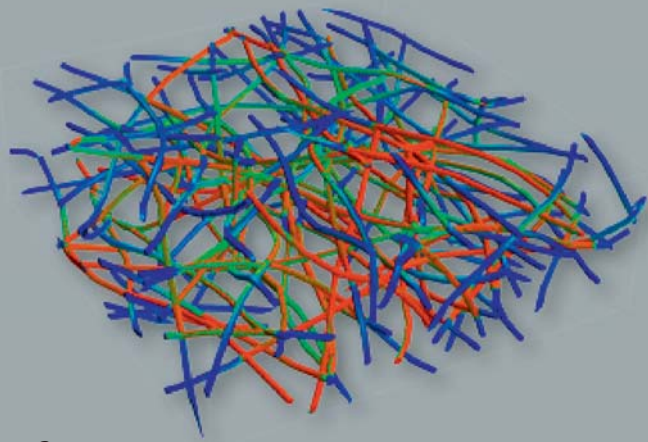
2

MICROMECHANICAL SIMULATION OF THE RESILIENCE OF NONWOVENS

Nonwovens are an important component of different products of several uses, e. g. transport of humidity in sanitary products, insulation materials or filters. Nonwovens are usually produced on large engineering facilities. For this, experimental studies of design with regard to the optimization of these nonwoven-structures prove to be very difficult. There are so many parameters of design, as for example fiber properties, surface weight or type of nonwoven bonding and finishing that are affecting the properties of nonwovens. For the change of one single parameter, e. g. the material of fiber, it is necessary to adapt the whole process of fabrication from the spinning of the fibers via their stacking to the nonwoven hardening. Following the production of such a prototype a time consuming and cost-intensive characterization of the properties of nonwovens carried out experimentally has to be done. For this reason detailed studies considering several parameters of design are uneconomic.

Thus, micromechanical models of simulation are developed at Fraunhofer ITWM in cooperation with Procter & Gamble Service GmbH (P&G). By means of these models it is possible to forecast numerically the effective properties of nonwovens for diverse parameters of design. To virtually modify and optimize individual parameters in this connection it is only necessary to adapt the corresponding inputs of the computer model.

In this case, the focus of the numerical predictions is primarily lying on the time-dependent behavior of the nonwovens. The dynamic properties can be determined by means of numerical simulation of cyclic measurements. In doing so, a good correspondence of simulation and measurements is obtained. Compared to experiments the required computational time for the simulation in case of low frequencies does not change. Therefore, we can obtain rapid forecasts for the long-term behavior (month till years) and the corresponding resilience of nonwovens using numerical models. A lot of material variants can be simulated and studied within a few hours. The fact that not only effective (macroscopic) properties of nonwovens can be computed, but also local physical values such as distribution of tensile stresses in binding agents and fibres is a further advantage of this micromechanical approach. So, the simulation contributes to a better understanding of the properties of nonwovens.

Future designs deal with an extension of the models with regard to simulation of the production processes. By this, a fully digitalized layout design of nonwovens from the manufacturing process till the optimization of functionality is possible.

1 *Microstructure model of a nonwoven with a typical anisotropic distribution of fiber directions, generated at the computer*

