

Selected Publications of Dr. Eric von Lieres

Peer-Reviewed Journals

1. Täuber, S.; Golze, C.; Ho, P.; von Lieres, E.; Grünberger, A.: *dMSCC: A microfluidic platform for microbial single-cell cultivation under dynamic environmental medium conditions*, Lab on a Chip, accepted.
2. Chernomor, O.; Peters, L.; Schneidewind, J.; Loeschcke, A.; Knieps-Grünhagen, E.; Schmitz, F.; von Lieres, E.; Kutta, R.; Svensson, V.; Jäger, K.-E.; Drepper, T.; von Haeseler, A.; Krauss, U.: *Complex evolution of light-dependent protochlorophyllide oxidoreductases in aerobic anoxygenic phototrophs: origin, phylogeny and function*, Molecular Biology and Evolution, accepted.
3. Roush, D.; Asthagiri, D.; Babi, D.; Benner, S.; Bilodeau, C.; Carta, G.; Ernst, P.; Fedesco, M.; Fitzgibbon, S.; Flamm, M.; Hansen, E.; Hahn, T.; Hunt, S.; Insaído, F.; Lenhoff, A.; Lin, J.; Marke, H.; Marques, B.; Papadakis, E.; Popp, O.; Rolandi, P.; Schlegel, F.; Smith, B.; Staby, A.; Stenevang, M.; Sun, L.; Tessier, P.; von Lieres, E.; Welsh, J.; Willson, R.; Wang, G.; Wucherpennig, T.; Zavalov, O.: *Toward in silico CMC: An industrial collaborative approach to model-based process development*, Biotechnology and Bioengineering, in press.
4. Zhao, X.; Ploch, T.; Noack, S.; Wiechert, W.; Mitsos, A.; von Lieres, E.: *Analysis of the local well-posedness of optimization-constrained differential equations by local optimality conditions*, AIChE Journal **66,10** (2020), e16548.
5. Meyer, K.; Leweke, S.; von Lieres, E.; Huusom, J.; Abildskov, J.: *ChromaTech: A discontinuous Galerkin spectral element simulator for preparative liquid chromatography*, Computers and Chemical Engineering **41** (2020), 107012.
6. Beck, J.; Heymann, W.; von Lieres, E.; Hahn, R.: *Compartment model of mixing in a bubble trap and its impact on chromatographic separations*, Processes **8,7** (2020): 780.
7. Ploch, T.; von Lieres, E.; Wiechert, W.; Mitsos, A.; Hannemann-Tamás, R.: *Simulation of differential-algebraic equation systems with optimization criteria embedded in Modelica*, Computers and Chemical Engineering **140** (2020): 106920.
8. Velali, E.; Dippel, J.; Stute, B.; Handt, S.; Löwe, T.; von Lieres, E.: *Model-based performance analysis of pleated filters with non-woven layers*, Separation & Purification Technology **250** (2020), 117006.
9. He, Q.-L.; von Lieres, E.; Zhao, L.; Sun, Z.: *Model-based process design of a ternary protein separation using multi-step gradient ion-exchange SMB chromatography*, Computers and Chemical Engineering **138** (2020): 106851.
10. Täuber, S.; von Lieres, E.; Grünberger, A.: *Dynamic environmental control in microfluidic single-cell cultivations: From concepts to applications*, Small (2020): 1906670.
11. Ploch, T.; Zhao, X.; Hüser, J.; von Lieres, E.; Hannemann-Tamás, R.; Naumann, U.; Wiechert, W.; Mitsos, A.; Noack, S.: *Multi-scale dynamic modeling and simulation of a biorefinery*, Biotechnology and Bioengineering **116,10** (2019): 2561–2574.
12. Poonoosamy, J.; Westerwalbesloh, C.; Deissmann, G.; Mahrous, M.; Curti, E.; Churakov, S.; Klinkenberg, M.; Kohlheyer, D.; von Lieres, E.; Bosbach, D.; Prasianakis, N.: *A microfluidic experiment and complementary pore scale modelling diagnostics for assessing mineral precipitation and dissolution in confined spaces*, Chemical Geology **528** (2019): 1198264.

