Greeting

Dear Reader

This brochure gives an overview of the diverse activities at the Aachener Verfahrenstechnik (AVT). We introduce you to the visions of the individual working groups as well as our concept of integrated chemical engineering in Aachen. On the following pages, we present our new research initiatives and themes with the overall goal to develop solutions for the global challenges of the 21st century. A particular focus is the upcoming transition from fossil to renewable resources for the production of chemicals and fuels.

The collaboration of individual chemical engineering departments, forming the AVT, is reflected in the Process Engineering Bachelor and Master programs. With respect to research, the integrated approach is most visible in large strategic research alliances and programs such as the Cluster of Excellence “Tailor-Made Fuels from Biomass” and SFB 985 “Functional Microgels and Microgel Systems”.

AVT’s vision is to develop new processes and products through interaction across disciplinary borders. Close collaborations with the Forschungszentrum Jülich and the DWI - Leibniz Institute for Interactive Materials aim at developing new synergies in science and engineering disciplines.

We hope that you will find this brochure both entertaining and informative, and that it will motivate you to visit us in Aachen. We encourage collaborations to join forces solving the urgent scientific and technological challenges of the future.

Sincerely,

Matthias Wessling
On behalf of all AVT professors and staff
With its founding, AVT is prepared to meet the present and future challenges on both the university and research level. The collective expertise and resources of the departments provide a solid basis for the wide spectrum and interdisciplinary nature of the research projects. A wide range of process engineering topics can be investigated and studied using shared resources and contacts; therefore, the AVT is an innovative and reputable research partner for all process engineering tasks.

With over 220 employees, including more than 150 in the scientific field, the AVT has become a strong presence within RWTH. This contributes to an effective representation of interests within the university, as well as the German academic landscape. New contacts are formed with research collaboration partners in Aachen, Germany, and all over the world.

In addition, the teaching program has become stronger. Process engineering lectures were successfully incorporated earlier in the mechanical engineering curriculum. Thus a broader range of students can be motivated to join the process engineering field. The Process Engineering Master course has been carefully designed and structured in such a way that the course contents are closely interrelated and integrated.

The AVT consists of the following Institutes:

- **AVT.BioVT** – Prof. J. Büchs
  Biochemical Engineering
- **AVT.CSB** – Prof. W. Wiechert
  Computational Systems Biotechnology
- **AVT.CVT** – Prof. M. Wessling
  Chemical Process Engineering
- **AVT.EPT** – Prof. A. Spieß
  Enzyme Process Technology
- **AVT.FVT** – Prof. A. Jupke
  Fluid Process Engineering
- **AVT.MST** – Prof. A. E. Ismail
  Molecular Simulations and Transformation
- **AVT.MVT** – Prof. M. Modigell
  Mechanical Process Engineering
- **AVT.SVT** – Prof. A. Mitsos
  Process Systems Engineering

**In 2007 the five independent chemical engineering institutes at the RWTH Aachen University joined together to form the “Aachener Verfahrenstechnik (AVT).” The newly founded Enzyme Process Technology department joined the AVT in 2010. A further expansion of the AVT through the Computational Systems Biotechnology department provided the basis for the cooperation with the Forschungszentrum Jülich.**

Recent changes within the AVT included the affiliation of the Chair for System Process Engineering, the Chair for Molecular Simulations and Transformations and the Chair for Fluid Process Engineering.
The AVT Research Network

**DWI - Leibniz Institute for Interactive Materials**

The AVT professors Antje Spieß and Matthias Wessling are members of the scientific board of the DWI. Hence, the AVT is working closely with the DWI by exchanging expertise and resources, forming a synergy between RWTH and the affiliated institutes.

**Forschungszentrum Jülich**

As part of the Jülich Aachen Research Alliance (JARA), the RWTH Aachen University and the Forschungszentrum Jülich have joined forces to overcome the insularity of the university and non-university research and teaching. Specific research areas have been combined in such a way that an effective complementation of expertise is possible.
Joint Projects

The AVT joins forces with several partners from research and industry to bundle their know-how, staff and equipment in order to raise scientific research onto the next level. Two of the most prominent examples are the Cluster of Excellence “Tailor-Made Fuels From Biomass” and the SFB 958 “Functional Microgels and Microgel Systems”.

