

LIST OF PUBLICATIONS

Monographs and Book Contributions

- [P1] Zeiser, T.; Freund, H.; Bernsdorf, J.; Lammers, P.; Brenner, G.; Durst, F.: *Detailed Simulation of Transport Processes in Reacting Multi-Species Flow Through Complex Geometries by Means of the Lattice Boltzmann Method*, (in: Krause, E.; Jäger, W. (Eds.), *High Performance Computing in Science and Engineering '01*), Springer, Berlin (2002) 442-452.
- [P2] Zeiser, T.; Freund, H.; Bernsdorf, J.; Brenner, G.; Durst, F.: *CFD Calculations of Flow, Dispersion and Chemical Reactions in Fixed Bed Tubular Reactors Using the Lattice Boltzmann Method*, (in: Breuer, M.; Durst, F.; Zenger, C. (Eds.), *High Performance Scientific and Engineering Computing, Lecture Notes in Computational Science and Engineering, Vol. 21*), Springer, Berlin (2002) 53-62.
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- [P5] Freund, H.; Sundmacher, K.: *Process Intensification, 2. Phase Level*, (in: Elvers, B. (Editor-in-Chief), *Ullmann's Encyclopedia of Industrial Chemistry*), Wiley-VCH, Weinheim (2011) 1-27.
- [P6] Freund, H.; Sundmacher, K.: *Process Intensification, 3. Process Unit Level*, (in: Elvers, B. (Editor-in-Chief), *Ullmann's Encyclopedia of Industrial Chemistry*), Wiley-VCH, Weinheim (2011) 1-24.
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Journal Articles (with peer review)

- [P8] Hess, S.; Freund, H.; Liauw, M.A.; Emig, G.: *Butane Oxidation to Maleic Anhydride over a VPO Catalyst Following the Riser Regenerator Approach*, Stud. Surf. Sci. Catal. 133 (2001) 205-210.
- [P9] Zeiser, T.; Steven, M.; Freund, H.; Lammers, P.; Brenner, G.; Durst, F.; Bernsdorf, J.: *Analysis of the Flow Field and Pressure Drop in Fixed Bed Reactors with the Help of Lattice Boltzmann Simulations*, Philos. T. Roy. Soc. A 360(1792) (2002) 507-520.
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- [P11] Heinen, C.; Tillich, J.; Buggisch, H.; Zeiser, T.; Freund, H.: *MRI Investigation and Complementary Numerical Simulations of Flow Through Random Bead Packings with Low Aspect Ratio*, Magn. Reson. Imaging 23(2) (2005) 369-370.
- [P12] Freund, H.; Bauer, J.; Zeiser, T.; Emig, G.: *Detailed Simulation of Transport Processes in Fixed-Beds*, Ind. Eng. Chem. Res. 44(16) (2005) 6423-6434.
- [P13] Freund, H.; Sundmacher, K.: *Towards a Methodology for the Systematic Analysis and Design of Efficient Chemical Processes – Part I: From Unit Operations to Elementary Process Functions*, Chem. Eng. Process. 47(12) (2008) 2051-2060.²
- [P14] Steyer, F.; Freund, H.; Sundmacher, K.: *A Novel Reactive Distillation Process for the Indirect Hydration of Cyclohexene to Cyclohexanol Using a Reactive Entrainer*, Ind. Eng. Chem. Res. 47(23) (2008) 9581-9587.
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- [P17] Inayat, A.; Freund, H.; Zeiser, T.; Schwieger, W.: *Determining the Specific Surface Area of Ceramic Foams: The Tetraikadehedra Model Revisited*, Chem. Eng. Sci. 66(6) (2011) 1179-1188.
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- [P19] Ahamed Imam, R.; Freund, H.; Sundmacher, K.: *Dynamics of Liquid-Liquid Systems Based on Linear Thermodynamics of Irreversible Processes*, Comput. Chem. Eng. 35(4) (2011) 630-637.

¹ Chemical Engineering Science (Elsevier) Most Cited Paper 2003-2006 Award

² In the Journal's quarterly TOP 25 in 7 out of 11 quarters from 10/2008 - 06/2011 (provided by ScienceDirect)

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- [P21] Inayat, A.; Schwerdtfeger, J.; Freund, H.; Körner, C.; Singer, R.F.; Schwieger, W.: *Periodic Open-Cell Foams: Pressure Drop Measurements and Modeling of an Ideal Tetrakaidecahedra Packing*, Chem. Eng. Sci. 66(12) (2011) 2758-2763.³
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- [P25] Ye, K.; Freund, H.; Sundmacher, K.: *Modeling Vapor-Liquid and Vapor-Liquid-Liquid Equilibria of {Water (H₂O) + Methanol (MeOH) + Dimethyl ether (DME) + Carbon Dioxide (CO₂)} Quaternary Systems Using the Peng-Robinson EoS with Wong-Sandler Mixing Rule*, J. Chem. Thermodyn. 43(12) (2011) 2002-2014.
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- [P31] Bianchi, E.; Heidig, T.; Visconti, C.G.; Groppi, G.; Freund, H.; Tronconi, E.: *An Appraisal of the Heat Transfer Properties of Metallic Open-Cell Foams for Strongly Exo-/Endothermic Catalytic Processes in Tubular Reactors*, Chem. Eng. J. 198-199 (2012) 512-528.
- [P32] Peschel, A.; Jörke, A.; Freund, H.; Sundmacher, K.: *Model-Based Development of Optimal Reaction Concepts for Plant Wide Process Intensification*, Comput. Aided Chem. Eng. 31 (2012) 150-154.
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- [P34] Chen, L.; Chen, L.; Ye, Y.; Qi, Z.; Freund, H.; Sundmacher, K.: *Co-Solvent Intensification Effect on Aromatic Alcohol Oxidation*, Catal. Commun. 28 (2012) 143-146.
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- [P39] Heidig, T.; Zeiser, T.; Schwieger, W.; Freund, H.: *Ortsaufgelöste Simulation des externen Stofftransports in komplexen Katalysatorträgergeometrien*, Chem.-Ing.-Tech. 86(4) (2014) 554-560.
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- [P45] Bianchi, E.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Numerical Simulation of Heat Transfer in the Near-Wall Region of Tubular Reactors Packed with Open-Cell Foams*, Chem. Eng. J. 264 (2015) 268-279.
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- [P48] Bianchi, E.; Schwieger, W.; Freund, H.: *Assessment of Periodic Open Cellular Structures for Enhanced Heat Conduction in Catalytic Fixed-Bed Reactors*, Adv. Eng. Mater. 18(4) (2016) 608-614.
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- [P53] Maußner, J.; Pietschak, A.; Freund, H.: *A New Analytical Approximation to the Extended Brinkman Equation*, Chem. Eng. Sci. 171 (2017) 495-499.
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- [P59] Xie, M.; Freund, H.: *Rigorous Design of Multiphase Reactors: Identification of Optimal Conditions for Mass Transfer Limited Reactions*, Chem. Eng. Process. 124 (2018) 174-185.
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- [P61] Maußner, J.; Freund, H.: *Optimization Under Uncertainty in Chemical Engineering: Comparative Evaluation of Unscented Transformation Methods and Cubature Rules*, Chem. Eng. Sci. 183 (2018) 329-345.
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- [P65] Maußner, J.; Freund, H.: *Efficient Calculation of Constraint Back-offs for Optimization Under Uncertainty: A Case Study on Maleic Anhydride Synthesis*, Chem. Eng. Sci. 192 (2018) 306-317.
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- [P67] Kaiser, M.; Freund, H.: *A Multimodular Pseudoheterogeneous Model Framework for Optimal Design of Catalytic Reactors Exemplified by Methanol Synthesis*, Chem. Eng. Sci. 206 (2019) 401-423.
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- [P73] Pietschak, A.; Maußner, J.; Dixon, A.G.; Freund, H.: *Comparative Evaluation of Heat Transfer Correlations with Different Fluid Property Considerations for Fixed-Bed Reactor Modeling*, Int. J. Heat Mass Tran. 148 (2020) 119099.
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- [P76] Pietschak, A.; Dixon, A.G.; Freund, H.: *A New Heat Transfer Correlation Suited for the Design of Fixed-Bed Reactors via Numerical Optimization*, Chem. Eng. Sci. 220 (2020) 115614.
- [P77] Fischer, K.L.; Freund, H.: *On the Optimal Design of Load Flexible Fixed Bed Reactors: Integration of Dynamics into the Design Problem*, Chem. Eng. J. 393 (2020) 124722.
- [P78] Delgado Otalvaro, N.; Kaiser, M.; Herrera Delgado, K.; Wild, S.; Sauer, J.; Freund, H.: *Optimization of the Direct Synthesis of Dimethyl Ether from CO₂ Rich Synthesis Gas: Closing the Loop between Experimental Investigations and Model-Based Reactor Design*, React. Chem. Eng. (2020) in press.