2 *Computed local stresses in the fibers (red: high stresses, blue: low stresses), of the compressed nonwoven; these stresses are essentially influencing the properties of nonwoven.*
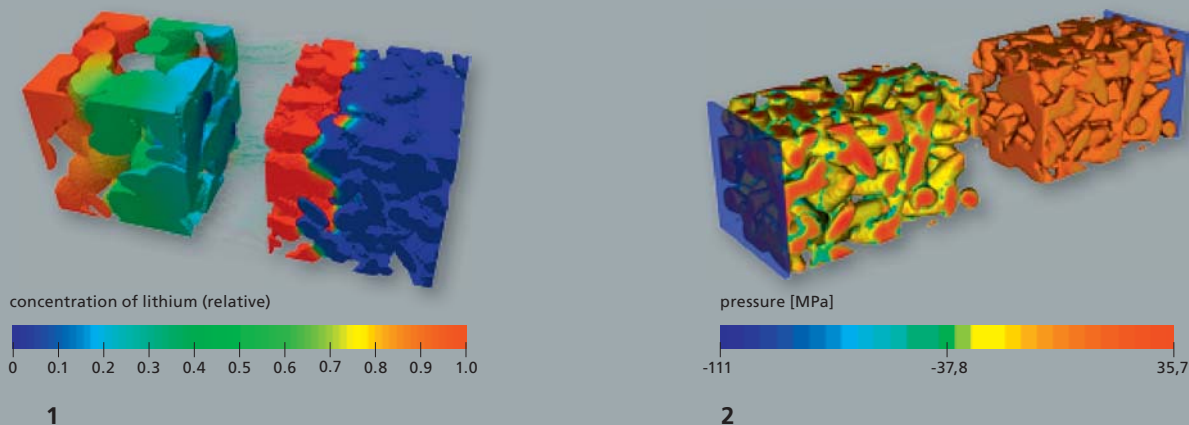
1   **2**   **3**
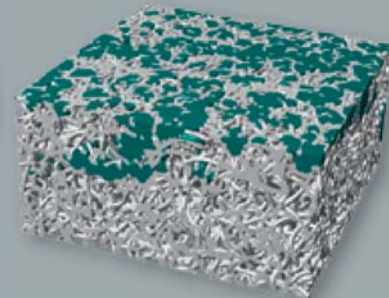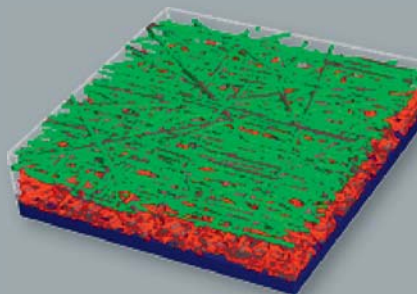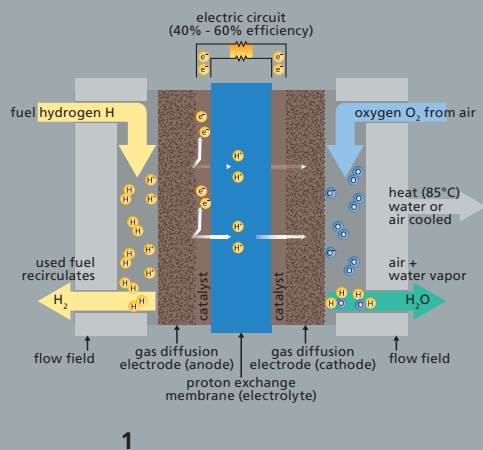
OPTIMIZATION OF THE GAS DIFFUSION LAYER TO BE USED WITH PEM-FUEL CELLS

1 *PEM fuel cells*

2 *Model of a gas diffusion layer and micro-porous layer*

3 *Porosimetry – simulation of water imbibition*

Hydrogen as an alternative energy source will play an important role in the future due to the decentralization of energy supply systems and declining oil reserves. The stored energy in hydrogen can be transformed into utilizable electric energy by fuel cells. Generally speaking, a fuel cell works as follows: molecular hydrogen, which is led to the anode, splits by disposal of two electrons into H^+-ions. While electrons are used by an external electric circuit in order to produce energy, H^+-protons diffuse to the cathode through an electrolytic membrane. At the cathode, the protons and the recirculating electrons react with oxygen from the air yielding water.

In order to guarantee optimal supply of oxygen to the cathode and removal of emerging water, a so called gas diffusion layer is installed between the cathode and the air supply channel. Usually, this layer is a nonwoven made of carbon fibers and a micro-porous layer made of carbon black. To enable water removal, the layer is made hydrophobic. Within the research cooperation 'OPTIGAA 2' supported by the BMBF, the Fraunhofer ITWM works on modelling of gas diffusion layers using the software GeoDict and computing material properties like flow resistance and effective diffusion. Change of material properties subject to varying water saturations of the diffusion layer are of special interest. Saturation dependent material parameters can be identified in an easy and efficient way by the pore morphology method.

The goal of the research cooperation is to establish the computer-aided design of fuel cells. Therefore, methods are developed in cooperation with research partners, which allow a scale transition between microstructure, fuel cell and fuel cell stacks. Consequently, material parameters of different gas diffusion layers, which are calculated at the ITWM, can be used in CFD-simulations of the fuel cell. Hence, it is possible to study the influence of different component designs on the whole cell stack.

concentration of lithium (relative)

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

1

pressure [MPa]

-111   -37,8   35,7

2

ELECTROCHEMICAL SIMULATION OF LITHIUM ION BATTERIES: VOLUME-CHANGING AND PHASE-SEPARATING ELECTRODE MATERIALS

The strong increase of electromobility demands the continued development and improvement of the key component of an electric car: the lithium ion battery as electrochemical energy storage system. To improve its life-time and reliability is a key issue which requires a profound understanding of the limiting degradation mechanisms. One major degradation effect is due to volume change by certain anode materials during intercalation of lithium ions: Silicon, for instance, which is a promising new anode material due to its high gravimetric energy density, changes its volume by 300 percent. The resulting mechanical stresses can lead to cracks within electrode material and eventually to a capacity loss.

