

CAPE tools for a sustainable world



# ESCAPE 22

The 22nd European Symposium on Computer Aided Process Engineering

## Conference programme

17–20 June 2012, University College London, UK



Working Party on  
Computer Aided Process Engineering

**IChemE** ADVANCING  
CHEMICAL  
ENGINEERING  
WORLDWIDE

# The 22nd European Symposium on Computer Aided Process Engineering

17–20 June 2012

University College London, UK



## CAPE tools for a sustainable world

IChemE and the European Working Party on Computer Aided Process Engineering are pleased to welcome you to London to participate in the 22nd European Symposium on Computer Aided Process Engineering (*ESCAPE 22*). London offers many attractions for visitors and delegates and will host the 2012 Olympics starting in late July. *ESCAPE 22* will be held at University College London, in London's academic quarter, Bloomsbury, which is right in the heart of London just a few minutes' walk from major attractions including Oxford Street and the British Museum.

The conference follows the well established series of *ESCAPE* conferences sponsored by the EFCE Working Party on Computer Aided Process Engineering (CAPE). Recent conferences have been hosted in Krakow, Poland (2009), Ischia, Italy (2010), and Porto Carras, Greece (2011).

*ESCAPE 22* will focus strongly on the important role of CAPE in design and operation in the process industries from the molecular scale through to managing complex manufacturing sites. In addition, the programme will address the implications of strategic planning, corporate finance, supply chain issues and the increasingly important area of sustainability audits. The close proximity of the conference venue to the City of London provides an opportunity for perspectives from the financial world. The conference will highlight the need for CAPE practitioners to embrace the three components of sustainable development: environmental, social and economic progress and will emphasise the role of systematic and sophisticated CAPE tools in delivering these goals. This will bring CAPE to the attention of new audiences.

The conference will take place in London, the UK's capital city. London is served by five international airports and the Eurostar service in addition to major road and rail networks. A range of accommodation options to suit all budgets will be available close to the conference venue in the heart of London.



Professor David Bogle  
Chairman  
Organising committee *ESCAPE 22*

# Plenary and keynote speakers



## Plenary speaker: Joan F Brennecke, University of Notre Dame, US

Joan F Brennecke is the Keating-Crawford Professor of Chemical Engineering at the University of Notre Dame and Director of the Centre for Sustainable Energy. She joined Notre Dame after completing her PhD (1989) and Masters (1987) degrees at the University of Illinois at Urbana-Champaign and her Bachelor degree (1984) at the University of Texas at Austin, US.

Her research interests are primarily in the development of less environmentally harmful solvents. These include supercritical fluids and ionic liquids. In developing these solvents, Dr Brennecke's primary interests are in the measurement and modelling of thermodynamics, thermophysical properties, phase behaviour and separations. Major awards include 2001 *Ipatieff Prize* from the American Chemical Society, the 2006 *Professional Progress Award* from the American Institute of Chemical Engineers, the *J M Prausnitz Award* at the Eleventh International Conference on Properties and Phase Equilibria in Greece in May, 2007, the 2008 *Stieglitz Award* from the American Chemical Society, and the 2009 E O Lawrence Award from the US Department of Energy.



## Plenary speaker: Prof Sir William Wakeham, UK

Professor Wakeham retired as Vice-Chancellor of the University of Southampton, UK in September 2009 after eight years in the post. He began his career in physics at Exeter University, UK at both undergraduate and doctoral level. In 1971, after a postdoctoral period in the US at Brown University, he took up a lectureship in the chemical engineering department at Imperial College London, UK where he became a professor in 1983 and head of department in 1988. His academic publications include six books and about 400 peer-reviewed papers.

From 1996 to 2001 he was Pro-Rector (Research), Deputy Rector and Pro-Rector (Resources) at Imperial. Among other activities he oversaw its merger with a series of medical schools and stimulated its entrepreneurial activities.

He is a fellow of the UK's Royal Academy of Engineering a Vice-President and its International Secretary. Sir William is also an IChemE Fellow and its President during 2011-2012. He is a Fellow of the Institution of Engineering and Technology and the Institute of Physics.

He is a Council Member of the UK's Engineering and Physical Sciences Research Council and Chair of its Audit Committee. He was made a Knight Bachelor in 2009 for services to chemical engineering and higher education.

## Theme: Tools for sustainable development



## Keynote speaker: Will Day, Pricewaterhouse Coopers, UK

As an independent consultant, and as Special Advisor to UNDP, Day has helped facilitate cross sector engagement between government, companies and civil society organisations in various parts of the world, with a strong focus on the role of the private sector in development. As a faculty member of the University of Cambridge programme for Sustainability Leadership, he has focussed on the identification, analysis and the communication, to senior business and government clients, of global mega trends, and their potential social and economic impacts.

Day was Chair of the UK Sustainable Development Commission until March 2011. He combines that with his role at Cambridge, and as Sustainability Advisor for PwC. He is also a Board member of the Overseas Development Institute.

## Theme: Product and process design



## Keynote speaker: Prof Xavier Joulia, ENSIACET, FRA

Xavier Joulia is professor of Chemical Engineering at ENSIACET (Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques Et Technologiques), in Toulouse, France. He completed his PhD (1981) and obtained a DSc (1987) in Chemical Engineering from the Institut National Polytechnique de Toulouse, France (INPT). Joulia currently heads the Computer and Chemical Engineering educational department of ENSIACET and leads the computer aided process analysis research team of the Laboratoire de Génie Chimique.

The author, or co-author, of more than 120 papers in the CAPE field, Joulia chaired the organising committee for ESCAPE 2 at Toulouse, in 1992. He is the French representative on the CAPE Working Party of the European Federation of Chemical Engineering.

Joulia was involved in the spin out of the chemical engineering software company, ProSim S.A., in 1989 through technology transfer activities. He remains actively involved in ProSim through the provision of scientific support.

## Theme: Systems biology and healthcare engineering



### Keynote speaker: Prof Andreas Linninger, University of Illinois, US

Andreas Linninger is Professor of Chemical Engineering and Bioengineering and Director of the Laboratory for Product and Process Design at the University of Illinois in Chicago, US. He received his Diploma and PhD degrees in Chemical Engineering from the Vienna University of Technology, Austria, before postgraduate training at the Rijksuniversiteit Gent, Belgium, the University of California at Berkeley, US and the Massachusetts Institute of Technology, US. His research interests include computer-aided process synthesis, mathematical modelling of complex systems and design under uncertainty. He has published more than 100 papers on parameter estimation in distributed systems, synthesis of distillative separation networks, integrated design and control, process design for the environment and computational fluid mechanics methods in biological systems.

## Theme: Multi-scale modelling and simulation



### Keynote speaker: Prof Hans Kuipers, University of Eindhoven, NL

Hans Kuipers graduated from the Department of Chemical Engineering at the Technical University of Twente in 1985. His PhD (1990) focussed on detailed micro balance modelling of gas-fluidised beds. In the same year he was appointed as assistant professor in the reaction engineering group headed by Prof. W.P.M. van Swaaij. In 1994 he was appointed as associate professor in the same group. In August 1999 he became fulltime professor in fundamentals of chemical reaction engineering at the chemical engineering department at the University of Twente, NL where he currently teaches introductory and advanced courses on transport phenomena and applied process technology. His research interests are in the area of multiphase reactors.

## Theme: Operations and control



### Keynote speaker: Prof Nina Thornhill, Imperial College London, UK

Nina Thornhill holds the ABB/RAEng Research Chair in Process Automation in the Department of Chemical Engineering at Imperial College London, UK. She studied physics at Oxford and joined University College London (UCL), UK in the Department of Electronic and Electrical Engineering after six years with ICI. She moved to Imperial in 2007 having been involved with the Imperial/UCL Centre for Process Systems Engineering for many years. Her research addresses industrial data analysis using time series analysis and signal processing for applications in oil and gas, chemicals and electricity supply, and has included secondments with BP and ABB.

# Technical programme

*ESCAPE 22* will be chaired by Professor David Bogle and co-chaired by Professor Mike Fairweather – University of Leeds, UK and Dr Robert Low – Mexichem Fluor Ltd., UK.

In addition to the thought-provoking line up of invited keynote speakers, *ESCAPE 22* will feature over 120 peer reviewed technical papers submitted by organisations from across Europe and farther afield. Contributions were invited under the following themes:

**Theme 1:** Tools for sustainable development

**Theme 2:** Tools for energy management

**Theme 3:** Tools for financial business and management decision making

**Theme 4:** Product and process design

**Theme 5:** Operations, control and process safety

**Theme 6:** Multi-scale modelling and simulation

**Theme 7:** Computational and numerical solution strategies

**Theme 8:** Systems biology and healthcare engineering

**Theme 9:** CAPE in education



# Programme overview

## Sunday 17 June 2012

10:00	CAPE Working Party workshop (members only)	Wilkins Haldane room
12:40	Lunch for Working Party members	Wilkins Haldane room
14:00	CAPE Working Party business meeting (members only)	Wilkins Haldane room
17:30	Delegate registration	South cloisters
18:00	Welcome reception (free to attend)	South cloisters

## Monday 18 June 2012

08:00	Delegate registration	South cloisters
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	Cruciform lecture theatre	Gustave Tuck lecture theatre	Chadwick lecture theatre	Jeremy Bentham room
09:30	Welcome and opening remarks			
09:50	EFCE Excellence in CAPE Award			
10:15	Plenary speaker: <b>Joan F Brenneck</b> Ionic liquids for CO <sub>2</sub> capture: From process modelling to quantum calculations			
11:00	Refreshment break, viewing of posters and exhibition – North and South cloisters			
11:30		Keynote speaker: <b>Professor Nina Thornhill</b> Imperial College London, UK	Keynote speaker: <b>Professor Andreas Linninger</b> University of Illinois, US	Keynote speaker: <b>Will Day</b> PriceWaterhouse Coopers, UK
12:00		Operations, control and process safety (Part 1)	Systems biology and healthcare engineering	Tools for sustainable development (Part 1)
13:00	Lunch, viewing of posters and exhibition North and South cloisters			
14:30		Operations, control and process safety (Part 1 cont'd)	Product and process design	Tools for sustainable development (Part 1 cont'd)
15:30	Refreshment break, viewing of posters and exhibition – North and South cloisters			
16:00		Operations, control and process safety (Part 2)	Systems biology and healthcare engineering	Tools for energy management
18:00	Close of day one			

## Tuesday 19 June 2012

	Cruciform lecture theatre	Gustave Tuck lecture theatre	Chadwick lecture theatre	Jeremy Bentham room
08:35	Introduction and welcome			
08:40	ESCAPE 23 presentations			
08:50	Plenary speaker: Professor Sir William Wakeham			
09:35	Delegates move to parallel sessions			
09:40		Operations, control and process safety (Part 3)	Product and process design (Part 2)	Tools for sustainable development (Part 2)
10:40	Refreshment break, viewing of posters and exhibition – North and South cloisters			
11:10		Operations, control and process safety (Part 3 cont'd)	Product and process design (Part 2 cont'd)	Tools for sustainable development (Part 2 cont'd)
12:30	Lunch, viewing of posters and exhibition North and South cloisters			
14:00		Tools for financial business and management decision making (Part 1)	CAPE in education (sponsored by EURECHA)	Tools for sustainable development (Part 3)
15:20	Refreshment break, viewing of posters and exhibition – North and South cloisters			
15:50		Keynote speaker: Professor Xavier Joulia, ENSIACET, France	Keynote speaker: Professor Hans Kuipers, University of Eindhoven, NL	Keynote speaker: Peter Bongers, Unilever R&D, NL
16:15		Product and process design (Part 3)	Multi-scale modelling and simulation (Part 1)	Computation and numerical solution strategies (Part 1)
17:55	Close of day two			
	ESCAPE 22 gala dinner (ticket only)			

## Wednesday 20 June 2012

08:00 Delegate registration

	Cruciform lecture theatre	Gustave Tuck lecture theatre	Chadwick lecture theatre	Jeremy Bentham room
08:45	Plenary speaker			
09:35	Delegates move to parallel sessions			
09:40		Tools for energy management (Part 2)	Multi-scale modelling and simulation (Part 2)	Product and process design (Part 4)
11:00	Refreshment break, viewing of posters and exhibition – North and South cloisters			
11:25		Computation and numerical solution strategies (Part 2)	Tools for financial business and management decision making (Part 2)	Product and process design (Part 4 cont'd)
12:45	Lunch, viewing of posters and exhibition North and South cloisters			
13:40		Operations, control and process safety (Part 4)	Tools for financial business and management decision making (Part 3)	Computation and numerical strategies (Part 2)
15:40	Delegates move to Cruciform lecture theatre			
	Awards and closing formalities			
16:15	End of conference			



# Conference programme

(Please note that the programme may be subject to alteration without notice)

## Sunday 17 June 2012

Time		Location
10:00	CAPE Working Party workshop (members only)	Wilkins Haldane room
12:40	Lunch for Working Party members	Wilkins Haldane room
14:00	CAPE Working Party business meeting (members only)	Wilkins Haldane room
17:30	Delegate registration	South cloisters
18:00	Welcome reception (free to attend)	South cloisters

