Imperial College London

UCL

The latest news from the Centre for Process Systems Engineering

NEWSLETTER

Welcome to the Autumn Edition

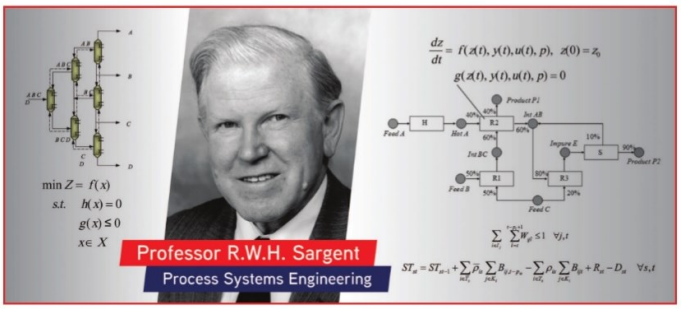
Issue 14 October 2016

Message from CPSE Director, Professor Nilay Shah

Welcome to the Autumn edition of the CPSE Newsletter. We remember Chris Floudas who sadly passed away in August. Chris had a great impact in the process systems community and especially to the CPSE academics whom he supervised for PhDs. I would like to welcome the four new academics: Marc Deisenroth, Federico Galvanin, Gonzalo Guillén-Gosálbez and Alex Kiparissides. I would also like to wish James Keirstead every success as he leaves to take up a post at Cambridge Assessment. This Newsletter includes an article on "The Commercial Potential Of Industrial Excess Heat" by my Postdoctoral Researcher Romain Lambert. The next CPSE Annual Industrial Consortium Meeting will take place on 1st and 2nd December 2016. Also we have the 23rd Professor Roger Sargent Lecture which will be delivered by Jay H. Lee from KAIST. The programme will include IChemE's MM Sharma Medal for Lifetime Achievement for Roger Sargent.

This is my last message as the Director of the Centre as I will be stepping down and passing on the reins to Claire Adjiman. It has been a great pleasure to see CPSE grow in size and breadth, while continuing to excel in both fundamentals and applications. I leave it in the capable hands of Claire, however, I will remain part of CPSE.

AIChE Highlight: Tribute to Founders



The **September issue** of the AIChE Journal is dedicated to Professor Roger W.H. Sargent, recognized as the father of Process Systems Engineering. In the opening article of this fourth Founders Tribute, the issue editors, **Professor Ignacio Grossmann** of Carnegie Mellon University; **Professor Michael Doherty** of University of California, Santa Barbara; and **Professor Costas Pantelides** of Imperial College London, review Professor Sargent's work through five decades.

"He has helped to expand the scope of chemical engineering by providing a strong systems component to it, and by establishing strong multidisciplinary links with fields such as numerical analysis, mathematical programming, control theory, and operations research." Professor I. E. Grossmann.

http://www.aiche.org/resources/publications/cep/2016/september/aiche-journal-highlight-tribute-founders-roger-sargent

New CPSE Director

Professor Claire S. Adjiman

Professor Nilay Shah will be stepping down as CPSE Director to take up the post of the Head of Department of Chemical Engineering at Imperial College London. Professor Claire S. Adjiman will be the new CPSE Director. A Professor of Chemical Engineering, Professor Adjiman is also the Director of the Institute for Molecular Science and Engineering. She obtained an MEng in Chemical Engineering (Imperial College London) and a PhD in Chemical Engineering (Princeton University). She has received many awards including: Fellow of the Royal Academy of Engineering, Fellow of the Institution of Chemical Engineers, Chartered Engineer, EPSRC Leadership Fellowship (2012-2017), Henry E. Armstrong Memorial Lecture of the Society of Chemical Industry (2011), Philip Leverhulme Trust Prize for Engineering (2009), Research Excellence Award for Molecular Systems Engineering team, Imperial College (2009), Rector's Excellence Award, Imperial College (2007), Royal Academy of Engineering ICI Fellowship (1998-2003) and Porter Ogden Jacobus Honorific Fellowship, Princeton University (1997). *Continues on page 2.*

Remembering Professor Christodoulos A. Floudas

Professor C. A. Floudas

It is with great sadness to report that Professor Christodoulos A. Floudas died on 14th August 2016. Professor Floudas was the director of the Texas A&M Energy Institute and the Erle Nye '59 Chair Professor for Engineering Excellence in the Artie McFerrin Department of Chemical Engineering at Texas A&M University. He passed away at age 56 whilst on vacation with his family in Greece. He is survived by his wife of 30 years, Fotini Floudas, as well as their daughter, Ismini Floudas.

