

LIST OF PUBLICATIONS of Gregor D. Wehinger

For more information on publication and review activities, see:

Google Scholar: <https://scholar.google.com/citations?user=fIV0a0QAAAAJ&hl=de>

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Web of Science ResearcherID: AAF-1335-2020

Publications in *peer-reviewed journals*

1. S. Flaischlen, T. Turek, G. D. Wehinger (2023) Local structure effects on hydrodynamics in slender fixed bed reactors: Spheres and rings. *Chemical Engineering Journal*, 475, 146342. <https://doi.org/10.1016/j.cej.2023.146342>
2. M. Kutscherauer, S. Anderson, S. Böcklein, G. Mestl, T. Turek, G. D. Wehinger (2023) A conjugated heat and mass transfer model to implement reaction in particle-resolved CFD simulations of catalytic fixed bed reactors. Accepted in *Engineering Applications of Computational Fluid Mechanics*, doi: 10.26434/chemrxiv-2023-cqrb6
3. G. R. George, M. Bockelmann, L. Schmalhorst, D. Beton, A. Gerstle, A. Lindermeir, G. D. Wehinger (2023) Optimization of metal foam pellet shape in packed beds for improved radial heat transfer using particle-resolved computational fluid dynamics. *Chemical Engineering and Processing - Process Intensification*, 188, 109357. <https://doi.org/10.1016/j.cep.2023.109357>
4. M. Kutscherauer, P. Reinold, S. Böcklein, G. Mestl, T. Turek, G. D. Wehinger (2023) How Temperature Measurement Impacts Pressure Drop and Heat Transport in Slender Fixed Beds of Raschig Rings. *ACS Engineering Au*, 3 (1), 45-58. <https://doi.org/10.1021/acsengineeringau.2c00039>
5. G. R. George, M. Bockelmann, L. Schmalhorst, D. Beton, A. Gerstle, A. Lindermeir, G. D. Wehinger (2022) Radial heat transport in a fixed-bed reactor made of metallic foam pellets: Experiment and Particle-resolved Computational Fluid Dynamics. *International Journal of Heat and Mass Transfer*, 197, 123376. <https://doi.org/10.1016/j.ijheatmasstransfer.2022.123376>
6. B. Kreitz, G. D. Wehinger, C. F. Goldsmith, T. Turek (2022) Microkinetic Modeling of the Transient CO₂ Methanation with DFT-Based Uncertainties in a Berty Reactor, *ChemCatChem*, 14 (18), e202200570. <https://doi.org/10.1002/cctc.202200570>
7. K. Kuhlmann, C. Sinn, J. M. U. Siebert, G. D. Wehinger, J. Thöming, G. R. Pesch (2022) From μ CT data to CFD: an open-source workflow for engineering applications. *Engineering Applications of Computational Fluid Mechanics*, 16 (1), 1706-1723. <https://doi.org/10.1080/19942060.2022.2109758>
8. S. D. Anderson, B. Kreitz, T. Turek, G. D. Wehinger (2022) Assessment of Concentration and Temperature Distribution in a Berty Reactor for an Exothermic Reaction. *Industrial & Engineering Chemistry Research*, 61 (30), 10790-10803. <https://doi.org/10.1021/acs.iecr.2c01459>
9. G. D. Wehinger (2022). Improving the radial heat transport and heat distribution in catalytic gas-solid reactors. *Chemical Engineering and Processing-Process Intensification*, 177, 108996. <https://doi.org/10.1016/j.cep.2022.108996>
10. G. D. Wehinger, F. Scharf (2022) Thermal radiation effects on heat transfer in slender packed-bed reactors: Particle-resolved CFD simulations and 2D modeling *Chemical Engineering Research and Design*. 184, 24-38. <https://doi.org/10.1016/j.cherd.2022.05.034>
11. G. D. Wehinger, M. Ambrosetti, R. Cheula, Z. B. Ding, M. Isoz, B. Kreitz, B. Kuhlmann, M. Kutscherauer, K. Niyogi, J. Poissonier, R. Réocreux, D. Rudolf, J. Wagner, R. Zimmermann, M. Bracconi, H. Freund, U. Krewer, M. Maestri (2022). Quo vadis multiscale modeling in reaction engineering? – A perspective. *Chemical Engineering Research and Design*. 184, 39-58 <https://doi.org/10.1016/j.cherd.2022.05.030>
12. G. R. George, M. Bockelmann, L. Schmalhorst, D. Beton, A. Gerstle, A. Lindermeir, G. D. Wehinger (2022). Influence of Foam Morphology on Flow and Heat Transport in a Random Packed Bed with Metallic Foam Pellets—An Investigation Using CFD. *Materials*, 15(11), 3754. <https://doi.org/10.3390/ma15113754>
13. G. D. Wehinger, B. Kreitz, C. F. Goldsmith (2022) Non-Idealities in Lab-Scale Kinetic Testing: A Theoretical Study of a Modular Temkin Reactor. *Catalysts*, 12(3), 349, <https://doi.org/10.3390/catal12030349>

