

## Prof. Alexander Mitsos, Ph.D.

(\*12/10/1976, married, one child: 2010)

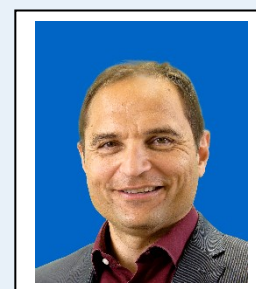
RWTH Aachen University

Aachener Verfahrenstechnik

Process Systems Engineering

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### Working group vision and contribution to catalaix

My research vision is the rational design and operation of novel chemical & energy systems using existing and/or new analysis & optimization methodologies. Our research is at the intersection of Process Systems Engineering, Energy Systems, and Computational Engineering. We work alone, in disciplinary teams and interdisciplinary teams, especially with Chemists, Biologists Mathematicians and Computer Scientists. We are at the forefront of numerical optimization and machine learning within chemical engineering.

Within catalaix, my aim is to develop tools for i) rational integrated product process for circularity and ii) integrated design of process and catalyst. To achieve this goal, I will lead the collaboration between on the one hand experts in machine learning and on the other hand technology specialists (from chemistry, biology and chemical engineering).

### Current & Previous Positions

Since 2012	<b>Full Professor (W3) and Director Process Systems Engineering (AVT.SVT)</b> , RWTH Aachen University
Since 2017	<b>Laboratory Director</b> Energy Systems Engineering (IEK-10), Forschungszentrum Jülich
2009-2012	<b>Rockwell International Assistant Professor</b> (Mechanical Engineering), Massachusetts Institute of Technology
2008-2008	<b>Junior Research Group Leader</b> (AICES), RWTH Aachen University
2006-2007	<b>Senior Engineer</b> , Cambridge (MA) USA, RES Group/Numerica Technology

### Education

2001-2006	<b>Ph.D.</b> , Paul I. Barton, Chemical Engineering with Minor in Optimization, Massachusetts Institute of Technology, Cambridge (MA) USA
1994-1999	<b>Diploma in Chemical Engineering (with distinction)</b> , Karlsruhe University, Germany

### Fellowships and Awards

2016	AICHe CAST Outstanding <b>Young Researcher Award</b>
2014	Journal of Global Optimization, <b>best paper</b>
2010	<b>Rockwell International Career Development Professor</b>
2010	<b>Best practice award</b> Research & Discovery, bioIT world
2003-2004	<b>Martin Fellow</b> for Sustainable Development
2000	Dechema Gesellschaft für Chemische Technik und Biotechnologie, <b>Price for short and efficient studies</b>

## Contributions to the science system

- Since 2000 -active member in several (inter)national professional societies, including Dechema/Processnet, American Institute of Chemical Engineers, INFORMS, Mathematical Optimization Society, Society of Industrial and Applied Mathematics, American Chemical Society, and Technical Chamber of Greece.
- member of several professional boards; e.g. deputy spokesperson for Modellgestützte Prozessentwicklung und -optimierung (Processnet) and the German academic representative to the European Computer Aided Process Engineering Working Party.
- several positions of trust in journals and professional societies, e.g., editor in the prestigious journal AAAS Science Advances and the specialized journals Journal of Global Optimization and Computers & Chemical Engineering.
- member of numerous programming committees and editorial boards; the programming chair (2020-2022) for the Computing and Systems Technology Division of the American Institute of Chemical Engineers.

## Selected Projects

- Since 2021 **Spokesperson/coordinator** DFG project SPP 2331 Machine Learning in Chemical Engineering (chemengml.org/)
- Since 2019 **Director** (for RWTH) of Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE hds-lee.de)
- Since 2016 **Director** BMBF Kopernikus-Projekt SynErgie
- Since 2012 **PI and vice-spokesperson** DFG project CRC 985 Functional Microgels and Microgel Systems