It was the main goal of the AiF project ALIB (Expansion of lithium ion battery cells) to be able to asses these effects reliably. The electrochemical simulation models that are available in our software BEST (Battery and Electrochemistry Simulation Tool) were extended to capture the effects of volume change. It is the main purpose of BEST to compute ion and charge transport within a battery in order to make predictive statements on the battery behavior. The simulations can be performed within the 3d electrode microstructure as obtained, for instance, from imaging techniques. In a collaboration with colleagues from Helmholtz-Institute Ulm the models have been extended such that it is possible to describe the lithium-concentration-dependent change in volume as well as the build-up of mechanical stresses. Additionally the influence of the inhomogeneous stress distribution on ion transport and intercalation reaction is considered. The electrochemical-mechanical system is solved numerically by coupling the battery solver BEST to our structural mechanics solver FeelMath, which solves the mechanical equations using a highly efficient Fourier method.

Besides that, certain electrode materials display a phase-separation behavior into a lithium-rich and a lithium-poor phase for certain states-of-charge. It is believed that this enhances the effect of mechanical degradation. By adding a phase-field model we could simulate electrochemistry, mechanics and phase-separation including electrolyte and electrode microstructure in a fully coupled way. Hence it is possible to predict the mechanics-affected battery performance as well as to estimate the risk for mechanical degradation.

1 *Simulated concentration distribution within the electrode material. While ions in the left electrode move by pure diffusion, they show a phase-separation behavior in the right electrode into clearly separated lithium-rich (red) and lithium-poor (blue) phases.*

2 *Simulated distribution of pressure within the electrode matrix due to inhomogenous lithium ion distribution.*
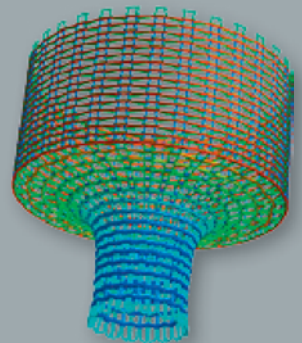
⬤➕⊖**BEST**
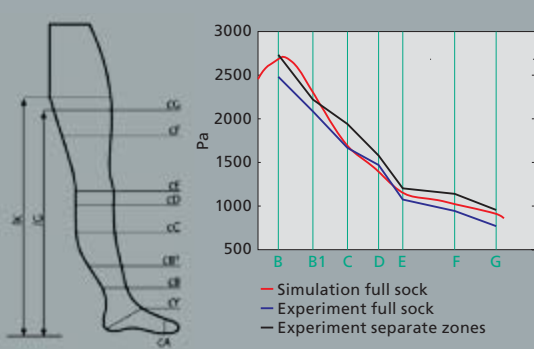
input (leg size (lenght, circumference), pressure profile)
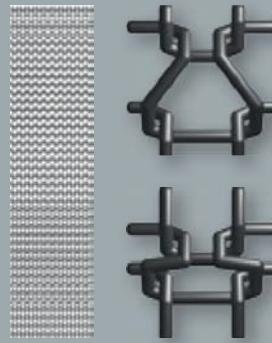
design optimization of the knitted textile

back transformation in the machine control parameters

1

MODELLING, SIMULATION AND OPTIMIZATION OF KNITTED COMPRESSIBLE STOCKINGS

**1** *Optimization of the knitting machine parameters for patient specific compressible stockings*

The company BSN medical is manufacturing different products from diverse knitted fabrics, among others tubular knitted compression stockings. The fact that despite of the same basic design diverse models can be developed from the same material is the particular characteristic of these compression stockings. An important characteristic of design of all compression stockings is that in addition to the yarn of the construction another yarn is added; only through the interaction of both yarns the final properties come into being.

 The aim of BSN Medical is to standardize and automatize the process of development that is strongly controlled by experience today. It should be possible for example that a specific compression stocking made from a newly-created material is designed virtually so that for the novel product the original characteristics of compression can be kept. Furthermore, machine parameters can be determined, to modify the compression at defined positions in case of unchanged material. Finally the possibility to design patient-specific stockings at the computer should be created. For this aim, ITWM developed special algorithms and implemented them into the own calculation tool TexMath. The numerical methods are based on the finite-element-method with non-linear truss-elements that is extended to frictional contact between yarns in this tool. The friction force is modelled by means of the Euler-Eytelwein law and the non linear problems are solved by two separate Newton procedures, for the elastic deformation and the sliding under friction force. By means of this computation programme the procedure of virtual knitting of a compression stocking is simulated and presented visually using different threads and parameters of the machine during the production. The virtual stockings resulting hereof are extended again in another simulation in order to get force-strain curves for a knitted sample. The simulated force-strain curve coincides well with the measured one. Furthermore the stocking, knitted virtually, is put on a virtual leg. This is done by means of seven measurements at seven zones of the leg along the leg's axis. Usually, on each line between every two zones, a value of the pressure on the leg is prescribed in the norms. So, for each given leg with known diameter at each of seven zones, the stocking can be verified in advance by means of the created pressure profile onto the leg.