Proceeding Articles

- [P79] Freund, H.; Klemm, E.; Emig, G.; Zeiser, T.; Brenner, G.; Durst, F.: *Detailed 3D-Simulations of Single Phase Reacting Flow in Randomly Packed Beds with Low Aspect Ratios*, (in: *Proceedings of the 3rd European Congress of Chemical Engineering, Nuremberg, Germany, June 2001 – CD-ROM*), Abstract in: *Chem. Ing. Tech.* 73(6) (2001) 685.
- [P80] Beronov, K.; Zeiser, T.; Freund, H.; Bernsdorf, J.; Brenner, G.; Durst, F.: *Packed Bed Reactor Flow Statistics for a Low Tube to Particle Diameter Ratio Obtained from 3D Lattice Boltzmann Simulations*, (in: Bennacer, R.; Mohamed, A.A. (Eds.), *Proceedings of the 1st International Conference on Applications of Porous Media, Djerba, Tunisia, June 2002*), (2002) 1-13.
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Further Publications

- [P89] Sundmacher, K.; Freund, H.; Hergersberg, P.: *Kurzer Prozess im chemischen Reaktor*, Max-Planck-Forschung (2) (2007) 52-57.
- [P90] Zeiser, T.; Hager, G.; Wellein, G.; Inayat, A.; Schwieger, W.; Heidig, T.; Freund, H.: *Selecting an Appropriate Computational Platform for Supporting the Development of New Catalyst Carriers*, inSiDE 7(1) (2009) 12-16.
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- [P94] Enzenberger, F.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Additive Manufacturing of Tailor-Made Components for Applications in Process Engineering*, Process Technology & Components (2015) 48-51.

Patents

- [Pat1] Schwieger, W.; Freund, H.; Bösmann, A.; Do, G.: *Additively Manufactured Cellular Components as Adjustable Static Mixers*, DE 102016008759A1.
- [Pat2] Schwieger, W.; Freund, H.; Bösmann, A.; Do, G.: *Electrophoretic Coating of Additively Manufactured Cellular Structures for Use as Switchable Catalyst Systems*, DE 102016009272A1.
- [Pat3] Freund, H.; Frind, R.; Henkel, T.; Kaiser, M.; Schuhmann, T.; Seuffert, W.; Werner, S.: *Reactor and Method for Maximizing Methanol Yield by Using Catalyst Layers*, DE 102017001520A1 and WO 2018149811A1 and CN 108424351A.

Conference Contributions: Oral Presentations

- [C1] Freund, H.; Hess, S.; Liauw, M.; Emig, G.: *Kinetische Untersuchungen zur Butanoxidation unter besonderer Berücksichtigung der Furanbildung*, 1. Erlanger VPO-Symposium, Erlangen, Germany, June 2000.
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- [C6] Zeiser, T.; Freund, H.; Steven, M.; Lammers, P.; Brenner, G.; Durst, F.; Bernsdorf, J.: *Simulation of Single Phase Reacting Flows in Randomly Packed Beds with Low Aspect Ratios - Application of the Lattice Boltzmann Method in Chemical Engineering*, International Conference on Discrete Simulation of Fluid Dynamics, Cargese, Corse, France, July 2001.
- [C7] Beronov, K.; Zeiser, T.; Freund, H.; Bernsdorf, J.; Brenner, G.; Durst, F.: *Packed Bed Reactor Flow Statistics for a Low Tube to Particle Diameter Ratio Obtained from 3D Lattice Boltzmann Simulations*, 1st International Conference on Applications of Porous Media, Djerba, Tunisia, June 2002.
- [C8] Freund, H.; Zeiser, T.; Huber, F.; Klemm, E.; Brenner, G.; Durst, F.; Emig, G.: *Numerical Simulations of Single Phase Reacting Flows in Randomly Packed Fixed-Bed Reactors and Experimental Validation*, 17th International Symposium on Chemical Reaction Engineering, Hong Kong, China, August 2002.
- [C9] Freund, H.; Zeiser, T.; Klemm, E.; Durst, F.; Emig, G.: *Lattice Boltzmann CFD Simulation of Reacting Flow in Isothermal Fixed-Bed Reactors*, AIChE Annual Meeting, San Francisco, CA, USA, November 2003.
- [C10] Zeiser, T.; Freund, H.; Heinen, C.; Tillich, J.: *Transportvorgänge in porösen Medien: Vergleich Lattice-Boltzmann-CFD-Simulation und NMR/MRI-Messung*, GVC Fachausschusssitzung CFD & Rheologie, Würzburg, Germany, March 2004.

- [C11] Freund, H.; Bauer, J.; Zeiser, T.; Emig, G.: *Ortsaufgelöste Simulation von Transportprozessen in durchströmten Schüttungen*, GVC/Dechema-Jahrestagungen, Wiesbaden, Germany, September 2005.
- [C12] Steyer, F.; Freund, H.; Sundmacher, K.: *Einsatz eines reaktiven Entrainers zur Synthese von Cyclohexanol in einem Prozess gekoppelter Reaktivdestillationskolonnen*, GVC/Dechema-Jahrestagungen, Wiesbaden, Germany, September 2006.
- [C13] Freund, H.; Bauer, J.; Zeiser, T.; Emig, G.: *Pore-Scale Simulation of Transport Processes in Fixed-Beds: Combining a Lattice Boltzmann CFD Method and a Particle Tracking Method*, AIChE Annual Meeting, San Francisco, CA, USA, November 2006.
- [C14] Sundmacher, K.; Freund, H.: *Process Intensification: Towards a Design Approach in Terms of Elementary Process Functions*, XIX Polish Conference of Chemical and Process Engineering, Rzeszow, Poland, September 2007.
- [C15] Chalakova, M.; Kaur, R.; Freund, H.; Mahajani, S.; Sundmacher, K.: *Innovative Reactive Distillation Process for the Production of the MTBE Substitute Isooctane from Isobutene*, DGMK International Conference “Opportunities and Challenges at the Interface between Petrochemistry and Refinery”, Hamburg, Germany, October 2007.
- [C16] Sundmacher, K.; Freund, H.: *Prozessintensivierung: Neue konzeptionelle Ansätze für die Prozessgestaltung und -führung*, ProcessNet-Jahrestagung, Aachen, Germany, October 2007.
- [C17] Freund, H.; Sundmacher, K.: *Systematic Analysis of Process Intensification Options: The Elementary Process Function Methodology*, AIChE Annual Meeting, Salt Lake City, UT, USA, November 2007.
- [C18] Agarwal, V.; Thotla, S.; Kaur, R.; Chalakova, M.; Freund, H.; Sundmacher, K.; Mahajani, S.: *Attainable Regions of Reactive Distillation*, Indo-German Workshop on Advances in Reaction and Separation Processes, Madras, India, February 2008.
- [C19] Katariya, A.; Steyer, F.; Freund, H.; Sundmacher, K.: *Process Intensification in Cyclohexanol Production: A Novel Integrated Process Scheme*, 18th International Congress of Chemical and Process Engineering, Prague, Czech Republic, August 2008.
- [C20] Freund, H.; Inayat, A.; Bauer, J.; Zeiser, T.; Schwieger, W.: *Local and Integral Transport Characteristics of Novel Consolidated and Unconsolidated Structures for Catalytic Applications*, 20th International Symposium on Chemical Reaction Engineering, Kyoto, Japan, September 2008.
- [C21] Freund, H.; Inayat, A.; Bauer, J.; Zeiser, T.; Schwieger, W.: *3D Simulation of the Local Flow Field in Ceramic Foam Structures*, AIChE Annual Meeting, Philadelphia, PA, USA, November 2008.

