# Astrid Boje — Curriculum Vitae

AstraZeneca, Pepparedsleden 1, 431 50 Mölndal, Sweden □ +46 (0)73 840 1129 • ⊠ astrid.boje@astrazeneca.com • ♂ aab64.github.io

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

W	/ork experience		
$\cap$	AstraZeneca	Sweden	
0	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.		
$\cap$	AstraZeneca	Sweden	
0	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.		
0	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.		
$\sim$	University of Cambridge	United Kingdom	
0	Ph.D. Student in Chemical Engineering and Biotechnology	2015–2019	
	Developed Monte Carlo methods (in-house C++ code: https://github.com/ucam-ceb-como/MOp balance equations for aerosol synthesis. Proposed reactor model for titanium dioxide synthesis	S) to solve population and new method to	
	improve performance of the stochastic solver.		
0	Helmholtz Zentrum Dresden Rossendorf Intern in Experimental Thermal Fluid Dynamics	Germany 2014	
	Developed 1D, dynamic, multicomponent model for a slurry bubble column reactor for Fischer-Tropsch synthesis.		
0	Mintek Graduate Engineer in Measurement and Control	South Africa 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	
0	Engineering Intern in Measurement and Control	2011–2012	
	Developed a temperature-dependent amperometry model for inclusion in a commercial cyanide m	easurement device.	
Т	eaching experience		
$\cap$	University of Cambridge	United Kingdom	
0	Supervisor for Partial Differential Equations Course	2019	
	Small-group teaching and tutorials for students in the Part IIA year of the Chemical Engineering	Tripos.	
A	Academic qualifications		

#### Churchill College, University of Cambridge

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.

**United Kingdom** 

#### Technical University of Berlin (TUB)

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)

M.Sc. Mathematics, A, "Excellent"

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)

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, LTFX, Linux, Microsoft Windows, MPI/OpenMP and parallel programming, Slurm.

# Achievements

0	Cambridge University Ph.D. Studentships Cambridge Centre for Advanced Research & Education in Singapore; Chemical Engineering & Biotechnology	<i>2015–2019</i> Department
0	COSSE Double Master's Programme	2013–2015
	Erasmus Mundus Scholarship	
0	Mintek	2011–2012
	Undergraduate Bursary	
0	University of Cape Town, Faculty of Engineering	2009–2012
	Entrance Scholarship (2009), Dean's Merit List (2010–2012)	
0	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.
- O 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

- O Bouchier, F., Boje, A., Reynolds, G., 2025. Life Cycle Assessment of Pharmaceutical Tablet Manufacturing: A Comparative Analysis and Systems Model Integration Framework. Submitted.
- Kjaer Jepsen, P., Martin De Juan, L., Boje, A., Sarangi, S., von Corswant, C., Sasic, S., 2024. Wurster fluidised-bed coating: Coarse-graining technique within CFD-DEM in conjunction with heat and mass transfer. Powder Technology 443, 119901. doi: 10.1016/j.powtec.2024.119901.
- 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.

#### Sweden 2013-2014

South Africa

### Germany

- 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<sub>2</sub> 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<sub>2</sub> synthesis in an industrial reactor. Poster presented at *Cambridge Particle Meeting*.