## Monday 18 June 2012

Time		Location
08:00	Delegate registration	South cloisters
09:30	Welcome remarks David Bogle - Chair of ESCAPE 22 organising committee, Jiri Klemes - acting chair EFCE working party and David Brown CEO, IChemE	Cruciform theatre
09:50	EFCE Excellence Award in recognition of an outstanding PHD thesis on CAPE 2012 Dr Jose Miguel Lainex Aguirre, Purdue University, US	Cruciform theatre
10:15	Plenary speaker Joan F Brennecke, University of Notre Dame, US Ionic liquids for CO <sub>2</sub> capture: From process modelling to quantum calculations	Cruciform theatre
11:00	Refreshment break, viewing of posters and exhibition	North and South cloisters
11:25	Delegates move to parallel sessions	

### Theme: Operations, control and process safety (Part 1) - Gustave Tuck lecture theatre

11:30	Keynote speaker: Professor Nina Thornhill, Imperial College London, UK
12:00	Regular and non regular production schedule of multi purpose batch plants <i>S Moniz<sup>1,3</sup>, A P Barbosa-Póvoa<sup>1</sup> and J Pinho de Sousa<sup>2,3</sup></i> <sup>1</sup> Centro de Estudos de Gestão, Instituto Superior Técnico, POR <sup>2</sup> INESC Porto, POR <sup>3</sup> Faculdade de Engenharia da Universidade do Porto, POR
12:20	An efficient unit-specific event-based continuous time MILP formulation for short-term scheduling multistage and multiproduct batch plants <i>J Li and C A Floudas</i> Princeton University, US
12:40	Solution methods for time-indexed MIP models for chemical production scheduling <i>S Zenner and C T Maravelias</i> Department of Chemical and Biological Engineering, University of Wisconsin, US

### Theme: Systems biology and healthcare engineering - Chadwick lecture theatre

11:30	Keynote paper: Professor Andreas Linninger, University of Illinois, US
12:00	A mathematical programming approach to community structure detection in complex networks <i>L Bennett, S Liu, L G Papageorgiou and S Tsokka</i> Department of Informatics, School of Natural and Mathematical Sciences, Kings College London, UK Centre for Process Systems Engineering Department, of Chemical Engineering, University College London, UK



- 12:20 Simulating bioreactor feature through CFD tool for the maturation of fresh 3D printed human organs  
*R A Rezende, V Mironov and J V Lopes da Silv*  
*Division of 3D Technologies, Renato Archer Information Technology Center, BRA*
- 12:40 Probabilistic optimal control of blood glucose under uncertainty  
*M De Paula and E Martínez*  
*INGAR(CONICET-UTN), ARG*

### Theme: Tools for sustainable development (Part 1) – Jeremy Bentham room

- 11:30 Keynote speaker: Will Day, PriceWaterhouse Coopers, UK
- 12:00 Metrics for evaluating the forest biorefinery supply chain performance  
*B Mansoornejad<sup>a</sup>, S Pistikopoulos<sup>b</sup> and P Stuart<sup>a</sup>*  
<sup>a</sup>*NSERC Environmental Design Engineering Chair in Process Integration, Department of Chemical Engineering, École Polytechnique – Montréal, CAN*  
<sup>b</sup>*Center for Process Systems Engineering, Imperial College, London UK*
- 12:20 Objective reduction in multi-criteria optimization of integrated bioethanol sugar supply chains  
*A Kostin<sup>a</sup>, G Guillén-Gozálbez<sup>a</sup>, F D Meleb and L Jiménez<sup>a</sup>*  
<sup>a</sup>*Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, ESP*  
<sup>b</sup>*Ingeniería de Procesos y Gestión Industrial, Universidad Nacional de Tucumán, ARG*
- 12:40 Water saving technologies for the efficient development of biorefineries  
*A Nikolakopoulos, P Karagiannakis, A Galanis and A Kokossis,*  
*School of Chemical Engineering, National Technical University of Athens, GRE*
- 13:00 Lunch, viewing of posters and exhibition North and South Cloisters
- 14:25 Delegates move to parallel sessions

### Theme: Operations, control and process safety (Part 1 cont'd) - Gustave Tuck lecture theatre

- 14:30 Dynamic behaviour and control of thermally coupled distillation columns  
*D Dwivedi<sup>1</sup>, I J Halvorsen<sup>2</sup> and S Skogestad<sup>1</sup>*  
<sup>1</sup>*Department of Chemical Engineering, Norwegian University of Science and Technology, NOR*  
<sup>2</sup>*Applied Cybernetics, SINTEF, Trondheim, NOR*
- 14:50 Exploiting grid adaptation and structure detection in multi-objective dynamic optimisation problems  
*F Logist<sup>1,2</sup>, F Assassa<sup>1,3</sup>, J Van Impe<sup>2</sup> and W Marquardt<sup>1</sup>*  
<sup>1</sup>*AVT – Process Systems Engineering, Aachener Verfahrenstechnik, RWTH Aachen University, DEU*  
<sup>2</sup>*BioTeC & OPTEC, Department of Chemical Engineering, Katholieke Universiteit Leuven, BEL*  
<sup>3</sup>*German Research School for Simulation Sciences GmbH, DEU*
- 15:10 Dynamics of reactive distillation for the production of ethyl acetate: experiments at a pilot plant and modelling  
*M F Fernandez<sup>a,b,c,d,e</sup>, B Barroso<sup>e</sup>, X M Meyer<sup>a</sup>, M Meyer<sup>a</sup>, M V Le Lann<sup>b,c</sup>, G Le Roux<sup>d</sup> and M Brehelin<sup>e</sup>*  
<sup>a</sup>*Université de Toulouse, FRA*  
<sup>b</sup>*CNRS; LAAS; FRA*  
<sup>c</sup>*Université de Toulouse; UPS, FRA*  
<sup>d</sup>*Department of Chemical Engineering, Polytechnic School of the University of São Paulo, BRA*  
<sup>e</sup>*Rhodia Recherches & Technologies – CRTL, FRA*

### Theme: Product and process design - Chadwick lecture theatre

- 14:30 Incorporating topographical characteristics in molecular signature descriptors  
*R H Herring, N G Chemmangattuvalappil, C B Roberts and M R Eden*  
*Department of Chemical Engineering, Auburn University, US*
- 14:50 On the design of optimal solvent mixtures using generalised disjunctive programming  
*P Akula, P M Kleniati and C S Adjiman*  
*Centre for Process Systems Engineering, Imperial College London, UK*

- 15:10 Impact of fouling on flexible design and operation of MSF desalination process with variable freshwater demand  
*E A M Hawaidi and I M Mujtaba*  
*School of Engineering Design & Technology, University of Bradford, UK*

### Theme: Tools for sustainable development (Part 1 cont'd) – Jeremy Bentham room

- 14:30 Economic value and environmental impact analysis tool for sustainable biorefinery design  
*E Martinez Hernandez<sup>1</sup>, G Campbell<sup>2</sup> and J Sadhukhan<sup>3</sup>*  
*<sup>1</sup>Centre for Process Integration, University of Manchester, UK*  
*<sup>2</sup>Satake Centre for Grain Process Engineering, University of Manchester, UK*  
*<sup>3</sup>Centre for Environmental Strategy, University of Surrey, UK*
- 14:50 BIOpt: A Library of models for optimisation of biofuel production processes  
*M Martín<sup>a</sup> and I E Grossmann<sup>b</sup>*  
*<sup>a</sup>Departamento de Ingeniería Química, Universidad de Salamanca, ESP*  
*<sup>b</sup>Chemical Engineering Department, Carnegie Mellon University, US*
- 15:10 A simulated annealing algorithm for the design and planning of supply chains with economic and environmental objectives  
*N C Martins<sup>a,c</sup>, T Pinto-Varela<sup>a,b</sup> and A P Barbósa-Póvoa<sup>b</sup>*  
*<sup>a</sup>Unidade de Modelação e Optimização de Sistemas Energéticos (DMS- INETI), POR*  
*<sup>b</sup>Centro de Estudos de Gestão, Instituto Superior Técnico, Universidade Técnica de Lisboa, Av, POR*  
*<sup>c</sup>Centro de Matemática e Aplicações, POR*
- 15:30 Refreshment break, viewing of posters and exhibition North and South Cloisters
- 15:55 Delegates move to parallel sessions

### Theme: Operations, control and process safety (Part 2) - Gustave Tuck lecture theatre

- 16:00 Integrated model for refinery production and pipeline system scheduling  
*K Tong, Y Feng and G Rong*  
*Institute of Cyber-System and Control, Zhejiang University, CHN*
- 16:20 Rationalisation of alarm sensor allocation consistent with hazard scenarios  
*T Fuchino<sup>1</sup>, Y Shimada<sup>2</sup>, T Kitajima<sup>3</sup> and K Takeda<sup>4</sup>*  
*<sup>1</sup>Chemical Engineering Department, Tokyo Institute of Technology, JPN*  
*<sup>2</sup>Institute of Symbiotic Science and Technology, Tokyo University of Agriculture and Technology, JPN*  
*<sup>3</sup>Chemical Safety Research Group, National Institute of Occupational Safety and Health, JPN*  
*<sup>4</sup>Department of Materials Science and Chemical Engineering, Shizuoka University, JPN*
- 16:40 Reduction of alerts in automated systems based on a combined analysis of process connectivity and alarm logs  
*M Schlegel<sup>1,2</sup>, L Christiansen<sup>1</sup>, A Fay<sup>1</sup> and N F Thornhill<sup>2</sup>*  
*<sup>1</sup>Institut für Automatisierungstechnik, Universität der Bundeswehr, DEU*  
*<sup>2</sup>Centre for Process System Engineering (CPSE), Imperial College London, UK*
- 17:00 A generic framework for systematic design of process monitoring and control systems for crystallisation processes  
*N Afi Abdul Samad, K T Meisler, G Sin, K V Gernaey and R Gani*  
*Dept., of Chemical and Biochemical Engineering, Technical University of Denmark, DNK*
- 17:20 An advanced control solution for a fluid catalytic cracking unit: distributed model predictive control  
*M Iancu, M V Cristea and P S Agachi*  
*Chemical Engineering Department, Babes-Bolyai University, ROM*
- 17:40 Session closed
- 18:00 Close of day one

### Theme: Systems biology and healthcare engineering (Part 2) - Chadwick lecture theatre

- 16:00 A novel design of experiment technique based on multi-objective optimisation and its application for toxin kinetics model of hemodialysis patients  
*V Maheshwari<sup>1</sup>, L Samavedham<sup>1</sup>, G Pandu Rangaiah<sup>1</sup> and T Lau<sup>2</sup>*  
*<sup>1</sup>National University of Singapore, SGP*  
*<sup>2</sup>National University Hospital, SGP*

- 16:20 **Optimisation of protein a chromatography for antibody capture**  
*C Ng<sup>a</sup>, H Osuna-Sanchez<sup>c</sup>, EC Valéry<sup>c</sup>, D Bracewell<sup>a</sup> and E Sørensen<sup>b</sup>,*  
<sup>a</sup>The Advanced Centre for Biochemical Engineering, Department of Biochemical Engineering, University College London, UK  
<sup>b</sup> Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, UK  
<sup>c</sup> Novasep Process, FRA
- 16:40 **Multiscale modelling and simulation of simultaneous oxygen and nitric oxide uptake in the human lungs and its application to methemoglobin anemia**  
*T Sanyal and S Chakraborty*  
 Department of Chemical Engineering, Indian Institute of Technology, IND
- 17:00 **Thermodynamically constrained flux and control analysis of Escherichia. Coli**  
*L A Martinez, M Binns and C Theodoropoulos*  
 School of Chemical Engineering and Analytical Science, University of Manchester, UK
- 17:20 **In silico analysis to explore the effect of various carbon sources on ethanol production in zymomonas mobilis**  
*H Widiastuti<sup>1</sup>, I A Karimi<sup>1</sup> and D Y Lee<sup>1,2</sup>*  
<sup>1</sup>Dept of Chemical and Biomolecular Engineering, National University of Singapore, SGP  
<sup>2</sup>Bioprocessing Technology Institute, Agency for Science, Technology and Research, SGP
- 17:40 **Economic and environmental assessment of integrated 1st and 2nd generation sugarcane bioethanol production. Different 2nd generation process alternatives**  
*T L Junqueira<sup>ab</sup>, M O S Dias<sup>ab</sup>, O Cavalett<sup>a</sup>, C D F Jesus<sup>a</sup>, M P Cunha<sup>a</sup>, C E V Rossell<sup>ab</sup>, R M Filho<sup>ab</sup>, Antonio Bonomi<sup>ab</sup>*  
<sup>a</sup> Laboratório Nacional de Ciência e Tecnologia do Bioetanol (CTBE), BRA  
<sup>b</sup> Faculdade de Engenharia Química, Universidade Estadual de Campinas (Unicamp), BRA
- 18:00 **Close of day one**