- [C22] Freund, H.; Heidig, T.; Inayat, A.; Zeiser, T.; Schwieger, W.: *Ortsaufgelöste Simulation der Strömung in offenporigen keramischen Schaumstrukturen*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, June 2009.
- [C23] Kumar, R.; Katariya, A.; Freund, H.; Sundmacher, K.: *Development of a Novel Reactive Distillation Process for Cyclohexanol Production: Miniplant Experiments and Complementary Process Simulations*, 2nd International Congress on Green Process Engineering, Venice, Italy, June 2009.
- [C24] Peschel, A.; Freund, H.; Sundmacher, K.: *Systematik zur modellgestützten Ermittlung der optimalen Reaktionsführung am Beispiel der SO₂-Oxidation*, ProcessNet-Jahrestagung, Mannheim, Germany, September 2009.
- [C25] Peschel, A.; Freund, H.; Sundmacher, K.: *Systematic Analysis, Design and Optimization of Gas Phase Reaction Processes*, AIChE Annual Meeting, Nashville, TN, USA, November 2009.
- [C26] Sundmacher, K.; Freund, H.: *Process Systems Engineering and Process Intensification: Rival Brothers or Best Buddies?*, CAPE Forum, Aachen, Germany, March 2010.
- [C27] Freund, H.: *Modellgestützter Reaktorentwurf auf der Basis der optimalen Reaktionsführung*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2010.⁴
- [C28] Qi, Z.; Tong, L.; Yuan, W.; Freund, H.; Sundmacher, K.: *Novel Green Processes Intensified by Direct and Indirect Auxiliary Reactions*, The 2nd International Symposium on Sustainable Chemical Product and Process Engineering, Hangzhou, China, May 2010.
- [C29] Peschel, A.; Freund, H.; Sundmacher, K.: *Methodology for the Design of Optimal Chemical Reactors Based on the Concept of Elementary Process Functions*, 21st International Symposium on Chemical Reaction Engineering, Philadelphia, PA, USA, June 2010.
- [C30] Sundmacher, K.; Freund, H.: *Process Intensification: Design of Optimal Process Routes in the Thermodynamic State Space*, PSE Asia 2010 – The 5th International Symposium on Design, Operation and Control of Chemical Processes, Singapore, July 2010.
- [C31] Thotla, S.; Freund, H.; Sundmacher, K.: *Entrainer Based Reactive Divided Wall Columns*, 19th International Conference on Chemical Reactors, Vienna, Austria, September 2010.
- [C32] Inayat, A.; Freund, H.; Zeiser, T.; Schwieger, W.: *Predicting the Specific Surface Area and Pressure Drop of Ceramic Foam Catalyst Supports*, International Conference on Cellular Materials, Dresden, Germany, October 2010.

⁴ Plenary Talk on the Occasion of the Hanns Hofmann Award of the ProcessNet Reaction Engineering Division

- [C33] Freund, H.; Kumar, R.; Katariya, A.; Sundmacher, K.: *Intensification Options for Different Hierarchical Process Levels Illustrated in the Conceptual Design of a Novel Cyclohexanol Production Process*, AIChE Annual Meeting, Salt Lake City, UT, USA, November 2010.
- [C34] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Optimal Reactor Design for the Hydroformylation of Higher Olefins in a Multiphase System*, 3rd European Process Intensification Conference, Manchester, UK, June 2011.
- [C35] Zhou, T.; Chen, L.; Ye, Y.; Qi, Z.; Freund, H.; Sundmacher, K.: *Screening Ionic Liquids for Toluene/Isooctane Extraction by COSMO-RS*, International Conference on Process Intensification for Sustainable Chemical Industries, Beijing, China, June 2011.
- [C36] Chen, L.; Chen, L.; Ye, Y.; Qi, Z.; Freund, H.; Sundmacher, K.: *Highly Selective Oxidation of Cyclohexanol to Cyclohexanone in Ionic Liquids*, 6th Asia Pacific Chemical Reaction Engineering Symposium, Beijing, China, September 2011.
- [C37] Peschel, A.; Karst, F.; Freund, H.; Sundmacher, K.: *Optimal Reactor Design for Ethylene Oxide Production*, 8th European Congress of Chemical Engineering, Berlin, Germany, September 2011.
- [C38] Inayat, A.; Freund, H.; Schwieger, W.: *Periodic Open-Cell Foams as Model Systems for the Description of the Pressure Drop in Reticulated Foams*, 8th European Congress of Chemical Engineering, Berlin, Germany, September 2011.
- [C39] Freund, H.; Peschel, A.; Hentschel, B.; Sundmacher, K.: *Optimal Reactor Design and Operation for Multiphase Systems*, 8th European Congress of Chemical Engineering, Berlin, Germany, September 2011.
- [C40] Schwieger, W.; Inayat, A.; Lopez, S.; Freund, H.; Schwab, A.; Zeiser, T.: *Solid Foam Monoliths as Supports for Zeolite Catalysts*, 36th International Conference on Advanced Ceramics and Composites, Daytona Beach, FL, USA, January 2012.
- [C41] Bianchi, E.; Heidig, T.; Visconti, C.G.; Groppi, G.; Freund, H.; Tronconi, E.: *Characterization of Geometry and Heat Transfer Properties of Metal Foams for Intensification of Catalytic Processes*, 15th International Congress on Catalysis, Munich, Germany, July 2012.
- [C42] Peschel, A.; Jörke, A.; Sundmacher, K.; Freund, H.: *Optimal Reaction Concept and Plant Wide Optimization of the Ethylene Oxide Process*, 22nd International Symposium on Chemical Reaction Engineering, Maastricht, Netherlands, September 2012.⁵
- [C43] Bianchi, E.; Heidig, T.; Visconti, C.G.; Groppi, G.; Freund, H.; Tronconi, E.: *Heat Transfer Properties of Metal Foam Supports for Process Intensification of Catalytic Tubular Reactors*, 22nd International Symposium on Chemical Reaction Engineering, Maastricht, Netherlands, September 2012.

⁵ Keynote Lecture

- [C44] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Optimal Reactor Design for the Hydroformylation of Long Chain Olefins*, 22nd International Symposium on Chemical Reaction Engineering, Maastricht, Netherlands, September 2012.
- [C45] Lopez, S.; Inayat, A.; Freund, H.; Selvam, T.; Schwieger, W.: *Zeolite Containing Materials with Hierarchical Porous Structures*, ProcessNet-Jahrestagung, Karlsruhe, Germany, September 2012.
- [C46] Freund, H.; Peschel, A.; Sundmacher, K.: *Process Intensification in Ethylene Oxide Production: Optimal Reactor Design From a Process Point of View*, AIChE Annual Meeting, Pittsburgh, PA, USA, October 2012.
- [C47] Schwieger, W.; Lopez, S.; Inayat, A.; Thangaraj, S.; Schwab, A.; Freund, H.: *Hierarchical Structuring of Catalytic Reactors Using Solid Foam Monoliths: Preparation and Characterization*, International Conference on Cellular Materials, Dresden, Germany, November 2012.
- [C48] Freund, H.; Inayat, A.; Heidig, T.; Zeiser, T.; Schwieger, W.: *Hierarchical Structuring of Catalytic Reactors Using Solid Foam Monoliths: Modelling and Simulation*, International Conference on Cellular Materials, Dresden, Germany, November 2012.
- [C49] Ye, K.; Freund, H.; Sundmacher, K.: *Azeotropic Mixture Separation by Phase Behavior Tuning Using Pressurized CO₂*, 9th European Congress of Chemical Engineering, The Hague, Netherlands, April 2013.
- [C50] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Optimale Reaktionsführung der Hydroformylierung langkettiger Olefine in innovativen Lösungsmittelsystemen*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2013.
- [C51] Bianchi, E.; Heidig, T.; Visconti, C.G.; Groppi, G.; Schwieger, W.; Freund, H.; Tronconi, E.: *Heat Transfer Properties of Metal Foam Supports for Structured Catalysts*, 4th International Conference on Structured Catalysts and Reactors, Beijing, China, September 2013.
- [C52] Schwieger, W.; Lopez, S.; Inayat, A.; Thangaraj, S.; Schwab, A.; Freund, H.: *Open Cellular Monoliths for Structured Catalytic Reactors: Preparation and Characterization*, AIChE Annual Meeting, San Francisco, CA, USA, November 2013.
- [C53] Freund, H.; Heidig, T.; Zeiser, T.; Schwieger, W.: *Open Cellular Monoliths for Structured Catalytic Reactors: Modeling and Simulation*, AIChE Annual Meeting, San Francisco, CA, USA, November 2013.
- [C54] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Optimal Reactor Design for the Hydroformylation of Long Chain Olefins in Thermomorphic Solvent Systems*, AIChE Annual Meeting, San Francisco, CA, USA, November 2013.
- [C55] Bianchi, E.; Visconti, C.G.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Open-Cell Metal Foams As Enhanced Catalyst Supports for Heat Transfer Intensification in Tubular Reactors*, AIChE Annual Meeting, San Francisco, CA, USA, November 2013.