13. Lindemann, D.; Westerwalbesloh, C.; Kohlheyer, D.; Grünberger, A.; von Lieres, E.: *Microbial single-cell growth response at defined carbon limiting growth conditions*, RSC Advances **9** (2019): 14040–14050.
14. Ho, P.; Westerwalbesloh, C.; Kaganovitch, E.; Grünberger, A.; Neubauer, P.; Kohlheyer, D.; von Lieres, E.: *Reproduction of large-scale bioreactor conditions on microfluidic chips*, Microorganisms **7,4** (2019): 105.
15. Kuzmak, A.; Carmali, S.; von Lieres, E.; Russell, A.; Kondrat, S.: *Can enzyme proximity accelerate cascade reactions?*, Scientific Reports **9** (2019): 455.
16. Burmeister, A.; Hilgers, F.; Langner, A.; Westerwalbesloh, C.; Kerkhoff, Y.; Tenhaef, N.; Drepper, T.; Kohlheyer, D.; von Lieres, E.; Noack, S.; Grünberger, A.: *A microfluidic co-cultivation platform to investigate microbial interactions at defined microenvironments*, Lab on a Chip **19** (2019): 98–110.
17. Velali, E.; Stute, B.; Leuthold, M.; von Lieres, E.: *Model-based performance analysis and scale-up of membrane adsorbers with a cassettes format designed for parallel operation*, Chemical Engineering Science **192** (2018), 103–113.
18. Bühler, J.; von Lieres, E.; Huber, G.: *Model based design of long distance tracer transport experiments in plants*, Frontiers in Plant Science **9** (2018), 773.
19. Loomba, V.; Huber, G.; von Lieres, E.: *Single-cell computational analysis of light harvesting in a flat-panel photo-bioreactor*, Biotechnology for Biofuels **11** (2018), 149.
20. Leweke, S.; von Lieres, E.: *Chromatography Analysis and Design Toolkit (CADET)*, Computers and Chemical Engineering **113** (2018), 274–294.
21. He, Q.-L.; Leweke, S.; von Lieres, E.: *Efficient numerical simulation of simulated moving bed chromatography with a single-column solver*, Computers and Chemical Engineering **111** (2018), 183–198.
22. Freier, L.; von Lieres, E.: *Robust multi-objective global optimization of stochastic processes with a case study in gradient elution chromatography*, Biotechnology Journal **13,1** (2018), 1700257.
23. Morschett, H.; Lomba, V.; Huber, G.; Wiechert, W.; von Lieres, E.; Oldiges, M.: *Laboratory scale photobiotechnology – Current trends and future perspectives*, FEMS Microbiology Letters **365,1** (2018), fnx238.
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25. 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 **1525** (2017), 60–70.
26. Zhao, X.; Noack, S.; Wiechert, W.; von Lieres, E.: *Dynamic flux balance analysis with nonlinear objective function*, Journal of Mathematical Biology **75,6** (2017), 1487–1515.
27. 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.
28. Freier, L.; von Lieres, E.: *Multi-objective global optimization (MOGO): Algorithm and case study in gradient elution chromatography*, Biotechnology Journal **12,7** (2017), 1600613.
29. 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.

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31. 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.
32. Poshyvailo, L.; von Lieres, E.; Kondrat, S.: *Does metabolite channeling accelerate enzyme-catalyzed cascade reactions?*, PLOS ONE **12,2** (2017), 1–17.
33. 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), 1127–1133.
34. 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.
35. Jussen, D.; Soltner, H.; Stute, B.; Wiechert, W.; von Lieres, E.; Pohl, M.: *μMORE: A microfluidic magnetic oscillation reactor for accelerated parameter optimization in biocatalysis*, Journal of Biotechnology **231** (2016), 174–182.
36. 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.
37. 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.
38. 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.
39. 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.
40. 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.
41. 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.
42. 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.
43. 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.
44. 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.
45. 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.

46. 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.
47. Baraibar, Á.; von Lieres, E.; Wiechert, W.; Pohl, M.; Rother, D.: *Effective production of (S)- α -hydroxy ketones: A reaction engineering approach*, Topics in Catalysis **57,5** (2014), 401–411.
48. 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.
49. 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.
50. 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.
51. 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.
52. 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.
53. 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.
54. 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.
55. 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.
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57. 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.
58. 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.
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65. 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.
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73. 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 (84th 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 14th 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 9th International MODELICA Conference (Munich, Germany, September 3–5, 2012).
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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.; Tsitouras, C. (Editors): ICNAAM 2010: 8th 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 7th 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.
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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 3rd European symposium on computer modeling and simulation* (Athens, Greece, November 25–27, 2009), IEEE computer society, Los Alamitos (USA), 2009.
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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.; Schmitt, 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 6th EUROSIM congress on modelling and simulation* (Ljubljana, Slovenia, September 9–13, 2007).
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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 5th 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.: *Probeentnahmevorrichtung und Verfahren zur Entnahme einer Probe aus einem Bioreaktor*, patent application (reference number EP20130000277 20130119).