Worldwide increasing carbon dioxide emissions, a rising energy demand and limited availability of fossil energy resources constitute major challenges facing society today. Renewable raw materials are attaining increasing interest in this context.

The Cluster of Excellence “Tailor-Made Fuels From Biomass” (TMFB) started in 2007 with the aim to produce new synthetic fuels from biomass. 17 institutes from RWTH Aachen University and two external partners from biology, chemistry, chemical and combustion engineering combined their knowledge to implement the vision of the cluster.

The TMFB Cluster takes an interdisciplinary research approach towards new synthetic fuels based on biomass feedstock. Novel catalytic systems, reaction solvents and tightly integrated production processes are considered to create new tailor-made fuels most efficiently. Several different production routes are targeted in order to explore new potentials for future mobility.

Within the cluster of excellence TMFB, AVT aims at the realization of the complete process chain from biomass to itaconic acid platform chemical.

The mechanical disruption of plant biomass is performed by a screw press at the AVT.MVT. This facilitates the subsequent enzymatic degradation of biopolymers, the main focus of the AVT.EPT. The degradation of plant cellulose to sugars and their fermentation to itaconic acid are simultaneous processes in a bioreactor (AVT.BioVT). Fermentation and purification processes are integrated in a membrane bioreactor (AVT.CVT). The resulting in-situ, cell-free fermentation broth is further purified through electrodialysis. In a final step, the pure itaconic acid is extracted (AVT.FVT), serving as a precursor for the synthesis of novel biofuels. For the entire process chain, AVT.SVT is involved in the model-based evaluation of reaction pathways for fuel production and the subsequent conceptual process design. In the area of product design, systematic methods are developed to predict combustion characteristics of possible fuels due to their molecular structure.

In the future, the interconnections between the individual process steps will become increasingly important to optimize the overall process in the new biorefinery.
SFB 985: Functional Microgels and Microgel Systems

Within the Collaborative Research Centre 985, we focus on microgels, a group of highly functional macromolecules that combine openness with interactive responsiveness. Microgels are promising candidates to add advanced functionality to material systems such as sensors and actuators, functionalization of surfaces or volumes, controlled uptake and release of active ingredients, or functionalization as nano-reactors. SFB 985 brings together research groups from polymer science, chemical engineering and life sciences, with three AVT chairs involved.

**Project B5 (CVT)** aims at reaction control in membrane-based microfluidic devices to control the size, topology and internal structures of microgels to produce monodisperse microgels. With the goal of scaling-up microgel production, the device design focuses on easy parallelization and operation.

In **project B6 (CVT)** membrane filtration processes for concentration, separation and purification of microgels are investigated to minimize adsorption of microgels on membranes. Particular emphasis lies in hydrodynamic conditions, membrane porosity and colloidal interactions as well as the visualization of fouling layers.

**Project C4 (CVT)** develops processes to pattern and assemble membranes with poly-electrolyte-microgel layers. Being used for molecular separations, these membranes require control of the active layer in terms of charge density while retaining selective permeability and high flux.

**Project C1 (EPT)** explores applications of responsive microgels as emulsifiers for biphasic enzyme-catalyzed reaction systems to understand relations between microgel properties and emulsion stability, influence of microgels on mass transfer and reaction or deactivation kinetics.

**Project B4 (SVT)** investigates kinetic mechanisms during microgel formation by developing a mathematical model to quantitatively predict microgel formation processes following the MEXA methodology.

Within **project G2 (SVT)**, the focus is on model-based evaluation of in-line measurements taken during microgel polymerizations to identify concentrations and particle sizes.
The establishment of the AVT as an umbrella organization for all chemical engineering departments in Aachen prompted the need for a shared facility. In this way expertise and resources can be shared more effectively. The main focus of all the AVT institutes is the process technology of renewable resources, leading to the concept of the ‘Center for Next Generation Processes and Products (NGP²)’ in Aachen.

