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Plant and Mechanical Engineering

Germany and in Worldwide, plant and mechanical engineering are facing a major test: in addition to solutions for CO2-neutral and digital technologies, resilient value creation structures must also be developed and deployed. We are meeting these challenges and contributing our technological expertise, for example by simulating plants or creating digital twins.

Healing Pigments Against Corrosion

Corrosion shortens the service life of metallic surfaces on aircraft and automobiles. The VIPCOAT project (Virtual Open Innovation Platform for Active Protective Coatings Guided by Modeling and Optimization), which is funded by the European Union, is looking for new solutions for corrosion protection.

Corrosion is more than rusting: it is the electrochemical reaction of base metals with oxygen or other components from the environment. To stop this process, chromates are used in aerospace, for example, but they are toxic, carcinogenic and harmful to the environment. In the search for chromate-free alternatives, the Fraunhofer ITWM contributes its expertise in the two departments "Optimization" and "Image Processing".

Project Manager Dr. Natalia Konchakova (HEREON) visited Dr. Katja Schladitz (left) and Dr. Peter Klein at the Fraunhofer ITWM.

Turning Pollutant into Advantage

The outer skin of aircraft is damaged by stone chipping, for example, and thus suffers cracks and scratches through which water penetrates. This leads to corrosion. "The idea: to turn water as a source of danger into an advantage, namely by using anti-corrosion pigments that react with water and release ions that close the crack," says Dr. Katja Schladitz from the "Image Processing" department. With each scratch, channels are created through which the water flows in, but also out again. In the process, it dissolves the anti-corrosion pigments consisting of salts from the coated outer skin of the aircraft and repairs it layer by layer. The crack virtually closes itself when the aircraft is left in the rain for a certain period of time. "Active-reactice" is the name given to this mechanism.

The VIPCOAT researchers want to find out exactly how the optimal layer is composed by reproducing the microstructure of chromate-free coatings, including the transport channels, and optimizing the composition. Information about the size, shape and arrangement of the corrosion inhibitors is obtained from 3D images taken at the German Electron Synchrotron (DESY) in Hamburg.

Detect Particles

The preparation of the paint samples and their 3D imaging are complex because the particles are very small. In order to correctly capture their shape, one has to resolve them extremely high. This end very small samples (100 µm diameter) have to be prepared and placed stably for measurement. In the resulting 3D images, the particles have to be identified. This step is also complex because the sizes vary greatly, but the gray values of different types of particles are sometimes identical or do not differ significantly from that of air.

VIPCOAT

www.itwm.fraunhofer.de/pr-vipcoat1

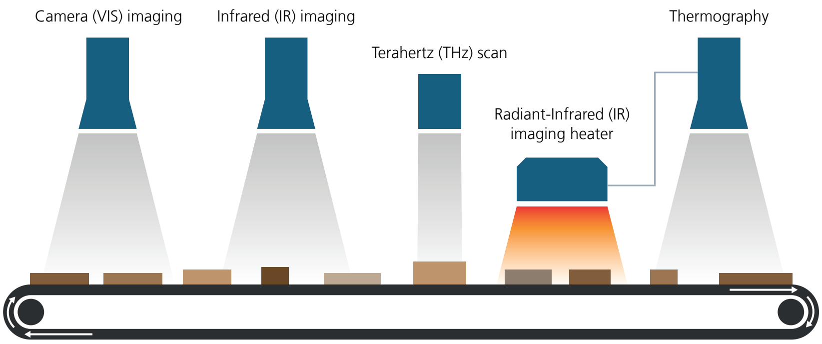
Recycling that's easy – with ASKIVIT save more wood from bulky waste

Some valuable raw materials are hidden in our bulky waste: non-ferrous metals, as well as wood and wood-based materials can be found in mountains of old cupboards. Recycling of these materials is useful from both an economic and an ecological perspective. In the "ASKIVIT" project, our researchers are developing an automated sorting system of bulky waste that is based on various imaging and processing techniques as well as artificial intelligence (AI).

In Germany alone, two million tons of bulky waste are generated every year. But not all of it is waste: depending on the regional disposal concept, up to fifty percent of the bulky waste consists of wood. This raw material is increasingly in demand; in order to protect the ecologically valuable forests from excessive deforestation, the use of waste wood is becoming more and more important.