Professor Floudas previously served Princeton University for 29 years and was the Stephen C. Macaleer '63 Professor in Engineering and Applied Science, Emeritus, and Professor of Chemical and Biological Engineering, Emeritus at Princeton. Born in Ioannina, Greece, he earned a Diploma of Chemical Engineering from Aristotle University of Thessaloniki in 1982 and a Ph.D. in Chemical Engineering from Carnegie Mellon University in 1986, studying under Professor I. E. Grossmann (an academic son of Professor Roger Sargent).

Professor Floudas was a leading figure in the field of process systems engineering. He was a friend of CPSE having visited us many times, including a sabbatical in the early 1990s and having delivered the 2008 Professor Roger Sargent Lecture. He influenced many and was a wonderful mentor. Three CPSE academics: Professor Claire Adjiman, Dr Peter DiMaggio and Dr Ruth Misener undertook PhDs under his guidance. Several CPSE students also took up postdoctoral positions in his group. He will be greatly missed.

CPSE Says Farewell to Academic Dr James Keirstead

Dr James Keirstead

CPSE academic Dr James Keirstead has left Imperial College London to take up a post of Principal Data Scientist at Cambridge Assessment.

Dr Keirstead joined CPSE in 2013 and was a Lecturer in the Department of Civil and Environmental Engineering. Previously he was a Research Fellow and Team Leader of the BP Urban Energy Systems project and lead editor of the resulting book Urban Energy Systems: An Integrated Approach (Earthscan, 2013). His research focused primarily on urban energy systems and the challenges that cities face in order to satisfy the social and economic goals of populations. Using a range of modelling methodologies, he investigates the technological and policy options that are available to cities as they try to address the challenges of providing reliable, cost-effective and environmentally -benign forms of Energy provision. Dr Keirstead was also interested in urban resource consumption and the industrial ecology of cities, as well as urban sustainability indicators and UK micro-generation and domestic energy consumption issues. We will miss you James and wish you all the best!

New CPSE Director

Continuing from page 1. Professor Adjiman's research interests are on systematic methodologies for integrated molecular and process design for reactive processes: development of modelling and optimisation tools and applications (*e.g.* solvent design for re actions or CO_2 capture, risk management). Model-based assessment of design of energy conversion systems including solid oxide fuel cells. Development of property prediction techniques integrating different scales of modelling (from quantum mechanics to advanced equations of state). Global analysis techniques, such as global optimisation and safety analysis.

For an introduction to her work, watch Claire's Inaugural Lecture entitled "Molecules on best behaviour: The Engineering of Molecular Systems"

In the next edition of the Newsletter we will cover the legacy of Professor Nilay Shah and his impact on CPSE.

CPSE Welcomes Four New Academics

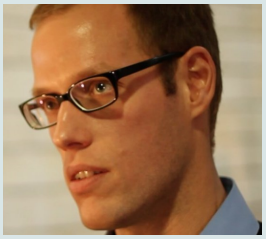
The number of CPSE academics has grow following the affiliation of four new members from both Imperial College London and University College London

Dr Federico Galvanin
UCL

Dr Federico Galvanin received a bachelor degree in Chemical Engineering in 2006 and a PhD degree in 2010 at the University of Padova. After post-doctoral activity in Padova focusing on the optimal design of clinical tests for the identification of physiological models, he has been working as a post-doc Research Associate at University College of London (UK) since 2014. In September 2015 he became a Lecturer in the Department of Chemical Engineering at the UCL. Federico's main areas of expertise are in the field of model identification including optimal design of experiments (theory and applications) for the development of chemical, biological and physiological models.

Dr Alexandros Kiparissides (former CPSE PhD student), UCL

Dr Alexandros (Alex) Kiparissides is a Lecturer in Biochemical Engineering at University College London, having joined UCL in 2015. His current research focuses on the development of novel computational approaches able to integrate, organize and guide experimental (and modeling) information across multiple scales, i.e. all the way from metabolic regulation to bioprocess monitoring and control. His research explores the boundaries between traditional Process Systems Engineering, Systems Biology and Applied Biotechnology. Alex obtained a Diploma in Chemical Engineering from the Aristotle University of Thessaloniki and received his PhD in Bioprocess Systems Engineering from Imperial College London.



