



Issue 02|17

Dear Friends, Alumni, and Fellows of d|b|t|a,



© TU Berlin/Pressestelle/
Philipp Arnoldt

Following our initial d|b|t|a newsletter six months ago, I received a lot of positive feedback from you. Thank you! The nice responses and the upcoming d|b|t|a Alumni Meeting encouraged us to prepare the second newsletter now. During the last half year, we were able to strengthen our research efforts, present our results at numerous conferences and in dozens of conference papers and journal articles. A new mini-plant has been taken into operation in our lab, a second is under construction, and we successfully completed some projects. Of course, we also started new ones, for example an international cooperation called BIO-CM on the usage of bio-methane for chemicals production. The project is coordinated by d|b|t|a and partners from Columbia, Brazil, and Latvian are involved.

During the last few months we gave several courses in Poland, Brazil, Columbia, and Great Britain, which further increased the number of users of MOSAICmodeling and strengthened our international network. Somebody may wonder why I wrote "MOSAICmodeling". Given a brand name conflict we recently had to rechristen our software package. Beside the hard work, we also had some nice team events. For sure, the highlight was our d|b|t|a summer party on Berlin's largest lake "Müggelsee". As you can see, we have been quite active in various fields. I do look forward to meeting some of you at our first "d|b|t|a Alumni Meeting" in November. The meeting will be a nice occasion to inform you about our current research activities, refresh contacts, meeting old and new friends. To those of you who cannot attend the alumni meeting this year: We will hold the next one in two or three years time.

Kind regards,

Jens-Uwe Repke, 7th November 2017

Content

» Projects	2
» Dissertations	3
» Team	4
» d b t a International	5
» d b t a Lab	5
» Events	6
» MOSAIC News	6

SELECTED PROJECTS



» Organic Solvent Nanofiltration with Ceramic Membranes

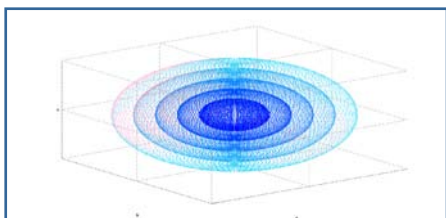
Contact: Kai Lechner

» *Process Intensification, OSN, Ceramic Membranes, Modeling, Separation* «

Liquid mixtures of organic solvents and solutes are commonly purified or concentrated through the application of common thermal separation processes such as extraction or distillation, which is by far the most widely employed unit operation for solvent regeneration. Separation is achieved by evaporating more volatile components, which results in a comparatively high energy requirement in order to attain the separation objectives. Hence, organic solvent nanofiltration (OSN) may represent an energy efficient separation technology regarding process intensification in pharmaceutical and specialty chemicals industries. However, due to the absence of thermodynamic knowledge, process understanding, and the lack of appropriate predictive tools to select nanofiltration membranes, extensive experimental screening is still required to assess the feasibility of a process within the scope of process synthesis or retrofitting. Therefore, the German Federal Ministry of Economic

Affairs and Energy funds the research project ESIMEM (03ET1279G) to reveal and investigate mass transfer principles within polymeric and ceramic membranes with the objective to develop heuristics and short-cut methods to establish nanofiltration as a widely accepted unit operation in chemical engineering.

In recent years, research has been done on the development of microporous ceramic membranes appropriate to nanofiltration applications, owing to their higher chemical and thermal resistance compared to polymeric membranes. Since the prediction of volume flux and retention of these membranes is still difficult due to uncertain interactions between membrane surface groups and permeating molecules, d|b|t|a launched filtration experiments with standardized component systems to generate reliable data in order to establish and develop a suitable mass transfer model for OSN with ceramic membranes within the ESIMEM project.



» Convergence Analysis on Large Nonlinear Equation Systems

Contact: Saskia Bublitz

» *Convergence Analysis, Process Simulation, Reformulation, Decomposition* «

Everybody, who ever tried to solve process simulation with hundreds of variables simultaneously, has probably run into convergence problems at some point. To find a good initial guess or change the system structure in order to overcome these issues can end in a time-consuming manual procedure. Fortunately, methods exist, which rearrange the system automatically. Decomposition methods split the system into smaller sub systems, called „blocks“, which can be solved simultaneously one after another. The condition number of the lower dimensional blocks typically decreases and the numerical cost is reduced. Well-known representatives are the Dulmage-Mendelsohn decomposition and the Bordered Block Transformation, which have already been implemented into MOSAICmodeling. Through automatic equation reformulation, intelligent estimation of initial values, preconditioning by scaling, and unit transformation the convergence performance can be further improved. Regarding these restructuring strategies, a method is now under develop-

ment to evaluate their efficiency. An “efficiency coefficient“ will be calculated depending on the initial guess and the model structure, which serves as a measure for the convergence probability and helps to select the most robust restructuring method for the initialized system.

