

## Selected Publications of Dr. Eric von Lieres

### Peer-Reviewed Journals

1. Diedrich, J.; Heymann, W.; Leweke, S.; Kunert, C.; Johnson, W.; Hunt, S.; Todd, B.; von Lieres, E.: *Multi-state steric mass-action model and case study on complex high loading behavior of mAb on ion exchange tentacle resin*, Journal of Chromatography A, accepted.
2. Freier, L.; von Lieres, E.: *Robust multi-objective global optimization of stochastic processes with a case study in gradient elution chromatography*, Biotechnology Journal, accepted.
3. Hemmerich, J.; Freier, L.; Wiechert, W.; von Lieres, E.; Oldiges, M.: *Generic protocol for optimization of heterologous protein production using automated microbioreactor technology*, Journal of Visualized Experiments, accepted.
4. Freier, L.; Wiechert, W.; von Lieres, E.: *Kriging with trend functions nonlinear in their parameters: Theory and application in enzyme kinetics*, Engineering in Life Sciences **17,8** (2017), 916–922.
5. Freier, L.; von Lieres, E.: *Multi-objective global optimization (MOGO): Algorithm and case study in gradient elution chromatography*, Biotechnology Journal **12,7** (2017), 1600613.
6. Westerwalbesloh, C.; Grünberger, A.; Wiechert, W.; Kohlheyer, D.; von Lieres, E.: *Coarse graining bacteria colonies for modeling critical solute distributions in pico-liter bioreactors for bacterial studies on single-cell level*, Microbial Biotechnology **10,4** (2017), 845–857.
7. Zhao, X.; Noack, S.; Wiechert, W.; von Lieres, E.: *Dynamic flux balance analysis with nonlinear objective function*, Journal of Mathematical Biology (April 11, 2017), 1–29.
8. Bühler, J.; Huber, G.; von Lieres, E.: *Finite volume schemes for the numerical simulation of tracer transport in plants*, Mathematical Biosciences **288** (2017), 14–20.
9. Morschett, H.; Freier, L.; Rohde, J.; Wiechert, W.; von Lieres, E.; Oldiges, M.: *A framework for accelerated phototrophic bioprocess development: Integration of parallelized microscale cultivation, laboratory automation and Kriging-assisted experimental design*, Biotechnology for Biofuels **10,26** (2017), 1–13.
10. Poshyvailo, L.; von Lieres, E.; Kondrat, S.: *Does metabolite channeling accelerate enzyme-catalyzed cascade reactions?*, PLOS ONE **12,2** (2017), 1–17.
11. Kiefer, J.; Wei, G.; Ciacchi, L. C.; von Lieres, E.: *Irreversible damage of polymer membranes during attenuated total reflection infrared analysis*, Applied Spectroscopy **71,6** (2017), 1–7.
12. Freier, L.; Hemmerich, J.; Schöler, K.; Wiechert, W.; Oldiges, M.; von Lieres, E.: *Framework for Kriging based iterative experimental analysis and design: Optimization of secretory protein production in Corynebacterium glutamicum*, Engineering in Life Sciences **16** (2016): 538–549.
13. Jussen, D.; Soltner, H.; Stute, B.; Wiechert, W.; von Lieres, E.; Pohl, M.:  *$\mu$ MORE: A microfluidic magnetic oscillation reactor for accelerated parameter optimization in biocatalysis*, Journal of Biotechnology **231** (2016), 174–182.
14. Kondrat, S.; Zimmermann, O.; Wiechert, W.; von Lieres, E.: *Discrete-Continuous reaction-diffusion model with mobile point-like sources and sinks*, European Physical Journal E **39,11** (2016), 1–10.

