Sargent Centre for Process Systems Engineering

The Sargent Centre for Process Systems Engineering

Report no. 2

Imperial College London | UCL

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Directors' Foreword

In this latest Sargent Centre report, we have sought to bring together selected highlights of our collective research programme and of the wide range of activities in which our dynamic and innovative community has engaged in the past two years. The report is also an opportunity to meet our new members, who bring an exceptional wealth of new expertise and interests to the academic team at the Sargent Centre.

We hope that in discovering snapshots of our work you will get a sense for the myriad ways in which we are working with our partners to address the sustainability grand challenges facing the process and allied industries and wider society, from the transition to net zero, to the reinvention of industry around renewable feedstocks, and the provision of affordable and effective healthcare. Systems thinking and systems engineering methods have a critical role to play in addressing these complex interconnected issues. Indeed, in parallel to deploying systems approaches on global challenges, the Sargent Centre community continues to advance the fundamentals of process systems engineering, finding new ways to model complex systems, developing the machine learning tools that can support decision-making in a context that is often data-poor, and enabling a more resilient approach to uncertainty and risk.

Collaboration is at the heart of the Centre's programme: our internal and external collaborators, and particularly our Consortium Members and Major Partners, shape our research and help us to focus on the most impactful questions. You will see evidence of partners' engagement throughout our projects and we are grateful for the insights they share with us and the challenges they set us.

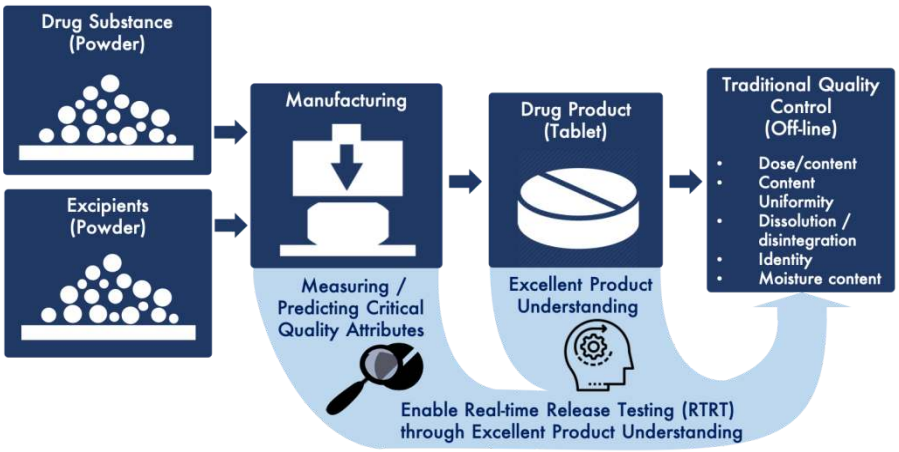
Looking back at all the achievements of the past year, we are particularly heartened by the enthusiasm and positive attitude with which members of the Sargent Centre community have reconnected in person after the isolation of the pandemic lockdowns and have worked together to provide an inclusive and diverse environment in which individuals can flourish.

We hope that you find the report interesting and we encourage you to get in touch if you'd like to find out more.

Professors Claire Adjiman and Nilay Shah

New Research Initiatives

Dr. Salvalaglio has been awarded a 5-year ERC Consolidator Grant for his project **ht-MATTER**: High Throughput Modelling of Molecular Crystals Out of Equilibrium (EP/X033139/1). His research aims to answer questions regarding how molecular properties affect technologically relevant processes in the fields of chemical and biochemical engineering. Through ht-MATTER, he will develop an open, transparent and flexible molecular simulation platform that will deploy state-of-the advanced molecular simulation methods necessary to model the out-of-equilibrium processes that govern crystal precipitation from solution at the atomistic scale.



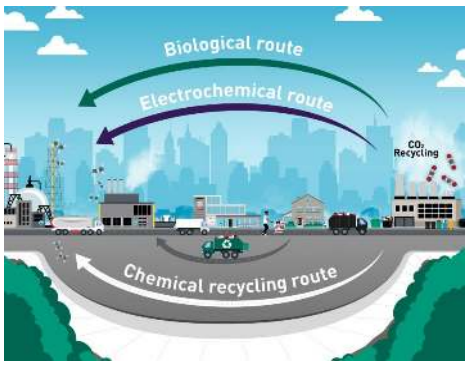
Professor Bogle is co-investigator on a 3-year EPSRC grant, **RIFTMaP**: Right First Time Manufacture of Pharmaceuticals (EP/V034723/1, 2021-2024), led by Professor Lister at Sheffield University with UCL, Strathclyde and Purdue Universities (funded by NSF) and a number of pharma, equipment and software companies exploring risk based digitalisation of formulated products manufacture. The project includes a significant element of work on two pilot plants for verification. Work continues with the University of Palermo and collaborating companies on the use of sea water and salt bitterns producing fresh water, electricity, and minerals (particularly Mg) as a circular economy system.

Dr. Papathanasiou was awarded a 3-year EPSRC New Investigator Award, **i-PREDICT**: Integrated adaPtive pRocEss DesIgn and ConTrol (EP/W035006/1, 2022-2025). She will work with industrial partners GSK and Pall on realising "Pharma 4.0" through the development and experimental validation of Industry 4.0-aligned frameworks for upstream in-process monitoring, optimisation and control. This research will create a roadmap towards the integration of product quality in bioprocess design. By considering the interplay between upstream and downstream operations, it will allow the design of variability-robust separation processes and enable seamless unit integration and downstream scale-up. The developed digital and mathematical tools will be validated experimentally, thereby closing the loop from in silico to in vitro.

Professors Kontoravdi and Shah are co-investigators in the WellcomeLEAP R3 project **Biofoundry-in-a-Box,** led by Professor Makatsoris at King's College London and in collaboration with Medicine at Imperial College London. The Biofoundry-in-a-Box is a modular, flexible and automated microfactory that enables rapid and on-demand access to a wide variety of RNA-based drug products, including mRNA and saRNA products. The project is aiming at compacting and modularizing mRNA product manufacture through intensification technologies for rapid and on-demand deployment and manufacture; overcoming mRNA substance manufacturing hurdles with innovative technologies; and evaluating the opportunity of smart manufacturing to transform manufacturing methods towards commercialization.

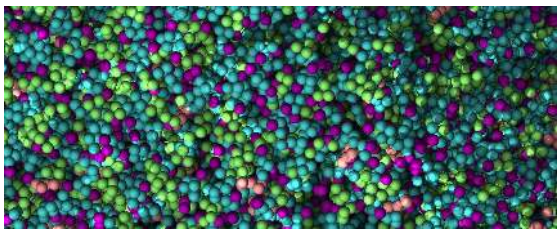
Professor Chachuat participates in the Marie Curie Training Network **digitalgaesation** (Agreement 955520, 2021-2025), led by Sargent Centre's alumnus Professor Bezzo (University of Padova). The project aims to develop a digitalisation approach to optimising control and operation of microalgea cultivation processes. Two early-career researchers joined the Sargent Centre in 2021 on research projects in collaboration with Siemens PSE (Marco Sandrin) and the Department of Life Sciences at Imperial College London (Giovanni Consoli).

Academics from the Sargent Centre (Professors Chachuat, Mac Dowell & Shah) are co-investigators in the 4-year UKRI-funded **Centre for Circular Chemical Economy** (EP/V011863/1) since 2021. The Centre's vision is to transform the UK's chemical industry into a fossil-independent, climate-positive and environmentally-friendly circular chemical economy. We lead one of the three themes of this project on Process Integration & Whole System Optimization, where we assess the performance of alternative routes to key chemicals (e.g. olefins) from CO2 streams, solid waste and biomass, and investigate the trade-offs inherent to chemical circularity to guide the selection and deployment of chemical recycling technologies.



Drs. del Rio Chanona and Cardin and Professor Shah are co-Investigators on the new **Hitachi-Imperial Centre for Decarbonisation and Natural Climate Solutions**, announced in late 2022. The Centre will work on fundamental and applied research, addressing key challenges in decarbonisation and climate repair in order to achieve a net-zero future and will help train the next generation of net-zero scientists and engineers. Initial research projects will focus on carbon management, the decarbonisation of energy and transport, CO2 removal and biodiversity, with a focus on new technologies and nature-based solutions.

A 3-year extension (2021-24) to the Shell-Imperial Digital Rocks (SDR) Programme (£8m, 2016-21) led by Professor Maitland, was put in place with Professors Blunt and Trusler as co-Directors. The programme outputs form the basis of a step-change in the way sub-surface reservoir systems (and multiphase fluid-filled porous media in general) through a combination of rock-fluid molecular imaging and X-ray micro/macro tomography with molecular, pore-scale and core scale modelling in a multi-scale molecular to reservoir scale-up methodology.



ADOPT (EP/W003317/1, 2022-2026) is a 4-year UKRI-funded international collaboration between the Sargent Centre and the JARA Center for Simulation and Data Science, co-led by Professors Chachuat and Mitsos with 13 co-investigators (including Professors Adjiman, Bogle, Misener, Pantelides & Wiesemann and Drs. Charitopoulos & Parpas). The main objective of ADOPT is to integrate deterministic global optimisation with surrogate models and machine learning in order to enable transformational changes in our capability to tackle complex decision-making problems. ADOPT will seek to demonstrate these theoretical and algorithmic advances through industrial use cases, including computer-aided molecular and process design (CAMPD), enterprise-wide optimisation (EWO), and computational fluid dynamics (CFD). The software companies GUROBI Optimization, MOSEK ApS, OCTERACT & Siemens PSE are partnering with ADOPT.