Previously, a concept has been introduced to generate initial values in the environment of known solutions belonging to three-dimensional test systems, which were then examined on convergence. The initial value generation was performed on spheres as shown in the figure. The most efficient restructuring methods were found by possessing the highest convergence probability (convergent iterations/all iterations) for a constant sphere radius. This concept could be further extended to find dependencies between the convergence probability and other quantities as the condition number, the system dimension and the number of highly linked variables. Eventually, the restructuring efficiency at the initial point will be predictable by their determination.

The fruitful cooperation between dbt|a and X-Visual Technologies in Berlin is continuing with a 6 month long project "Interoperability in plant design – industry 4.0", which starts in November 2017. After successfully implementing a prototypical interface for the data exchange between X-Visual's P&ID tool PlantEngineer and the PlantDesign feature of MOSAICmodeling for creating 3D plant models, the focus is now on the development of a central data model for storing life-cycle data of chemical plants. Financial support was realized by the Transfer BONUS funding of the IBB's digitalization initiative. Improving interoperability of heterogeneous CAE tools applied in basic and detailed engineering is of major importance for the digitalization in the process industries. The goal is

As part of a project with thyssenkrupp Industrial Solutions AG, a process for the desulfurization of coke oven gas is being investigated and refined. The objective is an energy and resource efficient process that should remove hydrogen sulfide, hydrogen cyanide and sulfur dioxide simultaneously. For this purpose an experimental setup for wide catalyst screening and the identification of kinetic data was built and commissioned to investigate and improve wet oxidative desulfurization processes. Additionally, parameter estimation was carried out to gain kinetic information from experimental data. Based on nine dynamic experiments kinetic parameters of 18 reac-

Biogas is a methane-rich gas produced from the decomposition of organic residues under anaerobic conditions and commonly used as a renewable energy source. The Oxidative Coupling of Methane (OCM) alternatively enables its utilization for producing valuable base chemicals. The aim of the BIOCM project is to investigate the production of ethylene from the methane in biogas via OCM. A Bio-OCM process is being conceptualized and evaluated regarding technical, economical, and environmental aspects by a multi-disciplinary team of 4 research institutes worldwide. The 3-year project is funded through the ERANet-LAC 2nd Joint Call on Research and Innovation. Besides being

the conceptual development of a central data storage format that enables the consistent, error-free transfer of life-cycle planning data between these tools via standardized and platform independent data interfaces. Hereby, special attention is paid to a suitable change management with respect to changes in the planning procedure and the development of common namespaces and data hierarchies. First steps for developing a centralized data model are planned for storing data of dynamic process simulations, 2D diagrams, and 3D plant models, but the data model should be expandable to other planning fields like process automation or electrical planning. The project will be handled by the main developer of the MOSAICmodeling environment, Gregor Tolksdorf.

tions have successfully been identified by using a model-based parameter determination algorithm, which has been developed at dbt|a. The results from the preliminary investigations were used to design a continuous and multifunctional pilot plant, which uses - among others - a new approach for the regeneration of the reduced scrubbing solution. For the first time, a jet zone loop reactor was introduced into this type of process. First experiments show that the proof of concept is successful. With the knowledge of the process behavior a holistic process model is developed, which should be validated by experimental data.

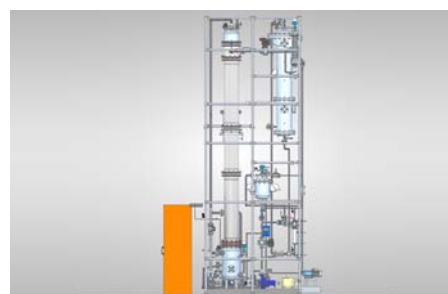
the project coordinator, dbt|a leads the work packages related to reaction and product purification. The Department of Chemical and Environmental Engineering in the National University of Colombia is focused on the synthesis of zeolites to be applied as adsorbents in gas separations. The Laboratory of Biochemical Engineering in Mauá Institute of Technology in Brazil leads the effluent treatment work package, aiming at the efficient and stable production of biogas feedstock. The Institute of Energy Systems and Environment in the Riga Technical University, Latvia, is focused on the Life Cycle Analysis and comparative studies of the process chain.



