



## Issue 01|17

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



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Philipp Arnoldt

I am pleased to present you d|b|t|a's first newsletter. Henceforth, we would like to inform you biannually about recent developments in personnel, research fields, and activities of our chair. Additionally, we hope d|b|t|a's newsletter will help intensifying the exchange with you – our friends and colleagues. Please, keep in mind that this is our very first newsletter. Any comments and suggestions on missing items and topics are always welcome. Naturally, feel free to contact me, also in case you would like to opt out of receiving the newsletter. A lot has happened since our last gathering more than a year ago and my appointment as new professor of the Process Dynamics and Operations Group (d|b|t|a). We reorganized the chair, integrated new colleagues, transferred equipment, test rigs and projects to TU Berlin, coped with ongoing projects both in Ber-

lin and Freiberg, initiated new research projects, strengthened the contacts to existing cooperation partners, and established new ones. Of course, we have also been highly active in teaching and received feedback from our students that we are offering very interesting but also challenging courses. As a special event, earlier this year, we had a first department retreat, during which we discussed and defined – amongst other things – our four strategic research clusters:

- » Transport Phenomena
- » Intensified Processes
- » Model Development
- » Methods for Process Design and Operations

I do hope, you will enjoy reading our first newsletter and find it both informative and interesting. Before closing, I would like to announce the upcoming “d|b|t|a Alumni Meeting”, which we are planning to hold in autumn this year. Further information thereon will follow soon.

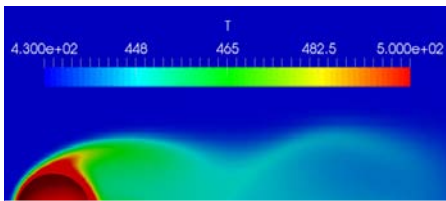
Kind regards,

Jens-Uwe Repke, 31th March 2017

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# SELECTED PROJECTS



» Numerical Investigation of Heat Transfer Mechanisms of a Spherical Particle rolling across a Flat Plate

Contact: Georg Brösigke

» *CFD, Direct Numerical Simulation, Rolling Sphere, Heat Transfer* «

The heat transfer between particles and walls has been topic of research for several decades. In most cases, existing correlations were developed empirically for special conditions and applications like fluidised beds. With a deeper fundamental understanding of the occurring heat transfer mechanisms both design of existing and development of innovative apparatuses, could be more straightforward since the mentioned existing correlations cannot be applied flawlessly to other conditions, due to specific simplifications and assumptions. The aim of this work is to investigate the fundamental heat transfer mechanisms between spherical particles rolling on a plate on the microscale with the lowest le-

vel of simplifications. For the identification of the dominating heat transfer mechanisms an approach with Computational Fluid Dynamics (CFD) simulations is chosen. The fundamental investigations are performed using a basic geometry of a moving sphere on a plate. Due to the lack of a solver, which is able to describe the system of a moving sphere on a plate, a new solver is developed in OpenFOAM®. Analogically to literature, the heat conduction through the gas layer between sphere and plate is identified as the dominating mechanism in laminar flow regime. In the ongoing work, the influence of turbulence on heat transfer is investigated via Direct Numerical Simulation.



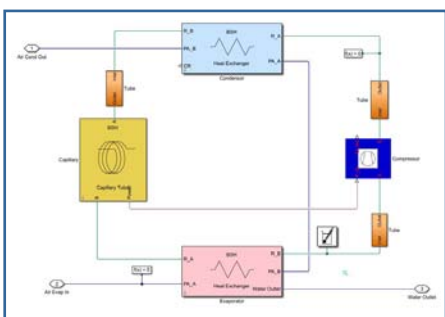
» Design and Construction of a Mobile Pilot Plant for the Absorption of CO<sub>2</sub> from Industrial Gases

Contact: Robert Wilhelm

» *Modular Pilot Plant, CO<sub>2</sub> Absorption, Process Design* «

The removal of carbon dioxide from industrial gases is of great interest and is an important technology in order to face reduction of gas emissions. One common method for the CO<sub>2</sub> removal is the application of reactive amine solutions in absorption/desorption processes. However, most available amine solutions suffer from their sensitivity to acid components and high heats for the regeneration. Therefore, a novel amine solution has been developed by thyssenkrupp Industrial solutions AG, Germany in order to increase the efficiency of the absorption/desorption process. In addition, non-optimal operation conditions for the process lead to increa-

sed costs for the whole process. Regarding changing conditions and the application of the pilot plant for novel amine solution without detailed thermodynamic knowledge require a flexible and reliable design of the process. For this purpose a modular and transportable pilot plant is designed and constructed at Process Dynamics and Operations Group. The plant can be easily assembled and transported to various industry sites. Under real operation conditions and the application of various fluid systems dynamic test campaigns at a steel mill in Duisburg are planned to gather experimental results and experience for the subsequent scale-up.



