Astrid Boje — Curriculum Vitae

AstraZeneca, Pepparedsleden 1, 431 50 Mölndal, Sweden
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Associate principal scientist with a focus on process modelling at AstraZeneca. Chemical engineer. Background in stochastic population balance and first-principles-informed kinetic modelling. Dual master's in mathematics, scientific computing.

Experience

Work experience

- **AstraZeneca** — **Sweden**
  Associate Principal Scientist – Digital Science, Pharmaceutical Technology & Development — *2023–*
  Develop mechanistic and data-driven models, process digital twins and accessible web applications to support sustainable development, scale-up, and reduced lead times in oral and inhalable product development through to on-market.
- **AstraZeneca** — **Sweden**
  Senior Scientist – Oral Product Development, Pharmaceutical Technology & Development — *2021–2023*
  Developed mechanistic and data-driven models, process digital twins and accessible web applications to support sustainable development, scale-up, and reduced lead times in oral product development.
- **Chalmers University of Technology** — **Sweden**
  Postdoc in Chemical Physics — *2020–2021*
  Developed first-principles-informed, multiscale models for studying chemical kinetics in nanoreactors and on surfaces. Developed simulation tools in Python and Matlab (https://github.com/aab64), with calculations in VASP.
- **University of Cambridge** — **United Kingdom**
  Ph.D. Student in Chemical Engineering and Biotechnology — *2015–2019*
  Developed Monte Carlo methods (in-house C++ code: https://github.com/ucam-ceb-como/MOpS) to solve population balance equations for aerosol synthesis. Proposed reactor model for titanium dioxide synthesis and new method to improve performance of the stochastic solver.
- **Helmholtz Zentrum Dresden Rossendorf** — **Germany**
  Intern in Experimental Thermal Fluid Dynamics — *2014*
  Developed 1D, dynamic, multicomponent model for a slurry bubble column reactor for Fischer-Tropsch synthesis.
- **Mintek** — **South Africa**
  Graduate Engineer in Measurement and Control — *2013*
  Researched viability of thickener control. Documented models developed for the control framework (in-house C++ code). Contributed to on-site testing and data analysis for a flotation reagent controller.
- **Mintek** — **South Africa**
  Engineering Intern in Measurement and Control — *2011–2012*
  Developed a temperature-dependent amperometry model for inclusion in a commercial cyanide measurement device.

Teaching experience

- **University of Cambridge** — **United Kingdom**
  Supervisor for Partial Differential Equations Course — *2019*
  Small-group teaching and tutorials for students in the Part IIA year of the Chemical Engineering Tripos.

Academic qualifications

- **Churchill College, University of Cambridge** — **United Kingdom**
  Ph.D. Chemical Engineering — *2015–2021*
  Modelling of combustion synthesis using stochastic methods for better understanding of the titanium dioxide process. Some research work conducted at the Cambridge CARES facilities at the National University of Singapore.
  Supervisor: Prof. Markus Kraft.

- **Technical University of Berlin (TUB)** **Germany**
  M.Sc. Scientific Computing, 1.2, "Sehr Gut" *2014–2015*
  Coursework in control theory, differential algebraic equations, optimal control of partial differential equations, and model order reduction. Thesis on convergence of stochastic coagulating particle systems with Weierstrass Institute of Applied Analysis and Stochastics (WIAS).
  Supervisors: Dr. Robert Patterson (WIAS) and Prof. Dr. Wolfgang König (TUB, WIAS).
- **Royal Institute of Technology (KTH)** **Sweden**
  M.Sc. Mathematics, A, "Excellent" *2013–2014*
  Coursework covered stochastic differential equations, parallel and high-performance computing, fast numerical algorithms, mathematical modelling, finite element and finite volume methods, and non-linear optimisation.
- **University of Cape Town (UCT)** **South Africa**
  B.Sc. Eng. Hons. (Chemical Engineering), First Class *2009–2012*
  Coursework included mathematics, physics, chemistry, thermodynamics, numerical methods, process design, modelling, and control, and post-graduate level coursework in optimisation. Honours project modelling Fischer Tropsch synthesis.
  Supervisor: Prof. Klaus Moller.