### Theme: Tools for energy management – Jeremy Bentham room

- 16:00 **Integration of strategic and operational decision making for continuous power-intensive processes**  
*S Mitra<sup>1</sup>, I E Grossmann<sup>1</sup>, J M Pinto<sup>2</sup> and N Arora<sup>3</sup>*  
<sup>1</sup>Chemical Engineering, Carnegie Mellon University, US  
<sup>2</sup> Praxair Inc., Danbury, US  
<sup>3</sup> Praxair, Inc., Tonawanda, US
- 16:20 **Deterministic optimisation of short-term scheduling for hydroelectric power generation**  
*M G Marcovecchio<sup>a,b</sup>, A Q Novais<sup>a</sup>, R M Lim<sup>a</sup> and I E Grossmann<sup>c</sup>*  
<sup>a</sup>Unidade de Modelação e Optimização de Sistemas Energéticos, POR  
<sup>b</sup>INGAR/CONICET, Instituto de Desarrollo y Diseño, ARG  
<sup>c</sup>Chemical Engineering Department, Carnegie Mellon University, US
- 16:40 **Control strategies for flexible operation of power plant integrated with CO<sub>2</sub> capture plant**  
*Y J Lin<sup>a</sup>, D S Hill Wong<sup>a</sup> S Shang Jang<sup>a</sup> and J Jang Ou<sup>b</sup>*  
<sup>a</sup> National Tsing-Hua University, TWN  
<sup>b</sup> China Steel Corporation, TWN
- 17:00 **Carbon dioxide liquefaction process for ship transportation**  
*U Lee, S Yang, Y Lim and C Han*  
 Intelligent Process System Laboratory, Seoul National University, KOR
- 17:20 **Combining coal, natural gas and nuclear heat for liquid fuels production with reduced CO<sub>2</sub> emissions**  
*Y K Salkuyeh and T A Adams II*  
 Department of Chemical Engineering, McMaster University, CAN
- 17:40 **Effective coordination of simultaneous delivery flows into receipt terminals of multiproduct pipelines**  
*V G C, D C Cafaro, C A Méndez and J Cerdá*  
 INTEC (UNL -CONICET), ARG

## Tuesday 19 June 2012

(Please note that the programme may be subject to alteration without notice)

Time		Location
08:00	Delegate registration. Open for queries and late registrations	South cloisters
08:35	Introduction and welcome	Cruciform theatre
08:40	ESCAPE 23 presentations	Cruciform theatre
08:50	Plenary speaker <i>Prof Sir William Wakeham, IChemE past president, UK</i>	Cruciform theatre
09:35	Delegates move to parallel sessions	

### Theme: Operations, control and process safety (Part 3) - Gustave Tuck lecture theatre

- 09:40 Reliable batch-to-batch iterative learning control of a fed-batch fermentation process  
*J Jewaratnam<sup>1</sup>, J Zhang<sup>1</sup>, A Hussain<sup>2</sup> and J Morris<sup>1</sup>*  
<sup>1</sup>School of Chemical Engineering and Advanced Material, Newcastle University, UK  
<sup>2</sup>Department of Chemical Engineering, University of Malaya, Kuala Lumpur, MAY
- 10:00 Investigation in to the application of PLS in MPC schemes  
*O Onel and B Lennox*  
*School of Electrical and Electronic Engineering, University of Manchester, UK*
- 10:20 Dynamic validation of model for post-combustion chemical absorption CO<sub>2</sub> capture plant  
*C Biliyok<sup>a</sup>, A Lawal<sup>b</sup>, M Wang<sup>a</sup> and F Siebert<sup>c</sup>*  
<sup>a</sup>Process Systems Engineering Group, Cranfield University, UK  
<sup>b</sup>Parsons Brinckerhoff, UK  
<sup>c</sup>Separation Research Programme, University of Texas at Austin, US

### Theme: Product and process design (Part 2) - Chadwick lecture theatre

- 09:40 A genetic algorithm (GA)-based rational approach for design of discrete microfluidic networks  
*J Maddala, S A Vanapalli and R Rengaswamy*  
*Texas Tech University, US*
- 10:00 Model-based conceptual design and tool support for the development of continuous chemical processes  
*J Steimel and S Engell*  
*Process Dynamics and Operations Group Technische Universität Dortmund, DEU*
- 10:20 A general framework for latent variable model inversion to support product and process design  
*E Tomba<sup>1</sup>, S García-Muñoz<sup>2</sup>, P Facco<sup>1</sup>, F Bezzo<sup>1</sup> and M Barolo<sup>1</sup>*  
<sup>1</sup>CAPE-Lab, Università di Padova, ITA  
<sup>2</sup>Pfizer Worldwide R&D, US

### Theme: Tools for sustainable development (Part 2) – Jeremy Bentham room

- 09:40 Sustainable development of the hydrological basin of Lake Koronia using mathematical programming and statistical analysis  
*V Manakou<sup>1</sup>, P Tsiakis<sup>2</sup>, T Tsiakis<sup>3</sup> and A Kungolos<sup>1</sup>*  
<sup>1</sup>Department of Planning and Regional Development, University of Thessaly, GRE  
<sup>2</sup>Wipro Consulting Service, UK  
<sup>3</sup>Department of Marketing, ATEI Thessalonikis, GRE
- 10:00 Integration of single-plant water networks into an eco-industrial park  
*E Rubio-Castro<sup>1</sup>, J M Ponce-Ortega<sup>1</sup>, M Serna-González<sup>1</sup> and M M. El-Halwagi<sup>2</sup>*  
<sup>1</sup>Chemical Engineering Dept., Universidad Michocana de San Nicolás de Hidalgo, MEX  
<sup>2</sup>Chemical Engineering Dept., Texas A&M University, College Station, US
- 10:20 Optimal water network synthesis with membrane separation-based regenerators  
*C S Khor, B Chachuat and N Shah*  
*Centre for Process Systems Engineering, Imperial College London, UK*
- 10.40 Refreshment break, viewing of posters and exhibition, North and South Cloisters
- 11.05 Delegates move to parallel sessions

### Theme: Operations, control and process safety (Part 3 cont'd) - Gustave Tuck lecture theatre

- 11:10 PID control of RO desalination process  
*M M AlDhaifallah<sup>a</sup>, K M Sassi<sup>b</sup> and I M Mujtaba<sup>b</sup>*  
<sup>a</sup>King Fahd University of Petroleum and Minerals, SAU  
<sup>b</sup>School of Engineering Design & Technology, University of Bradford, UK
- 11:30 Alternative learning control of batch chemical processes based on time-varying perturbation models  
*N Sanzida and Z K Nagy*  
*Dept of Chemical Engineering, Institute of Particle Science and Engineering, Loughborough University, UK*
- 11:50 Closed-loop control of crystal shape in cooling crystallisation of L-Glutamic acid  
*C Y Ma and X Z Wang*  
*University of Leeds, UK*
- 12:10 Optimal operation of RO System with daily variation of freshwater demand and seawater temperature  
*K M Sassi and I M Mujtaba*  
*School of Engineering Design & Technology, University of Bradford, UK*

### Theme: Product and process design (Part 2 cont'd) - Chadwick lecture theatre

- 11:10 Modular design in optimisation-based process synthesis  
*A Harwardt, M Skiborowski and W Marquardt*  
*AVT - Process Systems Engineering, RWTH Aachen University, DEU*
- 11:30 Thermally-coupled reactive distillation systems with minimum number of reboilers: Optimisation using differential evolution  
*M Vázquez-Ojeda<sup>a</sup>, J G Segovia-Hernández<sup>a</sup>, S Hernández<sup>a</sup>, A Hernández-Aguirre<sup>b</sup> and R Maya-Yescas<sup>c</sup>*  
<sup>a</sup>Universidad de Guanajuato, MEX  
<sup>b</sup>CIMAT, A.C., MEX  
<sup>c</sup>Universidad Michoacana de San Nicolás Hidalgo, MEX
- 11:50 Innovative biodiesel production in reactive dividing-wall columns  
*A A Kiss<sup>1</sup>, J G Segovia-Hernández<sup>2</sup>, E Y Miranda-Galindo<sup>2</sup> and S Hernández<sup>2</sup>*  
<sup>1</sup>AkzoNobel Research, Development & Innovation, Process Technology ECG, NL  
<sup>2</sup>Universidad de Guanajuato, Campus Guanajuato, MEX

### Theme: Tools for sustainable development (Part 2 cont'd) – Jeremy Bentham room

- 11:10 Environomic optimal design and synthesis of energy conversion systems in urban areas  
*L Gerber, S Fazlollahi and F Maréchal*  
*Ecole Polytechnique Fédérale de Lausanne, SUI*
- 11:30 Towards defining a quantitative methodology to enhance the sustainability performance of major international events  
*O Parkes, D Bogle, P Lettieri*  
*University College London, UK*
- 11:50 Design of an IRCC with CO<sub>2</sub> capture utilising a mixed integer optimisation method  
*R Anantharaman<sup>1</sup>, E L Johnsen<sup>2</sup>, B Nygreen<sup>2</sup> and T Gundersen<sup>3</sup>*  
<sup>1</sup>SINTEF Energy Research, NOR  
<sup>2</sup>Department of Industrial Economics, NTNU, NOR  
<sup>3</sup>Department of Energy and Process Engineering, NTNU, NOR
- 12:10 Multi-period least cost optimisation model of an integrated CO<sub>2</sub> capture, transportation and storage infrastructure for the UK  
*N Elahi, N Shah and A Korre*  
*Imperial College London, UK*
- 12.30 Lunch, viewing of posters and exhibiton, North and South Cloisters
- 13.55 Delegates move to parallel sessions

### Theme: Tools for financial business and management decision making (Part 1) - Gustave Tuck lecture theatre

- 14:00 **Planperfect: An integrated production planning and decision support tool for pharmaceutical plants**  
*N Susarla and I A Karimi*  
*National University of Singapore, SGP*
- 14:20 **Risk pooling strategy in pharmaceutical for clinical trial supply chain**  
*Y Chen, J M Láinez, J F Pekny and G V Reklaitis*  
*School of Chemical Engineering, Purdue University, US*
- 14:40 **Production planning of batch and semi-continuous bioprocesses across multiple biopharmaceutical facilities**  
*C Siganporia<sup>a</sup>, S Ghosh<sup>b</sup>, T Daszkowski<sup>b</sup>, L Papageorgiou<sup>c</sup> and S S Farid<sup>a</sup>*  
*<sup>a</sup>The Advanced Centre for Biochemical Engineering, University College London, UK*  
*<sup>b</sup>Bayer Technology Services, US*  
*<sup>c</sup>Department of Chemical Engineering, University College London, UK*
- 15:00 **Integrated scheduling and control of continuous multi-product plants with product-dependent processing sequences**  
*K Frankl, J Brenner and W Marquardt*  
*RWTH Aachen University, DEU*

### Theme: CAPE in education (sponsored by EURECHA) - Chadwick lecture theatre

- 14:20 **Virtual and augmented reality as tools to train industrial operators**  
*S Nazir, R Totaro, S Brambilla, S Colombo and D Manca*  
*Dipartimento di Chimica, ITA*
- 14:40 **Use of distributed simulation environment for supply chain decision making training**  
*J Silvente, M Á Zamarripa and A Espuña.*  
*Chemical Engineering Department, Universitat Politècnica de Catalunya (UPC), ESP*
- 15:00 **Bridging the experience gap – How do we migrate skills and knowledge between the generations?**  
*R Calder, P Richmond and I Willets*  
*Invensys Operations Management, UK*
- 15:20 **Session closed**

### Theme: Tools for sustainable development (Part 3) – Jeremy Bentham room

- 14:00 **Integrated assessment of carbon capture and storage technologies in coal-based power generation using CAPE tools**  
*C C Cormos and P S Agachi*  
*Babes-Bolyai University, ROU*
- 14:20 **Sustainability analysis of a reactive distillation process**  
*E Zondervan<sup>a</sup>, A D Bojarski<sup>b</sup>, A B. de Haan<sup>a</sup>, A Espuña<sup>b</sup> and L Puigjaner<sup>b</sup>*  
*<sup>a</sup>Dept of Chemistry and Chemical Engineering, Eindhoven University of Technology, NL*  
*<sup>b</sup>Chemical Engineering Department, Universitat Politècnica de Catalunya, ESP*
- 14:40 **Multi-level design and selection of optimum working fluids and ORC systems for power and heat cogeneration from low enthalpy renewable sources**  
*A I Papadopoulos<sup>1</sup>, M Stijepovic<sup>2</sup>, P Linke<sup>2</sup>, P Seferlis<sup>3</sup> and S Voutetakis<sup>1</sup>*  
*<sup>1</sup>Chemical Process Engineering Research Institute, GRE*  
*<sup>2</sup>Chemical Engineering Department, Texas A&M University at Qatar, QTR*  
*<sup>3</sup>Department of Mechanical Engineering, Aristotle University of Thessaloniki, GRE*
- 15:00 **Choosing the suitable carbon dioxide storage location in sedimentary basins of Korea**  
*U Zahid<sup>1</sup>, Y Lim<sup>1</sup> and C Han<sup>1</sup>*  
*<sup>1</sup>School of Chemical and Biological Engineering, Seoul National University, KOR*
- 15.20 **Refreshment break, viewing of posters and exhibition, North and South cloisters**
- 15.45 **Delegates move to parallel sessions**