- [C56] Schwieger, W.; Lopez, S.; Inayat, A.; Thangaraj, S.; Schwab, A.; Freund, H.: *Hierarchical Zeolites and Zeolite Composites for Structured Catalytic Reactors*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, April 2014.
- [C57] Bianchi, E.; Visconti, C.G.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Enhancing the Heat Transfer within Catalytic Reactors by Optimization of Novel Structured Supports*, 21st International Conference on Chemical Reactors, Delft, Netherlands, September 2014.
- [C58] Zarekar, S.; Heidig, T.; Freund, H.: *3D Simulation of Laminar Fluid Flow in Open Cellular Monoliths for Structured Catalytic Reactors*, 21st International Conference on Chemical Reactors, Delft, Netherlands, September 2014.
- [C59] Bianchi, E.; Visconti, C.G.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Heat Transfer Properties of Metal Foam Supports for Structured Catalytic Reactors*, ProcessNet-Jahrestagung, Aachen, Germany, October 2014.
- [C60] Inayat, A.; Freund, H.; Schwieger, W.: *Open Cellular Materials as Catalyst Support: A Description of Morphology, Fluid Dynamics and Catalytic Performance*, 3rd International Conference on Cellular Materials, Dresden, Germany, October 2014.
- [C61] Klumpp, M.; Inayat, A.; Schwerdtfeger, J.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.: *Periodic Open Cellular Structures with Cubic Unit Cell Geometry: Effect of Porosity and Cell Orientation on the Pressure Drop*, 3rd International Conference on Cellular Materials, Dresden, Germany, October 2014.
- [C62] Enzenberger, F.; Schwarz, A.; Freund, H.; Schwieger, W.; Körner, C.; Wasserscheid, P.: *Periodic Open Cellular Structures for Enhanced Efficiency in Catalytic Applications*, 3rd International Conference on Cellular Materials, Dresden, Germany, October 2014.
- [C63] Freund, H.; Inayat, A.; Klumpp, M.; Heidig, T.; Bianchi, E.; Schwieger, W.: *Open-Cell Foam Supports for Structured Catalytic Reactors*, AIChE Annual Meeting, Atlanta, GA, USA, November 2014.
- [C64] Inayat, A.; Klumpp, M.; Freund, H.; Schwieger, W.; Petasch, U.; Adler, J.; Semu, D.T.; Michaelis, A.: *Periodic Cellular Metallic Structures & Porous Ceramic Foams: Novel Structures and Manufacturing Processes for Catalysts and Reactors*, ACHEMA, Frankfurt, Germany, June 2015.
- [C65] Enzenberger, F.; Lodes, M.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Efficiency Enhanced Process Equipment Made by Additive Manufacturing Technologies*, ACHEMA, Frankfurt, Germany, June 2015.
- [C66] Busse, C.; Inayat, A.; Freund, H.; Schwieger, W.: *Heat Transfer in Periodic Open Cellular Structures Produced via Additive Manufacturing*, 9th International Conference on Porous Metals and Metallic Foams, Barcelona, Spain, August 2015.

- [C67] Enzenberger, F.; Lodes, M.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Efficiency-Enhanced Structured Reactors Made by Selective Electron Beam Melting*, 10th European Congress of Chemical Engineering, Nice, France, September 2015.
- [C68] Heidig, T.; Zeiser, T.; Schwieger, W.; Freund, H.: *Parallel Particle Tracking: Detailed Mass Transport Simulation in Periodic Cellular Structures*, European Symposium on Chemical Reaction Engineering, Fürstenfeldbruck, Germany, October 2015.
- [C69] Xie, M.; Freund, H.: *Model-Based Optimization of Reaction and Process Conditions for the Reactive Absorption of Carbon Dioxide*, AIChE Annual Meeting, Salt Lake City, UT, USA, November 2015.
- [C70] Busse, C.; Inayat, A.; Freund, H.; Schwieger, W.: *Periodische offene zellulare Strukturen als Katalysatorträger für die katalytische Oxidation von Methanol zu Formaldehyd: Charakterisierung des Wärmeübergangs*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2016.
- [C71] Xie, M.; Freund, H.: *Design and Operation of Heterogeneous Catalytic Reactors to Achieve Overall Optimality over the Whole Catalyst Lifetime*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2016.
- [C72] Razza, S.; Heidig, T.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Optimized Heat Transfer Performance of Catalytic Reactors with Novel Structured Supports: Aspects for Proper Design*, 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, USA, June 2016.
- [C73] Lämmermann, M.; Schwieger, W.; Freund, H.: *Experimental Investigation of Gas-Liquid Distribution in Periodic Open Cellular Structures and their Application as Catalyst Support for Hydrodesulfurization of Dibenzothiophen*, 5th International Conference on Structured Catalysts and Reactors, San Sebastian, Spain, June 2016.
- [C74] Razza, S.; Heidig, T.; Bianchi, E.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Heat Transfer Performance of Structured Catalytic Reactors Packed with Metal Foam Supports: Influence of Wall Coupling*, 5th International Conference on Structured Catalysts and Reactors, San Sebastian, Spain, June 2016.
- [C75] Moioli, E.; Schmid, L.; Wasserscheid, P.; Freund, H.: *Guidelines for Proper Reactor Design for Aldehyde-Ammonias Production*, 22nd International Congress of Chemical and Process Engineering, Prague, Czech Republic, August 2016.
- [C76] Zorludemir, G.; McCann, N.; Täschler, C.; Wasserscheid, P.; Freund, H.: *The Mechanism of Acetonitrile Dimerization – A Theoretical Study*, 22nd International Congress of Chemical and Process Engineering, Prague, Czech Republic, August 2016.
- [C77] Freund, H.; Inayat, A.; Klumpp, M.; Heidig, T.; Bianchi, E.; Schwieger, W.: *Periodic Open Cellular Structures for Catalytic Reactors: Interaction of Structuring and Transport Processes*, ProcessNet-Jahrestagung, Aachen, Germany, September 2016.

- [C78] Lämmermann, M.; Schwieger, W.; Freund, H.: *Untersuchung der Gas-Flüssig-Verteilung in periodisch offenzelligen Strukturen als Katalysatorträger in Rieselbettreaktoren*, ProcessNet-Jahrestagung, Aachen, Germany, September 2016.
- [C79] Busse, C.; Salbaum, T.; Freund, H.; Schwieger, W.: *Additiv gefertigte zellulare Strukturen als Katalysatorträger für stark exotherme Reaktionen – Einfluss der geometrischen Eigenschaften auf den Wärmeübergang*, ProcessNet-Jahrestagung, Aachen, Germany, September 2016.
- [C80] Xie, M.; Freund, H.: *Model-Based Identification of Optimal Integrated Reactor Concepts for Heterogeneous Catalytic Reaction Systems with Rapidly Deactivating Catalysts*, ProcessNet-Jahrestagung, Aachen, Germany, September 2016.
- [C81] Ganzer, G.; Freund, H.: *Statistical Activity Variations in Diluted Catalyst Beds: Influence on Reactor Behavior*, AIChE Annual Meeting, San Francisco, CA, USA, November 2016.
- [C82] Kaiser, M.; Freund, H.: *Influence of Intraparticle Transport Processes on Optimal Reactor and Catalyst Design*, AIChE Annual Meeting, San Francisco, CA, USA, November 2016.
- [C83] Xie, M.; Freund, H.: *Model-Based Design of Optimal Reactors Considering Catalyst Deactivation*, AIChE Annual Meeting, San Francisco, CA, USA, November 2016.
- [C84] Moiola, E.; Schmid, L.; Wasserscheid, P.; Freund, H.: *A New Reaction Route for the Synthesis of 5-Ethyl-2-Methylpyridine*, 25th North American Catalysis Society Meeting, Denver, CO, USA, June 2017.
- [C85] Freund, H.; Hieringer, W.; McCann, N.; Taeschler, C.; Wasserscheid, P.; Zorludemir, G.: *Mechanistic Aspects of High Temperature Reactions of Acetonitrile*, 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, München, Germany, August 2017.
- [C86] Freund, H.: *Multiscale Modeling in Chemical Reaction Engineering*, European Summer School on Multiscale Modeling in Chemical Reaction Engineering, Chalkidiki, Greece, September 2017.
- [C87] Freund, H.; Körner, C.: *Additive Manufacturing of Tailor-Made Catalytic Reactors*, International Congress Engineering of Advanced Materials, Erlangen, Germany, October 2017.⁶
- [C88] Freund, H.; Lämmermann, M.; Busse, C.; Schwieger, W.: *Additive Manufacturing for Process Intensification: Tailor-Made Design of Catalyst Supports for Single Phase and Multiphase Reaction Systems*, AIChE Annual Meeting, Minneapolis, MN, USA, November 2017.