» Dynamic Process Simulation of a Heat Pump Tumble Drier

Contact: Xenia Gabrisch

» *Heat Pump, Dynamic Simulation, Two-Phase Viscosity* «

Within the scope of a project with the BSH Home Appliance Group, a dynamic process simulation of a heat pump tumble drier is to be developed. The vision will be make a model-based development of household driers possible and being able to simulate effects of e.g. new components, geometries or process control and reveal optimization potential. A long tube with very small diameter serves as throttling device within the heat pump of the tumble drier. Building a physical and predictive model of the throttle, the characteristics of the refrigerant in the two-phase region are fundamental. For the dynamic viscosity several correlations exist but there is no ge-

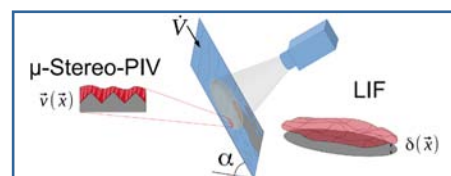
neral approach for fitting several refrigerants. Additionally, the experimental setup has an influence on which correlation matches the experimental data best. Thus, a test rig will be constructed in order to validate the model and identify the most accurate viscosity correlation for refrigerants being relevant for operation within the tumble drier. Besides, dynamic models of the remaining components of the heat pump have to be developed in order to validate the dynamic behavior. Following this, the remaining parts of the whole tumble drier are to be modeled and the whole system model is to be validated.

Several research projects at d|b|t|a focus on the experimental characterization of liquid films flowing over complex surfaces representative of structured packing material. The research aim is to gain a better understanding of fluid dynamics and mass transfer in structured packings for rectification and absorption processes, which might help enhancing their separation performance and energy efficiency. Hence, sophisticated and specifically adapted measurement techniques such as particle image velocimetry (PIV) and light-induced fluorescence are used to validate and extend ma-

D|b|t|a is part of the EU Horizon 2020 funded MEMERE-Project (see <https://www.spire2030.eu/memere>). The aim of this project and its eleven partners is to develop a new type of membrane reactor for the OCM reaction (Oxidative Coupling of Methane) - a highly exothermic and catalytic reaction where methane preferably reacts with low oxygen concentration to produce ethane and ethylene as desired products. The membrane is for dosing the oxygen along the catalytic bed, securing a selective methane conversion. A fixed-bed membrane reactor and a fluidized-bed reactor were (re-) constructed in miniplant scale at dbta.

thematical models. One investigation includes a micro PIV system to measure the velocity field inside a thin liquid film. The out of plane velocity is determined with a two-camera setup to analyse cross flow phenomena. Another project focuses on the development of a cell model to efficiently design structured packing columns based on a new measurement cell which substitutes common pilot plant scale investigations. This project is in cooperation with Prof. Grünewald from the Laboratory of Fluid Separation at the Ruhr-Universität Bochum.

These reactors enable the testing of new developed membranes and catalysts materials under real reactive conditions. The fluidized bed reactor is mainly used for catalyst screening and long-term stability tests, whereas the aim of the membrane reactor is to analyze and optimize reaction parameters and to maximize  $C_2$ -yield and  $CH_4$ -conversion. Developing a dense and yet  $O_2$ -selective membrane is a main target of the MEMERE project. The first dense membrane products have been already synthesized and tested under laboratory conditions and are currently being implemented in the miniplant reactors at d|b|t|a.



» Fundamental investigation of fluid dynamics in structured packing columns

Contact: Sören Gerke,  
Hannes Leuner

» *Liquid Film Flow, PIV, LIF, Structured Packings* «



» Miniplant Reactors for Oxidative Coupling of Methane

Contact: Tim Karsten

» *OCM, Membrane Reactors, dense/porous membranes* «

## RECENT DISSERTATIONS

### Dr.-Ing. Nataliya Yakut

January 2016, Ms Yakut defended her dissertation on "Closed-loop Realtime Experimental Design for Parameter Estimation and Model-based Design of a Man Machine Interface", which was part of the PROMETEI project and co-supervised by Prof. Wozny and Prof. Manzey.