### Theme: Product and process design (Part 3) - Gustave Tuck lecture theatre

- 15:50 Keynote speaker: Prof Xavier Joulia, ENSIACET, FRA
- 16:15 Separation of binary mixture using pressure swing distillation with heat integration  
*T Yamaki<sup>1</sup>, K Matsuda<sup>1</sup>, K Huang<sup>2</sup>, H Matsumoto<sup>3</sup> and M Nakaiwa<sup>4</sup>*  
<sup>1</sup>Department of Chemistry and Chemical Engineering, Yamagata University, JPN  
<sup>2</sup>School of Information Science and Technology, Beijing University of Chemical Technology, CHN  
<sup>3</sup>Department of Chemical Engineering, Tokyo Institute of Technology, JPN  
<sup>4</sup>AIST Tsukuba, National Institute of Advanced Industrial Science and Technology (AIST), JPN
- 16:35 Batch heteroazeotropic distillation with variable decanter hold-up: Feasibility studies  
*L Hégyel<sup>a,b,c</sup>, V Gerbaud<sup>b,c</sup> and P Láng<sup>a</sup>*  
<sup>a</sup>Budapest University of Technology and Economics, HUN  
<sup>b</sup>Université de Toulouse, FRA  
<sup>c</sup>CNRS, LGC (Laboratoire de Génie Chimique), FRA
- 16:55 Model based experimental design and parameter estimation for the mechanistic modelling of an industrial hydrophobic interaction chromatography step  
*E Close<sup>a,b</sup>, J Salm<sup>c</sup>, E Sørensen<sup>a</sup> and D Bracewell<sup>b</sup>*  
<sup>a</sup>Centre for Process Systems Engineering, University College London, UK  
<sup>b</sup>The Advanced Centre for Biochemical Engineering, University College London, UK  
<sup>c</sup>Pfizer Biopharmaceuticals, US
- 17:15 Dynamic modelling of margarine manufacturing  
*P Bongers and C Almeida*  
Unilever R&D Vlaardingen, NL
- 17:35 Removal and recovery of organic solvents from wastewater by distillation  
*G Modla and P Lang*  
Budapest University of Technology and Economics, Department of Building Services and Process Engineering, HUN
- 17:55 Close of day two

### Theme: Multi-scale modelling and simulation (Part 1) - Chadwick lecture theatre

- 15:50 Keynote speaker: Prof Hans Kuipers, University of Eindhoven, NL
- 16:15 Estimation of catalyst deactivation parameters of ethyl tert-butyl ether (ETBE) reactors based on industrial plant data  
*L Domingues<sup>a</sup>, C C Pinheiro<sup>a\*</sup>, N C Oliveira<sup>b</sup>, A Vilelas<sup>c</sup>, J Fernandes<sup>c</sup> and F Ribeiro<sup>a</sup>*  
<sup>a</sup>IBB – Instituto Superior Técnico/UTL, POR  
<sup>b</sup>GEPSI – PSE Group, University of Coimbra, POR  
<sup>c</sup>Repsol, POR
- 16:35 Reactor network analysis of claus furnace with detailed kinetics  
*F Manenti, A Cuoci, A Frassoldati, T Faravelli, S Pierucci, E Ranzi and G Buzzi-Ferraris*  
Politecnico di Milano, ITA
- 16:55 Multiscale modelling of spillover processes in heterogeneous catalytic systems  
*I S Fragkopoulos, I Bonis and C Theodoropoulos*  
School of Chemical Engineering and Analytical Science, University of Manchester, UK
- 17:15 A stochastic approach to improve the particle size distribution prediction of a classical emulsion polymerisation model  
*A Hosseini, A Eldin Bouaswaig and S Engell*  
Process Dynamics and Operations Group, Technische Universität Dortmund, DEU
- 17:35 Multi-scale simulation for high efficiency biodiesel production process intensification  
*J Sadhukhan*  
University of Surrey, UK
- 17:55 Close of day two



**Theme: Computational and numerical solution strategies (Part 1) – Jeremy Bentham  
room**

- 15:50 **Keynote speaker:** Peter Bongers, Unilever R&D, Vlaardingen, NL
- 16:15 **A new theoretical result for convex nonlinear generalised disjunctive programs and its applications**  
*J Pablo Ruiz and I E Grossmann*  
*Carnegie Mellon University, US*
- 16:35 **A generalisation of classical  $\alpha$ BB underestimation to include bilinear terms**  
*A Skjäl and T Westerlund*  
*Abo Akademi University, FIN*
- 16:55 **An index reduction method for solving differential algebraic equations**  
*K Alloula<sup>1</sup>, F Monfreda<sup>2</sup>, J P Belaud<sup>1</sup>, J C Yakoubsohn<sup>2</sup> and J M Le Lann<sup>1</sup>*  
*<sup>1</sup>Laboratoire de Génie Chimique (CNRS UMR 5503), INPT-ENSIACET, FRA*  
*<sup>2</sup>Institut de Mathématiques de Toulouse (CNRS UMR 5219), Université Paul, FRA*
- 17:15 **Linear MPC based on data-driven artificial neural networks for large scale nonlinear distributed parameter systems**  
*W Xie, I Bonis and C Theodoropoulos*  
*University of Manchester, UK*
- 17:35 **Surrogate based optimisation for design of pressure swing adsorption systems**  
*J Beck<sup>1</sup>, D Friedrich<sup>2</sup>, S Guillas<sup>3</sup>, S Brandani<sup>4</sup> and E S Fragay<sup>5</sup>*  
*<sup>1</sup>Centre for Process Systems Engineering, University College London, UK*  
*<sup>2</sup>Institute for Materials and Processes, Edinburgh University, UK*  
*<sup>3</sup>Department of Statistical Science, University College London, UK*  
*<sup>4</sup>Institute for Materials and Processes, Edinburgh University, UK*  
*<sup>5</sup>Centre for Process Systems Engineering, University College London, UK*
- 17:55 **Close of day two**
- 19.00 **Conference gala dinner (ticket only)**



## Wednesday 20 June 2012

(Please note that the programme may be subject to alteration without notice)

Time		Location
08:00	Delegate registration. Open for queries and late registrations	South cloisters
08:45	Plenary speaker	Cruciform theatre
09:35	Delegates move to parallel sessions	

### Theme: Tools for energy management (Part 2) - Gustave Tuck lecture theatre

- 09:40 Hydrogen production through steam electrolysis: A model-based study  
*Q Cai<sup>1</sup>, C S J Adjiman<sup>2</sup> and N P Brandon<sup>1</sup>*  
<sup>1</sup>Department of Earth Science and Engineering, Imperial College London, UK  
<sup>2</sup>Department of Chemical Engineering, Imperial College London, UK
- 10:00 Multi-objectives, multi-period optimisation of district heating networks using evolutionary algorithms and mixed integer linear programming (MILP)  
*S Fazlollahi<sup>1,2</sup> and F Marechal<sup>2</sup>*  
<sup>1</sup>Veolia Environnement Recherche et Innovation, FRA  
<sup>2</sup>Ecole Polytechnique federale de Lausanne, SUI
- 10:20 Targeting energy generation and carbon footprint for waste management and processing  
*P S Varbanov<sup>1</sup>, L U Ek<sup>1</sup>, J J Klemeš<sup>1</sup> and Z Kravanja<sup>2</sup>*  
<sup>1</sup>Centre for Process Integration and Intensification – CP2, University of Pannonia, HUN  
<sup>2</sup>Faculty of Chemistry and Chemical Engineering, University of Maribor, SVN
- 10:40 Selection of heat pump technologies for energy efficient distillation  
*A A Kiss<sup>1</sup> and S J Flores Landaeta<sup>1,2</sup>*  
<sup>1</sup>AkzoNobel Research, Development & Innovation, NL  
<sup>2</sup>Eindhoven University of Technology (TU/e), NL

### Theme: Multi-scale modelling and simulation (Part 2) - Chadwick lecture theatre

- 09:40 Simulation and analysis of crystallisation of high aspect ratio crystals with fragmentation  
*Á Borsos and B G Lakatos*  
 University of Pannonia, HUN
- 10:00 Modelling of cold traps for sodium purification in fast reactor  
*N Khatcherssian<sup>ab</sup>, C Latgé<sup>a</sup>, X Joulia<sup>b</sup>, T Gilardi<sup>a</sup> and X Meyer<sup>b</sup>*  
<sup>a</sup>CEA, DEN, Cadarache DTN/STPA/LIPC, FRA  
<sup>b</sup>Université de Toulouse-CNRS, FRA
- 10:20 HAZOP studies using a functional modelling framework  
*J L de la Mata and M Rodríguez*  
 Universidad Politécnica de Madrid, ESP
- 10:40 An online inverse problem for the simulation of extraction columns using population balances  
*H B Jildeh<sup>ab</sup>, M Attarakih<sup>ac</sup>, M Mickler<sup>ab</sup> and H J Barta<sup>b</sup>*  
<sup>a</sup>Chair of Separation Science and Technology, TU Kaiserslautern, DEU  
<sup>b</sup>Centre of Mathematical and Computational Modelling, TU Kaiserslautern, DEU  
<sup>c</sup>The University of Jordan, JOR

### Theme: Product and process design (Part 4) – Jeremy Bentham room

- 09:40 Using CAPE to develop a cost-effective process for converting natural gas into single cell protein  
*Q Shah, B Aufderheide and A M Al Taweel*  
 Process Engineering Programme of The University of Trinidad and Tobago, TTO
- 10:00 Multiobjective optimisation of membrane processes for chemicals ultrapurification  
*R Abejón, A Garea and A Irabien*  
 Dept. de Ingeniería Química y Química Inorgánica, Universidad de Cantabria, ESP
- 10:20 Economic and environmental evaluation of biodiesel production using process simulation and optimisation tools  
*R Brunet, D Carrasco, E Muñoz, G Guillén-Gosálbez, I Katakis and L Jiménez*  
 Universitat Rovira i Virgili, ESP

- 10:40 Optimal dynamic controllability in compressed-aided distillation schemes distillation using stochastic algorithms  
*J Cabrera-Ruiz<sup>a</sup>, J G Segovia-Hernández<sup>a</sup>, J R Alcántara-Ávila<sup>b</sup> and S Hernández<sup>a</sup>*  
<sup>a</sup>Universidad de Guanajuato, MEX  
<sup>b</sup>Kyoto University, JPN
- 11.00 Refreshment break, viewing of posters and exhibition, North and South Cloisters
- 11.20 Delegates move to parallel sessions

### Theme: Computation and numerical solution strategies (Part 2) - Gustave Tuck lecture theatre

- 11:25 Wavelet thresholding in optimal control problems  
*L S Santosa, A R Secchia and E C Biscaia Jr*  
*Universidade Federal do Rio de Janeiro, BRA*
- 11:45 Intelligent automation platform for bioprocess development  
*T Wu and Y Zhou*  
*University College London, UK*
- 12:05 SKU decomposition algorithms for the tactical planning in the fast moving consumer goods industry  
*M A H van Elzakker<sup>a</sup>, E Zondervan<sup>a</sup>, N B Raikar<sup>b</sup>, I E Grossmann<sup>c</sup> and P M M Bongers<sup>abd</sup>*  
<sup>a</sup>Department of Chemistry and Chemical Engineering, Eindhoven University of Technology, NL  
<sup>b</sup>Unilever R&D Vlaardingen, NL  
<sup>c</sup>Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, US  
<sup>d</sup>Hoogewerff Chair for Product-Driven Process Technology, Eindhoven University of Technology, NL
- 12:25 Efficient optimisation of simulated moving bed chromatographic processes using reduced order models  
*S Li<sup>a</sup>, L Feng<sup>a</sup>, P Benner<sup>ab</sup> and A Seidel-Morgenstern<sup>c</sup>*  
<sup>a</sup>Max-Planck-Institut für Dynamik of komplexer technischer Systeme, DEU  
<sup>b</sup>Fakultät für Mathematik, Technische Universität Chemnitz, DEU

### Theme: Tools for financial business and management decision making (Part 2) - Chadwick lecture theatre

- 11:25 Biopharmaceutical portfolio management optimisation under uncertainty  
*W Nie, Y Zhou, A S Simaria and S S Farid*  
*University College London, UK*
- 11:45 Operational and strategic alignment in the decision process of molecule substitution  
*J Heintz<sup>b</sup>, V Gerbauda<sup>b</sup> and J-P Belauda<sup>b</sup>*  
<sup>a</sup>Université de Toulouse, FRA  
<sup>b</sup>CNRS, LGC (Laboratoire de Génie Chimique), FRA
- 12:05 Transportation planning of oil products: an application of multi-agents auction-based protocol with improvements in the bidding strategy  
*RF Banaszewski<sup>a</sup>, K E Nogueira<sup>a</sup>, L V Arruda<sup>a</sup>, J M Simão<sup>a</sup>, C A Tacla<sup>a</sup>, S Relvas<sup>b</sup> and A P Barbosa-Póvoa<sup>b</sup>*  
<sup>a</sup>C PGEI-UTFPR, Universidade Tecnológica Federal do Paraná, BRA  
<sup>b</sup>CEG-IST, Instituto Superior Técnico, Universidade Técnica de Lisboa, POR
- 12:25 Network structure and logistics efficiency: a new approach to analyse supply chain system  
*S Liu, C Li, Y Feng and G Rong*  
*Department of Control Science and Engineering, Zhejiang University, CHN*

### Theme: Product and process design (Part 4 cont'd) – Jeremy Bentham room

- 11:25 A new graphical exergy targeting representation for processes operating above and below ambient temperature  
*D M Correa and T Gundersen*  
*Norwegian University of Science and Technology NTNU, NOR*