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- [C89] Freund, H.; Lämmermann, M.; Busse, C.; Schwieger, W.: *Additive Manufacturing of Tailor-Made Catalytic Reactors for Single Phase and Multiphase Reaction Systems*, 25th International Symposium on Chemical Reaction Engineering, Florence, Italy, May 2018.
- [C90] Freund, H.: *Heat Transfer Intensification in Catalytic Reactors by Optimized Catalyst Support Geometries*, 4th International Workshop on Methanation and 2nd Generation Fuels, Nuremberg, Germany, May 2018.⁷
- [C91] Freund, H.; Wachsen, O.; Sauer, J.: *Systematic Design of Tolerant Chemical Reactors and Processes*, ProcessNet-Jahrestagung, Aachen, Germany, September 2018.⁸
- [C92] Maußner, J.; Dreiser, C.; Wachsen, O.; Freund, H.: *Tolerant Chemical Reactor Design Exemplified on the Synthesis of Maleic Anhydride*, ProcessNet-Jahrestagung, Aachen, Germany, September 2018.
- [C93] Horak, G.; Lämmermann, M.; Schwieger, W.; Freund, H.: *Pressure Drop, Liquid Holdup and Liquid Distribution in Additively Manufactured Periodic Open Cellular Structures (POCS)*, ProcessNet-Jahrestagung, Aachen, Germany, September 2018.
- [C94] Do, G.; Schaack, S.; Schwieger, W.; Freund, H.: *interPOCS – A Sophisticated Structured System for in Operando Flow Control*, ProcessNet-Jahrestagung, Aachen, Germany, September 2018.
- [C95] Trunk, S.; Do, G.; Schwieger, W.; Freund, H.: *Numerical Investigations of Additively Manufactured Structures As Promising New Catalyst Supports with Adjustable Flow Characteristics*, ProcessNet-Jahrestagung, Aachen, Germany, September 2018.
- [C96] Pietschak, A.; Freund, H.: *2D Optimization of Fixed-Bed Reactors: Additional Degrees of Freedom for the Reactor Design to Increase Efficiency*, AIChE Annual Meeting, Pittsburgh, PA, USA, October 2018.
- [C97] Pietschak, A.; Kaiser, M.; Freund, H.: *Improved Fixed-Bed Transport Characteristics: A Shortcut Method to Optimize Catalyst Pellet Specifications*, AIChE Annual Meeting, Pittsburgh, PA, USA, October 2018.
- [C98] Warnecke, F.; Lin, L.; Haag, S.; Freund, H.: *Kinetic Modeling and Reaction Pathways of C₂ to C₇ Olefin Transformation over an H-ZSM-5 Catalyst*, AIChE Spring Meeting, New Orleans, LA, USA, April 2019.
- [C99] Ambrosetti, M.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Intensification of Non-Adiabatic Catalytic Processes with Packed Periodic Open Cellular Structures*, 2nd International Process Intensification Conference, Leuven, Belgium, May 2019.
- [C100] Littwin, G.; von Beyer, M.; Schwieger, W.; Freund, H.: *Transport Characteristics of Periodic Open Cellular Structures (POCS) in Multiphase Applications: Experiments and Modeling*, 6th International Conference on Structured Catalysts and Reactors, Bad Herrenalb, Germany, September 2019.

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- [C101] Ambrosetti, M.; Groppi, G.; Schwieger, W.; Tronconi, E.; Freund, H.: *Packed POCS: A New Opportunity for Process Intensification*, 6th International Conference on Structured Catalysts and Reactors, Bad Herrenalb, Germany, September 2019.
- [C102] Trunk, S.; Do, G.; Schwieger, W.; Freund, H.: *Numerical Investigations of Adjustable Mass Transport Characteristics in Interpenetrating Periodic Open Cellular Structures (interPOCS)*, 6th International Conference on Structured Catalysts and Reactors, Bad Herrenalb, Germany, September 2019.
- [C103] Trunk, S.; Do, G.; Schwieger, W.; Freund, H.: *Catalyst Support Structures with in operando Tunable Transport Properties Enabled by Additive Manufacturing*, 1st International Conference on Unconventional Catalysis, Reactors and Applications, Zaragoza, Spain, October 2019.
- [C104] Lin, L.; Warnecke, F.; Haag, S.; Renner, T.; Drosdzol, C.; Freund, H.: *Process Intensification in the Methanol-to-Propylene Process Enabled by Rigorous Kinetics*, AIChE Annual Meeting, Orlando, FL, USA, November 2019.
- [C105] Trunk, S.; Do, G.; Schwieger, W.; Freund, H.: *Additive Manufacturing of Catalyst Support Structures with in operando Adjustable Mass Transport and Flow Characteristics*, AIChE Annual Meeting, Orlando, FL, USA, November 2019.
- [C106] Lin, L.; Drosdzol, C.; Renner, T.; Haag, S.; Warnecke, F.; Freund, H.: *New Kinetic Model for Methanol-to-Propylene to Support Further Process Optimization*, 7th Maximising Propylene Yields Meeting, Barcelona, Spain, January 2020.

Conference Contributions: Poster Presentations

- [C107] Zeiser, T.; Li, Y.-W.; Freund, H.; Lammers, P.; Bernsdorf, J.; Brenner, G.; Klemm, E.; Emig, G.; Durst, F.: *Flow Field, Mass Transport and Selectivity of Chemical Reactions in Sphere-Packed Fixed-Bed Reactors*, 9th International Conference on Discrete Simulation of Fluid Dynamics, Santa Fe, NM, USA, August 2000.
- [C108] Freund, H.; Zeiser, T.; Steven, M.; Klemm, E.; Brenner, G.; Durst, F.; Emig, G.: *Detailed 3D-Simulations of Single Phase Reacting Flow in Randomly Packed Beds with Low Aspect Ratios*, 3rd European Congress of Chemical Engineering, Nuremberg, Germany, June 2001.
- [C109] Heinen, C.; Tillich, J.; Buggisch, H.; Zeiser, T.; Freund, H.: *MRI-Investigation and Complementary Numerical Simulations of Flow through Random Bead Packings with Low Aspect Ratio*, 7th International Conference on Recent Advances in MR Applications to Porous Media, Palaiseau, France, July 2004.
- [C110] Bauer, J.; Freund, H.; Zeiser, T.; Emig, G.: *Simulation von Stofftransportvorgängen in Festbetten mittels eines Particle-Tracking-Verfahrens*, GVC/Dechema-Jahrestagungen, Wiesbaden, Germany, September 2006.

- [C111] Freund, H.; Katariya, A.; Kumar, R.; Steyer, F.; Sundmacher, K.: *Application of Catalytic Distillation in a Novel Process Concept for the Production of Cyclohexanol*, DGMK International Conference “Opportunities and Challenges at the Interface between Petrochemistry and Refinery”, Hamburg, Germany, October 2007.
- [C112] Kumar, R.; Katariya, A.; Freund, H.; Sundmacher, K.: *A Continuous Reactive Distillation Process for the Production of Cyclohexanol from Cyclohexene*, AIChE Annual Meeting, Philadelphia, PA, USA, November 2008.
- [C113] Katariya, A.; Chalakova, M.; Freund, H.; Mahajani, S.; Sundmacher, K.: *Investigation of Isobutene Dimerization Process in Reactive Distillation Using Rigorous Three-Phase Non-Equilibrium Stage Model*, AIChE Annual Meeting, Philadelphia, PA, USA, November 2008.
- [C114] Inayat, A.; Freund, H.; Bauer, J.; Zeiser, T.; Schwieger, W.: *On the Characterization of Ceramic Foam Catalyst Supports*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, June 2009.
- [C115] Freund, H.; Peschel, A.; Sundmacher, K.: *Process Intensification in Terms of Elementary Process Functions*, 2nd European Process Intensification Conference, Venice, Italy, June 2009.
- [C116] Inayat, A.; Feldmeier, S.; Freund, H.; Zeiser, T.; Schwieger, W.: *Dip-Coated SiC Foams for Catalytic Applications*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2010.
- [C117] Peschel, A.; Freund, H.; Sundmacher, K.: *Systematik zum Entwurf und zur apparativen Gestaltung optimaler chemischer Reaktoren am Beispiel der SO₂-Oxidation*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2010.
- [C118] Inayat, A.; Feldmeier, S.; Freund, H.; Zeiser, T.; Schwieger, W.: *SiC Foams as Supports for Zeolite Catalyst Systems*, 16th International Zeolite Conference & 7th International Mesoporous Materials Symposium, Sorrento, Italy, July 2010.
- [C119] Thotla, S.; Katariya, A.; Freund, H.; Sundmacher, K.: *Cyclohexanol Production from Cyclohexene in a Reactive Divided Wall Column: A Feasibility Study*, 9th Distillation & Absorption Conference, Eindhoven, Netherlands, September 2010.
- [C120] Freund, H.; Kumar, R.; Katariya, A.; Sundmacher, K.: *Konzeptioneller Entwurf eines neuen Reaktivdestillationsprozesses zur Herstellung von Cyclohexanol aus Cyclohexen*, ProcessNet-Jahrestagung, Aachen, Germany, September 2010.
- [C121] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Modellbasierte Optimierung der zweiphasigen Hydroformylierung höherer Olefine in innovativen Lösungsmittelsystemen*, 44. Jahrestreffen Deutscher Katalytiker mit Jahrestreffen Reaktionstechnik, Weimar, Germany, March 2011.