Dr. Mercangoz, ABB Reader of Autonomous Industrial Systems at Imperial College London, was awarded an EPSRC grant (EP/W027860/1, 2022-2024) to investigate the grid integration of multi-vector energy storage systems, in collaboration with University of Manchester and University of Cambridge. As part of the project, the Autonomous Industrial Systems Lab will develop dynamic models and control and optimization algorithms for thermal and thermo-chemical electricity storage plants.

Professor Fraga is co-investigator on the EPSRC-funded project Elucidation of Unusual Nano-effects on Dissolution, Aggregation, and Denaturation Processes of Alpha Particles Generated by Fuel Debris Retrieval (EP/X022218/1, 2022-2025), co-led by Professor Angeli (UCL) and Professor Tsukahara (Tokyo Institute of Technology). The safe handling of nuclear fuel debris is challenging due to the lack of characterisation of how these debris evolve in time while being processed or awaiting processing. The original extraction of the debris, from for instance the site of the Fukushima-Daiichi nuclear power plant, and the subsequent processing create particles in solution, and potentially in the form of aerosols, due to both physical processing such as cutting and subsequent dissolution and aggregation of these particles. The aim of this project is to combine experimental expertise and resources with mathematical modelling to develop predictive models suitable for the prediction of distributions of nano-particles in solution arising from fuel debris.

Professors Adjiman, Galindo & Jackson are part of a new collaboration including partners from Greece, the UK, Austria, the Netherlands and Germany. This Horizon project (Agreement 101075727, 2022-2026), **HiRECORD** targets a reduction in the cost of CO2 capture, through scaling up of a highly modular rotating packed bed plant with an environmentally benign solvent. The contribution of the Molecular Systems Engineering (MSE) team will involve thermodynamic modelling using the molecular-based group-contribution SAFT Mie equation of state to predict solubility of CO2 in aqueous amine-based solvent systems saturated with SOx and NOx.

Following up on efforts to create machine-learned equations of state (DOI: 10.1021/acs.jpcb.0c05806), the MSE team has also signed a new project with BP and ICAM to further extend these ideas to other areas of prediction of thermophysical properties.

ReaxPro: Multiscale Software Platform Enabling the Bottom-up Design of Next-Generation Catalytic Processes

Contributed by Michail Stamatakis

Within the context of EU project ReaxPro, Professor Stamatakis and 9 partner institutions across Europe have been developing a comprehensive software solution for multiscale modelling of catalytic processes from electrons to reactors. The ReaxPro software platform enables the design of cost-efficient, environmentally friendly and sustainable processes, and aims at delivering measurable impact within the chemical industry, economy and society.

The chemical industry underpins virtually all sectors of the economy, from healthcare to construction, and is an integral part of a successful and sustainable industrial ecosystem. Essential to the chemical industry are catalytic materials, which accelerate reactions and are used by an estimated 85-90% of all chemical manufacturing operations. Yet, discovering catalytic materials and building catalytic processes is non-trivial. Reactive process design has largely been based on trial-and-error experimentation and similarly, reactor design has traditionally relied on empirical kinetics and data-based models. On the other hand, bottom-up physics-based modelling approaches are emerging as highly promising in the development of new catalytic materials and reactive processes. However, developing comprehensive multi-scale models is cumbersome and requires specific expertise at all levels, thereby raising significant barriers for the broad industrial uptake of such modelling methods.

Breaking the barriers

EU-funded project ReaxPro aims at empowering researchers and process developers to overcome these barriers, by delivering a software platform that is accessible to the generalist user, and which integrates catalytic materials modelling software with reactive process modelling at the industrial scale. As the basis for these development efforts, ReaxPro uses the commercial *ADF Modeling Suite* (developed by SCM, a Netherlands-based software company) for computational chemistry and materials science calculations at the electronic and atomistic scales, along with a set of academic software tools: *EON* (developed by Hannes Jónsson at the University of

Iceland and Graeme Henkelman at the University of Texas at Austin) for long timescale dynamics at the atomistic scale, *Zacros* (developed by Michail Stamatakis at UCL) for high-fidelity simulations of catalytic kinetics atthe mesoscale, and *CatalyticFOAM* (developed by Matteo Maestri at Politecnico di Milanofor heterogeneous reacting flows with detailed kinetic mechanisms at the macroscale. The academic tools have been upscaled into easy-to-learn, user friendly, interoperable software that is supported and well documented, and have been integrated into the *ADF Modeling Suite* towards an industry-ready solution for catalytic material and process design.

To ensure that the ReaxPro platform can be extended in a straightforward way in future efforts, a semantic interoperability layer enables cross-communication among the different simulation software components as well as data repositories. Interoperability is achieved by the use of the European Materials Modelling Ontology (EMMO), a broad and multidisciplinary effort towards the development of a standard representational framework (ontology) of materials modelling knowledge. In this context, the EMMO underpins the ReaxPro platform as the common vocabulary to describe its simulation workflows, including calculations, codes, models, simulation parameters, as well as relevant physical quantities. Additionally, the *SimPhoNy* package (developed by Fraunhofer) is used to facilitate (and realise) the actual communication between software components via the vocabulary of the ontology.

Proof of principle

As proof-of-concept, the ReaxPro consortium demonstrated the integrated approach on the CO oxidation reaction on Pt catalysts, relevant to gaseous emissions control. For this first test case, a reaction-diffusion formalism was used for the reactor level description, solving equations that express the mass conservation during the overall conversion of gaseous CO and O_2 into gaseous CO_2. In these mass balances, the rate-per-catalytic-site for the overall reaction was delivered by a machine-learning-based surrogate model, trained on detailed KMC simulations that used Zacros at the catalytic surface level. These KMC simulations considered the detailed reaction mechanism, by including additional elementary events, in particular, adsorption, desorption, diffusion and surface reactions. In turn, the rate constants of these elementary events, were derived via transition state theory expressions, parameterised by electronic/atomistic calculations. The latter used the ReaxFF potential and were performed by the *EON* module coupled to the *AMS Modeling Suite*. Thus, reactive processes were found in a semiautomated way via transition state searches, and further calculations were performed for the gas-phase configurations, as final states of desorption events, assuming the latter events are non-activated. Other case studies focusing on various materials, such as highly dilute alloys and zeolites, are ongoing in the ReaxPro partner labs.

Next steps and broader vision

The ReaxPro project aims at delivering a code base and software tools that will be useful for the entire materials and process modelling community. The inherent interoperability foundations of ReaxPro guarantee seamless integration with other codes and software solutions, making it e.g., possible to swap *Zacros* for a different KMC software package, which a user might be more familiar with. Developing such custom versions of the ReaxPro platform, also tailored to other potential applications, e.g., separations, or electrochemical processes, opens up exciting avenues for future development. Further towards maximising impact and ensuring the adoption of the project's deliverables, the ReaxPro software platform and associated services will be made available via the *European Materials Modelling Marketplace* through the consortium's partnership with ongoing EU projects MARKETPLACE and VIMMP. This marketplace will provide a one-stop shop for all materials modelling demands including translation, training, and simulation as a service, further facilitating the adoption of high-fidelity bottom-up modelling approaches for the development of next-generation chemical processes.

References:

- D Micale, C Ferroni, R Uglietti, M Bracconi, M Maestri (2022) Computational Fluid Dynamics of Reacting Flows at Surfaces: Methodologies and Applications. *Chemie Ingenieur Technik*. DOI: 10.1002/cite.202100196
- M Pineda, M Stamatakis (2022) Kinetic Monte Carlo simulations for heterogeneous catalysis: Fundamentals, current status and challenges. The Journal of Chemical Physics **156**, 120902. DOI: 10.1063/5.0083251

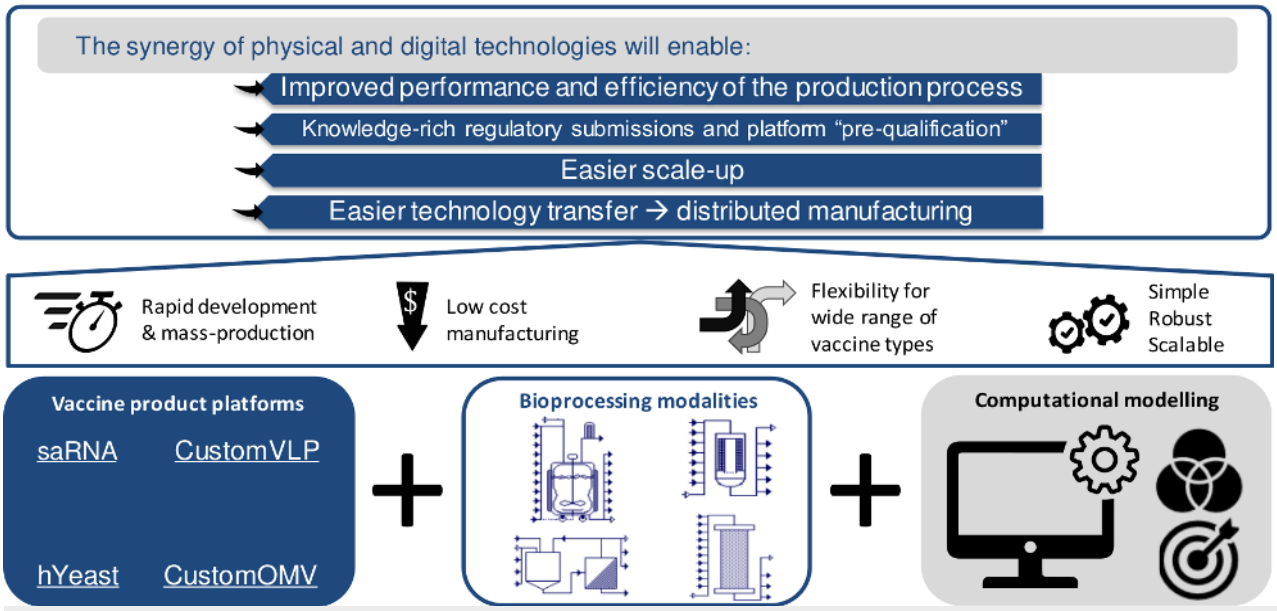
Optimisation of Vaccine Manufacturing and Supply Chain

Contributed by Cleo Kontoravdi & Nilay Shah

A team from the Sargent Centre, led by Professor Shah with Professor Kontoravdi, Dr. Papathanasiou and Dr. Kis, has played an important role in the Future Vaccine Manufacturing Research (FVMR) Hub coordinated by Imperial College London.