### Dr.-Ing. Sebastian Werk

In May 2016, Mr Werk presented his work on the "Application of Key Performance Indicators for Incorporating Uncertain Constraints into Process Control". His dissertation concludes dbta's series of dissertations in the PROMETEI project and was also co-supervised by Prof. Wozny and Prof. Manzey. Mr Werk developed the DoCCE framework as part of his PhD work, which is in regular use for chan-

ce constraint evaluation at d|b|t|a.

### Dr.-Ing. Diana C. Lopéz Cárdenas

In August 2016, Ms Lopéz defended her dissertation on the "Systematic Evaluation of Ill-posed problems in Model-based Parameter Estimation and Experimental Design" supervised by Prof. Wozny. Her subset selection framework for the regularization of parameter estimation problems has also become a popular tool at d|b|t|a to support the analysis of dynamic and steady-state experiments regarding the identifiability of parameters.

### Dr.-Ing. Michael Hoyer

In November 2016, Mr Hoyer presented his work on a membrane process for the purification of uranium contaminated sewage from mining sites. During his PhD, he constructed a

lab-scale membrane plant, conducted experimental investigations on it, and developed a model for the description of the observed phenomena.

### Dr.-Ing. Hilke-Marie Lorenz

In October 2016, Ms Lorenz successfully defended her Ph.D. thesis, which deals with the plant-wide retrofit of complex chemical processes, i.e. the modification and optimization of chemical plants that already exist. Ms. Lorenz developed a systematic approach to tackle the problem as opposed to the so far established experience-based approaches. The method includes a combination of heuristics and local mathematical optimization. Consequently, a toolbox was developed that combines the strategies and interfaces process simulation software.



# TEAM

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



» Dipl.-Ing. Hannes Leuner

Hannes Leuner studied Chemical Engineering at the Dresden University of Technology, University of Aberdeen, and Purdue University. His Master's thesis dealt with the development and evaluation of a botanical air filter, which improves indoor air quality in residential buildings. As part of his Ph.D. at d|b|t|a, he investigates the hydrodynamics and mass transfer in structured packings for rectification and absorption columns. Therefore, he conducts experimental research in a DFG-funded project including the light-induced fluorescence method.



» Dipl.-Ing. Sören Gerke

Sören Jakob Gerke studied Mechanical Engineering at TU Dresden. During his diploma thesis at the chair of Measurement and Sensor System Techniques (MST) he measured near-wall liquid film flow with a laser Doppler profile sensor. At d|b|t|a, he is currently working with particle image velocimetry techniques to identify vortices in liquid films induced by complex surface geometries of micro- and macro-structured packing materials as used in structured packing columns (funded by DFG).

as used in structured packing columns (funded by DFG).



» Xenia Gabrisch, M.Sc.

Xenia Gabrisch studied Computational Engineering Science at TU Berlin and wrote her Master's Thesis at BSH Hausgeräte GmbH. Based thereon the project "Dynamic Process Simulation of a Heat Pump Tumble Drier" was initiated at d|b|t|a in cooperation with BSH. In the scope of her dissertation she will deal with the modeling of tumble driers, the experimental validation of gained models, and subsequently model-based design optimization for tumble driers.



» Saskia Bublitz, M.Sc.

Saskia Bublitz completed her Master studies in Energy and Process Engineering at TU Berlin. She was motivated by solving convergence problems of a non-equilibrium rate-based stage model for rectification processes, which she dealt within her Master's Thesis. Now, she focuses on the development of automatic reformulation techniques for nonlinear equation systems to achieve robust numerical

performance. The automatic reformulation shall be a new feature of the modeling environment MOSAIC relieving modelers of the time-consuming challenge to solve convergence problems by him- or herself.



» Kai Lechner, M.Sc.

Kai graduated in Thermal Process Engineering at Freiberg University of Mining and Technology and concluded his studies with a Master's thesis on the modeling of absorption kinetics of carbon dioxide in green solvents. Since May 2015, he has been working as a research assistant on the investigation of organic solvent nanofiltration with ceramic membranes as a process alternative for pharmaceutical and specialty chemical industrial applications and joined d|b|t|a's team in January 2017. The research project is funded by the Federal Ministry for Economic Affairs and Energy.

# d|b|t|a INTERNATIONAL

## MOSAIC Workshop in Cracow

As part of the DAAD Program “Ostpartnerschaft” another MOSAIC Workshop was held at Politechnika Krakowska in February 2016. The workshop with roughly 40 participants focused on “Process Simulation and Optimization in Chemical Engineering” and talks were given by Prof. Wozny, Dr. Esche, and exercises were supervised by Markus Illner, Tim Karsten, and Gregor Tolksdorf.