The main focus of the NGP² research concept is to tackle the challenges evolving with the transition to renewable raw materials. Modified and complex raw materials demand for innovative process steps and process chains. Research at the AVT is characterized through its close links between fundamental research and application-oriented developments. In the planned biorefinery, process steps developed by the Cluster of Excellence „Tailor-Made Fuels from Biomass“ (TMFB) are integrated into the overall process and further optimized.

On 25th October 2010, the ‘Gemeinsame Wissenschaftskonferenz von Bund und Ländern’ allocated building funds of over 40 Mio. €. This launched the beginning of the in-depth planning phase. The construction and operation of the building has started in April 2014 and finishes in 2016.

The integrated NGP2 building will provide sufficient space for approximately 250 employees. This will include facilities not only for the AVT employees but also cooperation partners allowing more opportunities for intense collaboration. The design of the building includes centralized facilities such as workshops, analytical laboratories, seminar and conference rooms, a library, and an archive. This provides ample opportunities for informal discussions extending beyond individual departments. Apart from the centralized facilities, each department is allotted individual laboratories with respect to their specialized research projects. In this way each department is also able to focus on their individual research area.

Besides the presence of centralized facilities, each department has individually allotted laboratories, enabling the co-existence of different research branches under one roof. In this way specialized competencies of individual institutes are maintained and able to advance the state-of-the-art.

The overall initiative of the AVT is closely interlinked with the RWTH future concept, which within the framework of the Excellence Initiative, strives to realize a closer localization and networking of thematically similar research fields. As the
In 2010 the concept of ksg and Krawinkel Ingenieure for the NGP², won the competition with four other renowned competitors. In immediate locality to affiliated institutes on Campus Melaten, this new facility fulfills both the demands of the urban master plan and the functionality of a research center.

The typological structure of the building allows for the flexible usage of the available area, and provides highly efficient technical utilities, which are well structured and reach the consumer in the shortest possible way.

The external wall claddings will be covered with metal-coated panels, which on one hand reflect the external surroundings and on the other hand abstract the internal processes of the incorporated research chairs through slightly varying color shades.

The technical design implicitly conveys the majestic figure of mechanical bodywork for functional apparatus. This effect is amplified by the exposed concrete surfaces, which highlight special areas such as the three-story hall of the biorefinery, which is one of the main corner stones of the building.

Research facilities have a reputation to be purpose-oriented functional premises, where architectural design plays a subordinate role. With the VOF-success for the NGP², ksg has set new standards once more and continues a 15 year history of shaping the field of architecture for lab and institute buildings.

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Renewable raw materials such as wood and green biomass are becoming a favorable alternative to petroleum-based feedstocks. The utilization of a different feedstock, however, requires the development of tailored process concepts to fully exploit the synthesis power of nature. Such sustainable value-chains might also lead to novel functional materials and innovative products. So far, sustainable processes and renewable products play a secondary role in today’s market, which is due to a lack of fundamental process knowledge, missing innovations in equipment design and non-optimized process concepts. These aspects can be improved in the planned NGP² biorefinery.

As biorefinery processes are still in its infancy, any realization of a research-based biorefinery calls for very flexible equipment. The flexibility will be granted by modular unit operations, which can be connected to realize integrated processing setups. The unit operations are designed at the smallest scale allowing for closed recycle streams of solvents and catalysts. The investigations will demonstrate feasibility of the investigated processes and provide mass balance data to determine yields and intermediates which possibly require recycling or purging. The identification of bottlenecks helps to improve the productivity of a given process as well as to design innovative equipment. This objective is to be achieved by simulation and model-based optimization. Spectroscopic online analytics will be a key technology in order to provide in situ data of the investigated biorefinery processes.

The biorefinery will offer approximately 700 m² of experimental area. Lignocellulosic biomass such as wood, forest residues or green biomass are to be processed. The biomass is first mechanically comminuted and impregnated with catalysts and auxiliary agents. Subsequently, the molecular composite of lignin and carbohydrates is pretreated by liquid organic solvents and electrolytic media to enhance accessibility and establish fractionation. Afterwards, the carbohydrate fraction is converted by hydrolysis and fermentation into intermediates or products, while lignin is available as a byproduct. Following conversion, different downstream process steps such as distillation, membrane separation or crystallization are utilized in order to separate and purify the product from the fermentation broth and to recycle solvents, catalysts and unconverted substrate. The small-scale, flexible unit operations will also enable to estab-
lish hybrid processes and in situ product recovery for improved productivity of the biotechnological conversion.

