Imperial College London

UCL

The latest news from the Centre for Process Systems Engineering

NEWSLETTER

Welcome to the Spring Edition

Issue 9 March 2014

Message from CPSE Director, Professor Nilay Shah

It gives me great pleasure to welcome AkzoNobel to our Industrial Consortium. AkzoNobel is one of the largest global paints and coatings company and a major producer of specialty chemicals. We are looking forward to working with them! Since the last newsletter, we have had many activities, one of which was the Annual Industrial Consortium Meeting. It was exciting to see many of our member companies, academics, students and post docs interacting, especially, during the poster and recruitment sessions. I would like to thank Frank Doyle for delivering the 20th Professor Roger Sargent Lecture and Roger Sargent for coming. We received the results of our proposal for a new Centre for Doctoral Training in Process Systems Engineering. Unfortunately, despite being strong contender our application was not successful at this stage. Notwithstanding, to have been shortlisted to the interview stage from hundreds of Centres shows how close we were. I would like to stress my thanks again to my colleagues and industrial companies for their support. This has only renewed our energy and we will continue to look for new opportunities. I congratulate Geoff Maitland for being elected president of IChemE and to the students who won awards. The Newsletter includes an article on physical property prediction and we will follow up with further technical articles in future editions.

Twentieth Professor Roger W.H Sargent Lecture

From bottom left Professors: Francis J. Doyle III with four former/current CPSE Directors: Roger W.H Sargent, John Perkins, Nilay Shah (current Director) and Stratos Pistikopoulos

CPSE held the Twentieth Professor Roger W.H Sargent Lecture on 5th December 2013. The Lecture is an annual event the Centre inaugurated as a tribute to Professor Sargent's vision, leadership, significant technical contributions and to his legacy in the field of Process Systems Engineering. The Lecture titled "Engineering the Artificial Pancreas" was delivered by Professor Francis J. Doyle III, University of California, Santa Barbara. Prof Roger Sargent and his family attended the Lecture. Visitors also included national and international academics as well as industrial companies. The lecture theatre was packed with people sitting on the stairs eager to hear Prof Doyle's Lecture on this fascinating topic. *More on the lecture and Prof Doyle on page 2.*

New Industrial Consortium Member

AkzoNobel has joined our Industrial Consortium. AkzoNobel is a Global Fortune 500 company and has operations in more than 80 countries. It is also one of the largest global paints and coatings company and a major producer of specialty chemicals. Professor George Jackson is Akzonobel's academic 'friend' (the contact in CPSE). We are delighted to have our newest member and welcome AkzoNobel in our consortium. CPSE's Industrial Consortium has been running for nearly 25 years. We have 9 Multinational Companies and some have been members since the Centre was inaugurated in 1989. AkzoNobel joins ABB Corporate Research, BP, Petrobras, PSE, Praxair, Procter & Gamble, Shell Research & Technology and Syngenta.