The aim of this project is to reach a prescribed pressure profile for a deformed knitted fabric. At this, in case of indicated yarn characteristics, optimal machine parameters are searched for each zone in order to minimize the deviation of tension of the stocking with regard to the targeted pressure profile. It is a two-step procedure. In the first step, the virtual stocking is knitted and virtually put on the given leg. In the next step, the mesh size is optimized for each row in a gradient procedure, to minimize the deviation of the computed pressure profile to the wished one. The end result is a parameter set for an optimal stocking pattern.
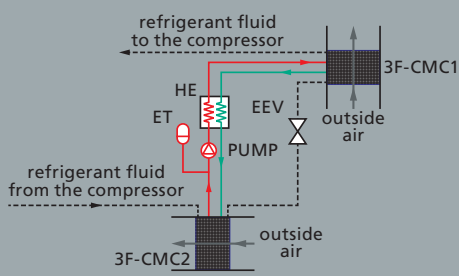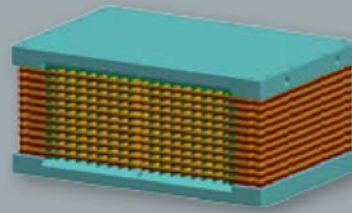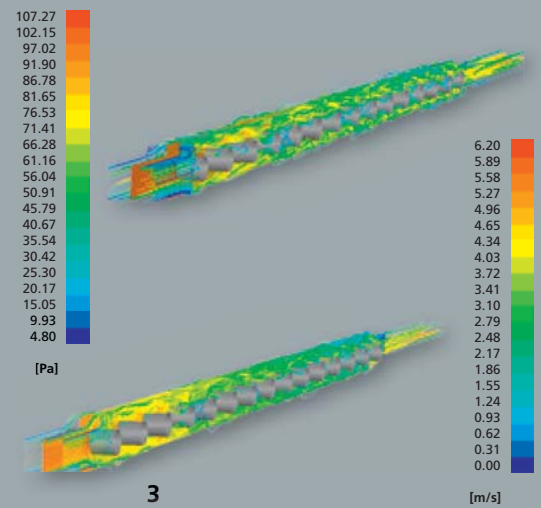
XERIC: INNOVATIVE CLIMATE-CONTROL SYSTEM FOR ELECTRIC VEHICLES

The project XERIC is funded within the Horizon 2020 EU program and aimed at developing a new climate-control system able to increase Battery Electric Vehicles (BEV) autonomy thanks to its better energy efficiency in comparison with traditional air conditioning systems. The climate-control system should be able to grant passengers' comfort in all weather conditions. The core of the system are innovative 3-Fluid-Combined Membrane Contactors (3F-CMCs) which simultaneously are crossed by air (to be sent to passengers vane), an aqueous desiccant solution (to dehumidify air) and a refrigerant (to control the desiccant temperature and partly to cool the air). Sensible and latent heat transfers between the air and the desiccant take place through a hydrophobic membrane which is permeable only to the vapour phase of water, while the refrigerant undergoes phase changes. The project partners work in close collaboration to achieve considerable power savings up to 35–40 %.

Within the project mathematical modeling and computer simulations tasks are assigned to Fraunhofer ITWM. The simulation results are used at different stages of the developments, aiming at optimizing the design and the performance of the 3F-CMC which consists of a stack of thin frames. High mechanical pressures occur due to the usage of the desiccant. High temperature gradients appear during the operation. Therefore, the first task of ITWM was to support proper sizing of the frames so that they mechanically sustain the pressures and the mechanical loads due to temperature gradients. Various studies on the mechanical stability were carried out in connection with this. Furthermore, the membranes separating air and desiccant are very thin and special spacers are used to support them in order to avoid deflection. These spacers, however, induce pressure losses in the air channel which need to be optimized also with respect to air resistance. Furthermore, simulations of heat and mass transfer processes are carried out to better understand the vapor concentration dynamics. The final task assigned to ITWM is the modeling of the frost formation. The new air conditioning system should work at a wide range of temperatures and humidity. Therefore, undesirable effects like frost formation should be studied in advance, and care should be taken to prevent them.

1 *Architecture of the air conditioning system with two 3F-CMCs*

2 *CAD design of the 3F-CMC prototype*

3 *Air pressure (top) and velocity distributions (bottom) for spacer geometry*

33