Manual selection of wood-containing parts from bulky waste is both costly and error-prone. Our researchers in the "Material Characterization and Testing" department seek to pursue the goal of ASKIVIT project: an intelligent system that sorts bulky waste accurately and without fatigue – even without the prior shredding.

Four different imaging methods are used successively in the measurement setup. The acquired images are analyzed by AI algorithms.



Terahertz Technology Allows You to See More

Valuable raw materials are not always directly visible: the materials to be recycled are often hidden by fabrics, such as upholstery. Techniques that only look at the visible surface are therefore not sufficient when examining bulky waste. "We therefore use a terahertz sensor that also detects hidden objects," explains Dr. Dovile Cibiraite-Lukenskiene from the project team. The terahertz sensor, which is designed as a line sensor, makes it possible to scan through non-metallic covers and thus create a kind of 3D image of the object.

An important part of our scientists' research work is to adapt the sensor geometry as well as the reconstruction algorithms to the irregular conditions of the bulky waste. Therefore, at the beginning of the project, the terahertz sensor will be used on well-defined samples, and later on actual bulky waste in a sorting plant.

One Common System

In order to reliably examine bulky waste, ASKIVIT combines several techniques – and several research institutes in the process. In

> ”Utilization pressure on wood as a resource is increasing and prices are rising. The development of new sources of waste wood is therefore crucial for the raw material supply of the wood-based materials industry.”

Dr.-Ing. Jochen Aderhold
Fraunhofer Institute for Wood Research, Wilhelm Klauditz Institute, WKI

addition to our terahertz sensor, other imaging techniques are used:

- conventional imaging technology in the visible spectral range (Fraunhofer IOSB)
- near-infrared spectroscopy (Fraunhofer IOSB)
- active heat flux thermography (Fraunhofer WKI)

Initially, each institute will develop and test its own technique; the goal of the project is to combine the individual techniques into a common system. With this future system, in which four different imaging techniques are used in succession, wood-containing parts will be reliably detected and classified using artificial intelligence. The AI algorithms are contributed by the Institute for Industrial Information Technology at the Karlsruhe KIT.

Economic Advantages

”With ASKIVIT, significantly more wood will be detected in bulky waste – and with less energy and personal resources than was previously required,” explains Dr. Dovile Cibiraite-Lukenskiene. The disposal companies benefit from the cost-efficient sorting as well as the increased amount of raw materials recovered. In addition, the wood-based materials industry becomes less dependent on fresh wood and companies that produce or process materials also benefit from the broader raw material base and increased efficiency in recovered wood.

www.itwm.fraunhofer.de/ASKIVIT_en

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Product Design Revolutionized by Programmable Materials

Research gives materials new extraordinary capabilities. The Fraunhofer Cluster of Excellence Programmable Materials CPM has been ensuring this since 2018. A team of seven around PD Dr. Heiko Andrä, Deputy Head of the Department "Flow and Material Simulation", provides the appropriate mathematics, simulation and optimization expertise from Fraunhofer ITWM.

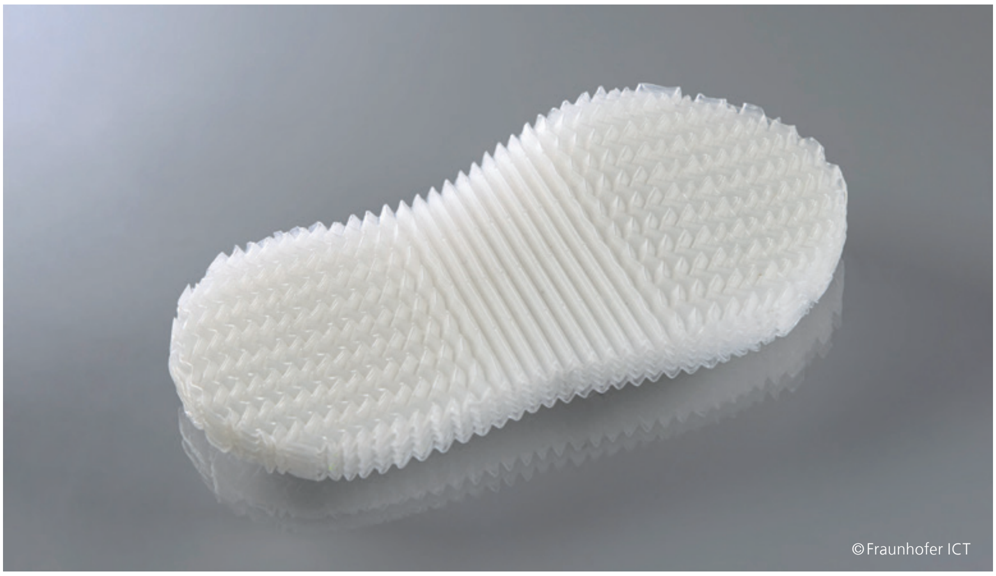
Running shoes with built-in cushioning that automatically adapts to the surface – whether forest floor or asphalt. Car seats that adapt to body tension or exterior components that quickly soften when they crash into pedestrians. Sound like dreams of the future? The cluster is about nothing less than the future of new materials.