The FVMR Hub has been researching innovative vaccine technologies and manufacturing processes to inform the manufacturing of future vaccine designs since 2018. The Hub has been outstanding in impacting the field of vaccine manufacturing, particularly in 2020. The Hub is funded by a £10 million grant from the Department of Health and Social Care to pursue vaccine research that impacts Official Development Assistance demographics (often known as lower- and middle-income countries, LMICs). The Hub consists of several UK universities, including the University of Bristol, the University of Nottingham, the University of Cambridge, and King's College London; UK-based research institutes such as the National Institute for Biological Standards and Controls (NIBSC), the Centre for Process Innovation (CPI), and the NHS Blood and Transplant. The Hub also collaborates directly with international vaccine manufacturers or research institutes in ODA countries, such as Incepta (Bangladesh), Vabiotech (Vietnam), Aimei Hissen (Dalian, China), Hilleman Laboratories (India), and theUganda Virus Research Institute (UVRI, Uganda), as well as the Developing Country Vaccine Manufacturing Network (DCVMN), which comprises over 40 vaccine manufacturing companies from developing countries.

The Hub team researches front-to-back vaccine supply chain issues, supported by modelling and cost analyses; quality control issues arising from innovative vaccine technologies; and innovative formulation strategies focusing on 4 pillar platform technologies: RNA vaccines, yeast-derived vaccines, baculovirus, and bacteria-derived outer membrane vesicles (GMMA). More than 20 pathogens are targeted by the Hub, including SARS-CoV-2 (causative agent of COVID-19), human papillomavirus, rabies, polio, cholera (cause of most epidemics in the decade prior to 2017), chikungunya virus, zika virus, and pneumococcal disease, amongst others. Each of these pathogens severely affects the economic and health welfare of many of the globe's population, particularly residents of developing countries.

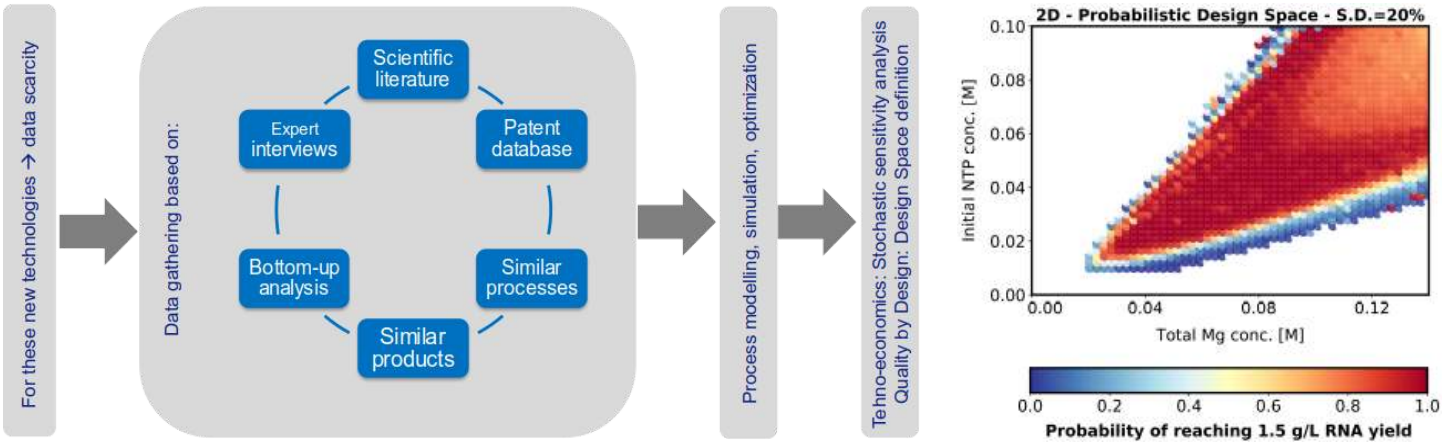


Systems approach to vaccine manufacturing optimisation

The outbreak and global pandemic of COVID-19 in early 2020 exemplifies the need for more rapid vaccine manufacturing and proves the impact of innovative vaccine technologies, such as RNA [1]. The FVMR Hub has directly been called on since the outbreak of COVID-19 to continue and expand upon business-as-usual activities, by focusing resources to support the Imperial self-amplifying RNA vaccine, engaging with the UK's Vaccine Task Force and MHRA (UK regulatory body) to assess and evaluate the saRNA COVID-19 vaccine candidate, supporting a clinical trial on a COVID-19 RNA vaccine candidate planned in Uganda, informing the world media on supply-chain issues and potential resolutions, informing the world media on COVID-19 vaccines and other vaccines, and training early career researchers as well as vaccine manufacturing staff from developing countries.

The team has modelled and optimised vaccine supply chains in developing countries, such as Kenya [2]. In in a follow-up work, the team quantified the resources, production scales and time required for producing RNA vaccines for the global pandemic demand, as well as the investment in manufacturing required to meet global demand for COVID-19 vaccines [1]. Such thought leadership on emerging technologies for low-cost and rapid vaccine manufacture and supply was acknowledged through the team's involvement in the Royal Society's highly influential DELVE initiative and >50 media interviews globally.

In addition to supply chain issues for RNA vaccines, quality control requires research to optimize this for broader vaccine production. Currently, quality control assessment is conducted using assays that can be refined to provide more detailed information on RNA integrity and quality. Modelling and optimisation including analysis of uncertainty can be used to identify efficient areas of operation which are highly likely to achieve product meeting target quality specifications – the "design space" [3,4]. Importantly, the template of the saRNA vaccine, supported by the newfound knowledge on dosing and reactogenicity, may be progressed to target other pathogens, including those present in developing regions as well as Disease X – the next pandemic.



Left: Quality by design framework **Right: Design space for mRNA vaccine production**

Follow-up funding: The team joined by Professor Chachuat has secured further COVID-19 UKRI funding for optimising the end-to-end vaccine supply chain including manufacturing of both RNA and viral vector vaccines [5,6]. More recently, the team has received funding from the Wellcome Leap programme to develop and optimise a continuous end-to-end process for RNA manufacturing, in a programme led by King's College London.

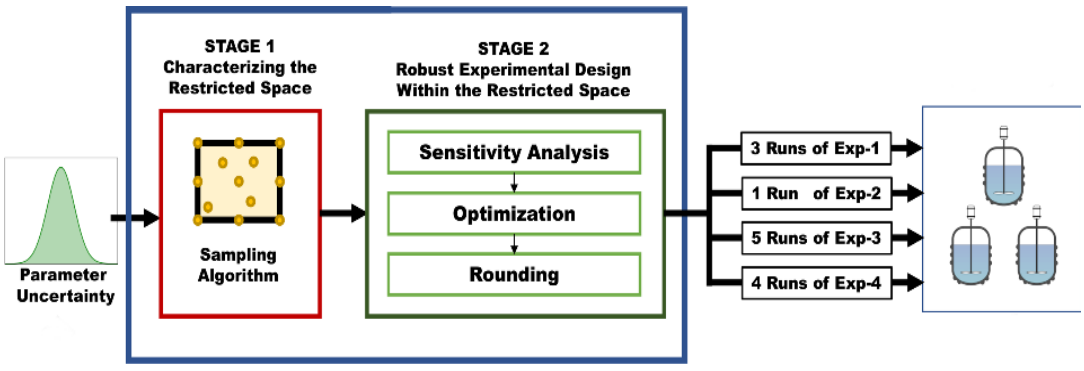
Awards: The members of the team were co-recipients of the Team Award of the IChemE Global Awards 2021, in recognition for their research contributions to the two UK FVMR Hubs led by Imperial and UCL/Oxford. The FVMR Hub also won an Imperial College President's Award for outstanding research team.

New Software Tools

A new version of kinetic Monte Carlo (KMC) software *Zacros* (v3.01) was released in October 2021 by the Stamatakis lab at UCL, which makes it possible to harness the power of supercomputers with thousands of CPU cores, towards simulating reaction kinetics of catalytic materials at unprecedented scales. This release is the culmination of a multi-year research effort (2015-2021), which developed a computational framework that couples the Graph-Theoretical KMC method with the Time-Warp algorithm. Learn more about the approach behind *Zacros* here: 10.1016/j.cpc.2021.108148. This disruptive approach enables detailed studies of heterogeneous catalysts at scales that were previously intractable and facilitates closer-than-ever comparisons of theory with experiments, towards the design of advanced catalytic materials for greener, more efficient, and more economical processes in the chemical industry.

Dr. Algaba with the Molecular Systems Engineering (MSE) group developed a new code, *ThermEST*, for the estimation of parameters for new groups to be employed within the SAFT-gamma Mie methodology. ThermEST, incorporates parallelisation to improve flexibility in relation to the number of interactions being parameterised, as well as the quantity of experimental data considered. Dr. Perdomo has developed the code *Reactive-HELD,* extending the Helmholtz free energy Lagrangian Dual (HELD) algorithm to incorporate charged and/or reactive systems.

The MSE group has continued to develop codes for crystal structure prediction and for its application. Specifically, new local minimisation codes, *CSO-RM* and *CSO-FM*, for structures containing rigid and flexible molecules respectively have been implemented. A new parameter estimation to construct transferable force field from computed reference data, *CrystalEstimator*. This code makes it possible to use larger datasets than previously possible (very detailed description of geometry and energetics for >300 crystal structures). A new workflow for the screening of co-crystallising agents has been proposed and implemented.