» Digitalization Project with X-Visual Technologies

Contact: Sandra Fillinger

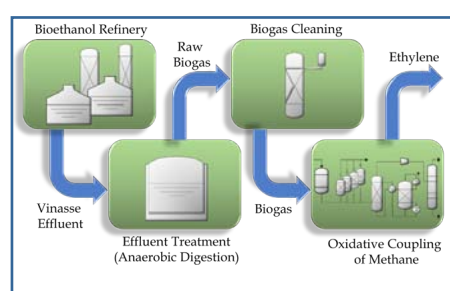
» *Digitalization, Centralized Data Model, Data Interface and Exchange, Life-Cycle Plant Data* «



» Oxisulf - Wet Oxidative Gas Desulfurization Processes

Contact: Stephan Holz

» *Gas Purification, H₂S Absorption, Liquid Phase Oxidation Processes* «



» Miniplant Reactors for Oxidative Coupling of Methane

Contact: Alberto Penteadó

» *Biogas Conversion, OCM, Green Ethylene, Cleaner Production, Renewable Resources* «

TEAM

» We welcome our new team members at d|b|t|a «



» Licianne Pimentel Santa Rosa, M.Sc.

Licianne Pimentel Santa Rosa, from the Industrial Engineering Graduate Program at the Federal University of Bahia, Brazil, is currently performing a sandwich PhD at d|b|t|a. She's developing a rigorous non-equilibrium model for a falling film absorber using MOSAIC modeling. Her PhD thesis is about modeling an industrial column containing trays, packing, and a falling film section for absorption using electrolytic solutions. Ms. Pimentel is a CAPES (Brazilian Government) scholarship grantee and the partnership between the institutions started thanks to the DAAD Summer School at UFBA in 2015.



» Joris Weigert, M.Sc.

Joris Weigert studied Energy and Process Engineering at TU Berlin. For his Master's thesis at d|b|t|a, he developed a state estimation algorithm on moving horizons supporting the real-time optimization of a hydroformylation mini-plant. In his upcoming research project, he will design a dynamic model for the chloralkali process and subsequent separation steps, which are part of the production of PVC. Based on these models, he will be able to develop an optimization environment aiming at the flexible operation of these processes.

» Happy Birthday Prof. Wozny! «

On the 1st of November the former head and founder of d|b|t|a, Professor Günter Wozny celebrated his 70th birthday. Prof. Repke and the d|b|t|a team warmly congratulate and wish him all the best for the future with interesting projects inside and outside of research. We are happy to still enjoy his regular visits at the department with good advice and always a cheerful mind. Beyond that, a special issue of the Journal Chemie Ingenieur Technik, released November 2017, is dedicated to Prof. Wozny and his outstanding contributions in the fields of chemical engineering and process systems engineering.



© TU Berlin/Pressestelle

RECENT DISSERTATIONS

On June 30th 2017, Joachim Kerber successfully defended his doctoral thesis on „Mass transfer and selectivity analysis of a dense membrane contactor for upgrading biogas“. He spent his time as a doctoral student at Prof. Repke's former group in Freiberg.

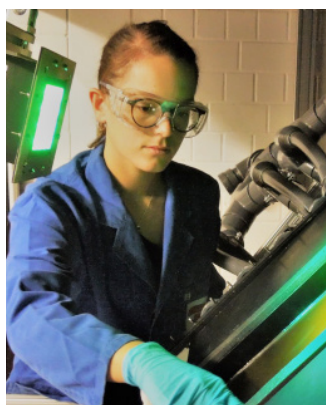
There he constructed a laboratory scale plant for his systematic investigations and also saw to a large part of the teaching. We congratulate Dr.-Ing. Kerber and wish him all the best for the future!



d|b|t|a INTERNATIONAL

International Student

Since August 2017 Martina Guidi has been working as a Master's student at d|b|t|a taking part in the Erasmus+ Programme. She studies chemical engineering at the University of Pisa in Italy and got in touch with d|b|t|a via Prof.-Ing. Elisabetta Brunazzi. Her topic is the enhanced film thickness measurement on structured packing materials for distillation and absorption columns under supervision of Hannes Leuner.



Prof. Repke in Colombia

Prof. Juarez-Romero from the Universidad Autonoma des Estado de Morelos in Cuernavanca, Mexico has been a guest at the d|b|t|a from November 2016 until January 2017. He investigates the modelling of the integrated heat exchange in absorption processes as part of an ongoing research project in Mexico.



MOSAICmodeling Workshop in Cracow

A long-standing tradition and research partnership between the TU Berlin and the Politechnika Krakowska is continuing. The 5th MOSAICmodeling workshop took place between the 18th and 29th of September 2017 in Cracow. The lectures and exercises dealt with the modeling, simulation, optimization, flowsheeting, and parameter estimation capabilities of MOSAICmodeling, which were applied to chemical and mechanical engineering themed applications.