In the Fraunhofer CPM, the competencies of various Fraunhofer institutes are bundled and work is carried out on various projects on the topic of "programmable materials". After four years, the first funding phase has ended. Since then, a lot has happened, also in the ITWM team.

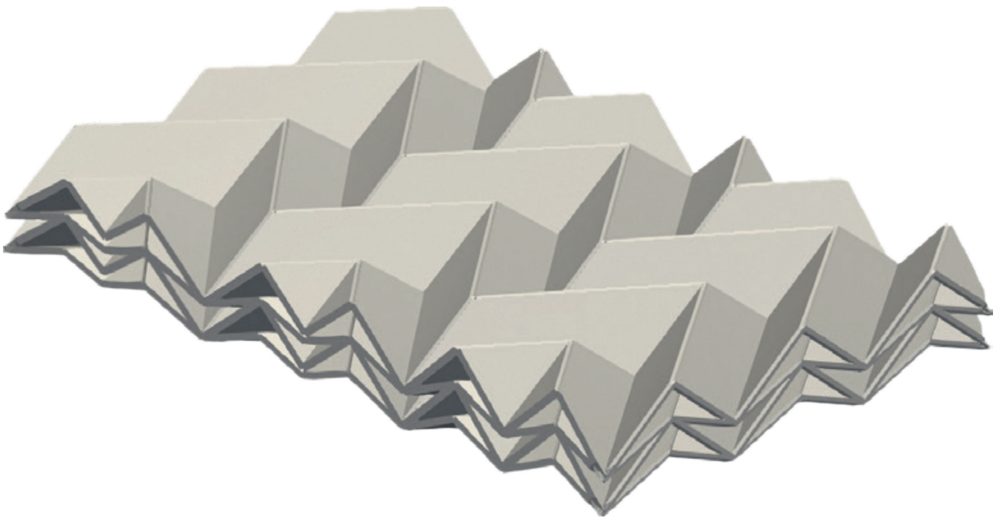
The Inner Values Count

New manufacturing processes such as 3D printing make it possible to produce targeted programmable structures in the micrometer range that have previously been developed on a computer.

In the case of "programmable materials", it is the internal structure that is important; through it, properties can be specifically controlled and the material behavior can change reversibly. Internally, they consist of a three-dimensional arrangement of many small individual cells. These serve as basic elements, are also called unit cells, and assemble them to



The Future of Materials: Product Design of a Plastic Sole Made of Programmable Material



form two- or three-dimensional lattices. In their development, the researchers are taking their inspiration from nature. Because just like there, each cell not only has its own structure, but also properties and functions that make up the material as a whole. The arrangement of thousands of cells offers options for designing novel materials with local behavior that adapts to external conditions. What makes the materials so special is that they respond to specific triggers from outside. Such switching triggers include temperature, load or humidity. But what do companies gain from this development?

Software Tools Make Developments Ready for Industry

"In our ideal scenario, an engineer comes to us with certain desired functions of the product, and our tools help to find a combination of unit cells so that the material composed of these specific unit cells performs the desired function," Andrä explains. "For this purpose, the ProgMatDesign and ProgMatSim software tools have been created in the CPM, which enable virtual experimentation by selecting and arranging the cells."