15. Püttmann, A.; Schnittert, S.; Leweke, S.; von Lieres, E.: *Utilizing algorithmic differentiation to efficiently compute chromatograms and parameter sensitivities*, Chemical Engineering Science **139** (2016), 152–162.
16. Leweke, S.; von Lieres, E.: *Fast arbitrary order moments and arbitrary precision solution of the general rate model of column liquid chromatography with linear isotherm*, Computers and Chemical Engineering **84** (2016), 350–362.
17. Kumar, V.; Leweke, S.; von Lieres, E.; Rathore, A.: *Mechanistic modeling of ion-exchange process chromatography of charge variants of monoclonal antibody products*, Journal of Chromatography A **1426** (2015), 140–153.
18. Grünberger, A.; Probst, C.; Helfrich, S.; Nanda, A.; Stute, B.; Wiechert, W.; von Lieres, E.; Nöh, K.; Frunzke, J.; Kohlheyer, D.: *Spatiotemporal microbial single-cell analysis using a high-throughput microfluidics cultivation platform*, Cytometry A **87,12** (2015), 1101–1115.
19. Westerwalbesloh, C.; Grünberger, A.; Stute, B.; Weber, S.; Wiechert, W.; Kohlheyer, D.; von Lieres, E.: *Modeling and CFD simulation of nutrient distribution in picoliter bioreactors for bacterial growth studies on single-cell level*, Lab on Chip **15** (2015), 4177–4186.
20. Kondrat, S.; Zimmermann, O.; Wiechert, W.; von Lieres, E.: *The effect of composition on diffusion of macromolecules in crowded environment*, Physical Biology **12** (2015), 046003.
21. Ghosh, P.; Lin, M.; Vogel, J. H.; Choy, D.; Haynes, C.; von Lieres, E.: *Zonal rate model for axial and radial flow membrane chromatography, part II: Model based scale-up*, Biotechnology and Bioengineering **111,8** (2014), 1587–1594.
22. Püttmann, A.; Nicolai, M.; Behr, M.; von Lieres, E.: *Stabilized space-time finite elements for high-definition simulation of packed bed chromatography*, Finite Elements in Analysis and Design **86** (2014), 1–11.
23. Choy, D.; Creagh, L.; von Lieres, E.; Haynes, C.: *A new mixed-mode model for interpreting and predicting protein elution during isoelectric chromatofocusing*, Biotechnology and Bioengineering **111,5** (2014), 925–936.
24. Ghosh, P.; Vahedipour, K.; Leuthold, M.; von Lieres, E.: *Model-based analysis and quantitative prediction of membrane chromatography: Extreme scale-up from 0.08 ml to 1200 ml*, Journal of Chromatography A **1332** (2014), 8–13.
25. Baraibar, Á.; von Lieres, E.; Wiechert, W.; Pohl, M.; Rother, D.: *Effective production of (S)- $\alpha$ -hydroxy ketones: A reaction engineering approach*, Topics in Catalysis **57,5** (2014), 401–411.
26. Kiefer, J.; Rasul, N. H.; Ghosh, P. K.; von Lieres, E.: *Surface and bulk porosity mapping of polymer membranes using infrared spectroscopy*, Journal of Membrane Science **452** (2014), 152–156.
27. Bühler, J.; von Lieres, E.; Huber, G.: *A family of compartmental models for long-distance tracer transport in plants*, Journal of Theoretical Biology **341** (2014), 131–142.
28. Ghosh, P.; Vahedipour, K.; Lin, M.; Vogel, J. H.; Haynes, C.; von Lieres, E.: *Computational fluid dynamic simulation of axial and radial flow membrane chromatography: Mechanisms of non-ideality and validation of the zonal rate model*, Journal of Chromatography A **1305** (2013), 114–122.
29. Sehl, T.; Hailes, H. C.; Ward, J. M.; Wardenga, R.; von Lieres, E.; Offermann, H.; Westphal, R.; Pohl, M.; Rother, D.: *Two steps in one pot: Enzyme cascade for the synthesis of nor(pseudo)ephedrine from inexpensive starting materials*, Angewandte Chemie International Edition **52,26** (2013), 6772–6775.