In addition to these research objectives, the NGP² biorefinery will also constitute an attractive part of the curriculum at the AVT and a key of interdisciplinary research in NGP². Bachelor and Master students will gain first-hand experience with technical process equipment. Projects from all scientific disciplines will be involved in further improvements of biorefinery processes. The cluster of excellence “Tailor-Made Fuels from Biomass” as the current project partner is clearly the start of such multidisciplinary research and development activities which will be intensified with further partners from academia and industry.

Facts & Figures

- raw material: lignocellulosic biomass (kg-scale)
- reactor volumes: 30-100 l
- temperature: <200°C
- pressure: <20 bar
- on-line analytics: spectroscopy (Raman, MIR, NIR, NMR, UV/vis), particle analysis, chromatography
- product separation and purification, e.g. by distillation, crystallization, extraction, and membrane technology
AVT.BioVT has three main research areas: characterization of shaken culture systems, fermentation technology and development of new methods for online process monitoring at all (bioreactor) scales.

Until recently, the handling of shaken bioreactors was primarily based on empirical research. AVT. BioVT has contributed significantly to an increased understanding of the cultivation conditions in microtiter plates and shaken flasks. The acquired knowledge from process monitoring and bioreactor characterization is supposed to simply the scale-up to the future production scale. The development and commercialization of several online monitoring tools for shake flasks and microtiter plates are main achievements of AVT.BioVT. These include RAMOS (Respiration Activity Monitoring System), COSBIOS (Continuously Operated Shaken BIOreactor System), and BioLector devices. In addition, techniques for fed-batch operations for small-scale cultures (e.g. FeedBeads, FeedPlates, SmartPlates) have been developed. Another successful commercialization is the so-called Flowerplate, a screening platform, which allows for the same oxygen transfer rates as in large scale fermenters.

An additional research field of the AVT.BioVT is the development of advanced process strategies for stirred tank fermentations. An important device in this research area is an unique bioreactor with a working volume of 50 L, pressure resistance of up to 10 bar, equipped with a calorimeter, a torque measurement device for the evaluation of the specific power input and several other measurement systems for process monitoring. This pressure fermenter enables the cultivation of fast-growing microorganisms with high biomass densities (> 100 g/L) without any limitation of the oxygen transfer rate (OTR). The development of fermentation integrated product recovery is investigated in collaboration with other AVT chairs.

AVT.BioVT has many years of experience in enzyme catalysis. After founding of the Chair of Enzyme Process Technology (AVT.EPT), AVT. BioVT has shifted its research on whole cell bio-transformation in solvent-based two-phase systems.

AVT. BioVT was founded in 1996 by Prof. Dr.-Ing. Jochen Büchs. Over the course of time, the Chair has developed a unique portfolio of new methods and techniques for the development of innovative biotechnological processes. AVT.BioVT cooperates with other universities, research institutes as well as leading companies within Germany and around the world.
Next to his responsibilities at the AVT.CSB, Prof. Wiechert is director of the IBG-1: Biotechnology at Forschungszentrum Jülich. The IBG-1 is engaged in the development of biotechnological production processes for bulk and fine chemicals, pharmaceuticals and proteins. The department of “Computational Systems Biotechnology” headed by Prof. Wiechert is using a systems biology measurement platform (metabolomics, fluxomics, proteomics) in combination with engineering approaches (process systems engineering, automation, modeling) for a fast targeted process development.

At the Jülich institute, both whole cell and cell free approaches are pursued. As central tools, quantitative bioanalytic methods (metabolomics, fluxomics, proteomics) and mathematical models are developed both for a detailed characterization of the complex biochemical networks inside a living cell and for the investigation of whole bioprocesses. The rational design of enzyme toolboxes for combinatorial biosynthesis paves the way to new chiral substances in industrial biotechnology up to the future establishment of synthetic pathways (synthetic biology). These projects are complemented by the development of microfluidic devices for single cell analysis with newly developed biosensors.
Projects within AVT.CVT can be separated into four research groups: Sustainable Processes (SusPro), Electrons to Chemicals (e2chem), Physics of Fouling (PoF) und Adaptive, interactive Membranes (Adact). Fundamental research and applied sciences are part of each research group.