With the help of optimization methods, each individual location in the component is given different parameters. The researchers from Fraunhofer IGD, Fraunhofer IWU and Fraunhofer ITWM are providing a web-based graphical user interface (ProgMatDesign) for designing the unit cells and programmable materials – it's easier to use than usual CAD software. "We are also building a database, where all the information on unit cells can be found, effectively the blanks for building the material. Using our in-house developed tool ProgMatSim, structures with optimal design are computed and used directly as input for 3D printing." A team then prints and tests the finished material, and it is recomputed if necessary. "Because it's not quite as ideal as in the digital twins yet realizable in practice on the 3D printer. The material sometimes warps or there are other interference aspects that don't show up in the virtual twin," Andrä says. But the mathematician is confident.

Mathematical Origami Art

Fraunhofer CPM is currently working on the scientific foundations and identifying potential applications of programmable metamaterials. In the process, cross-institute teams are also creating shape-morphing materials, which look like art, such as the origami materials that take on a desired shape when you pull on them. The individual cells are folded elements made of plastic films. In his doctoral thesis, Tobias Lichti, with the support of the Fraunhofer ICT and IWM, is computing the optimum size of the fold for each cell so that the origami material finally takes on the desired shape. This would not be possible without mathematics – in the end, the folded structures are hopefully at least as useful as they are beautifully shaped.

www.itwm.fraunhofer.de/programmable_materials

Origami mathematics: The individual cells are folded elements made of plastic foils.

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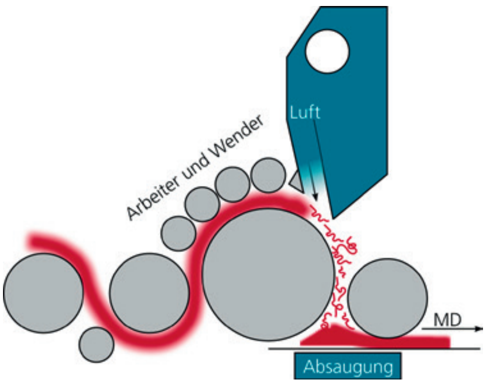
How Solutions From Our Departments "Flowed Together" in "ViDestoP"

Nonwovens are versatile and can be used in a wide range of applications – for example in medicine as protective clothing or in car interiors. Demand for the fabrics is growing, and with it the requirements for product properties. In an increasingly complex industry, the optimization of manufacturing processes is a key competence, which our researchers are addressing across departments in the "ViDestoP" project (Virtual Design and Stochastic Prototyping).

3 Departments, one project and a whole chain in view

Today, process and product optimization is usually carried out by trial-and-error tests directly on the production lines. This is a costly and time-consuming process due to the necessary production interruptions. In some areas of nonwovens production, digital twins and software solutions from our institute have already enabled virtual optimization. The interdisciplinary ViDestoP team has now extended the focus to the entire production chain.



Sketch of the airlay nonwoven production process

Simulation of Process and Product Properties

In the production of nonwovens of any kind, the interactions that occur between the fibers and air flows are particularly important for the end product. In the so-called "airlay process", individual fibers are first extracted from the plastic raw material and then swirled together by an air flow with the aid of a large cylinder. The highly turbulent air flow then deposits the fibers on a conveyor belt. There, they are compressed into a nonwoven fabric by an air suction system and further processed. Depending on the material and process properties, different nonwovens are produced in this way.

Our "Transport Processes" department has been simulating these dynamics of fibers in turbulent flows with the software FIDYST (Fiber Dynamics Simulation Tool) for years, focusing on energy consumption and fiber deposition on the conveyor belt. For the simulation of mechanical and thermal material properties, our "Flow and Material Simulation" department has also used the digital material laboratory GeoDict. The software can be used, for example, to calculate nonwoven properties such as permeability or conductivity and much more. In the ViDestoP project, these established ITWM software solutions for the process (FIDYST) and the material properties (GeoDict) were combined to form an integrated solution. Project manager Prof. Dr. Simone Gramsch emphasizes: "ViDestoP has not only closed the chain of our simulation tools, but also strengthened the connection between the departments and completely new ideas have emerged."

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Fiber Deposition as a Stochastic 3D Model Validated With 3D Printing

In the course of the process simulation, a novel 3D model was developed to represent the superimposition of the fibers, so that both the individual fiber deposition and the process parameters of the production plant are taken into account. With this model, it is possible for the first time to simulate a three-dimensional nonwoven with real thickness, width and a sufficiently large length. What then followed was new conceptual and methodological territory: to validate the simulated product properties, a team from the "Materials Characterization and Testing" department created 3D prints in various steps. Based on this work, the microscopic models of the simulations could in turn be adapted and refined. This procedure is called "stochastic prototyping", which also explains the title of the project.