- 11:45 **Process design optimisation strategy to develop energy and cost correlations of CO<sub>2</sub> capture processes**  
*L Tock and F Maréchal*  
*Industrial Energy Systems Laboratory, SUI*
- 12:05 **Novel MILP-based optimisation method for retrofitting heat exchanger networks**  
*M Pan, I Bulatov and R Smith*  
*Centre for Process Integration, School of Chemical Engineering and Analytical Science, University of Manchester, UK*
- 12:25 **Simultaneous process and working fluid optimisation for organic rankine cycles (ORC) using PCP-SAFT**  
*M Lampe<sup>a</sup>, J Groß<sup>b</sup> and A Bardow<sup>a</sup>*  
<sup>a</sup>*Institute of Technical Thermodynamics, RWTH Aachen University, DEU*  
<sup>b</sup>*Institute of Thermodynamics and Thermal Process Engineering, Universität Stuttgart, DEU*
- 12:45 **Lunch, viewing of posters and exhibiton, South and North Cloisters**
- 13:35 **Delegates move to parallel sessions**

### Theme: Operations, control and process safety (Part 4) - Gustave Tuck lecture theatre

- 13:40 **A stop-and-restart approach to hybrid dynamic optimisation problems**  
*I Mynttinen and P Li*  
*Ilmenau University of Technology, DEU*
- 14:00 **Parameter accuracy vs decorrelation in optimal experiment design: a multi-objective point of view**  
*D Telen, F Logist, E Van Derlinden and J F Van Impe*  
*BioTeC & OPTeC - Chemical Engineering Dept., Katholieke Universiteit Leuven, BEL*
- 14:20 **Analysing the effects of uncertainties on the economic performance of a chemical process plant using a probabilistic optimisation technique**  
*M Getu<sup>a</sup>, S Mahadzir<sup>b</sup> and M Lee<sup>c</sup>*  
<sup>a</sup>*Chemical Engineering Dept., Curtin University of Technology, MAL*  
<sup>b</sup>*Chemical Engineering Department, Universiti Teknologi PETRONAS, MAL*  
<sup>c</sup>*School of Chemical Engineering, Yeungnam University, KOR*
- 14:40 **Oil well drilling inside operational window – simulation and experimental control studies**  
*M P Vega<sup>a</sup>, M G Freitas<sup>a</sup>, N Ferreir<sup>a</sup>, de Araújo<sup>a</sup>, C M Scheid<sup>a</sup> and A L Martins<sup>b</sup>*  
<sup>a</sup>*DEQ - UFRRJ, BRA*  
<sup>b</sup>*PETROBRAS S.A./CENPES, BRA*
- 15:00 **Operational optimisation of low-temperature energy systems**  
*M M Morantes, M Jobson and N Zhang*  
*Centre for Process Integration, School of Chemical Engineering and Analytical Science, University of Manchester, UK*
- 15:20 **Improving dryer controllability and energy efficiency**  
*J C Atuonwu<sup>a</sup>, G van Straten<sup>a</sup>, H C van Deventer<sup>b</sup> and A J B van Boxtel<sup>a</sup>*  
<sup>a</sup>*Systems and Control Group, Wageningen University, NL*  
<sup>b</sup>*TNO, NL*

### Theme: Tools for financial business and management decision making (Part 3) - Chadwick lecture theatre

- 13:40 **Operational, tactical and strategic integration for enterprise decision-making**  
*E Muñoz<sup>a</sup>, E Capón<sup>a</sup>, J M Laínez<sup>b</sup>, M Moreno-Benito<sup>a</sup>, A Espuña<sup>a</sup> and L Puigjaner<sup>a</sup>*  
<sup>a</sup>*Department of Chemical Engineering, Universitat Politècnica de Catalunya, ESP*  
<sup>b</sup>*School of Chemical Engineering, Purdue University, US*
- 14:00 **Integration of mathematical programming and game theory optimisation in multi-objective competitive scenarios**  
*M Zamarripa<sup>a</sup>, A Aguirre<sup>b</sup>, C Méndez<sup>b</sup> and A Espuña<sup>a</sup>*  
<sup>a</sup>*Universitat Politècnica de Catalunya (UPC), Chem. Eng. Dept. ESP*  
<sup>b</sup>*INTEC (UNL-CONICET), ARG*

- 14:20 Optimum design and planning of resilient and uncertain closed-loop supply chains  
*L J Zeballos<sup>a,b</sup>, M I Gomes<sup>c</sup>, A P Barbosa-Povoa<sup>d</sup> and A Q Novais<sup>a</sup>*  
<sup>a</sup>UMOSE Laboratório Nacional de Energia e Geologia, Lisboa, POR  
<sup>b</sup>Universidad Nacional del Litoral – Fac. de Ingeniería Química, ARG  
<sup>c</sup>CMA, FCT, Universidade Nova de Lisboa, Monte de Caparica, POR  
<sup>d</sup>Centre for Management Studies, Instituto Superior Técnico, POR
- 14:40 A two-stage stochastic model for the design and planning of a multi-product closed loop supply chain  
*S Baptista<sup>a</sup>, M Isabel Gomes<sup>a</sup> and A P Barbosa-Povoa<sup>b</sup>*  
<sup>a</sup>Centro de Matemática e Aplicações, FCT, Universidade Nova de Lisboa, POR  
<sup>b</sup>CEG, IST-UTL, POR
- 15:00 Towards integrated production and distribution management  
*M E Cocco<sup>a</sup>, C A Méndez<sup>a</sup>, M Zamarripa<sup>b</sup> and A España<sup>b</sup>*  
<sup>a</sup>INTEC (UNL-CONICET), ARG  
<sup>b</sup>Chemical Engineering Department, Universitat Politècnica de Catalunya (UPC), ESP
- 15:20 Session closed

### Theme: Computation and numerical solution strategies (Part 2) – Jeremy Bentham room

- 13:40 Dual stochastic programming for data mining enhancement  
*A Ferrari<sup>1</sup>, S Gutierrez<sup>1</sup> and E C Biscaia Jr.<sup>2</sup>*  
<sup>1</sup>GISQyP – Chemical & Process Systems Engineering Group – IIQ – Universidad de la Republica, URY  
<sup>2</sup>LMSCP/PEQ/COPPE/UFRJ, BRA
- 14:00 Ontology approach to model construction  
*H Preisig and T Haug-Warberg*  
Norwegian University of Science and Technology, NOR
- 14:20 Effect of topology on parallel computing for optimising large scale logistics through binary PSO  
*Y Shimizu and T Miura*  
Dept of Mechanical Engineering, Toyohashi University of Technology, JPN
- 14:40 On the constrained maximum entropy solution of the population balance equation  
*M Attarakih<sup>a,b</sup> and H-J Bart<sup>b,c</sup>*  
<sup>a</sup>The University of Jordan, JOR  
<sup>b</sup>Chair of Separation Science and Technology, TU Kaiserslautern, DEU  
<sup>c</sup>Centre of Mathematical and Computational Modelling, TU Kaiserslautern, DEU
- 15:00 Deterministic global optimisation algorithm based on outer approximation for the parameter estimation of nonlinear dynamic biological systems  
*A Miró<sup>a</sup>, C Poz<sup>a</sup>, G Guillén-Gosálbez<sup>a</sup>, J A Egea<sup>b</sup> and L Jiménez<sup>a</sup>*  
<sup>a</sup>Departament d'Enginyeria Química, Universitat Rovira i Virgili, ESP  
<sup>b</sup>Departamento de Matemática Aplicada y Estadística, Universidad Politécnica de Cartagena, ESP
- 15:20 An approach to process monitoring under probabilistic constraints  
*S Werk<sup>a,b</sup>, T Barz<sup>a</sup>, G Wozny<sup>a</sup> and H Arellano-García<sup>a</sup>*  
<sup>a</sup>Berlin Institute of Technology, Chair of Process Dynamics and Operation, DEU  
<sup>b</sup>Berlin Institute of Technology, DEU
- 15.40 Delegates move to Cruciform lecture theatre
- 15.45 Awards, closing formalities
- 16.15 Close of conference

# Poster presentations

(Please note that the programme may be subject to alteration without notice)

## Theme: Tools for sustainable development

**Computer aided estimation of fugitive emission rates and occupational air concentration in process design**

*H M Ha, M Hurme<sup>b</sup> and N N N A Aziz<sup>a</sup>*

<sup>a</sup>*Universiti Teknologi Malaysia, Dept. Chemical Engineering, MAY*

<sup>b</sup>*Aalto University, School of Chemical Tech., FIN*

**Integrated tool for simulation and optimisation of a first and second generation ethanol-from-sugarcane production plant**

*F F Furlan<sup>a</sup>, C B B Costa<sup>a</sup>, A J G Cruz<sup>a</sup>, A R Secchi<sup>b</sup>, R P Soares<sup>c</sup> and R C Giordano<sup>a</sup>*

<sup>a</sup>*Department of Chemical Engineering, Federal University of São Carlos, BRA*

<sup>b</sup>*Chemical Engineering Program, COPPE, Federal University of Rio de Janeiro, BRA*

<sup>c</sup>*Department of Chemical Engineering, Federal University of Rio Grande do Sul, BRA*

**Computer aided evaluation of eco-efficiency of solvent-based algae oil extraction processes for biodiesel production**

*Y Pardo, Y Peralta, A Gonzalez and V Kafarov*

*Universidad Industrial de Santander, COL*

**Reliable and efficient targeting for optimal design of SWRO desalination processes**

*S Y Alnouri and P Linke*

*Department of Chemical Engineering, Texas A&M University at Qatar, QAT*

**A two-step optimisation approach for integrated water resources management**

*S Liu<sup>a</sup>, P Gikas<sup>b</sup> and L G Papageorgiou<sup>a</sup>*

<sup>a</sup>*Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, UK*

<sup>b</sup>*Department of Environmental Engineering, Technical University of Crete, GRE*

**Life cycle assessment and optimisation on the production of petrochemicals and energy from polymers for the Greater London Area**

*S M Al-Salema<sup>b</sup>, E Mechleri<sup>c</sup>, L G Papageorgiou<sup>c</sup> and P Lettieri<sup>a</sup>*

<sup>a</sup>*Department of Chemical Engineering, University College London, UK*

<sup>b</sup>*Petrochemical Processes Program Element, Petroleum Research and Studies Centre, KWT*

<sup>c</sup>*Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, UK*

**Comparative study of simulations and experimental results of biodiesel production using two types of reactive distillation columns**

*N L Da Silva, E L Martinez, L F Rios, T S S Dantas, M R Wolf Maciel and R Maciel Filho*

*School of Chemical Engineering, State University of Campinas (UNICAMP), BRA*

**Integrating economic and environmental aspects in the design and planning of supply chains: Two alternative methodologies**

*T Pinto-Varela<sup>a,b</sup>, F Martins<sup>c</sup> and A Barbosa-Povo<sup>a,b</sup>*

<sup>a</sup>*UMOSE/LNEG, POR*

<sup>b</sup>*CEG-IST Instituto Superior Técnico, Universidade Técnica de Lisboa, POR*

<sup>c</sup>*REQIMTE/ISEP, POR*

**Multi-objective optimisation of a membrane distillation system for desalination of sea water**

*S Sharma and G P Rangaiah*

*Department of Chemical & Biomolecular Engineering National University of Singapore, SGP*

**Development of a dynamic material flow analysis model for french copper cycle**

*M Bonnin<sup>a</sup>, C Azzaro-Pantel<sup>a</sup>, L Pibouleau<sup>a</sup>, S Domenech<sup>a</sup> and J Villeneuve<sup>b</sup>*

<sup>a</sup>*Laboratoire de Génie Chimique, FRA*

<sup>b</sup>*Bureau de Recherche Géologique et Minière, FRA*

**Incorporating CO<sub>2</sub> emission trading in the optimal design and planning of chemical supply chain networks under uncertainty**

*R Ruiz-Femenia<sup>a</sup>, R Salcedo-Díaz<sup>a</sup>, G Guillén-Gosálbez<sup>b</sup>, J A Caballero<sup>a</sup> and L Jiménez<sup>b</sup>*

<sup>a</sup>*Department of Chemical Engineering, University of Alicante, ESP*

<sup>b</sup>*Departament d'Enginyeria Química, Universitat Rovira i Virgili, ESP*

**Comparative techno-economic analysis of biodiesel production from microalgae via transesterification methods**

*B Z Bello, E Nwokoagbara and M Wang*

*Process Systems Engineering Group, School of Engineering, Cranfield University, UK*

**Optimisation of hybrid anaerobic-aerobic SBR-based systems**

*M Fuentes, N J Scenna and P A Aguirre*

*INGAR (CONICET-UTN), ARG*

**An integrated approach combining process simulation and life cycle assessment for ecoefficient process design**

*L F Morales-Mendoza, C Azzaro-Pantel, J-P Belaud, L Pibouleau and S Domenecha*

*Université de Toulouse, Laboratoire de Génie Chimique, FRA*

**Product and mixture design in latent variable space by chemometric techniques**

*S Hada<sup>a</sup>, N G Chemmangattuvalappil<sup>a,b</sup>, C B Roberts<sup>a</sup>, and M R Eden<sup>a</sup>*

*<sup>a</sup>Department of Chemical Engineering, Auburn University, US*

*<sup>b</sup>Department of Chemical and Environmental Eng., University of Nottingham, MAL*

**A bayesian network based approach for risk modeling to aid in development of sustainable biomass supply chains**

*J Amundson<sup>ab</sup>, W Faulkner<sup>b</sup>, S Sukumara<sup>c</sup>, J Seay<sup>c</sup> and F Badurdeen<sup>d</sup>*