- [C122] Peschel, A.; Hentschel, B.; Freund, H.; Sundmacher, K.: *Optimal Reactor Design for the Hydroformylation of Long Chain Alkenes in Biphasic Liquid Systems*, 21st European Symposium on Computer-Aided Process Engineering, Chalkidiki, Greece, May 2011.
- [C123] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Model Based Optimization of the Biphasic Hydroformylation of Higher Olefins in Innovative Solvent Systems*, 3rd European Process Intensification Conference, Manchester, UK, June 2011.
- [C124] Zhou, T.; Chen, L.; Qi, Z.; Freund, H.; Sundmacher, K.: *Mutual Solubility of Ionic Liquids and Water Predicted by COSMO-RS*, 8th European Congress of Chemical Engineering, Berlin, Germany, September 2011.
- [C125] Freund, H.; Peschel, A.; Sundmacher, K.: *Ermittlung der optimalen Reaktionsführung im prozesstechnischen Kontext am Beispiel der Ethylenoxidsynthese*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2012.
- [C126] Karst, F.; Freund, H.; Maestri, M.; Sundmacher, K.: *Incorporating Micro Reaction Kinetics in Dynamic Optimization: Intensified Reactor Concepts for the Catalytic Partial Oxidation (CPO) of Methane*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2012.
- [C127] Peschel, A.; Jörke, A.; Freund, H.; Sundmacher, K.: *Model-Based Development of Optimal Reaction Concepts for Plant Wide Process Intensification*, 11th International Symposium on Process Systems Engineering, Singapore, July 2012.
- [C128] Freund, H.; Peschel, A.; Sundmacher, K.: *Intensivierung des sauerstoffbasierten Ethylenoxid-Prozesses: Optimaler Reaktor für den Gesamtprozess*, ProcessNet-Jahrestagung, Karlsruhe, Germany, September 2012.
- [C129] Bianchi, E.; Visconti, C.G.; Schwieger, W.; Groppi, G.; Tronconi, E.; Freund, H.: *Modeling of Heat Transfer in Open-Cell Foams as Structured Catalyst Supports*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2013.
- [C130] Klumpp, M.; Inayat, A.; Schwerdtfeger, J.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.: *Periodic Cellular Structures with Ideal Cubic Cells: Effect of Porosity and Cell Orientation on Pressure Drop Behaviour*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2013.
- [C131] Enzenberger, F.; Knorr, T.; Peters, W.; Schwarz, A.; Schwerdtfeger, J.; Körner, C.; Singer, R.F.; Etzold, B.J.M.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Das Anwenderzentrum VerTec – Strukturierte Reaktoren aus dem 3D-Drucker*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2013.⁹
- [C132] Heidig, T.; Zeiser, T.; Schwieger, W.; Freund, H.: *Parallel Particle Tracking: Detailed Mass Transport Simulation in Complex Geometries*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2013.

⁹ Best Poster Award at the Annual Meeting 2013 of the German Reaction Engineering Division

- [C133] Enzenberger, F.; Lodes, M.; Peters, W.; Schwarz, A.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Tailor-made Components for Process Engineering Made by Selective Electron Beam Melting*, Fraunhofer Direct Digital Manufacturing Conference 2014, Berlin, Germany, March 2014.
- [C134] Klumpp, M.; Inayat, A.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.: *Periodic Open Cellular Structures with Cubic Unit Cell Geometry: Effect of Porosity and Cell Orientation on the Pressure Drop*, ProcessNet-Jahrestagung, Aachen, Germany, October 2014.
- [C135] Inayat, A.; Klumpp, M.; Freund, H.; Schwieger, W.: *Properties of Open-Cell Foams: Effect of Cell Geometry, Cell Periodicity and Strut Shape on the Pressure Drop*, ProcessNet-Jahrestagung, Aachen, Germany, October 2014.
- [C136] Do, G.; Scheiwein, A.; Schwarz, A.; Peters, W.; Enzenberger, F.; Bösmann, A.; Lodes, M.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Strukturierte Reaktoren zur hochdynamischen Wasserstoff-Freisetzung aus beladenen LOHC-Systemen*, ProcessNet-Jahrestagung, Aachen, Germany, October 2014.
- [C137] Inayat, A.; Klumpp, M.; Lämmermann, M.; Freund, H.; Schwieger, W.: *Pressure Drop Modeling in Open-Cell Foams: The Role of Geometric Tortuosity*, 9th International Conference on Porous Metals and Metallic Foams, Barcelona, Spain, August 2015.
- [C138] Moiola, E.; Aghalale, S.; Schmid, L.; Enzenberger, F.; Wasserscheid, P.; Freund, H.: *Influence of pH and Acid Type on the Reaction of Acetaldehyde with Ammonia*, 10th European Congress of Chemical Engineering, Nice, France, September 2015.
- [C139] Ganzer, G.; Daniel, A.; Heidig, T.; Freund, H.: *Statistical Activity Variations in Diluted Catalyst Beds*, European Symposium on Chemical Reaction Engineering, Fürstenfeldbruck, Germany, October 2015.
- [C140] Xie, M.; Freund, H.: *Model-Based Optimization of Reaction and Process Conditions for the Chemical Absorption of CO₂ Using Monoethanolamine*, European Symposium on Chemical Reaction Engineering, Fürstenfeldbruck, Germany, October 2015.
- [C141] Schwieger, W.; Machoke, A.; Inayat, A.; Selvam, T.; Inayat, A.; Freund, H.: *Cellular Supports for Catalytic Reactors: Design of Hierarchical Zeolites for Catalytically Active Composites*, European Symposium on Chemical Reaction Engineering, Fürstenfeldbruck, Germany, October 2015.
- [C142] Freund, H.; Inayat, A.; Klumpp, M.; Heidig, T.; Bianchi, E.; Schwieger, W.: *Cellular Supports for Catalytic Reactors: Interaction of Structuring and Transport Processes*, European Symposium on Chemical Reaction Engineering, Fürstenfeldbruck, Germany, October 2015.
- [C143] Busse, C.; Freund, H.; Schwieger, W.: *Periodic Open Cellular Structures as Catalyst Carriers for the Partial Oxidation of Methanol to Formaldehyde*, European Symposium on Chemical Reaction Engineering, Fürstenfeldbruck, Germany, October 2015.

- [C144] Lämmermann, M.; Bertelshofer, M.; Schwieger, W.; Freund, H.: *Experimental Investigation of Gas-Liquid-Distribution in Periodic Open Cellular Structures*, European Symposium on Chemical Reaction Engineering, Fürstfeldbruck, Germany, October 2015.
- [C145] Moiola, E.; Aghalale, S.; Schmid, L.; Enzenberger, F.; Wasserscheid, P.; Freund, H.: *Study of pH Effect on Acetaldehyde-Ammonia Reaction*, European Symposium on Chemical Reaction Engineering, Fürstfeldbruck, Germany, October 2015.
- [C146] Zorludemir, G.; Täschler, C.; McCann, N.; Wasserscheid, P.; Freund, H.: *Theoretical Study on the Mechanism of the Reaction of Acetonitrile with its Radical Form*, European Symposium on Chemical Reaction Engineering, Fürstfeldbruck, Germany, October 2015.
- [C147] Kaiser, M.; Sievi, G.; Freund, H.: *Efficient Solution Methods for Intraparticle Diffusion Suitable for Reactor Optimization*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2016.¹⁰
- [C148] Ganzer, G.; Daniel, A.; Freund, H.: *Influence of Statistical Activity Variations in Diluted Catalyst Beds on the Reactor Behavior*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2016.
- [C149] Lämmermann, M.; Schwieger, W.; Freund, H.: *Modellierung und experimentelle Validierung der Gas-Flüssig-Hydrodynamik in periodischen offenen zellularen Strukturen*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2016.
- [C150] Kreienbrink, D.; Inayat, A.; Klumpp, M.; Freund, H.; Schwieger, W.; Petasch, U.; Adler, J.; Semu, D.; Michaelis, A.: *Periodische offene zelluläre Strukturen & poröse keramische Schäume als Katalysatorträger in stark exothermen Reaktionen*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2016.
- [C151] Moiola, E.; Schmid, L.; Wasserscheid, P.; Freund, H.: *Guidelines for Optimal Dosing Strategies for Reactions of Aldehydes and Ammonia*, 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, USA, June 2016.
- [C152] Kaiser, M.; Sievi, G.; Freund, H.: *Efficient Solution Methods for Intraparticle Diffusion Suitable for Reactor Optimization*, 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, USA, June 2016.
- [C153] Enzenberger, F.; Lodes, M.; Körner, C.; Singer, R.F.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Tailor-Made Structured Reactors Made by Additive Manufacturing*, 5th International Conference on Structured Catalysts and Reactors, San Sebastian, Spain, June 2016.
- [C154] Busse, C.; Inayat, A.; Freund, H.; Schwieger, W.: *Heat Transfer Properties of Periodic Open Cellular Structures and their Impact on the Partial Oxidation of Methanol to Formaldehyde*, 5th International Conference on Structured Catalysts and Reactors, San Sebastian, Spain, June 2016.