This workshop laid the foundation for the further usage of MOSAICmodeling within a European project of the group of Prof. Michał Dyla. The workshop was organized and held by the former head of d|b|t|a, Prof. Günter Wozny, the founder of MOSAICmodeling. The first visit of Prof. Wozny already took place in June 1996 and we are looking forward to a further fruitful cooperation with the Politechnika Krakowska after more than 20 years.

d|b|t|a LAB EQUIPMENT

In this issue we will present you our rotary evaporator IKA RV10 digital V, which is used for research and lab work at our department. The rotary evaporator is meant to be used for vacuum distillation, a special distillation process under reduced pressure in the gas phase. Therefore, volatile components boil at a much lower temperatures due to the small difference between vapour and ambient pressure. Our rotary evaporator is equipped with an electrical vacuum pump reducing pressures to up to 30 mbar.

A vacuum controller recognizes changes in the vapour pressure and adjusts the vacuum automatically, which allows for operation without permanent supervision by the lab staff. The rotary evaporator is used for the TGO (Thermische Grundoperationen) lab separating an ethanol water system. Therein, students learn how to achieve high yields with different parameter settings. In another lab students distillate a caffeine solution, which has been extracted from energy drinks and coke using liquid-liquid extraction.



» IKA RV10 digital V

» Find more equipment in the next issue «

EVENTS



» Summer Party

On June 16th, 2017 d|b|t|a did a field trip to Berlin's largest lake "Müggelsee". We steered three rafts across the lake and anchored to have an extensive barbecue on the water. Although the day started out rainy, the weather remained stable throughout the rest of the day allowing for swimming and a day-long party on the rafts. Lots of laughter and fun made it an unforgettable summer event.



» Company Run 2017

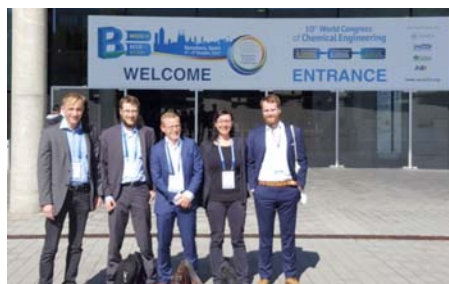
This year, d|b|t|a participated in the Berlin Company Run on June 21st, 2017. Six colleagues teamed up for the 5.5 km long race around the Tiergarten. They gave their best and have a remarkable performance to show for it. The evening faded away at one of the numerous snack bars and a well-deserved cool beer!

MOSAICmodeling NEWS

During the past six months the number of registered users of MOSAICmodeling increased from 1200 to about 1400. As part of summer schools in Salvador de Bahia (Brazil) and Cracow (Poland) many more students got into contact with the modeling, simulation, optimization, and code generation capabilities of MOSAICmodeling. Additionally, a dedicated workshop for our collaboration partner BSH Home Appliance Group was held in April, introducing them to d|b|t|a's modeling approach. As announced in the last newsletter, user-defined code generation export for optimization has been introduced, and the first unit operations in compliance to the Cape-Open standard were automatically created without manual programming interaction needed by the user. By compressing the model elements in the database, the size of the platform-independent xml models could be reduced by up to 90% - reducing the internet traffic between user and database at the same time. With the new and extended import interface the handling of result lists and variable specifications has significantly improved. Hierarchical modeling (compo-

sing systems of equation systems in a nested way) is now better reflected in the way the namespaces are introduced to equations and variables. Still on our agenda are features for handling large equation systems, such as reformulation, scaling, and further decomposition procedures and the option to display the condition numbers of (sub) systems at the initial point.

In October 2017 during the ESCAPE 27 conference in Barcelona (Spain) our group had four oral presentations featuring different aspects of MOSAICmodeling, showing the high versatility of our software in research and education.



» MOSAICmodeling at ESCAPE-27

» Find more Information on mosaic-modeling.de «

Publications

» Find recent publications of d|b|t|a members on:

www.dbta.tu-berlin.de/menue/publikationen

» Also follow us on ResearchGate:

www.researchgate.net/

Meet Us

» d|b|t|a members are joining:

- PAAT 2017
- Dt. Kälte- & Klimateagung
- ProcessNet: FluidverfahrenstechnikVT, Membranen
- ProcessNET: MPH, WSUE, CFD
- PSE 2018
- CHISA 2018
- Distillation & Absorption 2018

Edition Notice

d|b|t|a

Fachgebiet Dynamik und
Betrieb technischer Anlagen

Technische Universität Berlin
Straße des 17. Juni 135
Sekt. KWT 9
10623 Berlin

sekr@dbta.tu-berlin.de

www.dbta.tu-berlin.de