14. E. A. Daymo, M. Hettel, O. Deutschmann, G. D. Wehinger (2022). Accelerating particle-resolved CFD simulations of catalytic fixed-bed reactors with DUO. *Chemical Engineering Science*, 250, 117408. <https://doi.org/10.1016/j.ces.2021.117408>
15. M. Müller, M. Kutscherauer, S. Böcklein, G. D. Wehinger, T. Turek, G. Mestl (2022). Modeling the Selective Oxidation of n-Butane to Maleic Anhydride: From Active Site to Industrial Reactor. *Catalysis Today*, 387, 82-106. <https://doi.org/10.1016/j.cattod.2021.04.009>
16. M. Kutscherauer, S. Böcklein, G. Mestl, T. Turek, G. D. Wehinger (2022) An improved contact modification routine for a computationally efficient CFD simulation of packed beds. *Chemical Engineering Journal Advances*, 9, 100197. <https://doi.org/10.1016/j.ceja.2021.100197>
17. G. D. Wehinger, N. Paul, T. Six, A. Rix, J. Knossalla, R. Franke (2022) Instabilities in fixed bed reactors with downwards directed flow for the oligomerization of 1-butene. *Chemie Ingenieur Technik*. 94 (5), 663-670, <https://doi.org/10.1002/cite.202100165>
18. J. Friedland, M. Börnhorst, B. Kreitz, E. Moioli, G. D. Wehinger (2022) NaWuReT Colloquium: From PhD student to assistant professor – Early career chemical engineers in academia. *Chemie Ingenieur Technik*. 94 (5), 629-633, <https://doi.org/10.1002/cite.202100200>
19. B. Kreitz, K. Sargsyan, K. Blöndal, E. J. Mazeau, R. H. West, G. D. Wehinger, T. Turek, Goldsmith (2021). Quantifying the Impact of Parametric Uncertainty on Automatic Mechanism Generation for CO₂ Hydrogenation on Ni (111). *JACS Au*, 1, 1656-1673 <https://doi.org/10.1021/jacsau.1c00276>
20. E. Prumbohm, M. Becker, S. Flaischlen, G. D. Wehinger, T. Turek (2021) Flow field designs developed by comprehensive CFD model decrease system costs of vanadium redox-flow batteries. *Journal of Flow Chemistry*, 11, 461-481. <https://doi.org/10.1007/s41981-021-00165-2>
21. M. Börnhorst, J. Friedland, B. Kreitz, E. Moioli, G. D. Wehinger (2021). NaWuReT Workshop: Research in Reaction Engineering for and with Society. *Chemie Ingenieur Technik*. 93 (7), 1210-1213. <https://doi.org/10.1002/cite.202100017>
22. G. R. George, M. Bockelmann, L. Schmalhorst, D. Beton, A. Gerstle, L. Torkuhl, A. Lindermeir, G. D. Wehinger (2021). Workflow for computational fluid dynamics modeling of fixed-bed reactors packed with metal foam pellets: Hydrodynamics. *AIChE Journal*, e17284. <https://doi.org/10.1002/aic.17284>