Demonstrator as a Practical Test: Optimizing an Insulation Material

To prove the application of virtual design in optimizing nonwoven products, the researchers tested the process using a demonstrator. From the Design of Experiments (DoE), an optimal virtual microstructure for the insulation material was derived and validated by 3D printed fabrications. From this, clear conclusions for the manufacturing process can be derived in the industry. With this portfolio, the ViDestoP team is ideally equipped to support companies in the production of nonwovens by simulations in their questions through simulations.

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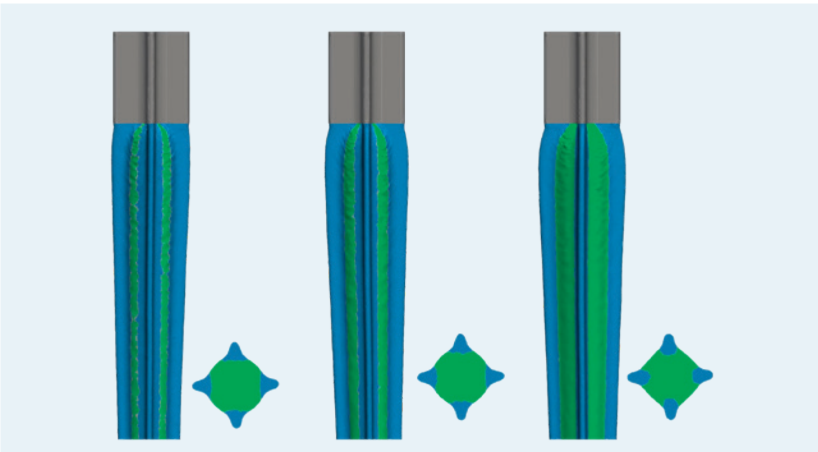
Extrusion Simulation of Bicomponent Synthetic Fibers

Not all fibers are round. But how do you make it run round anyway and spin a plastic fiber with a cloverleaf-shaped cross section, for example? A team from our department "Transport Processes" develops simulation methods for such complex tasks – our established software solutions MESHFREE and VISPI are used here.