Pydex is an open-source Python package for model-based optimal experiment design originally developed by Dr. Kusumo during his PhD thesis as part of the PharmaSEL-Prosperity partnership with Eli Lilly & Company. Its focus is on designing maximally informative experimental campaigns for model parameter precision, using a discretization approach and optimizing over experimental efforts. It can accounts for model uncertainties to compute risk-averse experimental campaigns, and it can also be combined with feasible space sampling techniques such as the code *DEUS* to enable safe optimal experimental campaigns. Learn more about *Pydex*: 10.1016/j.compchemeng.2022.107680, 10.1039/D1RE00465D

CANON is a C++ library for deterministic global optimization developed by PhD student Tanuj Karia with Professors Chachuat and Adjiman. It has the capability to reformulate mixed-integer polynomial models (MIPOP) into quadratically-constrained programming (MIQCP) models, which can be solved more reliably to global optimality using state-of-the-art codes such as *GUROBI*, *SCIP, BARON* or *ANTIGONE* through *GAMS*. Learn more about the algorithms behind *CANON* and their effectiveness: 10.1016/j.compchemeng.2022.107909

OMLT is a Python package for representing machine learning models (neural networks and gradient-boosted trees) within the *Pyomo* optimization environment (Ceccon, Jalving, et al., 2022), co-developed by the Computational Optimization Group. OMLT gets >15k PyPI downloads per month and won the 2022 COIN-OR Cup as the best contribution to open-source operations research software development. Learn more about OMLT: 10.48550/arXiv.2202.02414

Other open-source software packages recently developed by the group of Professor Misener include: *ENTMOOT*, a multiobjective black-box optimization tool that uses gradient-boosted trees with *GUROBI* as the underlying solver, and that is used in the BASF app store (10.1016/j.compchemeng.2021.107343); *GALINI*, a mixed-integer nonlinear optimisation solver that facilitates collaboration with Sandia National Laboratories; *ROmodel*, a modeling tool for robust optimisation problems in Pyomo.

Nature inspired methods for optimization have been available for many years. They are attractive because of their inspiration and because they are comparatively easy to implement. This new open access web book authored by Professor Fraga on Nature inspired methods for optimization -- A Julia primer for process engineering includes case studies, from industrial engineering with a focus on process engineering. All the code is available for readers to try and adapt for their particular applications. This book does not present state of the art research outcomes. It is primarily intended to demonstrate that simple optimization methods are able to solve complex problems in engineering. As such, the intended audience will include students at the Masters or Doctoral level in a wide range of research areas, not just engineering, and researchers or industrial practitioners wishing to learn more about Julia and nature inspired methods.

Integrated Development of Low-Carbon Energy Systems

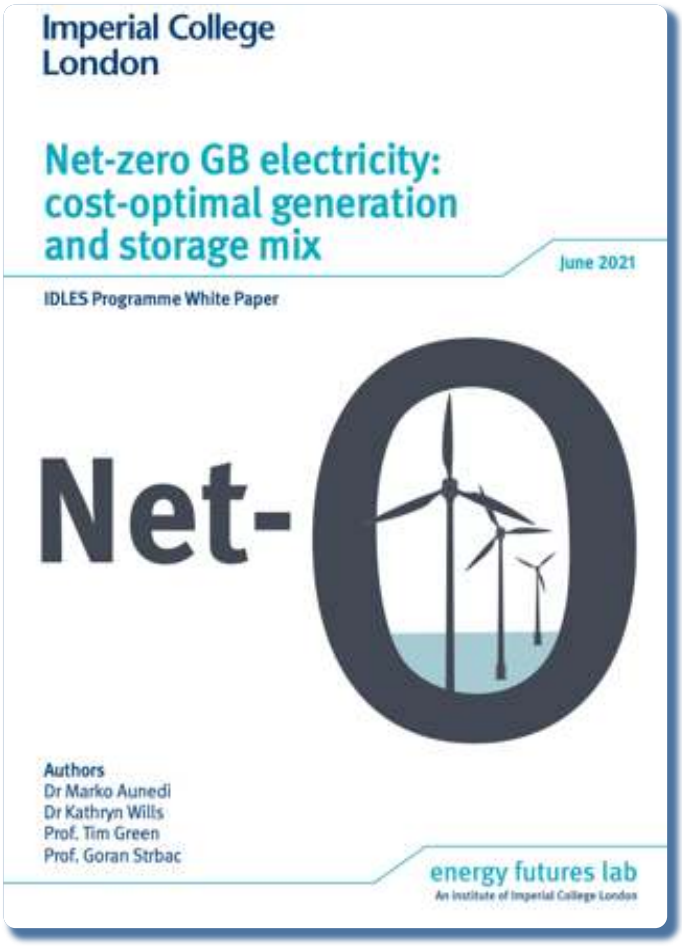
Contributed by Danny Huang & Wolfram Wiesemann

The Integrated Development of Low-Carbon Energy Systems (IDLES) Programme is a 5-year, EPSRC-funded programme that started in November 2018 and brings together academic researchers from 7 departments at Imperial College London to provide evidence to facilitate a cost-effective and secure transition to a zero-carbon future. IDLES is led by Professor Green from the Electrical & Electronic Engineering Department and comprises 14 co-investigators, including Professors Hawkes, Markides, Shah and Wiesemann from the Sargent Centre.

IDLES has whole-energy systems analysis at its core, aiming to create a set of linked models that can represent the complex interactions within the energy domain and support long-term strategic planning and operation of an integrated energy system. IDLES analyses across electricity, heat, gas, and hydrogen networks; and across energy uses in transport, buildings, water networks, and industrial processes; simulating various scenarios and case-studies. Energy consumption, exploitation of demand flexibility, stakeholder investment decisions, market design, incentivisation and policy objectives are all considered in the programme's analysis. IDLES is supported by a consortium of external partners, including lead industrial partners Hitachi, EDF Energy and National Grid ESO, and other large industrial companies, SMEs and public sector parties. These relationships help ensure that industrial and policy needs are embedded in the research programme and that research outcomes are readily and rapidly adopted by various key players in the energy industry.

Key Research Highlights

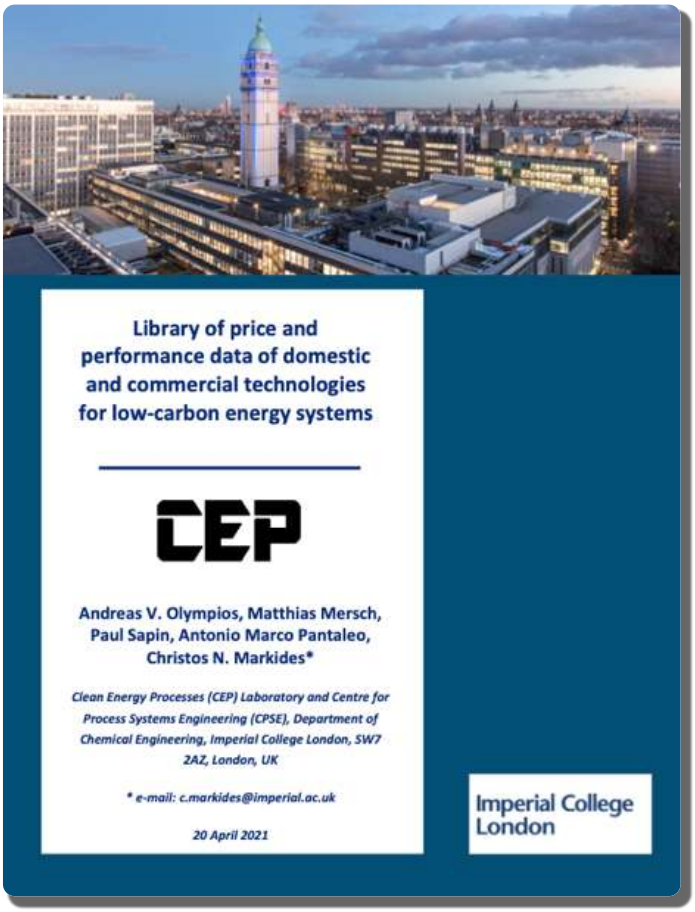
Some of the key research highlights of the programme so far include, firstly, a White Paper exploring cost - optimal portfolios of generation and storage technologies that could achieve a net-zero carbon emissions electricity system for Great Britain [1]. The report, launched in June 2021, identifies the scale of investment needed in various technologies and examines how system configuration and investment changes considering variations in the cost of available technologies and the availability of flexibility. Secondly, a Briefing Paper in October 2021 explored the impact of the COVID-19 pandemic on the UK's energy sector over the course of the first government-mandated national lockdown that began in March 2020 [2]. The paper aimed to determine what lessons can be learnt from that lockdown, given the unique set of challenges it presented in daily lives and the changes it brought about in energy demand, supply, and use.



Alongside publishing white/briefing papers, IDLES researchers have published a large number of academic papers. One, in particular, has received a great deal of attention in the media and policy circles. It is an international study into the markets mechanisms and policy drivers behind the rapidly falling price of offshore wind power [3], published in Nature Energy in July 2020. It was picked up by over 100 news outlets worldwide.

1. Aunedi, M., et al. "Net-Zero GB electricity: cost-optimal generation and storage mix", *Energy Futures Lab – Imperial College London*, IDLES Programme White Paper (2021) DOI: 10.25561/88966
2. Trask, A., et al. "Impacts of COVID-19 on the Energy System." *Energy Futures Lab Briefing Paper* (2021) DOI: 10.25561/91911
3. Jansen, Malte, et al. "Offshore wind competitiveness in mature markets without subsidy." *Nature Energy* 5.8 (July 2020): 614-622. DOI: 10.1038/s41560-020-0661-2

New Software Tools & Data



IDLES has placed a strong emphasis on making the models and data sets developed throughout the programme open source and on performing quality assurance. One of the key outputs is a comprehensive, open-access database of price and performance data for the characterisation of various small/medium-scale technologies (commercially available air-source and ground-source heat pumps, gas and electric boilers, water-storage cylinders, combined heat and power systems, solar-thermal collector and PV panels as well as compressors and heat exchangers), developed by Professor Markides' group and available on Zenodo. The library is also being regularly updated as new data become available.