23. G. D. Wehinger (2021). Young Scientists – Introducing Assistant Professor Gregor D. Wehinger. *Chemie Ingenieur Technik*. 93 (7), 1049-1057 <https://doi.org/10.1002/cite.202100039>
24. L. J. Frey, D. Vorländer, H. Ostsieker, D. Rasch, J. L. Lohse, M. Breitfeld, J. H. Grosch, G. D. Wehinger, J. Bahnemann, R. Krull (2021). 3D-printed micro bubble column reactor with integrated microsensors for biotechnological applications: From design to evaluation. *Scientific Reports*, 11 (1), 1-14. <https://doi.org/10.1038/s41598-021-86654-9>
25. B. Kreitz, G. D. Wehinger, C. F. Goldsmith, T. Turek (2021). Microkinetic Modeling of the CO₂ Desorption from Supported Multifaceted Ni Catalysts. *The Journal of Physical Chemistry C*, 125 (5), 2984-3000. <https://doi.org/10.1021/acs.jpcc.0c09985>
26. A. Schmidt, V. Montenegro, G. D. Wehinger (2021) Transient CFD Modeling of Matte Settling Behavior and Coalescence in an Industrial Copper Flash Smelting Furnace Settler. *Metallurgical and Materials Transactions B*, 52 (1), 405-413 <https://doi.org/10.1007/s11663-020-02026-0>
27. T. Eppinger, G. D. Wehinger (2021) A generalized contact modification for fixed-bed reactor CFD simulations. *Chemie Ingenieur Technik*, 93 (1-2), 143-153, <https://doi.org/10.1002/cite.202000182>
28. S. Flaischlen, M. Kutscherauer, G. D. Wehinger (2021) Local Structure Effects on Pressure Drop in Slender Fixed Beds of Spheres. *Chemie Ingenieur Technik*, 93 (1-2), 273-281 <https://doi.org/10.1002/cite.202000171>
29. N. Jurtz, S. Flaischlen, S. C. Scherf, M. Kraume, G. D. Wehinger (2020) Enhancing the Thermal Performance of Slender Packed Beds Through Internal Heat Fins. *Processes*, 8 (12), 1528, <https://doi.org/10.3390/pr8121528>
30. B. Kreitz, J. Brauns, G. D. Wehinger, T. Turek (2020). Modeling the Dynamic Power-to-Gas Process: Coupling Electrolysis with CO₂ Methanation. *Chemie Ingenieur Technik*, 92 (12), 1992-1997, <https://doi.org/10.1002/cite.202000019>
31. C. Sinn, F. Kranz, J. Wentrup, J. Thöming, G. D. Wehinger, G. R. Pesch (2020). CFD Simulations of Radiative Heat Transport in Open-Cell Foam Catalytic Reactors. *Catalysts*, 10 (6), 716. <https://doi.org/10.3390/catal10060716>
32. D. Emmel, J. Hofmann, T. Arlt, I. Manke, G. D. Wehinger, D. Schröder (2020) Understanding the Impact of Compression on the Active Area of Carbon Felt Electrodes for Redox Flow Batteries,