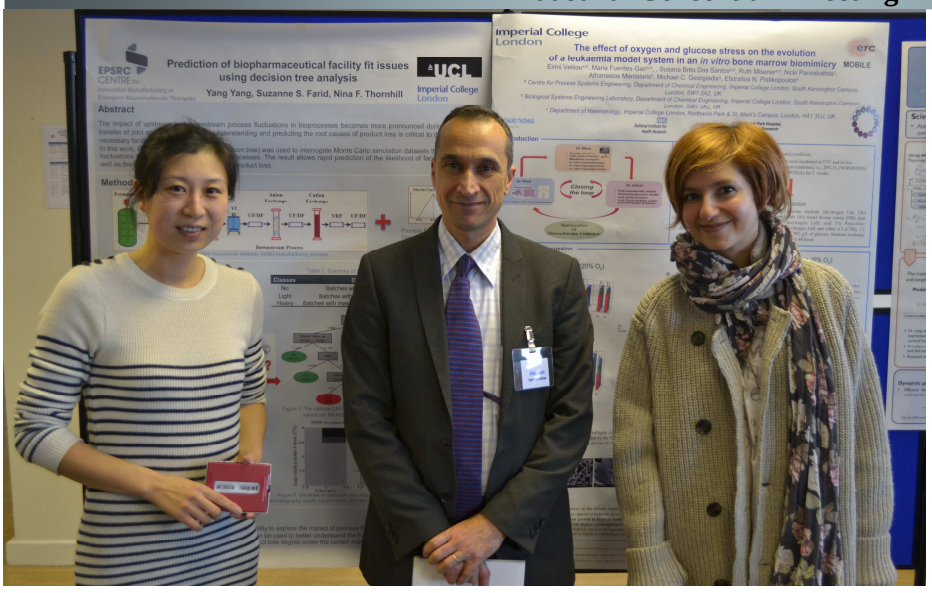
Engineering the Artificial Pancreas

Professor Francis J. Doyle III, holds the Duncan and Suzanne Mellichamp Chair in Process Control in the Department of Chemical Engineering, as well as appointments in the Electrical Engineering Department, and the Biomolecular Science and Engineering Program at UC, Santa Barbara. He is the Director of the UCSB/MIT/Caltech Institute for Collaborative Biotechnologies, and is the Associate Dean for Research in the College of Engineering. He is also the Great, Great Academic Grandson of Professor Roger Sargent and it was fitting that he should give the 20th Professor Roger Sargent Lecture.

In his lecture, Prof Doyle talked about Type 1 diabetes mellitus (T1DM) which is a chronic autoimmune disease affecting approximately 35 million individuals world-wide, with associated annual healthcare costs in the billions. In addition to the costs, the treatments are painful and requires patients to have either multiple daily insulin injections or continuous subcutaneous (SC) insulin infusion (CSII) delivered via an insulin infusion pump. Both treatment modes necessitate frequent blood glucose measurements to determine the daily insulin requirements for maintaining near-normal blood glucose levels. More than 30 years ago, the idea of an artificial endocrine pancreas for patients with type 1 diabetes mellitus (T1DM) was envisioned. The closed-loop concept consisted of an insulin syringe, a blood glucose analyzer, and a transmitter. In the ensuing years, a number of theoretical research studies were performed with numerical simulations to demonstrate the relevance of advanced process control design to the artificial pancreas, with delivery algorithms ranging from simple PID, to H-infinity, to model predictive control. With the advent of continuous glucose sensing, which reports interstitial glucose concentrations approximately every minute, and the development of hardware and algorithms to communicate with and control insulin pumps, the vision of closed-loop control of blood glucose is approaching a reality.

Prof Doyle discussed the work that he and his group are doing with medical doctors on clinical demonstrations of feedback control algorithms for the artificial pancreas. He highlighted the difficulties inherent in controlling physiological variables, the challenges with regulatory approval of such devices, and described a number of process systems engineering algorithms he and his group tested in clinical experiments for the artificial pancreas. *CPSE Consortium Members can download Prof Doyle's presentation from our website under "Members only" section: https://www3.imperial.ac.uk/centreforprocesssystemsengineering*

Industrial Consortium Meeting



CPSE Director, Prof Nilay Shah with Poster winners: Dr Yang Yang and Ms Nasim Elahi

The Annual Industrial Consortium kicked off with full swing on 5-6 Dec 2013. We had seven presentations from our academics and one from PhD student Hongxing Niu. The presentations were on many areas in process systems, including: Process Operations, Solvent Design for Reactions, Biological Systems Engineering, Energy Systems Engineering, Process Modelling and Numerical Methods, Molecular Systems Engineering and a focus talk on Bioprocess Modelling from Micro Metabolism/Biocatalysis to Macro (Reactor): Case Studies. The event also included 20 oral and poster presentations from PhD students and Post Docs. It was great to see many of our Industrial Consortium Members, although, the bad weather had meant that some could not travel into London. *Continues on page 3.*

Education

Industrial Consortium Meeting

Continues from page 2. CPSE Director, Professor Nilay Shah was pleased with the quality of posters and presented first prize to Dr Yang Yang who won £150 for her poster titled *'Prediction of biopharmaceutical facility fit issues using decision tree analysis'* (supervisor Prof N. Thornhill). Second prize of £100 went to Ms Nasim Elahi for her poster '*Multi-period least cost optimisation model of an integrated CCS network'* (supervisor Prof N. Shah). Third prize of £50 went to Mr Cristian Triana for his poster '*Optimal Energy Consumption in the Production of Bioethanol From Lignocellulosic Biomass'* (supervisors Dr E. Sorensen & Prof E. Fraga). The next Annual Industrial Consortium Meeting will be held on **4-5 December 2014**. During this meeting, we will have presentations which tackle topics of interest to our members. We will also have poster and recruitment sessions to foster interactions between our members, CPSE students and post docs. Please put these dates in your diary!

Doctoral Training in Process Systems Engineering

CPSE had applied for Doctoral Training in Process Systems Engineering. Despite our proposal having been shortlisted to the interview stage, unfortunately, we were not successful at this stage. However, there were hundreds of proposals submitted and to have been shortlisted shows that CPSE is a strong contender and only missed out by a small margin. CPSE Director, Professor Nilay Shah thanks Industrial companies for their invaluable support for our proposal and to CPSE staff who worked hard putting the application forward.