## Most important scientific contributions

1. A. L. Ziegler and C. Grutering and L. Poduschnick and A. Mitsos and L. M. Blank. "Co-feeding enhances the yield of methyl ketones". Journal of Industrial Microbiology and Biotechnology, Volume 50, Issue 1. (2023), <https://doi.org/10.1093/jimb/kuad029>.  
*Combination of experiments and simulation to improve the performance of microorganisms.*
2. A. M. Schweidtmann and J. M. Weber and C. Wende and L. Netze and A. Mitsos. "Obey validity limits of data-driven models through topological data analysis and one-class classification". Optimization and Engineering, volume 23, pages 855-876. (2022), <https://doi.org/10.1007/s11081-021-09608-0>.  
*A new method to identify the limits of machine learning models.*
3. A. M. Schweidtmann, D. Bongartz, D. Grothe, T. Kerkenhoff, X. Lin, J. Najman, and A. Mitsos. "Deterministic Global Optimization with Gaussian Processes Embedded". Mathematical Programming Computations, 13(3): 553–581. (2021), <http://DOI:10.1007/s12532-021-00204-y>.  
*A new numerical optimization algorithm that scales much better when optimizing with machine learning models.*
4. J. Burre, D. Bongartz, S. Deutz and C. Mebrahtu, O. Osterthun, R. Sun, S. Volker, A. Bardow, J. Klankermayer, R. Palkovit, and A. Mitsos. "Comparing pathways for electricity-based production of dimethoxymethane as a sustainable fuel." Energy and Environmental Science, 14: 3686–3699. (2021), <https://doi.org/10.1039/D1EE00689D>.  
*Combination of chemistry, chemical engineering and life-cycle analysis for production of synthetic fuels.*

5. A. M. Schweidtmann, J. G. Rittig, A. König, M. Grohe, A. Mitsos, M. Dahmen}, "Graph Neural Networks for Prediction of Fuel Ignition Quality". *Energy & Fuels*, volume 34, no. 9, pages 11395-11407. (2020), <https://doi.org/10.1021/acs.energyfuels.0c01533>.  
*A method for the prediction of combustion properties based on the fuel molecular structure.*
6. A. N. Ksiazkiewicz and L. Bering and F. Jung and N. A. Wolter and J. Viell and A. Mitsos and A. Pich, "Closing the 1-5  $\mu\text{m}$  Size Gap: Temperature-programmed, Fed-batch Synthesis of  $\mu\text{m}$ -sized Microgels". *Chemical Engineering Journal*, volume 379, page 122293. (2019), <http://dx.doi.org/10.1016/j.cej.2019.122293>.  
*Combination of mechanistic models, chemistry experiments and numerical simulation for optimal polymer properties.*
7. P. Joy and K. Rossow and F. Jung and H.-U. Moritz and W. Pauer and A. Mitsos and A. Mhamdi, "Model-based control of continuous emulsion co-polymerization in a lab-scale tubular reactor". *Journal of Process Control*, volume 75, pages 59-76. (2019), <https://doi.org/10.1016/j.jprocont.2018.12.014>.  
*Combination of mechanistic and data-driven models for the optimal use of a laboratory reactor.*
8. A. Tsoukalas and A. Mitsos. "Multivariate McCormick relaxations." *Journal of Global Optimization* 59.2-3: 633-662. (2014), DOI:10.1007/s10898-014-0176-0.  
*A new method for deriving convex relaxations of mathematical functions to be used in deterministic global optimization.*
9. A. Mitsos, B. Chachuat, and P. I. Barton. "McCormick-based relaxations of algorithms." *SIAM Journal on Optimization* 20.2: 573-601. (2009), <https://doi.org/10.1137/080717341>.  
*A new approach for the deterministic global optimization.*
10. A. Mitsos, I. N. Melas, P. Siminelakis, A. D. Chairakaki, J. Saez-Rodriguez, and L. G. Alexopoulos. "Identifying drug effects via pathway alterations using an integer linear programming optimization formulation on phosphoproteomic data." *PLOS Computational Biology* 5.12: e1000591. (2009), <https://doi.org/10.1371/journal.pcbi.1000591>.  
*Cooperation of systems biology and numerical optimization for the exploration of molecular effects of cancer drugs.*

## Patents

1. H. Zebian and A. Mitsos. A Double Pinch Criterion for Optimization of Regenerative Rankine Cycles. U.S. Patent 9,091,183. WO/2012/162187. May 2012.  
*Based on numerical optimization and engineering analysis, we identified how thermal power plants should be designed and operated.*
2. A. F. Ghoniem, A. Mitsos, Y. Shao-Horn, M. A. Habib, K. Mezghani, and R. Ben-Mansour. Integrated Polymeric-Ceramic Membrane Based Oxy-fuel Combustor. US Patent 9004909. 2015.  
*Combining material science, combustion, and chemical engineering, we proposed a new type of intensified unit operation combining separation and combustion.*