¹⁰ Best Poster Award at the Annual Meeting 2016 of the German Reaction Engineering Division

- [C155] Moioli, E.; Schmid, L.; Wasserscheid, P.; Freund, H.: *Kinetic Study of Reactions to Produce 5-Ethyl-2-Methylpyridine*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2017.
- [C156] Pietschak, A.; Kaiser, M.; Freund, H.: *A Shortcut Method for the Optimization of Catalyst Pellet Specifications During Reactor Design to Improve Catalyst Bed Transport Characteristics*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2017.
- [C157] Lämmermann, M.; Horak, G.; Schwieger, W.; Freund, H.: *Druckverlust und Flüssigkeitsholdup in zweiphasig durchströmten periodisch offenzelligen Strukturen (POCS): Modellierung und experimentelle Validierung*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2017.
- [C158] Teurer, S.; Schwieger, W.; Freund, H.: *Reaktionstechnische Untersuchungen zur Methandehydroaromatisierung*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2017.¹¹
- [C159] Strobel, V.; Freund, H.; Haumann, M.: *Towards a Mathematical Description of Supported Ionic Liquid Phase (SILP) Catalyzed Gas-Phase Reactions as a Basis for Numerical Modelling: Water-Gas Shift Reaction Case Study*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2017.
- [C160] Zorludemir, G.; Täschler, C.; McCann, N.; Wasserscheid, P.; Hieringer, W.; Freund, H.: *Reaction Mechanism and Kinetic Investigations of Nitrile Species*, European Summer School on Multiscale Modeling in Chemical Reaction Engineering, Chalkidiki, Greece, September 2017.
- [C161] Moioli, E.; Schmid, L.; Wasserscheid, P.; Freund, H.: *Kinetic Study of Reactions to Produce 5-Ethyl-2-Methylpyridine*, European Summer School on Multiscale Modeling in Chemical Reaction Engineering, Chalkidiki, Greece, September 2017.
- [C162] Pietschak, A.; Freund, H.: *Radial Optimization of Tubular Reactors: A Design Tool for the Development of Efficient Reactor Concepts*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2018.
- [C163] Maußner, J.; Dreiser, C.; Wachsen, O.; Freund, H.: *Reactor Design Under Uncertainty for Future Feedstocks*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2018.
- [C164] Trunk, S.; Do, G.; Schwieger, W.; Freund, H.: *Additively Manufactured Catalyst Support Structures with Adjustable Flow Field Characteristics*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2018.
- [C165] Pietschak, A.; Freund, H.: *2D Optimization of Tubular Reactors: A Novel Conceptual Design Tool*, 25th International Symposium on Chemical Reaction Engineering, Florence, Italy, May 2018.

¹¹ Best Poster Award at the Annual Meeting 2017 of the German Reaction Engineering Division

- [C166] Moiola, E.; Schmid, L.; Wasserscheid, P.; Freund, H.: *Reactor Design for Pyridine Base Production: Matching Transport Phenomena and Reaction Kinetics*, 25th International Symposium on Chemical Reaction Engineering, Florence, Italy, May 2018.
- [C167] Maußner, J.; Dreiser, C.; Wachsen, O.; Freund, H.: *Tolerante Prozesse – Optimale Auslegung bei unsicherer Rohstoffsituation*, Jahrestreffen Prozess-, Apparate- und Anlagentechnik, Köln, Germany, November 2018.
- [C168] Warnecke, F.; Lin, L.; Haag, S.; Freund, H.: *Kinetic Investigations on Olefin Interconversion and Hydrogen Transfer Reactions over an H-ZSM-5 Catalyst*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2019.
- [C169] Maußner, J.; Freund, H.: *Multi-Objective Reactor Design Under Uncertainty*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2019.
- [C170] Fischer, K.L.; Langer, M.R.; Freund, H.: *Dynamic CO₂ Methanation in a Wall-Cooled Fixed Bed Reactor: Comparative Evaluation of Reactor Models*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2019.
- [C171] Kaiser, M.; Freund, H.: *Model-Based Reactor Design Using a Modular Optimization Framework*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2019.
- [C172] Delgado Otalvaro, N.; Kaiser, M.; Herrera Delgado, K.; Wild, S.; Sauer, J.; Freund, H.: *Reaction Kinetic Modeling of the Direct Synthesis of DME, Model-Based Reactor Optimization and Experimental Validation*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2019.
- [C173] Trunk, S.; Do, G.; Schwieger, W.; Freund, H.: *In Operando Adjustable Mass Transport and Flow Characteristics in Additively Manufactured POCS*, Jahrestreffen Reaktionstechnik, Würzburg, Germany, May 2019.¹²
- [C174] Littwin, G.; Busse, C.; Schwieger, W.; Freund, H.: *Intensified Heat Transfer for Strongly Exo- or Endothermic Reactions with Additively Manufactured Periodic Open Cellular Structures*, 1st International Conference on Unconventional Catalysis, Reactors and Applications, Zaragoza, Spain, October 2019.

¹² Best Poster Award at the Annual Meeting 2019 of the German Reaction Engineering Division

Invited Talks

- [T1] Zeiser, T.; Freund, H.: *Lattice Boltzmann Methods - Theoretical Background and Applications in Chemical Engineering*, Seminar Talk, DFG Research Group FOR 338, Universität Karlsruhe, Karlsruhe, Germany, June 2002.
- [T2] Zeiser, T.; Freund, H.: *Möglichkeiten und Grenzen von Lattice-Boltzmann-Simulationen in der Verfahrenstechnik*, Degussa AG, Hanau, Germany, March 2003.
- [T3] Freund, H.; Zeiser, T.; Klemm, E.: *Numerische Simulation und Analyse lokaler Transportprozesse in Festbettreaktoren und experimentelle Validierung*, Degussa AG, Hanau, Germany, March 2003.
- [T4] Zeiser, T.; Freund, H.; Heinen, C.; Tillich, J.: *Strömungssimulation mit Lattice-Boltzmann-Verfahren auf Hochleistungsrechnern: Ein Vergleich mit NMR/MRI Messungen*, Seminar Talk, DFG Research Group FOR 338, Universität Karlsruhe, Karlsruhe, Germany, June 2004.
- [T5] Freund, H.: *Ortsaufgelöste Simulation von Transportprozessen in Festbettreaktoren*, Technical Chemistry Colloquium, Universität Dortmund, Dortmund, Germany, January 2005.
- [T6] Freund, H.: *Detaillierte Simulation der Struktur von Festbetten und der lokalen Transportprozesse*, Seminar Talk, Institut für Chemische Verfahrenstechnik, Universität Stuttgart, Stuttgart, Germany, January 2005.
- [T7] Freund, H.; Emig, G.: *Reaktionstechnische Untersuchungen heterogen katalysierter Gasphasenreaktionen – Stand des Wissens und neue Konzepte*, Degussa AG, Hanau, Germany, January 2006.
- [T8] Freund, H.: *Innovative Konzepte für die Reaktorsimulation*, Degussa AG, Hanau, Germany, January 2006.
- [T9] Freund, H.: *Ortsaufgelöste Simulation von Transportprozessen in durchströmten Festbetten*, Seminar Talk, Institut für Technische Mechanik, Technische Universität Clausthal, Clausthal-Zellerfeld, Germany, June 2007.
- [T10] Sundmacher, K.; Freund, H.: *Elementare Prozessfunktionen: Ein Weg zur systematischen Intensivierung chemischer Produktionsprozesse*, BASF SE, Ludwigshafen, Germany, April 2008.
- [T11] Freund, H.; Sundmacher, K.: *Systematische Analyse von Optionen zur Prozessintensivierung mittels Elementarer Prozessfunktionen*, Linde AG, Höllriegelskreuth, Germany, October 2008.
- [T12] Freund, H.: *Rationales Reaktordesign durch Multiskalenbetrachtung und modellgestützte Optimierung der Reaktionsführung*, AoC Colloquium “Catalytic Processes”, Evonik Degussa GmbH, Marl, Germany, September 2009.

