Sargent Centre for Process Systems Engineering

2023 SYMPOSIUM ON MODEL BASED DESIGN OF EXPERIMENTS

Friday 23 June 2023

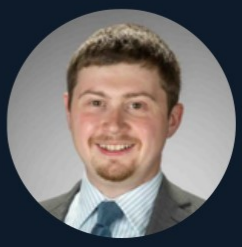
The Sargent Centre, Imperial College London

Programme

Kim McAuley
Queens University, Canada

Salvador Garcia
Eli Lilly &Co

Ruth Misener
Imperial College London



Alexander Dowling
Notre Dame University

Benoit Chachuat
Imperial College London

Daniel Rodriguez
Pfizer

Fabrizio Bezzo
University of Padova

Federico Galvanin
UCL

Federica Cattani
Syngenta

Enrico Sangoi
UCL

Brian Taylor
Astra Zeneca

Antonio del Rio Chanona
Imperial College London

PROGRAMME

The Sargent Centre, Imperial College London, Roderic Hill Building, Prince Consort Road, SW7 2BB

8.30	Registration (Roderic Hill lobby) and coffee (RODH 615) *Presentations in Lecture Theatre 3 - 3rd Floor, RODH 306*
9.00	Opening remarks - Prof Claire Adjiman, Imperial College London
9.05	Keynote presentation Sequential model-based design of experiments when some parameters are not estimable *Kim McAuley, Professor, Queen's University Canada*
Session 1	*Chair: Prof Claire Adjiman, Imperial College London*
9.50	Adoption of MBDoE approaches into new product development workflows *Salvador García-Muñoz, Senior Engineering Advisor, Eli Lilly & Co*
10.15	Pyomo.DoE: Enabling model-based design of experiments in the Pyomo ecosystem *Alexander Dowling, Associate Professor, University of Notre Dame*
10.40	Refreshments – 6th Floor RODH 615
Session 2	*Chair: Prof Benoit Chachuat, Imperial College London*
11.10	Partial least squares: Balancing accuracy with robustness *Ruth Misener, Professor, Imperial College London*
11.35	Model based design of experiments in autonomous model identification platforms: Recent developments and open challenges *Federico Galvanin, Associate Professor, UCL*
12.00	Tracking MBDoE research at University of Padova: Results, applications and open challenges *Fabrizio Bezzo, Professor, University of Padova*
12.25	Lunch and Posters – 6th Floor RODH 615
Session 3	*Chair: Dr Lauren Lee, Imperial College London*
13.45	Far from ideal: Exploring MBDoE for time consuming experiments with strong uncontrolled uncertainties (and limited understanding) *Federica Cattani, Technical Expert, Syngenta & Enrico Sangoi, Researcher, UCL*
14.10	Recent developments in effort based methods for optimal and robust experimental campaigns *Benoit Chachuat, Professor, Imperial College London*
14.35	Bringing Bayesian optimisation to high throughput experimentation as a tool for chemical synthesis *Daniel Rodriguez, API Process Modeller – Senior Scientist, Pfizer*
15.00	Refreshments – 6th Floor RODH 615

Session 4 *Chair: Dr Monica Tirapelle, UCL*

15.30 Applying design of experiments as a collaborative tool with kinetic modelling for API process development experimentation
Brian Taylor, Statistician, Astra Zeneca

15.55 Model-based design of experiments for automated model construction
Antonio del Rio Chanona, Senior Lecturer, Imperial College London

16.20 Poster session – 6th Floor RODH 615

17.00 Closing remarks and poster prizes

17.10 End

POSTER SESSION

1	Emmanuel Agunloye	UCL
	Applications of MBDoE techniques to a cloud-based platform for automated chemical manufacturing in flow reactor systems	
2	Gustavo Chaparro	Imperial College London
	Development of a physics-informed data-driven Equation of State for the Mie fluid	
3	Phillip Deussen	UCL
	A joint model-based design of experiments approach for the identification of Gaussian Process models in geological exploration	
4	Sarah Engell	Technical University of Denmark
	From Optimal Experimental Design to Safe Dose Guidance in Type 2 Diabetes	
5	Andrea Friso	UCL
	A Fisher information driven approach for online design of experiments	
6	Griffin Gui	Imperial College London
	Maximising the likelihood of obtaining accurate solvatochromic equations for reaction kinetics prediction	
7	Arun Pankajakshan	UCL
	Autonomous kinetic model identification using optimal experimental design and retrospective data analysis	
8	Mirko Pasquini	KTH Royal Institute of Technology
OBJ	*Model-based medium optimization in continuous perfusion cultures*	
9	Marco Sandrin	Imperial College London
	Exact designs of optimal experiment campaigns	
10	Enrico Sangoi	UCL
	On the development and application of a general model identification framework to biological systems	
11	Tom Savage	Imperial College London
	Multi-fidelity Data-Driven Design and Analysis of Reactor and Tube Simulations (DARTS)	
12	Lyu Wenyao	UCL
	Development of a Novel Framework for Automated Simultaneous Model Identification and Parameter Estimation in Kinetic Studies	