5MW Program

Monday, 26 of June

9:00–9:15	**Welcome – Arne Staby**	
9:15–10:30	**Session 1: Biophysics and Molecular Modeling** Chairs: Sophie Karkov (NN) and John Welsh (Rivanna Bioprocess Solutions)	
10’	**David Saleh** Boehringer Ingelheim/KIT	Multiscale modeling of polishing chromatography: A versatile tool for manufacturing assessment and process development
10’	**Julie Robinson** MSD	Multi-scale modeling: Bridging the gap between complexity, speed and HTS experimentation during early phase downstream process development
10’	**Lijuan Li** Takeda	Molecular Modeling to Support Process Development Decision and Create In-silico Developability Predictive Platform Across R&D
10:00–10:30	**Q&A**	
10:30–11:00	**Break**	

11:00–12:20	**Session 2: Mechanistic Modeling I** Chairs: Felix Wittkopp (Roche) and Jessica Lyall (Genentech)	
10’	**Katrin Paul** Novartis	Improving upstream process performance by combining flux balance analysis (FBA) with inhibition kinetics
10’	**Sara Canle Babío** Novo Nordisk	Mechanistic modeling of a dynamic cross-flow filtration for API recovery
10’	**Christian Krätzer** MSD	Kinetic model of a polysaccharide vaccine conjugation process
10’	**Till Briskot** Boehringer Ingelheim	Qualification of mechanistic models used for the development and regulatory filing of downstream processes
11:55–12:20	**Q&A**	
12:30–13:30	**Lunch**	
13:30–14:45	**Session 3: Mechanistic Modeling II.** Chairs: Felix Wittkopp (Roche) and Jessica Lyall (Genentech)	
10’	**Scott Altern** RPI*	Modeling of multimodal chromatography using high-throughput batch isotherm data
10’	**Eric Shierly** Regeneron	Exploring on-column conformational changes during HIC negative mode purification modeling
10’	**Dominik Hertweck** Roche	Application of Colloid Particle Adsorption Models for Flexible Downstream Process Development
10’	**Chyi-Shin Chen** Chugai	Modeling application for early-stage process optimization of a monoclonal antibody in mixed-mode chromatography
14:25–14:45	**Q&A**	
14:45–15:15	**Break**	
15:15–16:30	**Open mic discussions** Biophysics, molecular and mechanistic modeling and ideas related to day’s sessions	
16:30–18:00	**Break and poster preparation**	
18:00–19:30	**Dinner**	
19:30–21:30	**Poster Session**	

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9:00–10:20	**Session 4: Computational Fluid Dynamics** Chairs: Robert Todd (Digital Process Design) and Deenesh Babi (NN)	
10'	**Michael Martinetz** Boehringer Ingelheim	Precipitation – CFD and SDM experimental assisted troubleshooting to enhance production-scale process performance
10'	**Pavlos Kotidis** GSK	Use of computational fluid dynamic & mechanistic modeling in cell line selection and scale-up
10'	**Simone Dimartino** University of Edinburgh*	Machine learning for morphology optimization of perfectly ordered stationary phases
10'	**Tanja Hernández** Novartis	A probabilistic approach for diversion strategy development in continuous manufacturing
9:55–10:20	**Q&A**	
10:20–11:00	**Break**	
11:00–12:20	**Session 5: Plant Modeling** Chairs: Mariona Bertran (NN) and Robert Todd (DPD)	
10'	**Simon Lindahl** Novo Nordisk	Product and project allocation in primary pharmaceutical manufacturing
10'	**Suzanne Farid** UCL*	How can we best design facilities of the future to meet cost of goods, cost of development and sustainability priorities?
10'	**John Bagterp Jørgensen** DTU*	Modeling, simulation, control and uncertainty quantification for integrated optimization for upstream and downstream processes in mAb production
10'	**Tobias Overgaard** Novo Nordisk	A causal framework for performance analysis of full-scale pharmaceutical manufacturing systems
11:55–12:20	**Q&A**	

12:30–13:30	**Lunch**	
13:30–15:00	**Session 6: Invited Talks** Chairs: Arne Staby (NN) and David Roush (MSD)	
15'	**Abraham Lenhoff** University of Delaware*	The essential chemistry of electrostatic interactions of proteins
15'	**Todd Przybycien** RPI*	Implementation of the population balance model in CADET and application to the continuous antibody capture via precipitation
15'	**Shuichi Yamamoto** Yamaguchi University*	Simple and fast methods for determining parameters for model simulations of ion-exchange
15'	**Bernt Nilsson** Lund University*	Automatic modeling and optimization of a chromatography separation
14:40–15:00	**Q&A**	
15:00–15:30	**Break**	
15:30–16:45	**Open mic discussions** CFD, plant modeling and ideas related to the day's sessions	
16:45–17:00	**Closing Remarks – Arne Staby**	

List of Posters

1. **Jessica Emonts**, BOKU*: *Developing novel descriptors to capture spatial correlation of protein surface properties for purification applications*

2. **Anette Henriksen**, Novo Nordisk: *Antibody in-silico developbility assessment*

3. **Laila Sakhini**, Novo Nordisk: *Molecular Modeling to Support Process Development Decision and Create In-silico Developability Predictive Platform Across R&D*

4. **Tobias Hahn**, Cytiva: *Optimizing AAV5 full/empty separation through improved understanding of AAV-resin interaction*

5. **Sean Burgess**, Genentech: *"Using batch binding screens to identify an appropriate isotherm for multimodal chromatography models*

6. **Christian Frech**, HS Mannheim*: *Mechanistic modeling of cation exchange chromatography scale-up considering packing inhomogeneities*

7. **Janja Dermol-Cerne**, Novartis: *In-silico determination of excipient concentrations and pH during ultrafiltration and diafiltration process*

8. **Chris Gerberich**, GSK: *Modeling the Effect of Ionic Capacity on Cation Exchange Chromatography Separations of Biomolecules*

9. **Jürgen Beck**, BOKU*: *Challenges in parameter estimation for two-component protein adsorption using batch and small-scale column adsorption*

10. **Emmanouil Papadakis**, Novo Nordisk: *Optimization of industrial freeze drying process through a combination of model- and lab-based experiments*

11. **Nehal Patel**, Siemens: *End-to-end mechanistic models of integrated and continuous biomanufacturing processes*

12. **Rune Lorits**, Novo Nordisk: *Mechanistic modelling of industrial crystallization processes – Challenges and opportunities at the initial solution stage*

13. **Johannes Winderl**, Rentschler Biopharma: *Mechanistic model-based process development in a CDMO – client framework – a case study*

14. **Anton Ochoa Bique**, Novo Nordisk: *The three gears of success: a framework to tackle a need for expanding production capacity*

15. **Tim Thostrup Hybschmann**, EDR & Medeso: *Harnessing The Power of AI to Revolutionize the World of CFD Simulations*

16. **Juergen Fitschen**, Boehringer Ingelheim: *Computational Methods to Support Commercialization of intensified biopharmaceutical processes*

17. **Avik Sarkar**, MSD: *Advancing the maturity and impact of mechanistic predictive models in large-molecules manufacturing*