More models are expected to be made available by the IDLES Programme in 2023.

Outreach Activities

Several contributions have been made by the IDLES team in advocacy for science and engineering, including, firstly, the team published an article/brochure in conjunction with the educational company Futurum – "How do we prepare the UK for a zero-carbon future?" – aimed to inspire young people to pursue careers in STEM fields. It features input from all areas of IDLES and includes insights on career pathways. Secondly, IDLES regularly posts blogs summarising the latest research findings, which are targeted at individuals working in or interested in the energy sector. Thirdly, a podcast series 'Low Carbon Conversations' was created and hosted by PhD student Mr Cormac O'Malley, who delved into the challenges and opportunities facing different sectors as they strive to decarbonise. The podcast is intended to be highly accessible, and each episode features an interview with an Imperial College researcher discussing a different aspect of the energy transition.

Two demonstrators feature in IDLES as verification tools for the programme's modelling work, as teaching instruments and as a means of communicating more widely about energy systems. The first demonstrator, Wattown, is an interactive model of energy supply anddemand in a town of the near future, illustrating integration of renewable energy sources such as wind and solar and the installation of new

technologies into the national grid for energy storage. Wattown has been used at events such as the Great Exhibition Road Festival and Imperial Lates. The second demonstrator, the Hitachi-Imperial Digital Energy Demonstrator, is a research and teaching facility that provides researchers with state-of-the-art examples of energy network control. Within IDLES, it acts as a real-time testbed for the programme's findings and will make the outcomes from IDLES accessible to a broad range of stakeholders through realistic visualisations of the operation of zero carbon energy systems and demand-side response.

The Wattown demonstrator – an interactive model of energy supply and demand in a town of the near future, showing electricity supply and storage options.

Next Destinations

The IDLES co-investigators are proud to champion early career colleagues and assist in their development into future leaders. This is reflected by the prestigious positions many of the early career researchers have gone on to secure after working on IDLES. For example, Drs Man-Chung Yue and Huikang Liu joined the faculties of Hong Kong Polytechnic University and Shanghai University of Economics and Finance in 2020 and 2021, respectively, and Dr Stefano Moret joined ETH Zürich in September 2022, where he is now a Senior Scientist and the Principal Investigator of the RIMES (Robust Integrated Modelling for Energy and Engineering Systems) project. In September 2022, Dr Shahab Dehghan joined Newcastle University's School of Engineering as a Lecturer in Power System. And in October 2022, Dr Malte Jansen joined the Science and Policy Research Unit at the Business School of the University of Sussex as a Lecturer in Energy and Sustainability specialising in energy systems with high shares of renewables.

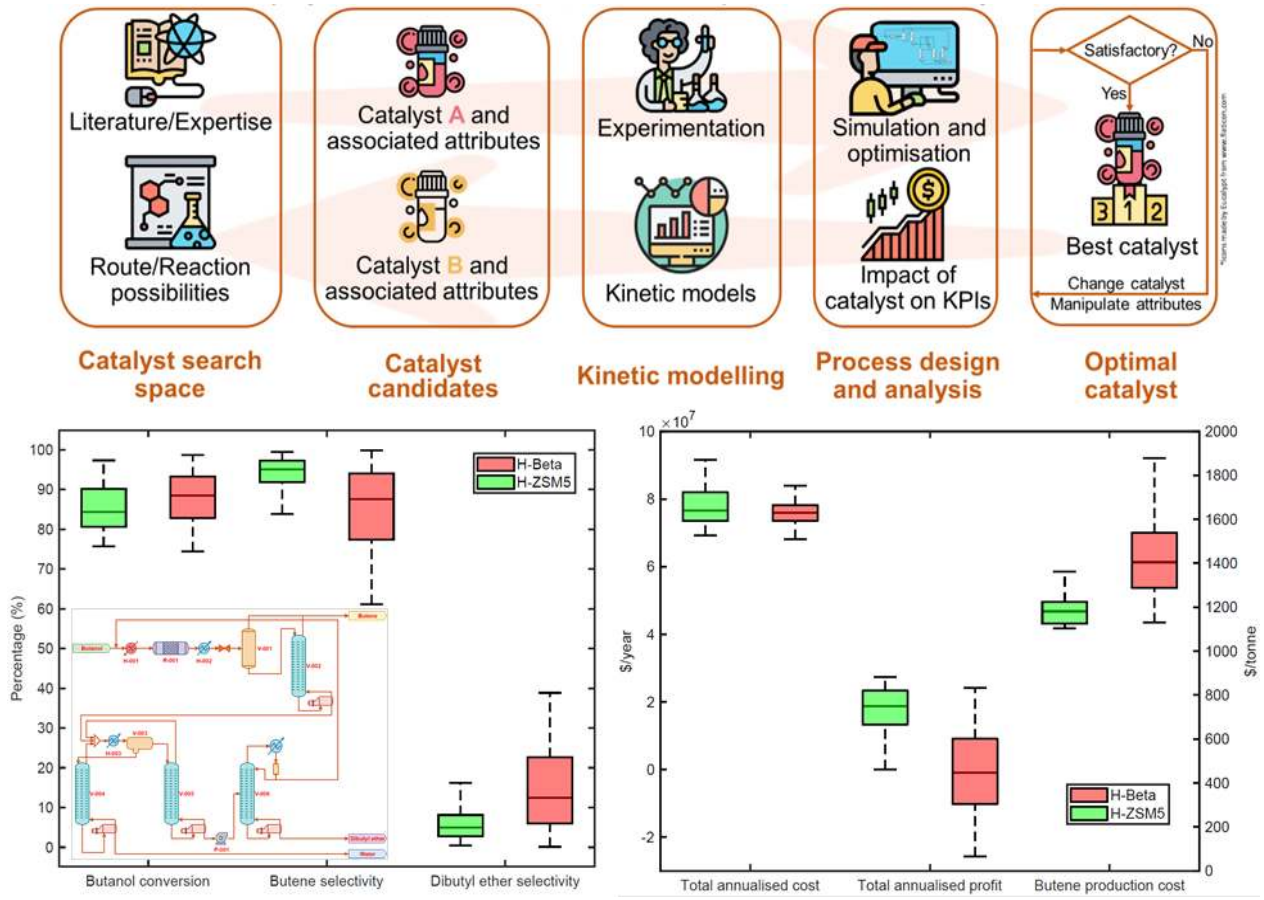
Systematic Strategy Towards Catalyst Selection and Design by Considering Whole Process Aspects

Contributed by Reza Abbasi, Federico Galvanin, Asterios Gavriilidis & Eva Sorensen

Replicating findings from laboratory experiments on a pilot scale can be difficult, even using a commercial catalyst, a problem that is further exacerbated at industrial scale. The volume and duration of production requires a robust catalyst in terms of efficiency, consistency, and durability, which in turn affects the cost and quality of the end product as well as process sustainability. In the early phases of process development, there may be considerable uncertainty about whether the required catalyst performance can be achieved at an industrial scale due to the many routes and/or process selection options, particularly associated with downstream processing, as a slight modification in the catalyst may substantially change the downstream separation processes. Even the best-performing catalyst in the laboratory may end up never being employed in industry as the intricacies of its implementation may render the process economically unviable or may need solvents, reagents, and/or conditions that are partially or wholly conflicting.

Process Systems Approach

This research uses cutting-edge process systems engineering methodologies to overcome current gaps in catalyst development by guiding initial lab-scale catalyst development towards commercially viable



A process-oriented approach towards catalyst selection or design (top), Comparison between two considered catalysts for the butanol dehydration process (inset) in terms of reaction performance and process-wide impacts on the KPIs (bottom). The box plots quantify the effect of uncertainty in estimated kinetic parameters on the KPIs.

options. The ultimate objective is to provide an *in-silico* methodology for evaluating the influence of a catalyst's attributes on the overall industrial process to guide experimentalists towards optimal targets when selecting or designing new catalysts. This technique reverses the typical catalyst design process by starting with the desired product and working backwards to the most promising catalyst attributes or best catalyst option to maximise production, minimise cost etc., depending on the main design objective. This approach reduces the time and resources needed to identify or synthesise a new catalyst, as ultimately its success depends on the impact of the catalyst on the final industrial process and not on what is achieved in the laboratory.

A Systematic Framework

Our methodology starts by first identifying catalyst candidates, with which initial experiments may be conducted with or without additional catalyst modifications. The experiments may not be required if the desired catalyst(s) is/are readily accessible and a trustworthy set of reaction kinetic data is available. The quality of the available data and the modelling approach dictate the choice of the kinetic model. Following initial kinetic model validation, the model predictions is evaluated using statistical analysis to estimate the associated uncertainty which must be accounted for in the following steps. The next step in the methodology is to perform process synthesis, followed by conceptual process design. For this, the computations require appropriate reaction routes, applicable kinetic models, and thermodynamic data. A potential process design space may be explored by considering various options for each process variable, such as the reactant and product requirements, catalyst properties, equipment configurations, operating conditions, and process route choices. In the next step of the methodology, Monte Carlo simulations are used to explore many selection criteria systematically. Process optimisation can be used if required to choose the optimal decision variables for which desired goals, such as cost and process sustainability, are minimised or maximised.