ACS Applied Energy Materials, 3 (5), 4384-4393 <https://doi.org/10.1021/acsaem.0c00075>

33. N. Jurtz, G. D. Wehinger, U. Srivastava, T. Henkel, M. Kraume (2020) Validation of pressure drop prediction and bed generation of fixed-beds with complex particle shapes using DEM and CFD, *AIChE Journal*, 66 (6), e16967, <https://doi.org/10.1002/aic.16967>
34. G. D. Wehinger, B. Kreitz, A. Nagy, T. Turek (2020) Characterization of the modular ILS Temkin reactor with experiments and computational fluid dynamics simulations, *Chemical Engineering Journal*, 389, 124342 <https://doi.org/10.1016/j.cej.2020.124342>
35. G. D. Wehinger, S. Flaischlen (2019) Computational Fluid Dynamics Modeling of Radiation in a Steam Methane Reforming Fixed-Bed Reactor, *Industrial & Engineering Chemistry Research*, 58, 31, 14410-14423 <https://doi.org/10.1021/acs.iecr.9b01265>
36. G. D. Wehinger, S. T. Kolaczkowski, L. Schmalhorst, D. Beton, L. Torkuhl (2019) Modeling fixed-bed reactors from metal-foam pellets with detailed CFD, *Chemical Engineering Journal*, 373, 709-719 <https://doi.org/10.1016/j.cej.2019.05.067>
37. S. Flaischlen, G. D. Wehinger (2019) Synthetic Packed-Bed Generation for CFD Simulations: Blender vs. STAR-CCM+, *ChemEngineering*, 3 (2), 52 <https://doi.org/10.3390/chemengineering3020052>
38. O. Deutschmann, R. Dittmeyer, J. Grunwaldt, G. Kolb, S. Löbbecke, G. D. Wehinger (2019), Trendbericht Technische Chemie, *Nachrichten aus der Chemie*, 67, 50-58 <https://doi.org/10.1002/nadc.20194088095>
39. E. Prumbohm, G. D. Wehinger (2019) Exploring Flow Characteristics in Vanadium Redox-Flow Batteries: Optical Measurements and CFD Simulations, *Chemie Ingenieur Technik*, 91 (6), 900-906 <https://doi.org/10.1002/cite.201800164>
40. B. Kreitz, J. Friedland, R. Güttel, G. D. Wehinger, T. Turek (2019) Dynamic Methanation of CO₂ – Effect of Concentration Forcing, *Chemie Ingenieur Technik*, 91(5), 576-582 <https://doi.org/10.1002/cite.201800191>
41. G. D. Wehinger (2019) Radiation Matters in Fixed-Bed CFD Simulations, *Chemie Ingenieur Technik*, 91 (5), 583-591 <https://doi.org/10.1002/cite.201800179>
42. B. Kreitz, G. D. Wehinger, T. Turek (2019) Dynamic simulation of the CO₂ methanation in a micro-structured fixed-bed reactor, *Chemical Engineering Science*, 195, 541-552 <https://doi.org/10.1016/j.ces.2018.09.053>
43. N. Jurtz, M. Kraume, G. D. Wehinger (2019) Advances in fixed-bed reactor modeling using particle-resolved computational fluid dynamics (CFD), *Reviews in Chemical Engineering*, 35 (2), 139-190 <https://doi.org/10.1515/revec-2017-0059>
44. A. Buße, M. Klee, G. D. Wehinger, T. Turek, G. Brenner (2017) 3D Modeling of a Catalyst Layer with Transport Pores for Fischer-Tropsch Synthesis, *Chemie Ingenieur Technik*, 89 (10), 1385-1390 <https://doi.org/10.1002/cite.201700066>
45. G. D. Wehinger, F. Klippe, M. Kraume (2017) Modeling pore processes for particle-resolved CFD simulations of catalytic fixed-bed reactors. *Computers & Chemical Engineering*, 101, 11-22 <https://doi.org/10.1016/j.compchemeng.2017.02.029>
46. G. D. Wehinger, C. Fütterer, M. Kraume (2017) Contact modifications for CFD simulations of fixed-bed reactors: cylindrical particles, *Industrial & Engineering Chemistry Research*, 56 (1), 87-99 <https://doi.org/10.1021/acs.iecr.6b03596>
47. G. D. Wehinger, M. Kraume (2017) CFD als Designtool für Festbettreaktoren mit kleinem Rohr-zu-Pelletdurchmesser-Verhältnis: Heute oder in Zukunft? *Chemie Ingenieur Technik*, 89 (4), 447-453 <https://doi.org/10.1002/cite.201600155>
48. G. D. Wehinger, M. Kraume, V. Berg, K. Mette, M. Behrens, R. Schlögl, O. Korup, R. Horn (2016) Investigating dry reforming of methane with spatial reactor profiles and particle-resolved CFD simulations, *AIChE Journal*, 62(12), 4436-4452 <https://doi.org/10.1002/aic.15520>
49. G. D. Wehinger, H. Heitmann, M. Kraume (2016). An artificial structure modeler for 3D CFD simulations of catalytic foams, *Chemical Engineering Journal*, 284, 543–556 <https://doi.org/10.1016/j.cej.2015.09.014>
50. T. Eppinger, G. D. Wehinger, N. Jurtz, R. Aglave, M. Kraume (2016) A numerical optimization study on the catalytic dry reforming of methane in a spatially resolved fixed-bed reactor. *Chemical Engineering Research and Design*, 115, 374-381 <https://doi.org/10.1016/j.cherd.2016.09.007>
51. G. D. Wehinger, T. Eppinger, M. Kraume (2015) Evaluating catalytic fixed-bed reactors for dry reforming of methane with detailed CFD, *Chemie Ingenieur Technik*, 87 (6), 734-745 <https://doi.org/10.1002/cite.201400153>