Technical skills

- **Programming languages:** C++, MATLAB, PYTHON.
- **Simulation tools:** ANSYS FLUENT, ASE, ASPEN HYSYS, COMSOL MULTIPHYSICS, gPROMS FORMULATED PRODUCTS, LIGGGHTS, VASP.
- **General proficiencies:** Git, HPC, LaTeX, Linux, Microsoft Windows, MPI/OpenMP and parallel programming, Slurm.

Achievements

- **Cambridge University Ph.D. Studentships** *2015–2019*
  Cambridge Centre for Advanced Research & Education in Singapore; Chemical Engineering & Biotechnology Department
- **COSSE Double Master's Programme** *2013–2015*
  Erasmus Mundus Scholarship
- **Mintek** *2011–2012*
  Undergraduate Bursary
- **University of Cape Town, Faculty of Engineering** *2009–2012*
  Entrance Scholarship (2009), Dean's Merit List (2010–2012)
- **Kwa-Zulu Natal Youth Dance Company** *2006–2008*
  Provincial ballet dancer

Extracurricular activities

- **Cambridge University Ballet Club** (2015–2016, 2018–2019). Performed in Don Quixote, 2019.
- **Churchill College Boat Club** (2015–2016, 2018–2019). Rowed in women's second boat, 2015–2016. Sub for women's first and second boats, 2018–2019.

Publications

- Engedahl, U., **Boje, A.**, Ström, H., Grönbeck, H., Hellman, A., 2024. Investigating the Composition of the Metal Dimer Site in Chabazite for Direct Methane-to-Methanol Conversion. *The Journal of Physical Chemistry C* 168, 3641–3651. doi: 10.1021/acs.jpcc.3c06635.
- Levin, S., Lerch, S., **Boje, A.**, Fritzsche, J., KK, S., Ström, H., Moth-Poulsen, K., Sundén, H., Hellman, A., Westerlund, F., Langhammer, C., 2022. Nanofluidic Trapping of Faceted Colloidal Nanocrystals for Parallel Single-Particle Catalysis. *ACS Nano* 19, 15206–15214. doi: 10.1021/acsnano.2c06505.
- **Boje, A.**, Kraft, M., 2022. Stochastic population balance methods for detailed modelling of flame-made aerosol particles. *Journal of Aerosol Science* 159, 105895. doi: 10.1016/j.jaerosci.2021.105895.
- **Boje, A.**, Taifan, W. E., Ström, H., Bučko, T., Baltrusaitis, J., Hellman, A., 2021. First-principles-informed energy span and microkinetic analysis of ethanol catalytic conversion to 1,3-butadiene on MgO. *Catalysis Science and Technology* 11, 6682–6694. doi: 10.1039/D1CY00419K.