Through a multidisciplinary collaboration with catalytic chemists, we have applied the methodology outlined above to a (bio)butanol dehydration process using H-ZSM5 and H-Beta catalysts. The results suggest that H-ZSM5 is a better option for this process when the catalysts are compared based on a fixed process design at the same conversions due to its higher selectivity toward the main product. However, for this process as for many other processes, due to the properties of the product stream from the reactor, and in particular the complex and costly downstream separation requirements associated with those properties, maximising the conversion in the reactor is the most economically viable option for either catalyst. Without sacrificing selectivity, the required conversion might be obtained by either conducting the reaction at higher temperatures; using a catalyst with greater activity; or increasing the reactor volume. As is typical for chemical processes, the findings suggest that raw materials account for the majority of the operating expenses. Reducing the use of fresh feed by recycling the unreacted and separated 1-butanol would therefore enhance economics.

Using information obtained by this methodology, process developers can select or design catalysts that are optimal for the overall industrial process, upstream *and* downstream, and not just what appears to be most promising from the point of view of the reaction at lab scale.

Funding:

The UK Catalysis Hub is kindly thanked for the resources and support provided via our membership of the UK Catalysis Hub Consortium and funded by EPSRC grant EP/R026815/1

Reference:

Abbasi, M. R. et al. (2022) Process-oriented approach towards catalyst design and optimisation, *Catalysis Communications*, **163**:106392.
DOI: 10.1016/j.catcom.2021.106392

Sargent Centre Researchers Recognized

Dr. Lai (PhD 2022) co-founded spin-out company Green Beads and won the £15k BP Women's Entrepreneurship Innovate Award in 2020. The company has developed micro-beads based on biodegradable non-toxic algae to replace environmentally damaging microplastics widely used in household products.

PhD student Manfredi di San Germano, co-supervised by Dr. Krishnan and Professor Ces, won a £300k Innovate UK Smart Grant for a cancer diagnostic startup he founded 9 months ago

Dr. Thiemann (PhD 2022) won the prestigious Christopher Wormald Prize of the Thermodynamics 2022 conference in Bath, awarded to the most meritorious graduate research in the field of thermodynamics. Further to that, his talk "Shaping the Ripples: Routes to Nanoengineering the Morphology of Graphene" received the best talk award at the Thomas Young Centre student day 2022.

Dr. Lee (PhD 2022) was selected to attend the Asian Deans Rising Stars forum in Melbourne, Australia. Her PhD thesis enabled the simultaneous optimisation of absorption/desorption processes and solvents for CO2 capture through fully-automated algorithms.

Dr. Ansari (PhD 2021) became chair of Chemical Engineering Postdoc and Fellows Committee and won the 2021-22 Imperial Postdoc and Fellows Development Centre Rep Award.

Dr Marinova (PhD 2020) won the 2020 Young Scientist Award of the British Association of Crystal Growth

PhD student Fanyi Duanmu (supervised by Professor Sorensen) was the recipients of the Best Poster Award at Distillation & Absorption 2022 conference in Toulouse, September 2022.

PhD student Niki Triantafyllou (supervised by Dr.) won the Best Poster Award at ESCAPE32 symposium in Toulouse, June 2022.

Sargent Centre Academics Recognized

Professor George Jackson FRS

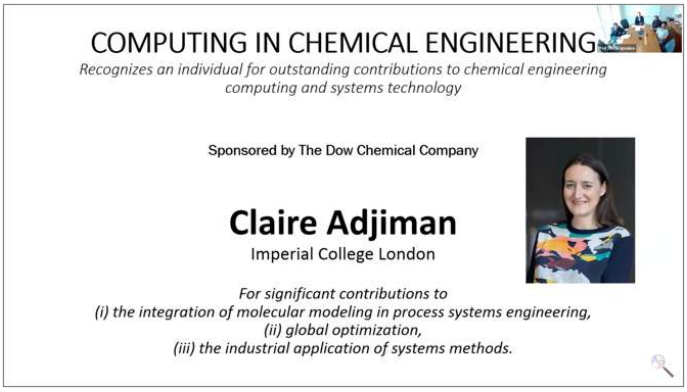
Congratulations to Professor Jackson on his election as Fellow of the Royal Society.

Congratulations to Professors Adjiman and Shah on getting elected as Fellows of American Academy of Arts & Sciences.

Congratulations to Professor Shah on being awarded OBE in 2020 for services to decarbonisation of the UK economy

Professor Maitland was awarded both the 2020 IChemE Ambassador Prize and the 2021 Royal Society of Chemistry Award for Exceptional Service.

Professor Kontoravdi won an Imperial President's Award for Excellence in Education for Research Supervision in 2021.



Professor Adjiman won the prestigious the 2021 Computers in Chemical Engineering Award of the AIChE CAST Division, recognising her outstanding contributions in the application of computing and systems technology to chemical engineering (prize-winning lecture at AIChE Annual Meeting).

Congratulations to Professor Misener, the 2020 Outstanding Young Researcher Award winner and to Dr. Tsay, the 2022 W. David Smith, Jr. Graduate Publication Award winner.

Professor Misener also became BASF/Royal Academy of Engineering Research Chair in Data-Driven Optimisation in March 2022, and also joined the BASF Strategic Partnership Committee as a key part of the major collaboration between Imperial and BASF

Professor Stamatakis, with co-workers from Cambridge, Tufts (USA), UCSB (USA) and Argonne (USA), won a 2022 Faraday Division Horizon Prize by the Royal Society of Chemistry "*for the development of single-atom alloys, a new class of catalysts that play a prominent role in the energy and sustainability fields*"

External Visibility and Outreach

Dr. Oluleye addressed the Parliamentary and Scientific Committee on the role of engineering in the decarbonisation of the UK economy. The panel event was chaired by Stephen Metcalfe MP who has been recently reappointed to the House of Commons Science and Technology Committee.

Professor Bogle was elected President of the Institution of Chemical Engineers (IChemE) for 2022/23 and stepped down as Scientific Vice President of the European Federation of Chemical Engineers (EFCE). He was lead author of a report on Engineering Ethics – Maintaining society's trust in the engineering profession for the Royal Academy of Engineering and the Engineering Council that was released in Feb 2022 and has resulted in a set of actions for the UK Engineering community.

Professors Maitland and Shah have been appointed to the Department of Business, Enterprise and Industrial Strategy (BEIS) Science Expert Group, advising the Chief Scientific Advisor on key engineering issues, especially energy systems. Professor Shah has also been appointed to the UK Government Hydrogen Advisory Council. Adopting a systems approach to policy making is an important aspect of these advisory roles

Department for Business Innovation & Skills

The MSE Group presented two stalls at the Exhibition Road Festival 2022. Benjamin Tan and Leticia Sanders de Almada featured crystallisation, using the tantalising example of chocolate to introduce and explain polymorphism, and Mohammad Muhieddine and Griffin Gui showcased computer-aided design for solvent selection, using the topical example CO2 capture with the help of Malak Wehbe, Ahmed Alyazidi, and Shubhani Paliwal (who was then an MSc student and has now joined the group as a PhD student).

Dr. Mercangoz organized the Chemical Engineering track for the 2022 Imperial Global Summer School, a programme introducing STEM students from around the world to engineering, physics, and medicine and life sciences.

Dr. Papathanasiou has been elected 2025 Program Coordinator for Area 10E of the Computers & Systems Technology (CAST) Division of AIChE. She has also been the Social Media Chair for CAST and an the Interim Secretary for the Computer Aided Process Engineering Special Interest Group of IChemE since 2022. She is a member of EPSRC-UKRI cross Strategic Advisory Team for ED&I between 2021-2023.

Professor Misener was the 2021 Program Coordinator for Area 10C (Systems and Process Operations) of CAST

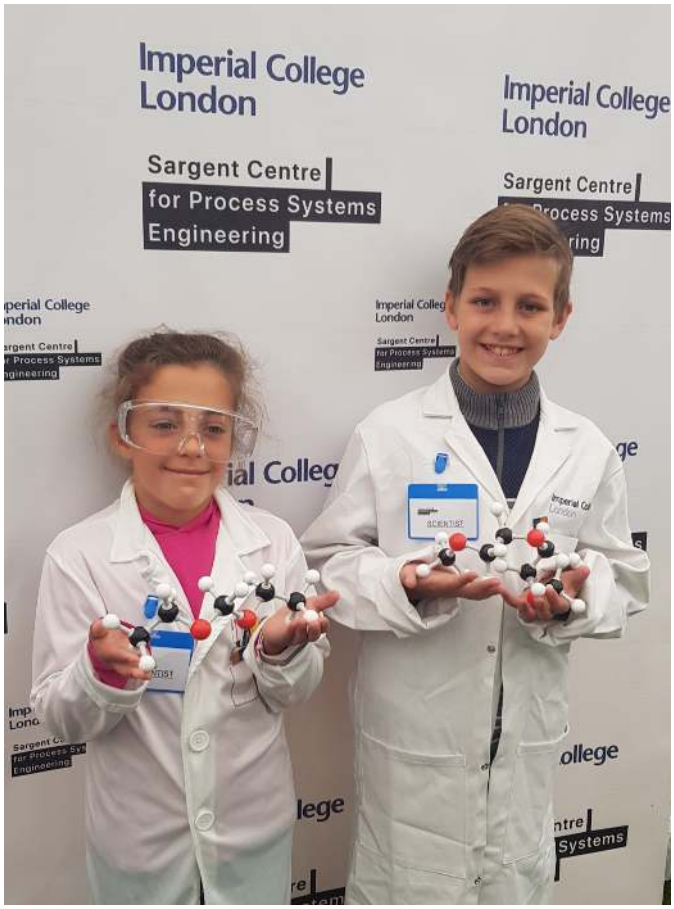
Professor Chachuat has joined the team of FIPSE Trustees in 2022, of which Professors Adjiman and Pantelides are also members.