Dr Marc Deisenroth
Imperial College London

Dr Marc Deisenroth is Lecturer in Statistical Machine Learning in the Department of Computing. Marc completed his PhD at the Karlsruhe Institute of Technology (Germany) in 2009. He conducted his PhD research at the Max Planck Institute for Biological Cybernetics (2006–2007) and at the University of Cambridge (2007–2009). Marc's research interests center around methodologies from modern Bayesian machine learning and their application autonomous control and robotic systems. Marc's goal is to increase the level of autonomy in robotic and control systems by modeling and accounting for uncertainty in a principled way. Potential applications include intelligent prostheses, autonomous robots, and healthcare assistants.

Dr Gonzalo Guillén-Gosálbez
Imperial College London

Dr Gonzalo Guillén-Gosálbez completed his MEng degree in Chemical Engineering at Universidad de Murcia in Spain following which he received his PhD from Universitat Politecnica de Catalunya in 2005. He then spent two years under the supervision of Professor Ignacio Grossmann (an Imperial College London alumnus) at Carnegie Mellon before joining Universitat Rovira Virgili in 2008 first as an Assistant Professor and then as an Associate Professor. In 2014 he joined the University of Manchester where he led the Computer Aided Process Engineering Lab (CAPE-Lab). Dr Guillén-Gosálbez's research interests lie at the interface of engineering, environmental sciences and computer aided systems design.

You can read more about the new CPSE academics on the CPSE Website:
http://www.imperial.ac.uk/process-systems-engineering/about-cpse/people/academic-staff/

Gas Research Innovation Centre

FAPESP (São Paulo Research Foundation) and BG Brasil, a BG Group company, announced the creation of the Gas Innovation Research Centre (GIC). The Centre will have its headquarters at University of São Paulo (USP). FAPESP invested R$27 million and BG Brasil have a further R$30 million. Together with the Sustainable Gas Institute (SGI), GIC will form a world-class centre for excellence for research on the current and future use of natural gas. Guided by three complementary lines of research: **Engineering, Energy Physics-Chemistry and Policy and Economy** – the centre will investigate low carbon emission energy generation, the increasing use of natural gas as fuel for ships, the prevention of fugitive emissions of methane gas, advanced combustion of natural gas, use in fuel cells, the conversion of natural gas into raw materials for the chemical industry, and the development of a natural gas supply chain for remote areas, among others. ***http://www3.imperial.ac.uk/newsandeventspggrp/imperialcollege/administration/energyfutureslab/newssummary/news_9-12-2015-8-51-4***

Professor Nilay Shah and Dr Gonzalo Guillén-Gosálbez were awarded an EPSRC pump-priming project that will focus on developing a systematic approach for the analysis of urban resource efficiency. This project is part of a wider collaboration (Data Science Institute, Grantham Institute, Institute for Security Science and Technology and the Energy Futures Laboratory) that ultimately seeks to develop data science tools that will allow us to rapidly organise and/or collate big data to produce knowledge on environmental change and security."

A paper by co-authored by **Professor Erich Müller** is featured on the cover of *Soft Matter* issue 48: *Modelling the superspreading of surfactant-laden droplets with computer simulation.* The paper describes how molecular dynamics simulation was used to provide a detailed description of droplet shape and surfactant dynamics during the superspreading process. **http://pubs.rsc.org/en/content/articlelanding/2015/sm/c5sm02090e#!divAbstract**

PhD student, Radu Baltean-Lugojan (supervisor Ruth Misener and Panos Parpas) participated in the annual Department of Computing Google Poster Competition. He was awarded 2nd in the 1st year category.

PSE@ResearchDayUK

Dr Chachuat, Professor Shah, and Miss Elnaz Jamili (winner of First Prize Oral Presentation)

On Tuesday 12th July 2016, CPSE hosted the Inaugural **PSE@ResearchDayUK** at Imperial College London. It was a great success with students participating from many universities. *Continues on page 5.*

Professor Geoff Maitland carried out a radio interview for ABC news, addressing both technical and policy issues for shale gas and coal seam gas. This took place at the international convention in Sydney on Unconventional Gas. Professor Maitland also provided a statement for **Science Media Centre** (reproduced in ***The Chemical Engineer***), was quoted in ***The Independent***, in a public release by **the IChemE Energy centre** and provided his views in the context of the **UN Climate Change Conference**.