*<sup>a</sup>Institute for Sustainable Manufacturing, Univ. of Kentucky, US*

*<sup>b</sup>Manufacturing Systems Engineering, Univ. of Kentucky, US*

*<sup>c</sup>Dept. of Chem. and Mat'ls Engineering, Univ. of Kentucky, US*

*<sup>d</sup>Dept. of Mechanical Engineering, Univ. of Kentucky, US*

**Multidisciplinary approach in developing region specific optimisation tool for sustainable biorefining**

*S Sukumara<sup>a</sup>, J Amundson<sup>b</sup>, W Faulkner<sup>b</sup>, F Badurdeen<sup>b,c</sup> and J Seay<sup>a</sup>*

*<sup>a</sup>Dept. of Chem and MSc Eng, University of Kentucky, US*

*<sup>b</sup>Institute for Sustainable Mfg, University of Kentucky, US*

*<sup>c</sup>Dept. of Mechanical Engineering, University of Kentucky, US*

**Automated environmental evaluation for the optimization of chemical processes**

*C M Torres, M Gadalla, J M Mateo-Sanz and Laureano Jiménez*

*Department of Chemical Engineering, Universtat Rovira i Virgili. ESP*

**Semantic formalism for waste and processing technology classifications using ontology models 1**

*N Trokanas<sup>a</sup>, T Raafat, F Cecelja<sup>a</sup>, A Kokossis<sup>b</sup>, and A Yang<sup>a</sup>*

*<sup>a</sup>PRISE, FEPS, University of Surrey, UK*

*<sup>b</sup>School of Engineering, National Technical University of Athens, GRE*

**Evaluation of different cogeneration systems in first and second generation ethanol production from sugarcane**

*M O S Dias<sup>a,b</sup>, T L Junqueira<sup>a,b</sup>, O Cavalett<sup>a</sup>, M P Cunha<sup>a</sup>, C D F Jesus<sup>a</sup>, P E Mantelatto<sup>a</sup>, C E V Rossell<sup>a,b</sup>, R Maciel Filho<sup>a,b</sup> and A Bonomi<sup>a,b</sup>*

*<sup>a</sup>Laboratório Nacional de Ciência e Tecnologia do Bioetanol (CTBE), BRA*

*<sup>b</sup>Faculdade de Engenharia Química, Universidade Estadual de Campinas (Unicamp),BRA*

**Economic and environmental assessment of integrated 1st and 2nd generation sugarcane bioethanol production evaluating different 2nd generation process alternatives**

*T L Junqueira<sup>ab</sup>, M OS Dias<sup>ab</sup>, O Cavalett<sup>a</sup>, C D F Jesus<sup>a</sup>, M P Cunha<sup>a</sup>, C E V Rossell<sup>ab</sup>, R M Filho<sup>ab</sup> and A Bonomi<sup>ab</sup>*

*<sup>a</sup>Laboratório Nacional de Ciência e Tecnologia do Bioetanol (CTBE), BRA*

*<sup>b</sup>Faculdade de Engenharia Química, Universidade Estadual de Campinas (Unicamp), BRA*

**Integrated modeling of sugarcane cultivation and ethanol fermentation from agriculture and engineering perspectives**

*Y Kikuchi<sup>a</sup>, R Suginobe<sup>a</sup>, Y Kanzaki<sup>a</sup>, S Ohara<sup>b</sup>, and M Hirao<sup>a</sup>*

*<sup>a</sup>Depart. of Chemical System Engineering, The University of Tokyo, JPN*

*<sup>b</sup>Asahi Group Holdings, Ltd., JPN*

**Evaluation of CO<sub>2</sub> capture process and operational challenges by dynamic simulation**

*A M Cormos, J Gaspar and P S Agachi*

*Babes – Bolyai University, Faculty of Chemistry and Chemical Engineering, ROM*

**An agent-based model for analyzing diffusion of biodiesel production schemes**

*R Yasuda and R Batres*

*Toyohashi Tech, JPN*



**Integration of process synthesis and location-transportation for the design of biomass conversion systems**

*T Miyazaki<sup>a</sup>, J Sugiura<sup>b</sup>, T Nagatomi<sup>c</sup>, and R Batres<sup>d</sup>*

<sup>a</sup> Corporate Manufacturing Engineering Center, Toshiba, JPN

<sup>b</sup> Fuji Xerox, JPN

<sup>c</sup> Hitachi, JPN

<sup>d</sup> Toyohashi Tech, JPN

**Identifying redundant environmental objectives in the design of heat-exchanger networks using rigorous dimensionality reduction techniques.**

*P Vaskan, G Guillén-Gosálbez and L Jiménez*

*Department of Chemical Engineering, University Rovira i Virgili ESP*

**Comparison of technology alternative for palm oil biodiesel production using exergy analysis**

*W Jaimes, P Acevedo and V Kafarov*

*Industrial University of Santander, COL*

**Nonlinear model predictive control applications**

*P Seferlis<sup>b</sup>, I Stavrakis<sup>a</sup> and A I Papadopoulos<sup>b</sup>*

<sup>a</sup> Dept., of Mechanical Engineering, Aristotle University of Thessaloniki, GRE

<sup>b</sup> Chemical Process Engineering Research Institute, Centre for Research and Technology-Hellas, GRE

**Utilisation of biomass feedstocks: A case study based on rice and sugar mills in Thailand**

*P Manakit, F Cecelja, A Yang and M Solda*

*PRISE Centre for Process and Information System Engineering, University of Surrey, UK*

**Computer-aided estimation of sustainability of biodiesel production from palm oil**

*D Martinez and V Kafarov*

*Industrial University of Santander, COL*

**Techno-economic optimisation of IGCC integrated with utility system for CO<sub>2</sub> emissions reduction**

*M Gharaie<sup>a</sup>, M Jobson<sup>a</sup>, M Hassan Panjeshahi<sup>b</sup> and N Zhang<sup>a</sup>*

<sup>a</sup> Centre for Process Integration, University of Manchester, UK

<sup>b</sup> Department of Chemical and Petroleum Engineering, University of Calgary, CAN

**Sustainable water desalination using waste heat: Optimisation of a liquid-liquid extraction process**

*E M Polykarpou and V Dua*

*Centre for Process Systems Engineering, Dept. of Chemical Engineering, University College London, UK*

**Dealing with uncertainties arising from environmental conscious multi-objective optimisation**

*H Mei Yao, M Oludayo Tade, and F Ali Mohammed*

*Department of Chemical Engineering, Curtin University, AUS*

**Life-cycle assessment of waste to energy technologies**

*Z Coventry<sup>a</sup>, R Tize<sup>b</sup> and A T Karunanithi<sup>a</sup>*

<sup>a</sup> University of Colorado Denver, US

<sup>b</sup> MWH, UK

**A life cycle cost analysis for sustainability of dimethyl ether production system from feasible raw materials**

*S Kim, B Joon Kang, N Jang and E Sup Yoon*

*School of Chemical and Biological Engineering, Institute of Chemical Processes, KOR*

**Simulation of the bioethanol process**

*J McMullen<sup>a</sup>, L Balcom<sup>b</sup> and R Calder<sup>b</sup>*

<sup>a</sup> Invensys, US

<sup>b</sup> Invensys, UK

**Combined heat and mass integration: A benchmarking case study**

*L Renard<sup>a</sup>, Z Périn-Levasseur<sup>b</sup>, L Salgueiro<sup>a</sup>, Luciana Savulescu<sup>b</sup>, F Maréchal<sup>a</sup> and M Benali<sup>b</sup>*

<sup>a</sup> EPFL/Industrial Energy Systems Laboratory, SUI

<sup>b</sup> Natural Resources Canada/CanmetENERGY, CAN

**Targeting the maximum carbon exchange for a total industrial site**

*S M Munir, Z A Manan and S R Wan Alwi*

*Process Systems Engineering Centre (PROSPECT), Universiti Teknologi Malaysia, MAY*

## Theme: Systems biology and healthcare engineering

**A mathematical programming approach to community structure detection in complex networks**

*L Bennett<sup>a</sup>, S Liu<sup>b</sup>, L G Papageorgiou<sup>b</sup> and S Tsoka<sup>a</sup>*

<sup>a</sup> Department of Informatics, School of Natural and Mathematical Sciences, King's College London, UK

<sup>b</sup> Centre for Process Systems Engineering, Dept. of Chemical Engineering, University College London, UK

**Improvements on adaptive predictive control with robust filter for blood glucose regulation in type I diabetic patients**

*G Campetelli, D Zumoffen and M Basualdo*

*Computer Aided for Process Engineering Group (CAPEG), ARG*

**Model-based optimal control of non-viral gene delivery**

*V Dua*

*Centre for Process Systems Engineering, University College London, UK*

**Model-based treatment of colon cancer in mice**

*M M Hadjiandreou and G D Mitsisa*

*Department of Electr. & Comp. Engin., University of Cyprus, CYP*

**Reconstruction of in silico metabolic models of desulfurising bacterial strains for comparative evaluation**

*S Aggarwal, G Reinaldi Ivan and I A Karimi*

*Department of Chemical and Biomolecular Engineering, National University of Singapore, SGP*

**An integrated computational model of powder release, dispersion, breakage, and deposition in a dry powder inhaler**

*J Milenkovic, A H Alexopoulos and C Kiparissides*

*Aristotle University of Thessaloniki and Chemical Process Engineering Research Institute, GRE*

**Automatic selection of the most promising enzymatic modulations for metabolic engineering: a multi-objective optimization approach**

*C Pozo<sup>a</sup>, G Guillén-Gosálbez<sup>a</sup>, L Jiménez<sup>a</sup>, A Sorribas<sup>b</sup>,*

<sup>a</sup> Department of Chemical Engineering, University Rovira i Virgili, Tarragona, ESP

<sup>b</sup> Departament de Ciències Mèdiques Bàsiques, Universitat de Lleida, Lleida, ESP

**Computational Investigation of counter-current reactors in a continuous hydrothermal flow synthesis system for reactor design Improvement**

*C Y Ma<sup>a</sup>, T Mahmud<sup>a</sup>, X Z Wang<sup>a</sup>, C J Tighe<sup>b</sup>, R I Guar<sup>b</sup> and J A Darr<sup>b</sup>*

<sup>a</sup> Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds, UK

<sup>b</sup> Department of Chemistry, University College London, UK

## Theme: Operations, control and process safety

**A new data driven index for control performance monitoring**

*T J Rato and M S Reis*

*CIEPQPF, Department of Chemical Engineering, University of Coimbra, POR*

**A signal processing approach for fault detection problem: Application to the DAMADICS actuator benchmark problem**

*G M de Almeida<sup>a</sup>, M S Reis<sup>b</sup> and S W Park<sup>c</sup>*

<sup>a</sup> Dept. of Chemical Engineering and Statistics, CAP, Federal University of Sao Joao, BRA

<sup>b</sup> Dept. of Chemical Engineering, FCTUC, University of Coimbra, POR

<sup>c</sup> Dept. of Chemical Engineering, Polytechnic School, University of Sao Paulo, BRA

**Efficient scheduling of complex multipurpose chemical batch processes**

*G M Kopanos<sup>a</sup>, M C Georgadis<sup>b</sup>, Efstratios, and N Pistikopoulos<sup>a</sup>*

<sup>a</sup> Imperial College London, Department of Chemical Engineering, London, UK

<sup>b</sup> Aristotle University of Thessaloniki, Department of Chemical Engineering, GRE

**Online feasibility and effectiveness of a spatio-temporal nonlinear model predictive control the case of methanol synthesis reactor**

*F Manenti<sup>a</sup>, S Cieri<sup>b</sup>, M Restelli<sup>b</sup>, N M Nascimento Lima<sup>c</sup>, L Z Linan<sup>c</sup>, and G Bozzano<sup>a</sup>*

<sup>a</sup> Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria Chimica, ITA

<sup>b</sup> Novartis Vaccines & Diagnostics, ITA

<sup>c</sup> University of Campinas (UNICAMP) Department of Chemical Processes, BRA

**MINLP model for optimal biocide dosing and maintenance scheduling of seawater cooled plants**

*F Nápoles-Rivera<sup>a</sup>, A Bin Mahfouz<sup>b</sup>, A Jiménez-Gutiérrez<sup>a</sup>, M M El-Halwagi<sup>b</sup> and J M Ponce-Ortega<sup>c</sup>*

<sup>a</sup> *Instituto Tecnológico de Celaya, MEX*

<sup>b</sup> *Texas A&M University, US*

<sup>c</sup> *Universidad Michoacana de San Nicolás de Hidalgo, MEX*

**Online real-time inference of ethanol composition in a mixed distillation column**

*C Gehlen, G G Koch, C M Franchi, R Hoffmann, and N P Gonçalves Salau*

*GIMOCAP/PPGEPRO/UFSM, BRA*

**Dynamic simulation of natural gas liquefaction process**

*K Song, C J Lee, J Jeon and C Han*

*School of Chemical and Biological Engineering, Seoul National University, KOR*

**Linking scheduling to control in an oil refinery**

*E Zondervan, J D J Hoekstra, S D P Flapper and A B de Haan*

*Eindhoven University of Technology, NL*

**A promising OPC-based computer system applied to fault diagnosis**

*J Silvente<sup>a</sup>, I Monroy<sup>b</sup>, G Escudero<sup>c</sup>, A Espuña<sup>a</sup> and M Graells<sup>b</sup>*