Equality, Diversity & Inclusion

Professor Bogle commissioned a report on Barriers to Doctoral Education by the UCL Doctoral School leading to actions aimed at reducing the barriers for minority doctoral applicants (across all disciplines).

Professor Deisenroth has been providing individual support for early-career researchers through mentorship programs at Deep Learning Indaba, Black in AI, and RSS. This ranges from providing feedback on CVs and research proposals to guidance on career planning. He is part of the advisory board of Queer in AI, an organization that raises awareness of and supports queer people in AI, and has been supporting Queer in AI by co-organizing events at conferences and co-developing guidelines for conferences to make them more queer friendly. He has also been chairing the Equity, Diversity and Inclusion (EDI) Committee in the Computer Science (CS) Department at UCL since 2021, with a view on identifying and removing barriers for marginalised groups in the CS department and a particular focus on race equality, LGBTQ+, gender equality, neurodiversity, and disability.

Professor Shah won the President's Medal for Excellence in Culture and Community in 2022 for his work chairing the Imperial History Group.



New Academic Members

Dr. Maximilian Besenhard, Department of Chemical Engineering, University College London
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Dr. Maximilian (Max) Besenhard is a Lecturer (Assistant Professor) in Digital in Manufacturing of Advanced Materials and programme lead for the same named MSc programme at the Department of Chemical Engineering, University College London. He has an interdisciplinary experimental and computational research background focussing on material science and pharmaceutical process development. His industrial and academic work has always combined experimental and computational work covering multiple areas including process scale-up and control, particle technology, as well as crystallisation and chromatography using techniques such as CFD, population balance modelling, statistical process control and multivariate data analysis/chemometrics, as well as flow sheet modelling for computational scale-up and process development. His expertise in process analytical and sensor technology, material science and reactor design, provides the background required for sensible (experimental) validation and fit for purpose testing of computational approaches. His current research focusses on solutions to empower digital manufacturing. Examples are i) Hybrid models for Artificially Intelligent systems combining mechanistic models where possible with machine learning strategies where not, ii) autonomous material discovery and process optimisation, iii) system engineering approaches to manufacture precisely engineered functional materials at small and large scales, iv) novel reactor designs facilitating novel synthetic procedures which yield novel (nano) materials.

Dr. Besenhard is a physicist by training who switched to chemical and pharma engineering for his PhD which focused on continuous pharma production at TU Graz. After ~6 years working for Siemens and the Research Centre Pharmaceutical Engineering (RCPE) in Austria, he returned to academia joining UCL in 2016. During his 5 years as a PDRA, he worked on the continuous syntheses of noble metal and magnetic nanoparticles for biomedical applications, multiphase and high temperature flow reactors synthesising advanced functional materials, sensor technology and real-time material characterisation, nature inspired nanomaterial tuning, and hybrid models combining mechanistic models with machine learning strategies to develop digital twins for HPLC. He joined the University of Leeds in 2021 as a lecturer (still visiting lecturer) and re-joined UCL in April 2022.

Dr. Michel-Alexandre Cardin, Dyson School of Design Engineering, Imperial College London
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Dr. Michel-Alexandre Cardin is a Senior Lecturer (Associate Professor) in Computational Aided Engineering at the Dyson School of Design Engineering, Imperial College London and Director of the Strategic Engineering Laboratory since 2019. His research focuses on the development and evaluation of new computational aided methodologies, digital

processes, and algorithms to support the design of engineering systems for uncertainty, sustainability, and resilience. His work has been recognized internationally through awards, research councils advisory, seminars, and consultancies (e.g., Institute of Industrial and Systems Engineers, UN SDG Impact Finance, Quantum Black a McKinsey Company). He has ongoing research collaborations and affiliations with institutions around the world such as ETH and MIT. He is currently an Associate Editor for the journals *IISE Transactions* and *ASME Journal of Mechanical Design*, and has served on the Editorial Boards of the INCOSE journal *Systems Engineering* and *IEEE Transactions on Engineering Management*. Before joining Imperial, Michel worked as a Quantitative Researcher in the hedge fund industry. From 2011 to 2018 he was as an Assistant Professor at the National University of Singapore. He holds a PhD in Engineering Systems and a Master of Science in Technology and Policy from MIT, a Master's in aerospace engineering from the University of Toronto, Honors BSc in Physics from McGill, and is a graduate of the Space Science Program at the International Space University.

Dr. Vasileos Charitopoulos, Department of Chemical Engineering, University College London
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Dr Vasileios Charitopoulos is a Lecturer (Assistant Professor) at the Department of Chemical Engineering, University College London. He leads the PRocess & energY Systems optiMisation (PRYSM) group with research focus on Optimisation under uncertainty method development, Integration of control with supply chain operations, energy systems optimisation decarbonisation strategies along with hybrid modelling applied to process & energy systems engineering. He is a Postgraduate (Research) Admissions Tutor at the Department of Chemical Engineering at UCL, a member of the Sargent Centre's management team, a member of the IChemE's Computer Aided Process Engineering (CAPE) Special Interest Group, and on the Editorial Board of Elsevier's Chemical Engineering Science.

Vasileios received his Diploma in Chemical Engineering from the National Technical University of Athens and PhD from UCL for which he was awarded the Springer Best PhD Thesis Award, UCL's Newton Prize and an honorable mention from the European Federation of Chemical Engineering (EFCE) for the Excellence Award in Recognition of an Outstanding PhD Thesis on CAPE. Before joining UCL, Vasileios was a research associate in the Energy Policy Research Group at the University of Cambridge. His research influence has been recognised on a number of occasions including the IChemE Best Young Researcher Global Award (Honorable Mention, 2022), his election as member of the UK BEIS Early Career Forum on CCUS (2020), as well as several UKRI research grants which enable collaborations with the UK, USA and Europe.

Dr. Antonio del Rio Chanona, Department of Chemical Engineering, Imperial College London
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Dr. Antonio del Rio Chanona is a Lecturer (Assistant Professor) at the Department of Chemical Engineering, Imperial College London and heads the Optimisation and Machine Learning for Process Systems Engineering group with research focus on Data-Driven Optimisation,

Reinforcement Learning, Control, and Hybrid Modelling applied to process systems engineering. He is a Director for Education and Continuous Learning at the Sargent Centre and the organiser of the Summer School on Data-Driven Optimisation and PSE@ ResearchDayUK 2022.

Antonio received his MEng from UNAM in Mexico, and his PhD from the University of Cambridge where he was awarded the Danckwerts-Pergamon Prize for the best doctoral thesis of his year. Antonio has received awards from the International Federation of Automatic Control (IFAC), the Association of European Operational Research Societies (EURO), and the Institution of Chemical Engineers (IChemE) in recognition for research in areas of process systems engineering, industrialisation of bioprocesses, and adoption of intelligent and autonomous learning algorithms to chemical engineering.

Dr. Mehmet Mercangöz, Department of Chemical Engineering, Imperial College London
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Dr. Mehmet Mercangöz received his BSc. and MSc. degrees from Boğaziçi University, İstanbul, Turkey and his Ph.D. degree from the University of California, Santa Barbara, USA all in Chemical Engineering. He is currently ABB Reader of Autonomous Industrial Systems at the Department of Chemical Engineering, Imperial College London, where he leads the Autonomous Industrial Systems Laboratory. Previously, he worked at the research and development organization of the engineering company ABB in Switzerland and he held a co-appointment as a lecturer at ETH Zurich at the Department of Information Technology and Electrical Engineering.

Mehmet's research activities extend over the fields of model predictive control, machine learning, and process optimization with a goal to realize increased levels of autonomous operation in the process and energy industries. He has worked on electrical variable speed drives for natural gas compressors as an emission free alternative for gas turbine drivers. The control solutions he helped develop for these applications are now responsible for the safe delivery of natural gas to many European countries. In other projects, he worked on the development of energy storage applications based on thermodynamic cycles, which are commercialised today by the company MAN Energy Solutions under license, and on the control and optimization of various manufacturing processes. Mehmet is the author of over 50 journal and conference publications and is listed as an inventor in 36 patents and patent applications.

Dr. Gbemi Oluleye, Centre for Environmental Policy, Imperial College London
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Twitter: @gbemi

Dr. Gbemi Oluleye is a Lecturer (Assistant Professor) at the Centre for Environmental Policy, Imperial College London, where she leads a transdisciplinary research called Modelling for the Adoption of Alternative Technological Systems (MAATS Lab), focusing on the development of novel theories and concepts at the interface of engineering, economics and policy implemented in optimisation tools to analyse uptake of

alternative fuels and technologies for decarbonising hard to abate sectors. Applications include synthesising cost-effective adoption pathways for advance energy and material efficiency, fuel and technology switching, carbon capture utilisation and storage, and direct air capture in the UK process industry and globally.

Dr. Oluleye received a BSc in Chemical Engineering from the Obafemi Awolowo University, Nigeria, an MSc in Advanced Chemical Process Design and PhD from the University of Manchester. She is also a visiting lecturer at the Centre for Process Integration, the University of Manchester, and the Research Theme Champion, Policy and Innovation, Energy Futures Lab.

Dr. Oluleye has established a high profile as an international leader in assessing the impact of interventions in policy and business models in accelerating uptake of technological solutions for clean manufacturing. She has been invited to be a member of BEIS strategic advisory board for the UK Industrial Decarbonisation and Hydrogen strategy, Member Assessing Low Carbon Transition (ACT) Technical Working Group on Industrial Decarbonisation, Keynote speaker at the Achieving Net Zero: Decarbonising Industry roundtable by the All-Party Parliamentary Climate Change Group, and presented evidence to support policy making at UK Government departments 4 times, parliament 3 times, and co-authored essays on achieving sustainable and clean manufacturing with a member of the House of Lords. She is also actively involved in several evidence based high impact activities to promote equal opportunities and improve diversity in energy research.