- Engedahl, U., **Boje, A.**, Ström, H., Grönbeck, H., Hellman, A., 2021. Complete Reaction Cycle for Methane-to-Methanol Conversion over Cu-SSZ-13: First-Principles Calculations and Microkinetic Modeling. *The Journal of Physical Chemistry C* 125, 14681–14688. doi: 10.1021/acs.jpcc.1c04062.
- Tiburski, C., **Boje, A.**, Nilsson, S., Say, Z., Fritzsche, J., Ström, H., Hellman, A., Langhammer, C., 2021. Light-Off in Plasmon-Mediated Photocatalysis. *ACS Nano* 15, 11535–11542. doi: 10.1021/acsnano.1c01537.
- Albinsson, D., **Boje, A.**, Nilsson, S., Tiburski, C., Hellman, A., Ström, H., Langhammer, C., 2020. Copper Catalysis at Operando Conditions–Bridging the Gap between Single Nanoparticle Probing and Catalyst-Bed-Averaging. *Nature Communications* 11, 4832. doi: 10.1038/s41467-020-18623-1.
- **Boje, A.**, Akroyd, J., Sutcliffe, S., Kraft, M., 2020. Study of industrial titania synthesis using a hybrid particle-number and detailed particle model. *Chemical Engineering Science* 219, 115615. doi: 10.1016/j.ces.2020.115615.
- **Boje, A.**, Akroyd, J., Kraft, M., 2019. A hybrid particle-number and particle model for efficient solution of population balance equations. *Journal of Computational Physics* 389, 189–218. doi: 10.1016/j.jcp.2019.03.033.
- **Boje, A.**, Akroyd, J., Sutcliffe, S., Edwards, J., Kraft, M., 2017. Detailed population balance modelling of TiO_2 synthesis in an industrial reactor. *Chemical Engineering Science* 164, 219–231. doi: 10.1016/j.ces.2017.02.019.

Conference Presentations

- **Boje, A.**, Taifan, W. E., Ström, H., Bučko, T., Baltrusaitis, J., Hellman, A., 2022. Kinetics of MgO-Catalyzed Ethanol Conversion to 1,3-Butadiene. Talk presented at *The 27th North American Catalysis Society Meeting*.
- **Boje, A.**, Taifan, W. E., Ström, H., Bučko, T., Baltrusaitis, J., Hellman, A., 2021. Kinetic modelling of ethanol conversion to 1,3-butadiene on MgO and implications for catalyst design. Talk presented at *AIChE Fall Meeting*.
- **Boje, A.**, Ström, H., Hellman, A., 2021. First-principles-informed kinetic modelling in operando catalysis studies: CO oxidation on metal nanoparticles. Talk presented at *AIChE Fall Meeting*.
- **Boje, A.**, Taifan, W. E., Ström, H., Bučko, T., Baltrusaitis, J., Hellman, A., 2021. Exploring the free energy landscape: Comparison of kinetic models for MgO-catalyzed ethanol conversion to 1,3-butadiene. Talk presented at *ACS Spring Meeting*.
- **Boje, A.**, Taifan, W. E., Ström, H., Bučko, T., Baltrusaitis, J., Hellman, A., 2021. Performance and predictions of kinetic models for MgO-catalyzed ethanol conversion to butadiene. Poster presented at *DPG Surface Science Meeting*.
- **Boje, A.**, Albinsson, D., Langhammer, C., Ström, H., Hellman, A., 2020. Multiscale modelling of CO oxidation on copper nanoparticles in nanoreactors. Talk presented at *ACS Postdoc Symposium (invited)*.
- **Boje, A.**, Albinsson, D., Langhammer, C., Ström, H., Hellman, A., 2020. Multiscale modelling of CO oxidation on copper nanoparticles in nanoreactors. Talk presented at *ACS CATL Division ChemistsLive (invited)*.
- **Boje, A.**, Albinsson, D., Langhammer, C., Ström, H., Hellman, A., 2020. Multiscale modelling of CO oxidation on copper nanoparticles in nanoreactors. Talk presented at *ACS Fall Meeting*.
- **Boje, A.**, Akroyd, J., Kraft, M., 2019. Detailed population balance modelling using a hybrid particle model. Talk presented at *AIChE Fall Meeting*.
- **Boje, A.**, Akroyd, J., Kraft, M., 2019. Using a hybrid particle-number and particle model to study inorganic combustion synthesis. Talk presented at *Combustion Aerosol Conference*.
- **Boje, A.**, Akroyd, J., Kraft, M., 2018. Numerical study of the evolution of particle size and morphology in an industrial titanium dioxide reactor. Talk presented at *AIChE Fall Meeting*.
- **Boje, A.**, Kraft, M., 2017. Computational study of temperature effects in TiO_2 synthesis in an industrial reactor. Poster presented at *Cambridge Particle Meeting*.