President of the Institution of Chemical Engineers

Professor Geoffrey Maitland has been elected President of the Institution of Chemical Engineers (IChemE) from May 2014. He is currently the Deputy President. IChemE is the global professional membership organisation for people with relevant experience or an interest in chemical engineering. They are the only organisation to award Chartered Chemical Engineer status. Founded in 1922 as a professional institution for chemical and process engineers, it has over 38,000 members across 120 countries.

Process Systems Engineering: an enhanced role in the curriculum?

Sir William Wakeham

Prof Sir William Wakeham, Senior Vice President of the Royal Academy of Engineering and Past President of the IChemE gave a webinar on 'Process Systems Engineering – An enhanced role in the curriculum' for the IChemE Computer Aided Process Engineering and Education Special Interest Groups.

The talk was chaired by Professor David Bogle and was interesting as it related to our recent grant proposal for Doctoral Training in Process Systems Engineering. Sir William considered the professional role of chemical engineers today, the challenges for the modern chemical engineering curriculum to prepare students appropriately, and the central role that Process Systems Engineering has to play. Sir William had given the plenary talk at the ESCAPE22 Conference held at UCL in 2012, and at this webinar developed these ideas further. He proposed a call to arms to ensure that we train all Chemical Engineers to be systems thinkers. Sir William stressed systems engineering is important for tackling the 'grand challenges' that face society and that can be solved by engineering. However, he points out that systems engineering is not being used as a framework but is only being introduced later on in courses as (another topic). Sir William who was also former Head of the Department of Chemical Engineering at Imperial would like to change this and include systems engineering in undergraduate university curricula. He urges those in education to recognise the importance of process systems engineering in the curriculum. He also asks the process systems engineering community to do more to promote the interdisciplinary field.

"I would argue that for too long systems engineering has been somewhat of a 'Cinderella' subject in the curriculum. Systems engineering is often seen as peripheral or an add-on to other aspects of an undergraduate programme, but this may be inappropriate if we are to prepare students for a leading role in the complex world of modern engineering."

With this in mind, it is unfortunate that CPSE was not awarded the grant for Doctoral Training in Process Systems Engineering. We feel that our objective to establish a Doctoral Training in Process Systems Engineering is important for chemical engineers, society and businesses. Our aim is to provide a structured programme of training and research which will impart systems thinking, modelling and quantitative analysis skills required to invent, design, optimise and operate future industrial systems molecular to the supply chain level. We hope to establish this soon and we will continue to do more to promote systems engineering.

Sir William, is a renowned Chemical Engineer, who's achievements and influence is respected world-wide. *You can view his talk titled "Process Systems Engineering: an enhanced role in the curriculum?" : http://www.tcetoday.com/*

CPSE Inaugural Lectures

During the summer of 2013, CPSE had 3 academics who gave inaugural lectures; Professor Claire Adjiman, Professor Amparo Galindo and Professor Erich A. Müller. Many of us attended their inaugurals and enjoyed their lectures and sharing this huge milestone in their careers. For the last newsletters, we featured an article on Professors Claire Adjiman's journeys to her inaugural. As promised, in this newsletter we have Professor Erich A. Müller's journey in his own words.

The next newsletter will feature Prof Amparo Galindo. If you have any questions you would like to ask her before the next publication, please email: s.selassie@imperial.ac.uk. In the mean time, you can view all 3 Inaugural Lectures on our website: http://www3.imperial.ac.uk/centreforprocessystemsengineering/newsandevents/inauguralllectures video

CPSE Industrial Consortium Members

ABB Corporate Research

AkzoNobel

BP

Petrobras

Praxair

PSE

Procter & Gamble

Shell Research & Technology

Syngenta

Companies and organisations wishing to learn more about the CPSE Consortium membership should contact CPSE Director, Professor Nilay Shah at n.shah@imperial.ac.uk

CPSE's Annual Consortium Meeting will take place on **4th and 5th December 2014**. This is strictly for Consortium Member Companies. To register, please contact Miss Senait Selassie: s.selassie@imperial.ac.uk

CPSE Inaugural Lecture

Professor Erich A. Müller 's journey, in his own words...

"Jiggling of Atoms"

Professor Erich A. Müller

One of the greatest achievements of the 20th century was the foundation of the atomic theory, the understanding that the macroscopic behaviour of matter is a direct consequence of the forces that act between atoms and molecules. The advent of the computer age paved the way for the in silico modelling of such interactions and the emergence of computer simulation as a scientific tool of unprecedented potential.