Ruth Misener was invited to speak at the annual Mixed Integer Programming workshop (23rd - 26th May 2016 at the University of Miami); the workshop was a single -track event of 25 invited talks on recent and typically unpublished work on MIP.

Dr Oleksiy Klymenko (supervisors Professor Nilay Shah and Dr Cleo Kontoravdi) will be leaving the Centre to take up the post of lecturer at the Department of Chemical and Process at the University of Surrey.

The Department of Chemical Engineering at Imperial College held a dinner celebration in December to honour the achievements of some of the long-serving members of staff: CPSE academic, Professor Geoffrey Maitland who has worked and has been associated with Imperial since 1974.

New CPSE Academic Dr Marc Deisenroth receives two prestigious Awards

Google Faculty Research Award for 2016

Dr Marc Deisenroth was awarded the Google Faculty Research Award for 2016. This one-year award supports the work of world-class, permanent faculty members at leading universities around the world with the aim of advancing cutting-edge research in computer science, engineering and related fields. For the 2016 awards, only 16% of the 950 proposals submitted were successful.

Dr Deisenroth received the Google Faculty Research Award in the category of Machine Learning. Among other topics, Marc's research focuses on scalable probabilistic models and data-efficient machine learning in the context of robotics and autonomous systems.

Microsoft PhD Scholarships

Marc Deisenroth was awarded with the Microsoft PhD Scholarship for his work on "Data-Efficient Reinforcement Learning from Image Pixels" The scholarship provides four-year funding for PhD students and the unique opportunity of working closely with researchers at Microsoft Research Cambridge.

This year, 17 scholarships have been awarded to researchers in six European countries. Applicants, who are PhD supervisors, collaborate with an assigned Microsoft Research co-supervisor to support a PhD student for up to three years as he/she carries out the proposed research project.

Sainsbury's Extended Their Partnership

Sainsbury's and Imperial College London have announced that they will continue to work together for another five years to help Sainsbury's meet its **20x20 sustainability** Plan. The deal is an extension of a project that was started in 2010 in which the **Centre for Process Systems Engineering** and the **Department of Chemical Engineering** worked with Sainsbury's to reduce the company's carbon footprint.

The work has led to the retailer making energy savings worth £2m, and 11 kilotons of CO_2, every year for the past five years. Working together they have focussed on three main areas; buildings (stores and distribution centres), transport logistics and food sourcing. This has led to the creation of multiple zero carbon stores across the UK, improved regional monitoring of carbon, empowered energy efficiency programs and increased use of low-carbon energy. With the continued partnership, it is estimated that the supermarket chain could see annual savings of £9m and emit 47.5 kilotons less of CO_2.

PSE@ResearchDayUK

Continuing from page 4. Professor Nilay Shah and Dr Benoît Chachuat started the PSE@ResearchDayUK because they wanted to bring together researchers from around the UK to explore the latest technological advances in core and emerging application areas in PSE and to build their personal networks for future collaborations. The event centred around a combination of talks and posters in which postgraduate students were invited to showcase their research results and share visions with leading researchers and academics. The Opening Lecture *"Ubiquitous Process Systems"* was delivered by Professor Costas Pantelides, Managing Director of PSE Ltd.

The winner of the oral presentation was Miss Elnaz Jamili, University College London (Supervisors Dr Vivek Dua and Dr Michail Stamatakis) for her talk on *"Modelling and optimal control for delivering of siRNAs"*, First prize for Poster Presentations was awarded to Mr Andres J. Calderon from University College London (Supervisor Professor Lazaros Papageorgiou) for his poster *"Water management in shale gas supply chains"*, Runner up was Ricardo Suarez-Heredia from University College London (supervisor Dr Alexandros Kyparissidis) for his poster. Students from University College London had won on every category! We would like to thank Dr Miao Guo and her team for taking on the role of judges. The date for the next PSE@ResearchDayUK will be announced soon.