30. Püttmann, A.; Schnittert, S.; Naumann, U.; von Lieres, E.: *Fast and accurate parameter sensitivities for the general rate model of column liquid chromatography*, Computers and Chemical Engineering **56** (2013), 46–57.
31. Borg, N.; Westerberg, K.; Andersson, N.; von Lieres, E.; Nilsson, B.: *Effects of uncertainties in experimental conditions on the estimation of adsorption model parameters in preparative chromatography*, Computers and Chemical Engineering **55** (2013), 148–157.
32. Stute, B.; Krupp, V.; von Lieres, E.: *Performance of iterative equation solvers for mass transfer problems in three-dimensional sphere packings in COMSOL*, Simulation Modelling Practice and Theory **33** (2013), 115–131.
33. Ghosh, P.; Vahedipour, K.; Lin, M.; Vogel, J. H.; Haynes, C.; von Lieres, E.: *Zonal rate model for axial and radial flow membrane chromatography, part I: Knowledge transfer across operating conditions and scales*, Biotechnology and Bioengineering **110,4** (2013), 1129–1141.
34. Gerhards, T.; Mackfeld, U.; von Lieres, E.; Wiechert, W.; Pohl, M.; Rother, D.: *Influence of organic solvents on enzymatic asymmetric carbonylations*, Advanced Synthesis & Catalysis **354,14-15** (2012), 2805–2820.
35. Winz, R.; Wiechert, W.; von Lieres, E.: *Surface bound adsorption in a microfluidic T-sensor: Numerical comparison and optimization of 2D and 3D models and of sensor designs*, Sensors and Actuators B: Chemical **170** (2012), 75–81.
36. Osberghaus, A.; Baumann, P.; Hepbildikler, S.; Nath, S.; Haindl, M.; von Lieres, E.; Hubbuch, J.: *Detection, quantification, and propagation of uncertainty in high throughput experimentation by Monte Carlo methods*, Chemical Engineering and Technology **35,8** (2012), 1456–1464.
37. Osberghaus, A.; Drechsel, K.; Hansen, S.; Hepbildikler, S.; Nath, S.; Haindl, M.; von Lieres, E.; Hubbuch, J.: *Model-integrated process development demonstrated on the optimization of a robotic cation exchange step*, Chemical Engineering Science **76** (2012), 129–139.
38. Osberghaus, A.; Hepbildikler, S.; Nath, S.; Haindl, M.; von Lieres, E.; Hubbuch, J.: *Optimizing a chromatographic three component separation: A comparison of mechanistic and empiric modeling approaches*, Journal of Chromatography A **1237** (2012), 86–95.
39. Osberghaus, A.; Hepbildikler, S.; Nath, S.; Haindl, M.; von Lieres, E.; Hubbuch, J.: *Determination of parameters for the steric mass action model – A comparison between two approaches*, Journal of Chromatography A **1233** (2012), 54–65.
40. Francis, P.; von Lieres, E.; Haynes, C.: *Zonal rate model for stacked membrane chromatography: II. Characterizing ion-exchange membrane chromatography under protein retention conditions*, Biotechnology and Bioengineering **109,3** (2012), 615–629.
41. Francis, P.; von Lieres, E.; Haynes, C.: *Zonal rate model for stacked membrane chromatography: I. Characterizing solute dispersion under flow-through conditions*, Journal of Chromatography A **1218,31** (2011), 5071–5078.
42. von Lieres, E.; Andersson, J.: *A fast and accurate solver for the general rate model of column liquid chromatography*, Computers and Chemical Engineering **34,8** (2010), 1180–1191.
43. von Lieres, E.; Wang, J.; Ulbricht, M.: *Model based quantification of internal flow distributions from breakthrough curves of flat sheet membrane chromatography modules*, Chemical Engineering and Technology **33,6** (2010), 960–968.
44. Siudak, A.; von Lieres, E.; Müller, C. H.: *Estimation, model discrimination, and experimental design for implicitly given nonlinear models of enzyme catalyzed chemical reactions*, Mathematica Slovaca **59,5** (2009), 593–610.

45. Susanto, A.; Treier, K.; Knieps-Grünhagen, E.; von Lieres, E.; Hubbuch, J.: *High throughput screening for the design and optimization of chromatographic processes: Automated optimization of chromatographic phase systems*, Chemical Engineering and Technology **32,1** (2009), 140–154.
46. Susanto, A.; Knieps-Grünhagen, E.; von Lieres, E.; Hubbuch, J.: *High throughput screening for the design and optimization of chromatographic processes: Assessment of model parameter determination from high throughput compatible data*, Chemical Engineering and Technology **31,12** (2008), 1846–1855.
47. Susanto, A.; Herrmann, T.; von Lieres, E.; Hubbuch, J.: *Investigation of pore diffusion hindrance of monoclonal antibody in hydrophobic interaction chromatography using confocal laser scanning microscopy*, Journal of Chromatography A **1149,2** (2007), 178–188.
48. Teske, C.; von Lieres, E.; Schröder, M.; Ladiwala, A.; Cramer, S. M.; Hubbuch, J.: *Competitive adsorption of labeled and native protein in confocal laser scanning microscopy*, Biotechnology and Bioengineering **95,1** (2006), 58–66.
49. Schröder, M.; von Lieres, E.; Hubbuch, J.: *Direct quantification of intraparticle protein diffusion in chromatographic media*, Journal of Physical Chemistry B **110,3** (2006), 1429–1436.
50. Bensch, M.; Schulze Wierling, P.; von Lieres, E.; Hubbuch, J.: *High throughput screening of chromatographic phases for rapid process development*, Chemical Engineering and Technology **28,11** (2005), 1274–1284.
51. Knosowski, Y.; von Lieres, E.; Schneider, A.: *Regularization of a non-characteristic Cauchy-problem for a parabolic equation in multiple dimensions*, Inverse Problems **15,3** (1999), 731–743.