<sup>a</sup> *Chemical Engineering Department, Universitat Politècnica de Catalunya, ESP*

<sup>b</sup> *Chemical Engineering Department, Universitat Politècnica de Catalunya, ESP*

<sup>c</sup> *Software Department, Universitat Politècnica de Catalunya, ESP*

**Quality assessment support system and its use in pharmaceutical plant operations**

*H Kawai<sup>a</sup>, T Kitajima<sup>b</sup>, T Fuchino<sup>c</sup>, H Seki<sup>a</sup> and Y Naka<sup>d</sup>*

<sup>a</sup> *Chemical Resources Laboratory, Tokyo Institute of Technology, JPN*

<sup>b</sup> *Institute of Engineering, Tokyo University of Agriculture and Technology, JPN*

<sup>c</sup> *Chemical Engineering Department, Tokyo Institute of Technology, JPN*

<sup>d</sup> *Techno Management Solutions Ltd., JPN*

**Shared resources management by price coordination**

*R Martíá, D Naviaa, D Sarabíaa, and C De Prada*

*Dep. of System and Engineering Control of Valladolid, ESP*

**A novel method for monitoring of separation performance in distillation columns**

*M Stuckert<sup>a</sup>, B Pluyers<sup>b</sup> and W Marquardt<sup>a</sup>*

<sup>a</sup> *Process Systems Engineering, RWTH Aachen University, DEU*

<sup>b</sup> *IPCOS NV, BEL,*

**Use case driven development of a risk management tool with business process model for chemical plants**

*T Kitajima<sup>a</sup>, T Fuchino<sup>b</sup>, Y Shimada<sup>c</sup> and L Yuanjin<sup>d</sup>*

<sup>a</sup> *Institute of Engineering, Tokyo University of Agriculture and Technology, JPN*

<sup>b</sup> *Chemical Engineering Department, Tokyo Institute of Technology, JPN*

<sup>c</sup> *Chemical Safety Research Group, National Institute of Occupational Safety and Health, JPN*

<sup>d</sup> *Techno Management Solutions Ltd., JPN*

**Aggregate model for refinery production planning**

*E Ejikeme-Ugwu and M Wang*

*Process Systems Engineering Group, School of Engineering, Cranfield University, UK*

**Control system performance monitoring based on optimal action selection**

*L Ávila, E Martínez*

*INGAR (CONICET-UTN), ARG*

**Run-to-run MPC tuning via gradient descent**

*G A Bunin, F Fraire Tirado, G François, and D Bonvin*

*Laboratoire d'Automatique, École Polytechnique Fédérale de Lausanne, SUI*

**Control of forced convection drying in food slabs**

*V M Cristea, A Irimita, G S Ostace and S P Agachi*

*Chemical Engineering Department, Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, ROM*

**Avoiding oversizing in plant-wide control designs for industrial processes**

*D Zumoffen<sup>ab</sup> and M Basualdo<sup>b</sup>*

<sup>a</sup> *Computer Aided for Process Engineering Group (CAPEG). French-Argentine International Center for Information and Systems Sciences, ARG*

<sup>b</sup> *Universidad Tecnológica Nacional (UTN). Facultad Regional Rosario (FRRo), ARG*

**A new dual modifier-adaptation approach for real-time optimisation with inaccurate models**

*A G Marchetti and M Basualdo*

*French-Argentine International Center for Information and Systems Sciences, CIFASIS-CONICET, ARG*

**Specifying risk level for constraint violation in stochastic systems - A case study on papermaking**

*A Ropponen and R Ritala*

*Department of Automation Science and Engineering, Tampere University of Technology, FIN*

**Analysis of dynamic behavior of a thermally coupled distillation column implemented on a process with recycles**

*D Mascote-Pérez<sup>a</sup>, A Sánchez-Hijar<sup>a</sup>, N Ramírez-Corona<sup>a</sup> and A Jiménez-Gutiérrez<sup>b</sup>*

<sup>a</sup> *Departamento de Ingeniería Química, Alimentos y Ambiental, Universidad de las Américas Puebla, MEX*

<sup>b</sup> *Departamento de Ingeniería Química, Instituto Tecnológico de Celaya, MEX*

**Ontology-based expert system for process supervision**

*E Musulin, F Roda and M Basualdo*

*GIAIP-CIFASIS, CONICET-UNR-UPCAM, ARG*

**Control performance assessment for a class of nonlinear multivariable systems**

*W Yu<sup>a</sup>, D I Wilson<sup>b</sup> and B R Young<sup>a</sup>*

<sup>a</sup> *Chemical and Materials Engineering, The University of Auckland, NZL*

<sup>b</sup> *Electrical & Electronic Engineering, Auckland University of Technology, NZL*

**Advanced control for anaerobic digestion processes: volatile solids soft sensor development**

*G Opong<sup>ab</sup>, M O'Brien<sup>a</sup>, M McEwan<sup>a</sup>, E B Martin OBE<sup>b</sup> and G A Montague<sup>b</sup>*

<sup>a</sup> *Perceptive Engineering Ltd, UK*

<sup>b</sup> *BBTC, CEAM, Newcastle University, UK*

**A novelty detection approach for detecting faulty batches in a photo-Fenton process**

*I Monroy<sup>a</sup>, E Yama<sup>la</sup>, G Escudero<sup>b</sup>, M Pérez-Moya<sup>a</sup> and M Graells<sup>a</sup>*

<sup>a</sup> *Chemical Engineering Department, Universitat Politècnica de Catalunya, ESP*

<sup>b</sup> *Software Department, Universitat Politècnica de Catalunya, ESP*

**Modeling and simulation of poly-lactic acid synthesis in batch process for biomedical applications**

*G A R Martinez<sup>ab</sup>, A J R Lasprilla<sup>ab</sup>, J E J Figueroa<sup>a</sup>, M I R Barbosa<sup>ab</sup>, A L Jardim<sup>ab</sup> and R M Filho<sup>ab</sup>*

<sup>a</sup> *Laboratory of Optimization, Design and Advanced Control. Department of Process and Product Development. School of Chemical Engineering State University of Campinas, BRA*

<sup>b</sup> *Institute of Biofabrication, University City 'Zeferino Vaz', BRA*

**Operational optimisation of crude oil distillation systems using artificial neural networks**

*L M Ochoa-Estopier, M Jobson, R Smith*

*University of Manchester, UK*

**Improvement of crude oil refinery gross margin using a NLP model of a crude distillation unit system**

*D C López<sup>a</sup>, L J Hoyos<sup>b</sup>, A Uribe<sup>b</sup>, S Chaparro<sup>b</sup>, H Arellano-García<sup>a</sup> and G Wozny<sup>a</sup>*

<sup>a</sup> *Process Dynamics and Operation, Berlin Institute of Technology, DEU*

<sup>b</sup> *ECOPETROL S.A., COL*

**Multivariate control chart with a deployed matrix for auto correlated data**

*A S Matos and D Ferreira*

*UNIDEMI, Departamento em Engenharia Mecânica e Industrial, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa POR*

**Towards enhanced weight selection for (N)MPC via multi-objective optimisation**

*M Vallerio, F Logist and J Van Impe*

*BioTeC & OPTEC Dept. of Chemical Engineering, Katholieke Universiteit Leuven, BEL*

**Exploiting plant and process flexibility at the operational level**

*M Á Zamarripa, J Silvente and A España*

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**Ontology approach to model construction**

*H A Preisig and T Haug-Warberg*

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**A comparison of predictive control and fuzzy-predictive hybrid control performance applied to a three-phase catalytic hydrogenation reactor**

*M C A F Rezende, N M N Lima and R Maciel Filho*

*Chemical Engineering School, State University of Campinas (UNICAMP), BRA*

**Neural networks for thermal runaway detection in batch and semibatch reactors**

*E Molga*

*Warsaw University of Technology, Chemical and Process Engineering Department, POL*

**Revamp of a fuel gas system to rectify operational problems using basic chemical and process control engineering concepts with an innovative method to control the boiler's fuel gas drum**

*M S El-Taji*

*Mathematical Modelling and Simulation, Fluor Ltd, UK*

**Comparison of different inversion methods in controller strategies**

*L R Toth, L Nagy and F Szeifert*

*University of Pannonia, Department of Process Engineering, HUN*

**APC application on an NGL plant**

*M S El-Taji*

*Mathematical Modelling and Simulation, Fluor Ltd, UK*

**Simulation and nonlinear analysis of the stagnant polymer layer in a LDPE tubular reactor**

*M Krasnyk<sup>ab</sup>, C Kunde<sup>c</sup> and M Mangold<sup>a</sup>*

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**A combined multi-parametric and dynamic programming approach for model predictive control of hybrid linear systems**

*P Rivotti, M Wittmann-Hohlbein and E N Pistikopoulos*

*Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, UK*

**Dynamics model based decoupler for distillation column in aspen dynamics™ and matlab™ simulink environment**

*Q H Lee, Z Ahmad, and N Aziz*

*School of Chemical Engineering, University Sains Malaysia, MAY*

Tuesday 19 June, 2012

**Theme: Tools for financial business and management decision making**

**Realising continuous improvement in pharmaceutical technical operations – business process model in Roche's parenterals production Kaiseraugst**

*H Sugiyama and R Schmidt*

*Steril Drug Product Manufacturing Kaiseraugst, Pharma Technical Operations Biologics, F. Hoffmann-La Roche Ltd, SUI*

**Integration in process industries via Unified Processing Core (UPC) in operational and logistic planning levels**

*R Hosseini and P Helo*

*University of Vaasa, Department of Production, FIN*

**Design and planning of downstream petroleum supply chains**

*L J Fernandes<sup>ab</sup>, S Relvas<sup>b</sup> and A P Barbosa-Póvoa<sup>b</sup>*

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**Application of semantic and lexical analysis to technology forecasting by trend analysis – thematic clusters in separation processes**

*R Sitarz<sup>ab</sup> and A Kraslawski<sup>ac</sup>*

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**Quotation tool for process equipment**

*M Ershov<sup>ac</sup>, Y Avramenko<sup>a</sup>, J Häkkinen<sup>b</sup>, A Kraslawski<sup>ad</sup> and I Beloglazov<sup>c</sup>*

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<sup>d</sup> *Technical University of Lodz, POL*

**Designing and planning of closed-loop supply chains for risk and economical optimisation**

*S R Cardoso, A P Barbosa-Póvoa and S Relvas*

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**Semantic support for industrial symbiosis process**

*T Raafat, F Cecelja, A Yang and N Trokanas*

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**Supply chain planning under uncertainty using genetic algorithms**

*M Zamarripa, J Silvente and A Espuña*

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**Multiproduct, multiechelon supply chain analysis under demand uncertainty and machine failure risk**

*M Muresan, C C Cormos and P S Agachi*

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**Synthesis and design of processing networks: Stochastic formulation and solution**

*A Quaglia<sup>a</sup>, B Sarup<sup>b</sup>, G Sin<sup>a</sup> and R Gani<sup>a</sup>*

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**Inventory management for multi-product tank farm systems using a MILP model with rolling horizon**

*C N Marques<sup>a</sup>, H A Matos<sup>a</sup> and S Relvas<sup>b</sup>*

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**MILP-based approach for the scheduling of automated manufacturing system with sequence-dependent transferring times**

*A M Aguirre<sup>a</sup>, C A Méndez<sup>a</sup>, P M Castro<sup>b</sup> and C De Prada<sup>c</sup>*

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<sup>b</sup> *UMOSE, Laboratório Nacional de Energia e Geologia, POR*

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**Carbon management in the chemical process arena – a multi-faceted CAPE problem**

*R Calder<sup>a</sup>, H Gulati<sup>b</sup> and D Thomas<sup>a</sup>*

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**Computer-aided design and evaluation of batch and continuous multi-mode biopharmaceutical manufacturing processes**

*J Pollock<sup>a</sup>, S V Ho<sup>b</sup> and S S Farid<sup>a</sup>*

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**A framework for the evaluation of investments in clean power-technologies**

*G Di Lorenzo, P Pilidis, J Witton and D Probert*

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**UOPSS: A new paradigm for modeling production planning & scheduling systems**

*D Zyngier<sup>a</sup> and J D Kelly<sup>b</sup>*

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**A spatially-explicit, multi-period MILP modelling framework for the optimal design of a hybrid biofuel supply chain**

*O Akgul<sup>a</sup>, N Shah<sup>b</sup> and L G Papageorgiou<sup>a</sup>*

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**Theme: Product and process design**

**Model-based optimisation in pharmaceutical technical operations – Yield measurement and increase in Roche's parenterals production Kaiseraugst**

*H Sugiyama and R Schmidt*

*Steril Drug Product Manufacturing Kaiseraugst, Pharma Technical Operations Biologics, F. Hoffmann-La Roche Ltd, SUI*

**Hybrid simulation-optimization logic based algorithms for the rigorous design of chemical process**

*J A Caballero<sup>a</sup>, M A Navarro<sup>a</sup> and I E Grossmann<sup>b</sup>*

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**Application of computer aided mixture design in paints and coatings**

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<sup>b</sup> Department of Chemical Engineering, Polytechnic School of the University of São Paulo, BRA