- [T13] Peschel, A.; Freund, H.; Sundmacher, K.: *Systematik zum Entwurf und zur apparativen Gestaltung optimaler chemischer Reaktoren am Beispiel der SO₂-Oxidation*, Seminar Talk, Institut für Mikroverfahrenstechnik, Karlsruher Institut für Technologie, Karlsruhe, Germany, December 2009.
- [T14] Freund, H.: *Methodology for the Design of Optimal Chemical Reactors Based on the Concept of Elementary Process Functions*, Seminar Talk, State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, China, September 2010.
- [T15] Freund, H.: *3D Simulation of Transport Processes in Chemical Reactors for the Evaluation of Local and Integral Transport Characteristics*, Seminar Talk, State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, China, September 2010.
- [T16] Freund, H.: *Computer-Aided Design and Evaluation of Foam Structures as Catalyst Support*, Seminar Talk, State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, China, September 2010.
- [T17] Freund, H.; Peschel, A.; Sundmacher, K.: *Modellgestützter Reaktorentwurf auf Basis der optimalen Reaktionsführung*, BASF SE, Ludwigshafen, Germany, October 2010.
- [T18] Freund, H.: *Innovative Methods for Reactor Simulation and Catalyst Support Design*, Seminar Talk, Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano, Milan, Italy, March 2011.
- [T19] Freund, H.: *Model-Based Design of Tailor-Made Reactors*, Seminar Talk, Cluster of Excellence Engineering of Advanced Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany, July 2011.
- [T20] Peschel, A.; Karst, F.; Freund, H.; Sundmacher, K.: *From the Dynamic Optimization of a Fluid Element to Optimal Technical Reactors*, Workshop DeMiR 2011 “From Detailed Microkinetics to the Reactor”, Technische Universität München, Garching, Germany, September 2011.
- [T21] Hentschel, B.; Peschel, A.; Freund, H.; Sundmacher, K.: *Rational Reactor Design for the Hydroformylation of Higher Olefins Based on a Dynamic Optimization Approach*, IChemE Symposium “Rational Catalyst and Process Design”, University of Oxford, Oxford, United Kingdom, September 2011.
- [T22] Freund, H.; Sundmacher, K.: *Intensification Options in the Conceptual Design of a Novel Cyclohexanol Production Process*, DSM, Geleen, Netherlands, October 2011.
- [T23] Freund, H.: *Model-Based Design of Tailor-Made Reactors*, 3rd Symposium “Engineering of Advanced Materials”, Oberhof, Germany, November 2011.
- [T24] Freund, H.: *Vom Fluidelement zum Reaktor: Modellgestützter Entwurf maßgeschneiderter Reaktoren*, Seminar Talk, AVT Colloquium, RWTH Aachen, Aachen, Germany, November 2011.

- [T25] Freund, H.: *Optimal Reactor Concepts for Plantwide Process Intensification*, Summer School “Engineering of Advanced Materials”, Kloster Banz, Bad Staffelstein, Germany, June 2012.
- [T26] Ye, K.; Freund, H.; Sundmacher, K.: *A New Process for Azeotropic Mixture Separation by Phase Behavior Tuning Using Pressurized CO₂*, Expert Meeting of Netherlands Group of Users of Technology for Separation – NL GUTS, Helmond, Netherlands, June 2013.
- [T27] Freund, H.: *Optimale Reaktionsführung: Methoden zur Ermittlung und Materialien zur Realisierung*, Evonik Industries AG, Marl, Germany, July 2013.
- [T28] Freund, H.: *Von der optimalen Reaktionsführung zum technischen Reaktor: Methoden, Werkzeuge und Materialien*, Air Liquide Forschung & Entwicklung GmbH, Frankfurt a.M., Germany, August 2013.
- [T29] Freund, H.: *Unlock the Full Potential of Reaction Systems by Optimal Reactor and Process Design – or – How To Navigate Molecules on the Optimal Process Route*, Chemelot Colloquium, Geleen, Netherlands, October 2013.
- [T30] Freund, H.: *Modellgestützter Entwurf maßgeschneiderter Reaktoren auf Basis der optimalen Reaktionsführung: Methoden, Werkzeuge und Materialien*, Seminar Talk, Institut für Katalysatorforschung und -technologie, Karlsruher Institut für Technologie, Karlsruhe, Germany, January 2014.
- [T31] Freund, H.: *A Systematic Approach to Process Intensification: Methods and Computational Tools for Optimal Reactor and Process Design*, Speaking engagement at a US-based company, USA, February 2014.
- [T32] Enzenberger, F.; Lodes, M.; Körner, C.; Freund, H.; Schwieger, W.; Wasserscheid, P.: *Tailor-made Structured Reactors Made by Selective Electron Beam Melting*, IChemE Symposium “Chemical Sciences in the 21st Century: The Role of 3D Printing”, University of Nottingham, Nottingham, United Kingdom, April 2014.
- [T33] Freund, H.: *Interaction of Structuring and Transport Processes in Catalytic Reactors*, 6th Symposium “Engineering of Advanced Materials”, Kloster Banz, Bad Staffelstein, Germany, November 2014.
- [T34] Schwieger, W.; Inayat, A.; Selvam, T.; Freund, H.: *Open Cellular Structures for Catalytic Reactors: Preparation and Characterization*, Seminar Talk, Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano, Milan, Italy, May 2015.
- [T35] Jia, Z.; Freund, H.: *Countless Possibilities of What Process Intensification Can Do*, AIChE Process Development Symposium, Houston, TX, USA, June 2015.
- [T36] Freund, H.: *Cellular Supports for Catalytic Reactors: Interaction of Structuring and Transport Processes*, Short Course “Structured Catalysts and Reactors” of the Graduate School “Advanced Materials and Processes”, Fürth, Germany, December 2015.

- [T37] Freund, H.: *Catalytic Reactors and Process Technology*, Seminar Talk, Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, USA, June 2016.
- [T38] Freund, H.: *Optimal Design of Tailor-Made Reactors and Structured Catalytic Materials*, Workshop Talk, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN, USA, August 2016.
- [T39] Freund, H.: *Open Cellular Structures for Catalytic Reactors: Interaction of Structuring and Transport Processes*, Seminar Talk, Verfahrenstechnisches Kolloquium, Zentrum für Umweltforschung und nachhaltige Technologien, Universität Bremen, Bremen, Germany, November 2016.
- [T40] Freund, H.: „*Das Ganze ist mehr als die Summe seiner Teile*“ – *Additive Fertigung optimierter Reaktoren für hocheffiziente Prozesse*, Seminar Talk, Kolloquium an der Fakultät Bio- und Chemieingenieurwesen, Technische Universität Dortmund, Dortmund, Germany, May 2017.
- [T41] Freund, H.: *Intensifying Chemical Reactors through Additive Manufacturing*, Workshop Talk, EUROPIC 12th Expert Meeting on Process Intensification, Visp, Switzerland, June 2017.
- [T42] Freund, H.: *Optimal Design of Catalytic Reactors and Structured Catalysts*, Catalysis Talks @ Heufeld, Clariant Produkte (Deutschland) GmbH, Heufeld, Germany, July 2017.
- [T43] Freund, H.: *Optimal Design of Catalytic Reactors and Structured Catalysts*, Seminar Talk, Dipartimento di Energia, Politecnico di Milano, Milan, Italy, March 2018.
- [T44] Freund, H.: *Process Intensification in Catalytic Reactors by Structured Catalyst Supports*, Guest Lecture, Process & Energy Department, TU Delft, Delft, Netherlands, March 2018.
- [T45] Freund, H.: *Additive Manufacturing of Tailor-Made Catalytic Reactors for Process Intensification*, Solvay Lyon Research & Innovation Center, Saint Fons, France, June 2018.
- [T46] Freund, H.: *Process Intensification via Structuring the Processing Space*, Workshop Talk, 7th EUROPIC Course “Process Intensification: Fundamentals & Applications”, INVITE, Leverkusen, Germany, October 2018.
- [T47] Freund, H.: *Optimal Design of Catalytic Reactors and Structured Catalysts*, Seminar Talk, Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, United Kingdom, November 2018.
- [T48] Freund, H.: *A Systematic Function-Based Approach to Optimal Reactor and Process Design*, Dial-A-Molecule – An EPSRC Grand Challenge Network Symposium “Predictive Scalability of Processes in Fine Chemical and Pharmaceutical Manufacturing”, GlaxoSmithKline, Stevenage, United Kingdom, November 2018.

- [T49] Freund, H.: *Structuring Concepts for Process Intensification in Catalytic Reactors*, Guest Lecture, Process & Energy Department, TU Delft, Delft, Netherlands, February 2019.
- [T50] Freund, H.: *Open Cellular Structures for Process Intensification in Catalytic Reactors (or: POCS for President)*, Scientific Colloquium on the Occasion of the Academic Farewell of Professor Wilhelm Schwieger, FAU Erlangen-Nürnberg, Erlangen, Germany, March 2019.
- [T51] Freund, H.: *Systematischer Entwurf toleranter chemischer Prozesse*, Impulsvortrag, DFG-Rundgespräch “Technische Chemie”, Universität Ulm, Ulm, Germany, April 2019.
- [T52] Freund, H.: *Catalytic Reactors and Process Technology*, DSM Nutritional Products Ltd., Sisseln, Switzerland, October 2019.
- [T53] Freund, H.: *Structure: Process Intensification in the Spatial Domain*, Workshop Talk, 8th EUROPIC Course “Process Intensification: Fundamentals & Applications”, TU Delft, Delft, Netherlands, November 2019.
- [T54] Freund, H.: *Structuring Concepts for Process Intensification in Catalytic Reactors*, Guest Lecture, Process & Energy Department, TU Delft, Delft, Netherlands, February 2020.
- [T55] Freund, H.: *Optimal Design of Catalytic Reactors and Structured Catalysts*, Seminar Talk, Department of Chemical Engineering, TU Delft, Delft, Netherlands, February 2020.