The projects in the SusPro research group include the development of a new enthalpy exchanger for the air conditioning in buildings, upgrading of biogas, environmentally friendly methods for water treatment and processing of renewable resources using electrodialysis and other membrane processes.

The “Electrons to Chemicals” (e2chem) research group aims at synthesizing both new membranes and membrane electrode assemblies, transforming electrons and renewable feedstock into chemicals. Specifically, electricity (from wind or solar), water and carbon dioxide are used to produce new aliphatic chemicals like methane, ethane etc.

The Adact research group aims at the production of new “adaptive, interactive membranes” and membrane based systems that are inspired by nature. This will significantly broaden membrane functionality in use today. One goal is to mimic the functionality of the glomerular barrier membrane in kidneys, and the protein rejection and salt passage by building layered architectures comprising functional polymers and cells. Such membranes will then be incorporated into miniaturized capsules in order to perform fluid contacting and molecular separations.

The “Physics of Fouling” (PoF) research group tackles the fundamental physico-chemical questions: how does membrane fouling during filtration occur, and how to prevent it? Three physical properties need to be considered: hydrodynamic conditions, particle properties and membrane characteristics. Through precise experimentation in the microfluidic domain, jamming phenomena and de-jamming during controlled flow instabilities will be elucidated.

Since 2010 Prof. Dr.-Ing. Matthias Wessling is the head of the Chair of Chemical Process Engineering (AVT.CVT). The core research field of the chair focuses on the development and application of membrane technology for current global challenges.
AVT.EPT’s primary focus is on the study of enzyme-catalyzed processes. This may range from basic research topics such as the mechanistic description of the interactions between the enzyme and the reaction medium to the interaction of reaction networks for the application of reactor design and integrated enzymatic processes.

Due to their selective catalytic effect, enzymes have an immense industrial potential in the field of fine chemicals and pharmaceutical products as well as bulk chemicals and fuels. Unlike conventional catalysts, enzymes are not only environmentally friendly and economically efficient, but may also offer a wide range of new synthetic routes. In the context of changing raw materials from petrochemicals to renewable resources, the use of selective biocatalytic processes is becoming an increasingly important key factor for sustainability.

Industry and publicly funded research projects within AVT.EPT can be categorized thematically into three groups. One group includes projects relating to the Cluster of Excellence “Tailor-Made Fuels from Biomass (TMFB)”, which addresses the enzymatic conversion of lignin and cellulose to new platform chemicals. Another focus is on the development and study of enzyme-catalyzed reactions in various reactor types and reaction media. The third group focuses on the modeling of reaction kinetics for a rational, quantitative understanding of enzyme-catalyzed processes. They are an essential prerequisite for the optimization of these processes.

There is a new impetus regarding the work of the AVT.EPT department in cooperation with the DWI - Leibniz Institute for Interactive Materials, which focuses on the control and design of enzyme-catalyzed reactions with responsive materials such as functional polymers.
Chemical products are more and more obtained from renewable resources. This change causes an increasing research demand especially for downstream and separation processes which contribute significantly to the investment and production costs and thereby determine the competitiveness of these processes.

At the chair of Fluid Process Engineering, AVT.FVT, the focus is on the development and optimization of low-temperature separation processes like extraction, crystallization, adsorption and chromatography, especially for applications based on biomass.

In the field of extraction, the main work strives to further development of simulation and design tools. With the programs developed at AVT.FVT, the operational limits and the separation efficiency of extraction columns can be predicted on the basis of single-drop experiments with the original chemical system. Recent studies on the residence time of drops in stirred compartments are carried out. Extraction in aqueous two-phase systems and reactive extraction is examined as well.
The mission of the Molecular Simulations and Transformations group is to model complex material interactions, with primary applications in the areas of renewable energy and interfacial systems. We also develop and implement new algorithms and models to further advance these goals.