The title of my lecture results from the comments of Richard Feynman, the 1965 physics Nobel laureate, who described the "jiggling of atoms" as a cartoon for the description of atomic motion and how this resulted in the understanding of the macroscopic observables of nature. Nowadays, we can model this behaviour on a computer, and my current research relies heavily on this basic starting point.

In the lecture, which can be watched online, I explore the origins of molecular dynamics simulations, from the first applications half a century ago, where computers were used to iteratively solve Newton's equations of motion for simple model systems to the modern paradigms that allow the study of the spontaneous self assembly of complex fluids. I discoursed on how molecular simulation provides invaluable insight on the behaviour of industrially, biologically and technologically important classes of fluids such as liquid crystals, amphiphiles and macromolecules. I ended the lecture by pointing out the very recent award of the 2013 Nobel prize to a trio of molecular modelers, in an attempt to point out the fast pace of this very topical field.

I have enjoyed my academic journey which began with my studies in Chemical Engineering at Universidad Simón Bolívar in Caracas, Venezuela. I had my first lecturer position there where I was in charge of the courses in thermodynamics. Since then, my research within CPSE has centred around the use of molecular modelling as a tool to help understand and design complex fluids. I continue to be fascinated with this area and it was a great privilege to be able to share my inaugural with family, friends and colleagues.

If you would like to see Professor Müller's Inaugural Lecture, please visit our website. http://www3.imperial.ac.uk/centreforprocesssystemsengineering

Young Entrepreneur Award

CPSE PhD student María Fuentes Gari won second prize at the 2nd Young Entrepreneur Award Competition (YEA). YEA is an international business plan competition organized by the Fourth Valley Concierge Corporation and Asia Innovators' Initiative (President: Nobuyuki Idei, Former CEO of Sony Corporation). There were 143 applications in total, from over 20 countries. María was presented the award in Tokyo on the 13th Dec for her project "Automated cell counting: the software." María is currently in the 3rd year of her PhD studies in Biological Systems Engineering (supervised by Professors Sakis Mantalaris and Stratos Pistikopoulos). The aim of her PhD is to develop a mathematical model of the cell cycle in leukemia (which plays a key role in chemotherapy outcomes) that is directly informed by patient-specific experimental data and that is coupled to an optimisation platform in order to predict the best chemotherapy treatment on an individual basis. We asked María to describe her project for the competition:

"In biological labs we need to measure cell growth often (daily to several times a day) to monitor the effect of a particular condition or simply to correlate cell numbers with the output of our mathematical models. This is done by counting cells manually under the microscope, which is very repetitive and time-taking, so the idea is to build a software to automatically count cells on microscope images without the need of a physical apparatus (which is the state of the art nowadays, but is quite expensive). As you can see, the project is not directly related to my research and is not something required to complete my PhD, but it's a struggle I faced that eventually turned into a potential business idea. I would like to take the opportunity to thank Professor Sakis Mantalaris for his support throughout the competition." http://www.asia-ii.org/yea/en/

6 PhD Students Pass their Viva

6 CPSE PhD students have passed their Viva exams. They will be graduating this year having successfully defended their thesis. We congratulate Romain Lambert, Eleni Pefani, Pedro Rivotti, Alexandra Krieger who are supervised by Prof Stratos Pistikopoulos; Mark Jennings who is supervised by Prof Nilay Shah; and Erini Siougkrou, supervised by Professors Claire Adjiman and Amparo Galindo.

PhD student Gabriel Lau, supervised jointly by Professors George Jackson, Erich Muller, Patricia Hunt (Chemistry, Imperial) and Ian Ford (Physics, UCL) has been awarded the Materials Design Graduate Research Prize for 2013. Gabriel's PhD work is within the DCT on Theory and Simulation of Materials. Gabriel received the award for showing independent thinking and originality. His poster titled *"interfacial tension of water nano droplets"* was presented at the Thermodynamics 2013 conference, an international biannual conference focussing on the fundamentals and applications of thermodynamics. He received the best poster award from around 200 entries.

Dr Benoit Chachuat has become Associate editor of The Journal of Process Control. He has also become Associate Editor of JOTA.

Ioscani Jimenez Del Val (supervisor Dr Cleo Kontoravdi) won the Dudley Newitt Prize for Computational/Theoretical Excellence.

More News!!

Susie Sou (supervised by Dr Cleo Kontoravdi) won the best poster prize at the recent UK Meeting of the European Society for Animal Cell Technology in Nottingham.