## MOSAIC Workshop in Bogota

In July 2016, Alberto Penteadó and Dr. Esche returned to the Universidad Nacional de Colombia in Bogota for a workshop on Advanced Modeling with MOSAIC. This time the focus was laid on custom model formulation and integration of MOSAIC-generated models into standard simulation software. The workshop was part of the joint DAAD PROCOL project between Prof. Alvaro Orjuela at UNdC and dbta.



## Visiting Prof. Dr. David Juárez-Romero

Prof. Juárez-Romero from the Universidad Autónoma del Estado de Morelos in Cuernavaca, 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.



# d|b|t|a LAB EQUIPMENT

At this point, we will – with each edition of the newsletter – present one of our numerous analytic devices, which are in use for student projects and research at d|b|t|a alike:

The 736 GP Titrino of Methrom is a compact, table-top titrator including operating unit, magnetic stirrer, dosing system, and autosampler. Important parameters such as injection amount, test tube capacity, drift, etc. are continuously monitored. The Titrino is also applicable for further analytic purposes, for example the Karl Fischer titration for water content or the quantification of non-ionic surfactants.

Recently, the titrator was used during the lab classes PAD (Process and

Plant Dynamics) and TGO (Thermal Unit Operations) for the determination of the carbon dioxide content in liquid samples via neutralization titration. The prepared liquid sample of a carbon dioxide-containing amine solution is dosed with barium chloride in an alkaline solution. The precipitating barium carbonate is dissolved in hydrochloric acid after washing and filtration. The amount of carbon dioxide is then determined through direct titration with sodium hydroxide solution. The measurement time for each sample is roughly 25 minutes. The associated autosampler can hold up to 16 samples, which can be measured successively without further operator interaction.



» Titrino Unit 736 GP by Methrom

» Find more equipment in the next issue «



## EVENTS



### » Students Meet Industry - Information Day

On November 24<sup>th</sup> 2016 the Process Dynamics and Operations Group (d|b|t|a) at Technische Universität Berlin hosted an information day initiated by the „Stiftung zur Förderung des Kokereiwesens in Technik und Wissenschaft“ (Foundation of the Coking Industry). The idea was to give an overview of the latest trends and prospects in the steel and coking industry together with large-scale plant construction. Experts from industry and science talked in various presenta-

tions about recent scientific topics and current issues in practice. Furthermore, graduates as well as professionals shared their experience and advice regarding their professional careers. At the subsequent get-together, students could inquire about career opportunities, discuss new technical developments, and establish new contacts with leading representatives of industry and science. The whole event attracted wide interest and shall be repeated.

## MOSAIC NEWS

2016 was quite a successful year for the MOSAIC team. The number of registered users surpassed 1200 – with a special celebration and gift for No. 1000 (see photo). In workshops in Cracow (Poland) and Bogota (Colombia) the modeling and code generation features of MOSAIC were presented with a focus on simulation and optimization in chemical engineering. MOSAIC itself made some major advancements. The server access was switched to a more secure protocol and several new features and improvements were introduced, which were released as part of MOSAIC 2.0. The new version comes with a revised user interface, a more convenient workflow, and the possibility to introduce units of measurements inside models. In 2017 we aim to extend this feature by implementing automatic dimensionality checks, guiding the user in identifying inconsistent equations. A novel “Plant-Design” feature, which enables the automatic constructive 3D design of Modular Process Units was successfully implemented as well as a cost estimation functionality for equipment and a physical property database. Additional

fields of research and development in the current year are the automatic generation and export of Unit Operations based on MOSAIC models and the possibility to create user-defined code exports for optimization. We are therefore happy to welcome Saskia Bublitz as an addition to the MOSAIC team to ensure continuation of MOSAIC’s development. You can find a presentation of Saskia in the newsletter’s “new member” section. The next MOSAIC workshop is scheduled for April at TU Berlin, during which partners from industry get an introduction into MOSAIC’s capabilities regarding modeling, system analysis, and simulation.



» 1000th MOSAIC user, Nora from Norway

» Find more Information on [mosaic-modeling.de](http://mosaic-modeling.de) «

## Publications

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

[www.dbta.tu-berlin.de/menue/publikationen](http://www.dbta.tu-berlin.de/menue/publikationen)

» Also follow us on ResearchGate:

[www.researchgate.net/](http://www.researchgate.net/)

## Meet Us

» d|b|t|a members are joining:

- AIChE Spring Meeting
- EuroPACT
- Students Meet Industry 2017
- ProcessNET: PAAT 2017
- Escape 27
- PRES'2017
- ICOM 2017

## Edition Notice

# d|b|t|a

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