Our work in renewable energy focuses mainly on the challenge of biomass dissolution. An abundant resource in nature, commercial biomass use has been hindered by our inability to efficiently reduce raw biomass into an exploitable form. As part of the Tailor-Made Fuels from Biomass Cluster of Excellence, we use both detailed molecular dynamics simulations and multiscale modeling to analyze the interactions between biomass and various solvent mixtures. Working closely with experimental colleagues, by identifying the key characteristics that lead to optimal biomass dissolution, we can develop more economically and energetically viable solvent media.

Interfacial simulations are another challenging front in the world of molecular simulations, in part because the material models usually used in such simulations have been developed for bulk simulations. The presence of the interface can lead to significant errors in the calculation of long-range electrostatic and dispersion forces, which can in turn cause potentially catastrophic wrong modeling results unless appropriate workarounds are employed. We have thus pioneered the development of multiple algorithms for the accurate calculation of these long-range forces on high-performance computing clusters. This work has enabled cutting-edge studies of wetting and spreading phenomena previously impossible with molecular simulations. We are also working on multiscale models to develop parameterization models for finite-element simulations using molecular simulations, thereby extending the capabilities of both techniques.
Mechanical Process Engineering

The Chair of Mechanical Process Engineering (AVT.MVT) is rooted in the former Chair for Mechanical Boundary Areas and the former Chair for Mathematical Methods in Chemical Engineering in the year 1992. Since 1994, Prof. Dr.-Ing. Michael Modigell is the Head of this Chair.

Research work at „Mechanical Process Engineering“ focuses on energy- and environmental technologies, rheology and the development of high resolution experimental measurement methods.

The MVT participates in two joint research projects that deal with the development of membrane based power plant processes for carbon capture and storage. Main tasks are the system development for high temperature air separation as well as process design and optimization. The simulation tools used for this purpose also find their application in the analysis of high temperature processes such as clinker-burning or the production of pigments.

Additionally the development of regenerative processes plays a role in the portfolio of MVT. In an EU funded project, biologic production of hydrogen from waste disposals is investigated, as well as its pretreatment by means of mechanical pulping.

The focus of the rheological work is on investigation of suspensions from semi solid metal alloys used in so-called thixo forming. The range of work reaches from experiments in self developed high temperature rheometers to simulate filling processes with the parameters determined in these experiments.

Fundamental research is performed on mass transport phenomena in falling liquid films. A luminescence based, non-invasive method has been developed that allows measurements of concentration distributions of absorbed gases in flowing liquids at high spatial and temporal resolutions. The results of experimental studies are used to develop mass transport models and to improve design methods for technical devices like film absorbers.
Within research cooperation programs with industrial and university partners. Ongoing research projects at AVT.SVT can be subdivided as follows:

- Major applications are processing of biomass, water desalination, polymers and (renewable) energy systems. These applications range over various time and length scales, such as the determination of promising reaction pathways for the conversion of biomass to fuels and the design of entire chemical processes using optimization methods.

The design and operation of chemical processes is challenging as different, even contradicting objectives exist, such as cost, flexibility and safety. Instead of identifying individual optima for each criterion, process design requires a comprehensive design approach. This includes computer-aided simulation and mathematical optimization.

The research of AVT.SVT covers a wide range of topics of process systems engineering, combining methods from engineering, mathematics and informatics. Our focus is on developing methods for mathematical modeling, conceptual process design, process operations and control, as well as connecting experiments and models.

Besides our fundamental research, the practical implementation and testing of the methods developed in various projects is of great importance. To this end, experimental work is being carried out within research cooperation programs with industrial and university partners. Ongoing research projects at AVT.SVT can be subdivided as follows:

- **Model-based experimental analysis**: Development of a methodology for model-based design and analysis of experiments for the modeling of kinetic phenomena in multiphase and reactive systems
- **Process synthesis**: Development of conceptual methods for model-based analysis, synthesis and optimisation of (integrated) reaction and separation processes
- **Optimisation-based process control and operations**: Methods, algorithms and applications for model-predictive control, monitoring and real time optimisation of batch and continuous polymerisation processes

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