Quantifying the value of CCS for the future electricity system

A new paper by Mac Dowell, N; Shah, N; Staffell, I; and Heuberger, C tackles the complex cost-benefit analysis.

Abstract: Many studies have quantified the cost of Carbon Capture and Storage (CCS) power plants, but relatively few discuss or appreciate the unique value this technology provides to the electricity system. CCS is routinely identified as a key factor in least-cost transitions to a low-carbon electricity system in 2050, one with significant value by providing dispatchable and low-carbon electricity. This paper investigates production, demand and stability characteristics of the current and future electricity system. We analyse the Carbon Intensity (CI) of electricity systems composed of unabated thermal (coal and gas), abated (CCS), and wind power plants for different levels of wind availability with a view to quantifying the value to the system of different generation mixes. As a thought experiment we consider the supply side of a UK-sized electricity system and compare the effect of combining wind and CCS capacity with unabated thermal power plants. The resulting capacity mix, system cost and CI are used to highlight the importance of differentiating between intermittent and firm low-carbon power generators. We observe that, in the absence of energy storage or demand side management, the deployment of intermittent renewable capacity cannot significantly displace unabated thermal power, and consequently can achieve only moderate reductions in overall CI. A system deploying sufficient wind capacity to meet peak demand can reduce CI from 0.78 tCO_2 /MWh, a level according to unabated fossil power generation, to 0.38 tCO_2 /MWh. The deployment of CCS power plants displaces unabated thermal plants, and whilst it is more costly than unabated thermal plus wind, this system can achieve an overall CI of 0.1 tCO_2/MWh. The need to evaluate CCS using a systemic perspective in order to appreciate its unique value is a core conclusion of this study. The paper was published in **Energy and Environmental Science**: *http://hdl.handle.net/10044/1/34750*

Building low-carbon bridges with Australia

Imperial College is working with Australia's CSIRO to fund research and development of clean fossil fuels. The collaboration will fund two new studentships to explore a solution where captured carbon can be stored in old underground oil and gas reservoirs. Once the oil or gas has been extracted from these pockets hundreds of metres underground it is hoped that they could be used as a storage site for carbon dioxide (CO_2). The projects will look at how natural gas, oil and CO_2 behave, and can be contained, in these empty reservoirs. Professor Geoffrey Maitland, is one of the academics collaborating in this exciting project: *"At Imperial we have a highly active CCS research environment and this unique opportunity to take our research out of the laboratory and into the field is truly exciting. Working with CSIRO also promotes knowledge sharing between likeminded researchers from different regional settings allowing a sustainable pathway for the development of CCS to be identified."*

http://www3.imperial.ac.uk/newsandeventspggrp/imperialcollege/administration/energyfutureslab/newssummary/news_19-8-2016-10-33-9

Compilation of Ideas from the Final Session of the 2015 CPSE Industrial Consortium Meeting

CPSE Members can access the document containing the ideas from the Final Session of the 2015 Consortium Meeting held on 4th Dec 2015. The ideas include:

- Technical challenges and predictions
- Communication challenges
- Process challenges

Please log onto the '**Members Only**' section of the website to download the document. The agenda for the next Annual Industrial Consortium Meeting can be found on page 7.

CPSE Annual Industrial Consortium Meeting
1st and 2nd December 2016

Day 1 - Thursday 1st December 2016

AM	Informal meetings between representatives of CPSE Industrial Consortium member companies and academic staff. To be arranged as required	
12:00 – 13:15	*Lunch*	
13:15 – 14:45	Research Presentations	
14:45 – 16:15	Research Poster Session and Student Recruitment Session	
16:15 – 16:30	Results of Best Poster Competition	
16:30 – 17:30	*Professor Roger Sargent Lecture Reception in Common Room (Room 228), Department of Chemical Engineering*	
17:30 – 18:30	23rd Professor Roger Sargent Lecture: The Programme will include the presentation of the IChemE's MM Sharma Medal for Lifetime Achievement to Professor Roger W. H. Sargent Mathematical Programming and Dynamic Programming: How they have been used in control and can be combined for further use in planning, scheduling and control of multi-scale stochastic systems	Professor Jay H. Lee, Korea Advanced Institute of Science and Technology (KAIST)
18:30 – 22:00	*Dinner at 170 Queen's Gate*	