52. G. D. Wehinger, T. Eppinger, M. Kraume (2015) Detailed numerical simulations of catalytic fixed-bed reactors: Heterogeneous dry reforming of methane, *Chemical Engineering Science*, 122, 197-209 <https://doi.org/10.1016/j.ces.2014.09.007>
53. G. D. Wehinger, T. Eppinger, M. Kraume (2014) Fluidic effects on kinetic parameter estimation in lab-scale catalysis testing—A critical evaluation based on computational fluid dynamics. *Chemical Engineering Science*, 111, 220-230 <https://doi.org/10.1016/j.ces.2014.02.025>
54. T. Eppinger, G. Wehinger, M. Kraume (2014) Parameter optimization for the oxidative coupling of methane in a fixed bed reactor by combination of response surface methodology and computational fluid dynamics, *Chemical Engineering Research and Design*, 92 (9), 1693-1703 <https://doi.org/10.1016/j.cherd.2013.12.017>
55. G. D. Wehinger, J. Peeters, S. Muzaferija, T. Eppinger, M. Kraume (2013). Numerical simulation of vertical liquid-film wave dynamics. *Chemical Engineering Science*, 104, 934-944 <https://doi.org/10.1016/j.ces.2013.10.027>

Book chapters, conference proceedings, and monographs with DOI

1. G. D. Wehinger (2023) Computational Fluid Dynamics. In *Kirk-Othmer Encyclopedia of Chemical Technology*. John Wiley & Sons, Inc. <https://doi.org/10.1002/0471238961>
2. S. Flaischlen, J. Martin, B. Kreitz, T. Turek & G. D. Wehinger (2020). Computational Fluid Dynamics Simulation of CO₂ Methanation in a Fixed-bed Profile Reactor. In *Computer Aided Chemical Engineering*, 48, 499-504. Elsevier. <https://doi.org/10.1016/B978-0-12-823377-1.50084-7>
3. B. Kreitz, G. D. Wehinger, F. Goldsmith & T. Turek (2020). Development of a Microkinetic Model for the CO₂ Methanation with an Automated Reaction Mechanism Generator. In *Computer Aided Chemical Engineering*, 48, 529-534. Elsevier. <https://doi.org/10.1016/B978-0-12-823377-1.50089-6>
4. G. D. Wehinger & S. Flaischlen (2020). Studying Computational Fluid Dynamics in a New Dimension with Virtual Reality. In *Computer Aided Chemical Engineering*, 48, 2041-2046. Elsevier. <https://doi.org/10.1016/B978-0-12-823377-1.50341-4>
5. G. D. Wehinger, U. Kunz, T. Turek (2018) *Reaktoren für spezielle technisch-chemische Prozesse: Elektrochemische Reaktoren*, in Handbuch Chemische Reaktoren, W. Reschetilowski (Ed.), Springer-Verlag GmbH, Deutschland https://doi.org/10.1007/978-3-662-56444-8_37-1
6. G. D. Wehinger (2016) *Particle-resolved CFD simulations of catalytic flow reactors*, Dissertation, Technische Universität Berlin, <http://dx.doi.org/10.14279/depositonce-5432>

Presentations at scientific conferences as speaker since 2017

1. G. D. Wehinger, T. Six, N. Paul, A. Rix, J. Knossalla, R. Franke (2023) Determining stable/unstable flow conditions in fixed bed reactors with downwards directed flows, *14th ECCE and 7th ECAB*, Berlin, Germany
2. G. D. Wehinger, N. Paul, T. Six, A. Rix, J. Knossalla, R. Franke (2022) Characterization of Stable Flow Conditions in Fixed Bed Reactors with Downwards Directed Flows, *AICHE Annual Meeting 2023*, Phoenix, AZ, USA
3. G. D. Wehinger, F. Scharf (2021) Heat Transfer in Slender Packed bed reactors: Effect of Radiation, *XXIV International Conference on Chemical Reactors (ChemReactor-24)*, online
4. G. D. Wehinger, N. Paul, T. Six, A. Rix, J. Knossalla, R. Franke (2021) Instabilities in fixed bed reactors with downwards directed flows for the oligomerization of 1-Butene, *ProcessNet Annual Meeting Reaction Engineering*, online
5. G. D. Wehinger & S. Flaischlen (2020) Using Virtual Reality to Gain Deeper Insights into Transport Phenomena in Process Engineering, *2020 Virtual AICHE Annual Meeting*, online
6. G. D. Wehinger & S. Flaischlen (2020) Studying Computational Fluid Dynamics in a New Dimension with Virtual Reality, *ESCAPE 30 Virtual Symposium*, online
7. G. D. Wehinger (2020) CFD simulations of thermal radiation in particle-resolved fixed-bed reactors, *ProcessNet Jahrestreffen CFD 2020*, Bamberg, Germany
8. G. D. Wehinger, S. T. Kolaczkowski, D. Beton, L. Schmalhorst, L. Torkuhl (2019) CFD model and experiments of fixed-bed reactors from metal-foam pellets, *ICOSCAR6*, Bad Herrenalb, Germany
9. G. D. Wehinger (2019) The Effect of Radiation in Particle-Resolved CFD Simulations of Fixed-Bed Reactors, *NASCRE4*, Houston, TX, USA