Dr Ruth Misener has been listed as *Top Reviewer* for the journal *Computers and Chemical Engineering;* this is a leading process systems engineering publication. Dr Misener also attend the *2nd Belgium Symposium on Tissue Engineering* with a travel grant from the European Science Foundation (€500). At the symposium, she won the *Best Poster* prize.

Dr Michail Stamatakis was named Top Reviewer for Computers& Chemical Engineering (CACE) in 2012-2013. CACE is published by Elsevier and is one of the influential Chemical Engineering journal covering, areas of Modelling, Numerical Analysis, Simulation and Process Systems Engineering.

PhD student Tareq Al-Ansari (co-supervisor Prof Nilay Shah) has won the Qatar Energy R&D Award for outstanding achievement for his PhD research which could impact Qatar Industry. He has been invited to receive the award on 18th March 2014 at the Qatar Energy R&D Forum. Well done Tareq!

Software Package Release - Catalysis Kinetic Monte Carlo Package "Zacros"

Accurate predictions of catalytic performance are essential for the development of efficient processes in the chemical industry. In a work published last December in the Journal of Chemical Physics [1], Dr Stamatakis and coworkers present a kinetic Monte Carlo framework and a software package, *Zacros* [2], which incorporates several sources of complexity encountered in catalytic systems. In particular, the framework can capture steric exclusion effects for multi-dentate species, complex reaction patterns involving adsorbates in specific binding configurations and neighbouring patterns, and adsorbate lateral interactions that involve many-body contributions. These advances push the frontiers of kinetic simulation of catalytic systems and contribute to the "rational catalyst design" paradigm.

References:

[1] Nielsen, J., M. d'Avezac, J. Hetherington and M. Stamatakis (2013). "Parallel Kinetic Monte Carlo Simulation Framework Incorporating Accurate Models of Adsorbate Lateral Interactions." Journal of Chemical Physics 139(22): 224706.
[2] Stamatakis, M. (2013) http://www.e-lucid.com/i/software/material_modelling/Zacros.html

CPSE and Dept Events

Distinguished Seminar Series 2013-14
All seminars will take place in Lecture Theatre 1, Department of Chemical Engineering, ACE Extension, South Kensington Campus

WEDNESDAY 26 MARCH 2014 (16:00)
"Process Integration Tools for Hybrid Power Systems,"
Professor Zainuddin Abdul Manan ,
Universiti Teknologi Malaysia

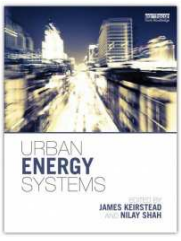
WEDNESDAY 7 MAY 2014 (16:00)
"Sustainable Energy and Resource Development in China,"
Professor Zheng Li, Tsinghua University

WEDNESDAY 14 MAY 2014 (16:00)
"*Process Integration Tools for Hybrid Power Systems***,"**
Professor Zainuddin Manan, Universiti Teknologi Malaysia

The CPSE Autumn Consortium Meeting will take place on **4th and 5th December 2014**. The programme will be available soon.

For our Events, please check: www3.imperial.ac.ukcentreforprocesssystemsengineering/newsandevents

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.



Events at Imperial and UCL that could be of interest

TUESDAY 07 Apr 2014 (18:00 - 19:30)

The Grantham Annual Lecture 2014 will be delivered by Paul Polman, CEO of Unilever, one of the world's largest consumer goods companies. In this lecture, he will argue that climate change is now the single greatest threat facing mankind. The need to act now is not just a moral calling, but an increasingly clear commercial imperative. We have recently reached a tipping point: the cost of inaction now exceeds the cost of action. The only future is a low carbon future. To meet this opportunity, exciting ideas are now emerging from governments, businesses and individuals. We all have a responsibility to play our part. There has never been a better time to create a better world. *More details, can be found at Imperial College website: http://www3.imperial.ac.uk/events*

TUESDAY 1 APRIL 2014 (18:00 - 19:30)

In this UCL ISR / UCL Energy Joint Public Lecture, Dr Christof Ruhl, Group Chief Economist and Vice President of BP plc will be speaking at the first joint public lecture with our partner institute UCL-Energy for 2014. Dr Ruhl manages BP's global Economics Team, which produces the annual Statistical Review of World Energy & Global Energy Outlook. In this lecture he will outline the major features of the BP Energy Outlook 2035, and the role of carbon pricing in seeking to encourage a transition to a low-carbon energy system. *More details, can be found at UCL website: http://events.ucl.ac.uk/calendar/date:2014-03-27/*