Dr. Dario Paccagnan, Department of Computing, Imperial College London
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Dario Paccagnan is a Lecturer (Assistant Professor) at the Department of Computing, Imperial College London since the Fall 2020. Before that, he was a postdoctoral fellow with the Center for Control, Dynamical Systems and Computation, University of California, Santa Barbara. He obtained his PhD from the Automatic Control Laboratory, ETH Zurich, Switzerland, in 2018. He received a BSc. and MSc. in Aerospace Engineering from the University of Padova, Italy, in 2011 and 2014, and a MSc. in Mathematical Modelling and Computation from the Technical University of Denmark in 2014; all with Honors.

Dario's interests are at the interface of game theory and control theory, with a focus on the design of behavior-influencing mechanisms for future mobility systems. Dario was a finalist for the 2019 EECI best PhD thesis award and was recognized with the SNSF Early Postdoc Mobility Fellowship, the SNSF Doc Mobility Fellowship, and the ETH medal for his doctoral work.

Dario has co-authored over 35 full length peer-reviewed publications most of which appearing in flagship venues in control theory (e.g., IEEE Transactions on Automatic Control), game theory (e.g., ACM Economics and Computation conference) and multiagent systems (e.g., AAMAS). Dario has a strong network of national and international collaborators, including ETH Zurich, MIT, Cornell, Stanford, HEC Montreal, TU Munich, TU Delft.

Dr. Maria Papathanasiou, Department of Chemical Engineering, Imperial College London
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Dr Maria Papathanasiou is a Lecturer (Assistant Professor) at the Department of Chemical Engineering, Imperial College London and leads the Life Science and Process Systems Engineering lab, focusing on the development of digital twins and control methodologies for process understanding, optimisation and automation. Applications include personalised therapies, (bio-) pharmaceuticals, energy & food systems engineering. She has received her 5-year Diploma in Chemical Engineering from the National Technical University of Athens and her MSc and PhD degrees in the Department of Chemical Engineering at Imperial College London. Prior to her permanent appointment with Imperial College London, she was a Visiting Scholar at the Artie McFerrin Department of Chemical Engineering and the Energy Institute at Texas A&M University.

Maria's research activities are supported by EPSRC, UKRI, as well as industrial partnerships with GSK, Pall Biologics, AstraZeneca, TrakCel Lt and others. Recent influential contributions include the development of supply chain models to address challenges related to efficient and speedy vaccine delivery during the COVID-19 pandemic. Outcomes of this work have contributed to Royal Society's DELVE report on SARS-CoV-2 vaccine development and implementation. she is a co-recipient of IChemE's Global Team Award and the Imperial College President's Awards for Excellence in Research (2021). she has co-authored over 35 full length and peer-reviewed conference publications and 3 book chapters that include contributions to Scientific Report Nature, AIChE Journal, and Computers & Chemical Engineering. She has strong international representation to scientific and industrial conferences with over 40 oral presentations, including invited talks.

Dr Papathanasiou serves as Social Media Chair for AIChE's CAST Division and was recently elected as the 2025 Programming Coordinator for CAST's Area 10E Information Management and Intelligent Systems. she is the Interim Secretary of IChemE's Computer Aided Process Engineering Special Interest Group. She is a member of EPSRC's Early Career Researcher Forum, and she is actively involved in Equality, Diversity & Inclusion (EDI) initiatives through EPSRC-UKRI cross-Strategic Advisory Teams EDI committee.

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Dr Calvin Tsay is a Lecturer (Assistant Professor) in the Computational Optimisation Group at the Department of Computing, Imperial College London. His research focuses on computational methods for optimisation and control with applications in machine learning and process systems engineering.

Calvin received his PhD degree in Chemical Engineering from the University of Texas at Austin, receiving the 2022 W. David Smith, Jr. Graduate Publication Award from the CAST Division of the American Institute of Chemical Engineers (AIChE). He previously received his BS/BA from Rice University (Houston, TX). Prior to his appointment as lecturer, he was an Imperial College Research Fellow and EPSRC David Clarke Fellow at the Department of Computing.

Courses and Events

Course on multivariate data analytics

This course provides an Introduction to modern day multivariate data analytics methods through lectures and hands-on workshops. The syllabus is geared towards general concepts on latent variable modelling (LVM) theory and advanced topics on the analysis of specific data scenarios (e.g. batch data, image analysis and chemometrics). LVM is a data-driven modelling technique particularly useful to understand processes where acquired data is abundant, complex, correlated and noisy. The course is delivered by Dr. Salvador Garcia Munoz, who has 20+ years of experience in the implementation of systems engineering tools to industrial problems ensures relevancy for the industry participants enabling them to lead the application of digital design tools for the development of new products and accelerated process design in their organisations.

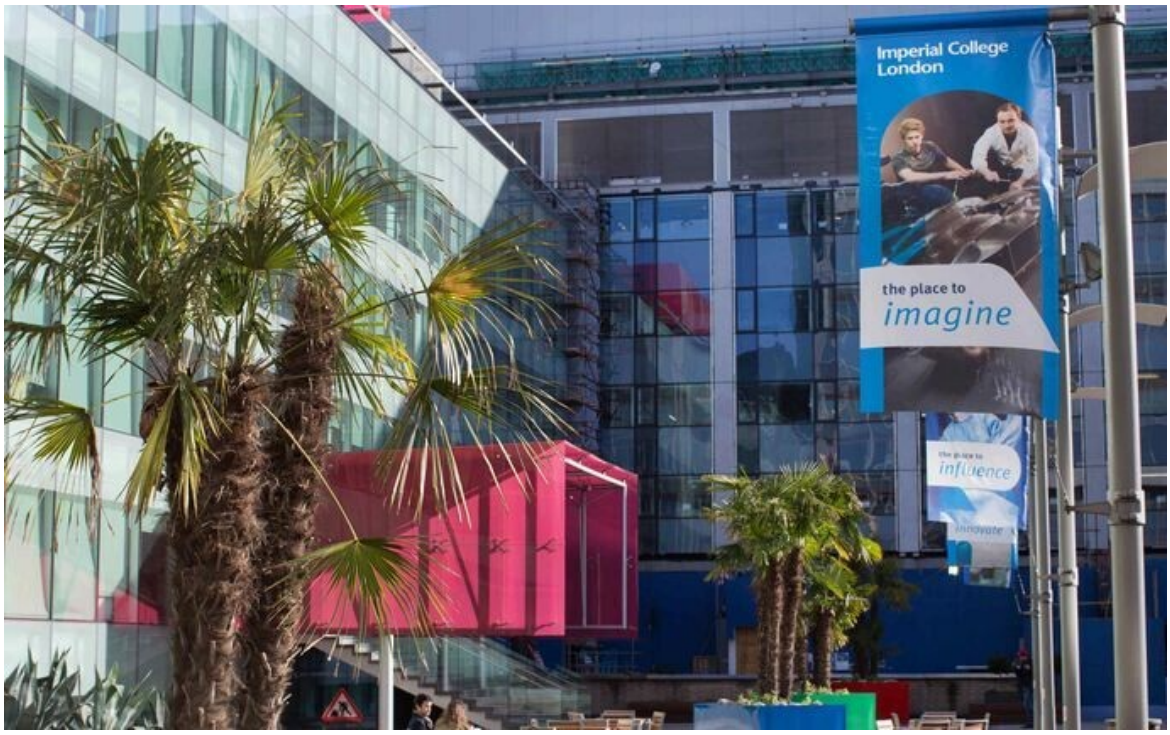
Mark you calendar: The next course is scheduled for **week commencing 15th May 2023**

Courses on optimization

These courses were developed with input from our industrial partners and provide a unique technical training in optimisation which has been growing in popularity with industrial companies from various sectors. They are offered every two years and delivered by academics and researchers from the Sargent Centre.

- The course ***Introduction to Optimisation*** is geared towards concepts in problem formulation and solution methods for linear, nonlinear and mixed-integer problems. Primarily focused on local optimisation methods, with a brief introduction to global optimisation, it gives participants an overview of the types of problems that can be solved with today's tools and allows them to get some hands-on experience.
- The course ***Advanced Optimisation*** builds on the introductory course and focuses on concepts in global optimisation, bilevel optimisation, multi objective optimisation, dynamic optimisation, optimisation under uncertainty.

Mark you calendar: The next course is scheduled for **week commencing 4th September 2023**



Sargent Centre Summer School

The 2022 summer school was organised on the topic of ***Data-driven optimisation and decision making***. Included in this one weeklong training were lectures on reinforcement learning, Bayesian optimisation, stochastic and robust optimisation, statistical learning and optimisation delivered by internal and external experts in the field. The summer school had over 120 attendees from 23 universities across UK and Europe as well as attendees from 13 business. It also provided a unique opportunity for networking with students and industry participants.

Sargent Centre Career Event

Throughout the year the Sargent Centre hosts and collaborates on several events designed to provide a range of opportunities for our students to connect with the industrial partners, explore careers, apply for internships and identify new research opportunities.

The annual career event is an excellent way to connect with our students and Postdocs in an informal setting, support their career exploration and get a privileged access to the exceptional cohort of young talents in your field. This collaborative event is open to students and Postdocs from Imperial College London as well as UCL, bringing together candidates with employers hiring for engineering positions. This year we had great contributions form representatives from Syngenta, BASF, Solvay and Recursion.

Mark you calendar: The next career event is planned for **June 2023**

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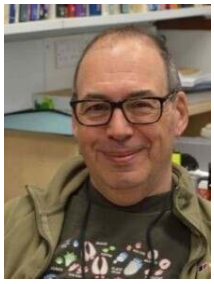

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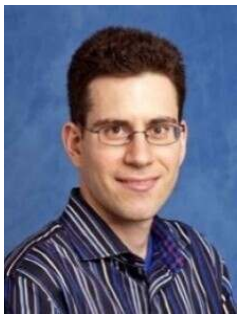

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