10. G. D. Wehinger (2019) Reactor modeling using particle-resolved computational fluid dynamics (CFD), invited talk at the *CFD Workshop* at *NASCRE4*, Houston, TX, USA
11. G. D. Wehinger, N. Jurtz, T. Eppinger, M. Kraume (2019) Was kann CFD leisten? Eine Bestandsaufnahme am Beispiel der rigorosen ortsauflösten Modellierung von Festbettreaktoren, *ProcessNet Jahrestreffen CFD 2019*, Frankfurt a.M., Germany
12. G. D. Wehinger, S. T. Kolaczkowski, D. Beton, R. Kolenbach, L. Torkuhl (2018) Digital Twins for exploring metal foams used as structured catalyst support, *Siemens Simcenter Conference 2018*, Prag, Czech Republic
13. G. D. Wehinger (2018) Particle-resolved modeling of fixed-bed reactors: Is this the silver bullet? Invited talk at *Evonik Catalysis Conference 2018*, Hanau, Germany
14. G. D. Wehinger (2018) Particle resolved CFD simulations of fixed bed reactors: pain or gain? Invited talk at *BASF R&D Reaction Engineering Colloquium*, Ludwigshafen, Germany
15. G. D. Wehinger (2018) Shaping transport phenomena inside fixed bed reactors, invited talk at *NaWuReT & YounGeCatS Summerschool 2018*, Frankfurt a.M., Germany
16. G. D. Wehinger, S. T. Kolaczkowski, D. Beton, R. Kolenbach, L. Torkuhl (2018) Particle-resolved CFD simulations of metal foams used as structured catalyst support, *ISCRE 25*, Florence, Italy
17. G. D. Wehinger (2018) Hanns Hofmann Award Lecture: Detailed modeling of fixed bed reactors – Challenges and applications, *ProcessNet Jahrestreffen Reaktionstechnik 2018*, Würzburg, Germany
18. G. D. Wehinger (2018) Modeling fixed-bed reactors with particle-resolved computational fluid dynamics (CFD), invited talk at *BIMoS Day*, TU Berlin und Berlin International Graduate School in Model and Simulation based Research (BIMoS), Berlin, Germany

In addition, I was invited to give talks at scientific colloquia at the following universities:

1. Karlsruhe Institute of Technology, invited by Prof. Grunwaldt, 2023
2. Clausthal University of Technology, invited by Prof. Langefeld, 2022
3. Helmut-Schmidt-Universität/UniBw H, invited by Prof. Schatz, 2022
4. Karlsruhe Institute of Technology, invited by Prof. Enders, 2022
5. TU Berlin, invited by Prof. Vrabec, 2022
6. RWTH Aachen, invited by Prof. Palkovits, 2021
7. Otto-von-Guericke Universität Magdeburg, invited by Prof. Sundmacher, 2021
8. TU Berlin, invited by Prof. Riediger, 2021
9. TU Bergakademie Freiberg, invited by Prof. Aneziris, 2020
10. Karlsruhe Institut für Technologie, invited by Prof. J. Sauer, 2019
11. Universität Bremen, invited by Prof. Thöming, 2019
12. Leibniz Universität Hannover, invited by Prof. Scheper, 2019
13. TU Clausthal, invited by Prof. Endres, 2018
14. FAU Erlangen-Nürnberg, invited by Prof. Freund, 2018
15. Karlsruhe Institut für Technologie, invited by Prof. Deutschmann, 2014