### Conference Proceedings

1. Kondrat, S.; Zimmermann, O.; von Lieres, E.: *Mehrskalenmodellierung von Reaktions-Diffusions-Prozessen in lebenden Systemen*, 18. Heiligenstädter Kolloquium, Technische Systeme für die Lebenswissenschaften (Heilbad Heiligenstadt, Germany, September 19–21, 2016).
2. Freier, L.; von Lieres, E.: *Kriging based iterative parameter estimation procedure for biotechnology applications with nonlinear trend functions*, MATHMOD (Vienna, Austria, February 18–20, 2015), IFAC-PapersOnLine **48,1** (2015): 574–579.
3. Püttmann, A.; Nicolai, M.; Behr, M.; von Lieres, E.: *A Finite Element Method for Spatially Resolved Simulation of Packed Bed Chromatography*, Proceedings in Applied Mathematics and Mechanics **13** (2013), 511–512 (84<sup>th</sup> Annual meeting of the international association of applied mathematics and mechanics, Novi Sad, Serbia, March 18–22, 2013).
4. Ghosh, P.; von Lieres, E.: *Mechanistic and semi-empirical approaches for modeling inhomogeneous flow in membrane chromatography capsules*, pp. 512–524 in *Proceedings of the 14<sup>th</sup> Aachener Membran-Kolloquium* (Aachen, Germany, November 7–8, 2012).
5. Zimmermann, O.; von Lieres, E.: *Mehrskalige Simulation räumlicher Inhomogenitäten in biochemischen Netzwerken*, 16. Heiligenstädter Kolloquium, Technische Systeme für die Lebenswissenschaften (Heilbad Heiligenstadt, Germany, September 24–26, 2012).

6. Hannemann-Tamás, R.; Tillack, J.; Schmitz, M.; Förster, M.; Wyes, J.; Nöh, K.; von Lieres, E.; Naumann, U.; Wiechert, W.; Marquardt, W.: *First- and second-order parameter sensitivities of a metabolically and isotopically non-stationary biochemical network model*, Proceedings of the 9<sup>th</sup> International MODELICA Conference (Munich, Germany, September 3–5, 2012).
7. Borg, N.; Westerberg, K.; Schnittert, S.; von Lieres, E.; Nilsson, B.: *Numerical analysis of model uncertainties as a result of experimental uncertainty – An example from preparative chromatography*, MATHMOD (Vienna, Austria, February 15–17, 2012).
8. Dalitz, R.; von Lieres, E.: *Reconstruction of high dimensional functions from irregularly spaced and error afflicted samples by Kriging*, ASIM conference (Winterthur, Switzerland, September 7–9, 2011).
9. von Lieres, E.: *Chromatography models with Langmuir and steric mass action adsorption isotherms are of differential index one*, pp. 1004–1007 in Simos, T. E.; Psihoyios, G.; Tsitoras, C. (Editors): ICNAAM 2010: 8<sup>th</sup> International conference of numerical analysis and applied mathematics (Rhodos, Greece, September 19–25, 2010).
10. Stute, B.; Joppich, W.; Wiechert, W.; von Lieres, E.: *Performance of iterative equation solvers for convection-diffusion-adsorption-problems in three-dimensional sphere packings in COMSOL*, Šnorek, M.; Buk, Z.; Čepeck, M.; Drchal, J. (Editors): *Proceedings of the 7<sup>th</sup> EUROSIM congress on modelling and simulation* (Prague, Czech Republic, September 6–10, 2010).
11. Winz, R.; Wiechert, W.; von Lieres, E.: *Surface bound adsorption in a microfluidic T-sensor: Numerical comparison and optimization of 2D and 3D models*, Proceedings of Eurosensors XXIV (Linz, Austria, September 5–8, 2010), Procedia Engineering **5** (2010), 1272–1275.
12. Droste, P.; von Lieres, E.; Wiechert, W.; Nöh, K.: *Customizable visualization on demand for hierarchically organized information in biochemical networks*, pp. 163–174 in Barneva, R. P.; Brimkov, V. E.; Hauptman, H. A.; Jorge, R. M. N.; Tavares, J. M. R. S. (Editors): *Computational modeling of objects presented in images: Proceedings of 2<sup>nd</sup> international symposium CompIMAGE 2010* (Buffalo-Niagara, USA, May 5–7 2010), Lecture notes in computer science 6026, Springer, Berlin, 2010.
13. Schnittert, S.; Winz, R.; von Lieres, E.: *Development of a 3D model for packed bed liquid chromatography in microcolumns*, pp. 193–197 in Al-Dabass, D.; Katsikas, S.; Koukos, I.; Abraham, A.; Zobel, R. (Editors): *Proceedings of UKSim 3<sup>rd</sup> European symposium on computer modeling and simulation* (Athens, Greece, November 25–27, 2009), IEEE computer society, Los Alamitos (USA), 2009.
14. Elsheikh, A.; Nöh, K.; von Lieres, E.: *Improving convergence of derivative-based parameter estimation with multistart parameter clustering based on DAE decomposition*, pp. 47–55 in Casella, F. (Editor): *Proceedings of the 7<sup>th</sup> international MODELICA conference* (Como, Italy, September 20–22, 2009), Linköping University Electronic Press, Linköping (Sweden), 2009.
15. Winz, R.; von Lieres, E.; Wiechert, W.: *Numerical analysis of the impact of geometric shape patterns on the performance of miniaturized chromatography systems*, in: *Proceedings of the COMSOL conference 2008* (Hannover, Germany, November 4–6, 2008).
16. von Lieres, E.; Frauen, C.; Nöh, K.: *Fast solution of chromatographic particle and column models on parallel computers*, International Journal of Pure and Applied Mathematics **42,3** (2007), 309–317.
17. Winz, R.; de los Rios Gonzalez, A.; von Lieres, E.; Schmittl, M.; Wiechert, W.: *Simulation of a micro-analytical device for adsorbing substances from a fluid*, pp. 736–741 in Petit, J.-M.; Squalli, O. (Editors): *Proceedings of the European COMSOL conference 2007* (Grenoble, France, October 23–24, 2007).