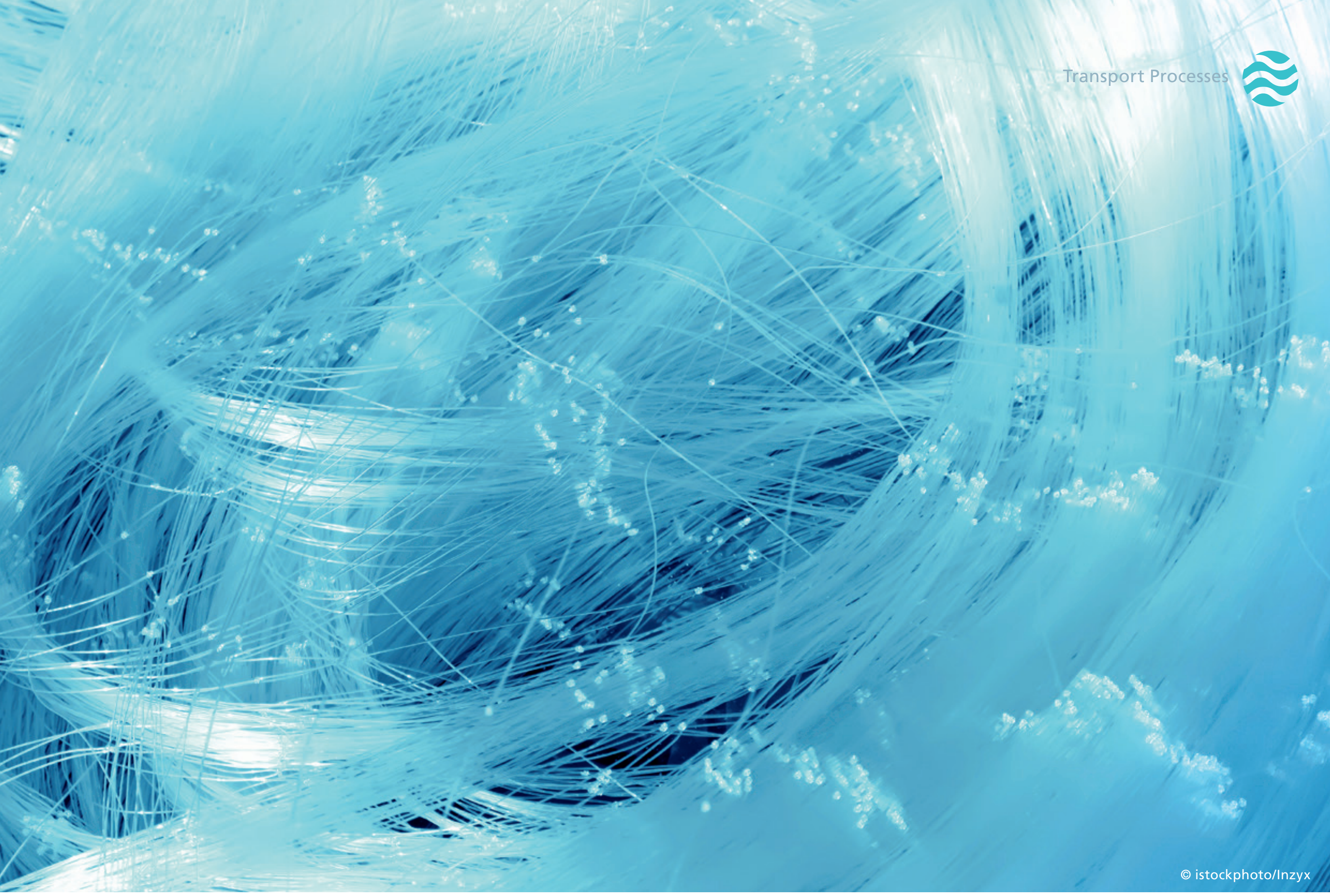
Three different BiGOFil fibers with different raw material properties: The graphic shows in each case the fiber spinning out of the die and the final fiber cross-section.

Today, everyday life without plastic fibers is unthinkable. We encounter them in almost all areas of life, whether in an oil filter or in a nonwoven medical face mask – and their composition varies depending on their function. In essence, however, they all depend on the fibers on a small scale and the production process on a large scale.

In spinning processes for the production of synthetic fibers, molten or dissolved mass is forced through fine nozzles and spun into fibers. These are usually passed through an air flow for curing. Known processes are melt spinning or dry spinning. What they all have in common is that it is always a demanding process in which all components must interact optimally. That is why our department "Transport Processes" has already developed software solutions that virtually map the spinning process as a digital twin. Such simulations save manufacturers cost- and time-intensive experiments, allow new insights and enable systematic parameter variations, which then support product design.

BiGOFil: Simulation of Plastic Fibers Using the Project Example

The work of the past decades has made our researchers world-leading experts in this field. Numerous projects have involved modeling, simulation and optimization. One example is the two-year BiGOFil project, which will be completed in 2022. Coalescence filters are used, for example, to filter fine oil droplets from an air flow. We are supporting our project partners in the development of special bicomponent fibers that are added to the filter to better drain off the collected oil. The shape of the fibers is particularly important for the



functional properties, which we can influence by designing the fine capillaries of the spinneret.

"We use two of our established ITWM tools and thus achieve an unprecedented simulation depth," says Dr. Christian Leithäuser, project manager BiGOFil. "Our VISPI solution simulates the spinning process as a whole. In the next step, our software MESHFREE is then called upon. It takes over the mesh-free detail simulations of a single fiber. In the process, several areas and properties can be taken into virtual view at the same time. For example, the temperature curve influences the shape and properties of the finished fiber.« The researchers then reflect the findings from this micro view back to the macro level: What does the fiber look like in the simulation and how must the nozzle therefore be designed?

Outlook: New Challenges From Bio-Based Materials

The portfolio expansion of the ITWM team can not only be applied to plastic fibers for filters, but may also help in the production of bio-based plastics in the future. The majority of materials produced so far are based on petroleum. That is set to change.