Day 2 - Friday 2nd December 2016

09:45 – 10:00	Registration	
10:00 – 10:15	Welcome and Introduction to CPSE and Update on Progress Since Last Meeting	
10:15 – 11:15	Industrial Technical Challenge Presentations	
11:15 – 11:30	*Break*	
11:30 – 12:30	CPSE Major Research Programmes and Proposals	
12:30 – 13:30	CPSE Consortium Company Member's Meeting	
13:30 – 14:00	Feedback from Company Members	All
14:00 – 14:45	CPSE Future Research Direction	
14:45 – 15:00	*Break*	
15:00 – 16:30	CPSE Research Programme Overview: Panel Discussion	
16:30 – 16:45	Final Comments and Meeting Close	

The Twenty Third Professor Roger W.H. Sargent Lecture
Thursday 1st December 2016 · 17:30

Mathematical Programming and Dynamic Programming: How they have been used in control and can be combined for further use in planning, scheduling and control of multi-scale stochastic systems

Professor Jay H. Lee
Korea Advanced Institute of Science and Technology (KAIST)

The Programme will include the presentation of the IChemE's MM Sharma Medal for Lifetime Achievement for Professor Roger W.H. Sargent

Abstract: Mathematical programming has been an important pillar of the process systems engineering discipline and has provided useful tools for making optimal decisions in many process design, operation planning/scheduling, and control problems. Dynamic programming has been the foundation of many classical optimal control methods, especially those addressing stochastic systems like the linear quadratic Gaussian method. In this talk, we will review how they have supported each other in the development of theories and tools for optimal control. This will be followed by a discussion on their shortcomings as individual methods for addressing multi-scale, stochastic decision problems and how they may be combined in a complementary manner to provide more general and powerful methods for solving such problems. Examples of multiple timescale planning scheduling problems in electric power grid operation and procurement in process industries will be presented to highlight the issues and illustrate the roles of the two respective approaches. **http://www.imperial.ac.uk/process-systems-engineering/courses-and-seminars/professor-roger-sargent-lecture/**

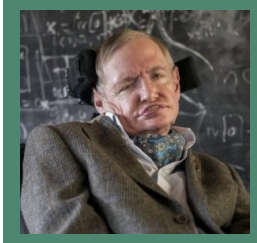
Dates For Your Diary!

CPSE Industrial Consortium Meeting

The Annual Industrial Consortium Meeting will take place on **1st and 2nd December 2016**.

The **Sustainable Gas Institute** has a new e-newsletter. Subscribe here or read the latest edition. Also, be sure to visit the SGI YouTube channel for their latest videos including their new 'Research in a nut-shell series'.

Events that might be of interest at Imperial College and University College London



An evening with Professor Stephen Hawking

17 Oct 2016, 18:00 - 19:00
Imperial College

Professor Stephen Hawking presents Quantum Black Holes, rescheduled from March 2016.

Two women on thin ice: climate change science meets contemporary art.

09:00 - 17:00, 1 November - 15 December 2016 - UCL

UCL Polar scientist Rachel Tilling and award-winning artist Zsuzsanna Ardó. Climate change science meets contemporary art.

Optimisation Courses

The CPSE Optimisation Courses tackle concepts in problems formulation and solution method in optimisation at basic and advanced levels. The courses are highly suitable for those in Industry and also individuals seeking to advance their knowledge in optimisation. We will be running these courses yearly.

- **Introduction to Optimisation**
- **Advanced Optimisation**

Cost of attendance:

- CPSE Consortium Member Companies can enrol up to two employees for free
- £900 per course and £1440 for both off (20%)
- The course is sponsored by an EPSRC Leadership Fellowship

To register for these courses, please email **Miss Senait Selassie:** s.selassie@imperial.ac.uk

Professor Nigel Brandon, Dr Adam Hawkes and their team at Sustainable Gas Institute published the second White Paper. The review paper assesses the current state of knowledge regarding the 'unburnable carbon' issue, and attempts to provide clarity by quantitatively defining the potential role of CCS in unlocking the unburnable carbon over the next 85 years.

The CPSE Newsletter aims to keep members of the Industrial Consortium, Staff and Students updated on Centre activities. If you have any comments, or would like to add to the next issue, please email: Miss Senait Selassie: s.selassie@imperial.ac.uk.

Highlights of PSE@ResearchDayUK 12th July 2016