18. Nöh, K.; Finke, M.; Wiechert, W.; von Lieres, E.: *Modeling and simulation of diffusion in chromatographic resin using spatially structured random media and a parallel cellular automaton*, in: Zupančič, B.; Karba, R.; Blažič, S. (Editors): *Proceedings of the 6<sup>th</sup> EUROSIM congress on modelling and simulation* (Ljubljana, Slovenia, September 9–13, 2007).
19. von Lieres, E.; Finke, M.; Buschmann, U.: *Simulation of hindered diffusion in spatially structured domains using a parallel cellular automaton*, in Troch, I.; Breitenecker, F. (Editors): *Proceedings of 5<sup>th</sup> MATHMOD* (Vienna, Austria, February 8–10, 2006), ARGESIM-Verlag, Vienna (Austria), 2006.
20. von Lieres, E.: *Modelling and simulation of cellular regulation for metabolic engineering*, pp. 35–47 in Feldmann, V.; Mühlfeld, K. (Editors): *Virtual worlds of precision. Computer-based simulations in the sciences and social sciences* (Oxford, England, January 10–12, 2003), Lit Verlag, Münster (Germany), 2005.
21. von Lieres, E.; Wiechert, W.: *Bayesian statistics and Markov chain Monte Carlo simulation: An alternative method for parameter identification and error estimation*, in Hamam, Y.; Attiya, G. (Editors): *Proceedings of 5<sup>th</sup> EUROSIM* (Paris, France, September 6–10, 2004).
22. von Lieres, E.; Petersen, S.; Wiechert, W.: *A Multi-scale modeling concept and computational tools for the integrative analysis of stationary metabolic data*, *Journal of Integrative Bioinformatics*, 2004 and pp. 105–118 in Hofestädt, R. (Editor): *Yearbook Bioinformatics 2004*, Informationsmanagement in der Biotechnologie e.V.

### Book Chapters / Other

1. von Lieres, E.: *Modellierung und Simulation chromatographischer Trennsysteme*, *GIT Labor-Fachzeitschrift* **54,1** (2010), 36–38.
2. Wiechert, W.; Haunschild, M. D.; Weitzel, M.; Nöh, K.; von Lieres, E.; Wahl, A.; Qeli, E.; Freisleben, B.: *Grid Computing for Systems Biology*, pp. 98–133 in Barth, T.; Schüll, A. (Editors): *Grid Computing: Konzepte – Technologien – Anwendungen*, Vieweg-Verlag, Wiesbaden (Germany), 2006.
3. Petersen, S.; von Lieres, E.; de Graaf, A. A.; Sahm, H.; Wiechert, W.: *A Multi-scale approach for the predictive modeling of metabolic regulation*, pp. 237–275 in Kholodenko, B. N.; Westerhoff, H. V. (Editors): *Metabolic engineering in the post genomic era*, Horizon Scientific Press, Wymondham (England), 2003.

### Patents

1. Mottyll, S.; Paczia, N.; von Lieres, E.: *Probeentnahmeverrichtung und Verfahren zur Entnahme einer Probe aus einem Bioreaktor*, patent application (reference number EP20130000277 20130119).