"One alternative, for example, is materials that are partly made from renewable raw materials and/or are biodegradable. Here, the industry is constantly looking for ways to replace the classic raw materials. Processing these novel materials is a challenge. This also requires modified production processes." Processes that the team will certainly be able to support with digital twins in the future.

www.itwm.fraunhofer.de/tv-process-design

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Process Engineering: Using AI for Industrial Processes

It is one of the great visions of the "Optimization" field: to make the next level of artificial intelligence (AI) usable for process engineering. In doing so, the researchers want to penetrate completely new regions.

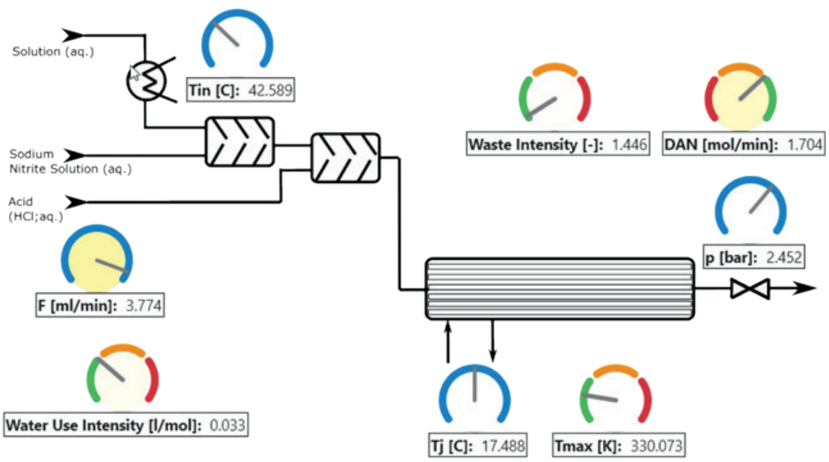
Whenever raw materials become a product, process engineering is used. Processes in this branch of industry are usually tried and tested over many years. The decision to intervene in work steps must be well thought out – wrong decisions can not only change the quality of a product, but also cause high costs.

AI Should Show Potential for Improvement Show

"AI is now very good at describing actual states," says Prof. Dr. Michael Bortz, head of the "Optimization – Technical Processes" department, and illustrates this with the example of speech recognition as used on cell phones: "It recognizes words that the user uses frequently and therefore suggests them as soon as he starts writing a certain sequence of letters. So the system is individually trained by the user and learns."

If AI is to be used to optimize production processes, there is more to it than that: optimization means finding combinations of degrees of freedom that lead to better results than those known to date. This requires rigorous physical models and optimization algorithms that come as close as possible to potential improvements. "The goal is for AI in process engineering to recognize where there is potential for improvement and thus provide the most concrete clues possible to take a closer look at specific processes," says Bortz. "Figuratively speaking: If I'm standing in the Alps and want to reach the highest point, AI should be able to tell me where to start from and how to reach the destination. Efforts to climb the second highest mountain only to see from there that there is an even higher one is not a satisfying result."

Schematic flow diagram of a chemical production process



Successful Projects Pave the Way

Bortz's team has gained experience in developing rigorous models for reliable, realistic predictions for the chemical company BASF SE, among others: In projects that have since been completed, a user-friendly interface to historical process data was created for a flowsheet simulator in order to calibrate the data for forecasts. In a current collaborative project, the aim is to use AI to numerically evaluate the processes calibrated in this way as

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The main plant of BASF SE in Ludwigshafen is the largest contiguous industrial complex in Europe. Fraunhofer ITWM is currently working with BASF SE in a joint project to realize virtual "what-if scenarios" with the help of AI.

effectively as possible, enabling users to quickly and intuitively realize virtual "what-if" scenarios. In this way, the effects of changes can be simulated before they are actually implemented.

AI Projects Underway

Bortz's team is also exploring the possibilities of AI for process engineering in the KEEN project (AI incubator labs in the process industry) – an innovation platform for the chemical industry that brings together startups, corporations and research institutions. Fraunhofer ITWM provided the first software prototypes as part of the project last year. For one of these, a neural network was trained in such a way that the software enables engineers to reverse forward planning. That is, instead of changing certain factors and then checking their impact on the product, it answers the question, "Here's what I want the product to be, how do I need to run the plant to get it?"

Bortz rates the potential of AI for process engineering as definitely high because, "In numerically complex simulations, information about where to look can save a lot of time. The more precise this information is, the more concretely we can provide assistance and optimize processes."

More information at www.itwm.fraunhofer.de/projectkeen

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