**A nonlinear programming approach to conceptual design of reaction–separation systems**

*S Recker and W Marquardt*

*Aachener Verfahrenstechnik, RWTH Aachen University, DEU*

**Optimal design of chemical processes with chance constraints**

*G Ostrovsky, N Zyatdinov and T Lapteva*

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**Predicting a wide variety of constant pure compound properties for long chain substances using a 'reference series' method**

*I Paster<sup>a</sup>, M Shacham<sup>a</sup> and N Brauner<sup>b</sup>*

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**Considering physical property uncertainties in process design**

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**Modeling of open-system process for sustainable production: case studies in metal cleaning process**

*E Kikuchi, Y Kikuchi and M Hirao*

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**High-boiling-point petroleum fractions upgrading using the centrifugal reactive–molecular distillation process over catalyst: Mathematical modeling and simulation including experimental validation**

*L P Tovar<sup>a</sup>, M R Wolf–Maciel<sup>a</sup>, C B Batistella<sup>a</sup>, A Winter<sup>a</sup>, R Maciel–Filho<sup>a</sup> and L C Medina<sup>b</sup>*

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**A novel method for designing flotation circuits**

*F D Sepulveda<sup>a</sup>, M A Elorza<sup>a</sup>, L A Cisternas<sup>ab</sup> and E D Gálvez<sup>bc</sup>*

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**Water and energy use in mineral processing: A case study in copper flotation**

*M Donoso<sup>a</sup>, M E Mellado<sup>b</sup>, E D Gálvez<sup>bc</sup>, and L A Cisternas<sup>ab</sup>*

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**Evaluation of the batch distillation process in the ethanol production**

*M E Alvarez<sup>a</sup>, E B Moraes<sup>a</sup>, J C Rodrigues<sup>ab</sup>, A J Bonon<sup>a</sup>, and M R Wolf-Maciel<sup>a</sup>*

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**Integrated operation and design of a simulated moving bed reactor**

*E Zondervan<sup>a</sup>, N Nikacevic<sup>b</sup>, H Khajuria<sup>c</sup>, E N Pistikopoulos<sup>c</sup> and A B. de Haan<sup>a</sup>*

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**Modeling and analysis of intensified processes for economic recovery of high-grade lactic acid**

*G Krishna<sup>a</sup>, G P Rangaiah<sup>a</sup>, S Lakshminarayanan<sup>a</sup>*

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**Economic analysis of an industrial refining unit involving hydrotreatment of whole crude oil in trickle bed reactor using gPROMS**

*A T Jarullah, I M Mujtaba, and A S Wood*

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**Design of glycerol etherification process by constructive nonlinear dynamics**

*E Vlad, C S Bildea and G Bozga*

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**An integrated framework for flowsheet synthesis and molecular design**

*S Bommareddy<sup>a</sup>, N G Chemmangattuvalappil<sup>ab</sup> and M R Eden<sup>a</sup>*

<sup>a</sup> Department of Chemical Engineering, Auburn University, US

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**Enhanced bioethanol dehydration in extractive dividing-wall columns**

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**Enhancing multi-component separation of aromatics with Kaibel columns and DWC**

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**Genetic algorithms in the design of configurations for distillation of quaternary mixtures using less than N-1 columns with thermally coupling**

*J Cortez-Gonzalez<sup>a</sup>, J G Segovia-Hernández<sup>a</sup>, S Hernández<sup>a</sup>, C Gutiérrez-Antonio<sup>b</sup>, A Briones-Ramírez<sup>c</sup> and B G Rong<sup>d</sup>*

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**Multiobjective optimisation in distillation with reactor-side for hydrodesulfurisation process of diesel**

*E Y Miranda-Galindo<sup>a</sup>, J G Segovia-Hernández<sup>a</sup>, S Hernández-Castro<sup>a</sup>, A Bonilla-Petriciolet<sup>b</sup> and G P Rangaiah<sup>c</sup>*

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**Design and optimisation of pressure swing distillation using a stochastic algorithm based in the Boltzmann distribution**

*J Cortez-González<sup>a</sup>, R Murrieta-Dueñas<sup>a</sup>, R Gutiérrez-Guerra<sup>a</sup>, J G Segovia-Hernández<sup>a</sup> and A Hernández-Aguirre<sup>b</sup>*

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**A neural network application in the design of emulsion-based products**

*A Dubbelboer<sup>a</sup>, E Zondervan<sup>a</sup>, J Meuldijk<sup>a</sup>, H Hoogland<sup>b</sup>, and P M M Bongers<sup>ab</sup>*

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**Cyclic distillation – towards energy efficient binary distillation**

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**An integrated framework for product formulation by computer aided mixture design**

*J Heintz<sup>ab</sup>, I Touche<sup>ab</sup>, M Teles dos Santos<sup>ab</sup> and V Gerbaud<sup>ab</sup>*

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**Analysis of the production of methyl esters by the two-step supercritical method using reactive distillation**

*F I Gomez-Castro<sup>a</sup>, V Rico-Ramirez<sup>b</sup>, J G Segovia-Hernandez<sup>a</sup> and S Hernandez-Castro<sup>a</sup>*

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**Environmental and economic optimisation of distillation structures to produce anhydrous ethanol**

*J R Alcántara-Avila, M Kano, and S Hasebe*

*Department of Chemical Engineering, Kyoto University, JPN*

**Ontology-driven description and engineering of autonomous systems: Application to process systems engineering**

*M Rodriguez, J Bermejo-Alonso, C Hernandez Corbato and R Sanz*

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**Design of experiments and sensitivity analysis for microalgal bioreactor systems**

*S J Yoo, S K Oh and J M Lee*

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**Process design of integrated reaction and membrane separation by organic solvent nanofiltration using evolutionary algorithms**

*P Schmidt<sup>a</sup>, M Becker<sup>b</sup>, M Priske<sup>b</sup>, B Hamers<sup>b</sup>, P Kreis<sup>b</sup> and A Górák<sup>a</sup>*

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**Reactive distillation processes used as unique operation or finishing stage: A comparison**

*J P Archenti, M S Diaz and P M Hoch*

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**New distillation sequences for bioethanol production by extractive distillation**

*M Errico and B G Rong*

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**Optimal design and control of trains of dividing wall columns for the separation of petrochemical mixtures**

*C Gutiérrez-Antonio<sup>a</sup>, S Hernández<sup>b</sup>, F I Gómez-Castro<sup>b</sup>, J G Segovia-Hernández<sup>b</sup>, J O Campos-Vargas<sup>b</sup> and A Briones-Ramírez<sup>c</sup>*

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**A sustainable design and simulation of waste sulfuric acid concentration process for semiconductor industry**

*K S Kshetrimayum, C Jeong, S Park and C Han*  
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**An integrated methodology for design of tailor-made blended products**

*N Alafiza Yunus, K V Gernaey, J M Woodley and R Gani*  
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**A framework for the design of reacting systems with phase transfer catalysis**

*C Piccolo<sup>a</sup>, A Shaw<sup>b</sup>, G Hodges<sup>b</sup>, P M Piccione<sup>b</sup>, J P O'Connell<sup>c</sup> and R Gani<sup>a</sup>*  
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**The solvent selection framework: solvents for organic synthesis, separation processes and ionic-liquids solvents**

*I Mitrofanov*  
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**Model-based assessment of process sensitivity and robustness in biopharmaceutical manufacturing**

*K Westerberg<sup>a</sup>, E B Hansen<sup>b</sup>, T B Hansen<sup>b</sup>, N Borg<sup>a</sup> and B Nilsson<sup>a</sup>*  
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**Modelling of two-stage ATAD bioreactor system by using artificial neural network**

*E G Kirilova and N G Vaklieva-Bancheva*  
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**Modeling and simulation of a PSA process using SiCHA for propylene/propane separation**

*M Khalighi, S Farooq and I A Karimi*  
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**Theme: Computational and numerical solution strategies**

**Linking correlations spanning adjacent applicability domains**

*TM Alsoudani and I D L Bogle*  
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**A novel hybrid simulation-optimisation approach for the optimal design of multicomponent distillation columns**

*J A Reyes-Labarta, J A Caballero and A Marcilla*  
*Department of Chemical Engineering, University of Alicante, ESP*

**Reduced rigorous models for efficient dynamic simulation and optimisation of distillation columns**

*A Valleriote, L Dorigo, A R Secchi and E C Biscaia Jr*  
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**State estimators for better bioprocesses operation**

*N P G Salau<sup>a</sup>, J O Trierweiler<sup>b</sup> and A R Secchi<sup>c</sup>*  
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**Practical aspects on nonlinear state estimation**

*N P G Salau<sup>a</sup>, J O Trierweiler<sup>b</sup> and A R Secchi<sup>c</sup>*  
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**Design of flotation circuits including uncertainty and water efficiency**

*N E Jamett<sup>a</sup>, J P Vielma<sup>b</sup> and L A Cisternas<sup>a,c</sup>*  
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**Heat integration in non-isothermal systems using an alternative disjunctive optimisation model**

Miguel A. Navarro-Amorós<sup>a</sup>, José A. Caballero<sup>a</sup> and Ignacio E. Grossmann<sup>b</sup>

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**Global solution of min-max optimisation problems for nonlinear dynamic systems**

Y Zhao and M A Stadtherr

Department of Chemical and Biomolecular Engineering, University of Notre Dame, US

**Evaluation of the batch distillation process in the ethanol production**

M E T Alvarez<sup>a</sup>, E B Moraes<sup>a</sup>, J C Rodrigues<sup>ab</sup>, A J Bonon<sup>a</sup> and M R Wolf-Maciel<sup>a</sup>

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**Rigorous computational methods for dimensionality reduction in multi-objective optimisation**

P J Copado-Méndez, G Guillén-Gosálbez and L Jiménez

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**An efficient adjoint-free dynamic optimisation methodology for batch processing using  
pontryagin's formulation**

T C Freitas<sup>a</sup>, T C do Quinto<sup>b</sup>, A R Secchi<sup>a</sup> and E C Biscaia Jr<sup>a</sup>

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**A fractional calculus application to biological reactive systems**

V Rico-Ramirez<sup>a</sup>, J Martinez-Lizardo<sup>a</sup>, G A Iglesias-Silva<sup>a</sup>, S Hernandez-Castro<sup>b</sup> and U M Diwekar<sup>c</sup>

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**Bounding the solutions of parametric ODEs: When Taylor models meet differential inequalities**

B Chachuat and M Villanueva

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**BzzMath: Library overview and recent advances in numerical methods**

G Buzzi-Ferraris and F Manenti

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**Identification and estimation of functional states in drinking water plant based on fuzzy clustering**

H M Sarmiento<sup>ab</sup> and C N Isaza<sup>b</sup>

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**Homotopy continuation solution method in nonlinear model predictive control applications**

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**Stochastic and hybrid approaches to solve integrated synthesis and operation of batch processes**

M Moreno-Benito and A Espuña

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**Model-based design of experiments for model identification using closed-loop set-point response**

Nataliya Barana, Günter Woznya and Harvey Arellano-Garcia

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**Development of a nonlinear model predictive control framework for a PEM fuel cell system**

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**A numerical tool for integrating renewable energy into total sites with variable supply and demand**

*S R W Alwi<sup>a</sup>, P Y Liew<sup>a</sup>, P S Varbanov<sup>b</sup>, Z A Manan<sup>a</sup> and J J Klemeš<sup>b</sup>*

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**An industrial perspective on the use of differential equation solvers for parameter estimation**

*A Shaw, D Dionisi, S Taylor and P M Piccione*

*Process Studies Group, Syngenta, UK*

**Explicit analytical expressions for convex hull of quadrilinear functions**

*S Balram, I A Karimi*

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**Parameter estimation of thermodynamic models for equilibrium of proteins solutions with salts**

*J L Borges<sup>a</sup>, A L H Costa<sup>b</sup>, T L M Alves<sup>a</sup> and F L P Pessoa<sup>c</sup>*

<sup>a</sup> *PEQ/COPPE/Federal University of Rio de Janeiro, BRA*

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**On the application of the cascade optimization algorithm in distributed computer networks and grids**

*D Du<sup>a</sup>, F Cecelja<sup>a</sup> and A Kokossis<sup>b</sup>*

<sup>a</sup> *PRISE, FEPS, Unversity of Surrey, UK*

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**Parameter estimation of dynamic grade transitions in a polyethylene plant**

*N Andersson<sup>a</sup>, P O Larsson<sup>b</sup>, J Åkesson<sup>b</sup>, S Skälén<sup>c</sup>, N Carlsson<sup>c</sup> and B Nilsson<sup>a</sup>*

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**A novel method for identification of critical points in flow sheet synthesis under uncertainty**

*M Kasaš, Z Kravanja and Z N Pintari*

*University of Maribor, Faculty of Chemistry and Chemical Engineering, SLO*

**A multi-level meta-heuristic algorithm for the optimisation of antibody purification processes**

*A S Simaria<sup>a</sup>, Y Gao<sup>b</sup>, R Turner<sup>b</sup> and S S Farid<sup>a</sup>*

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**A heuristic algorithm for the piecewise linear segmentation of multiple time-series for solar thermal systems inverse modelling**

*V V Lopes<sup>a</sup>, F Ferro<sup>a</sup>, M J Carvalho<sup>b</sup> and A Q Novais<sup>a</sup>*

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**Theme: CAPE in education (sponsored by EURECHA)**

**Computer-aided delivery of case-based learning activities in EBL within chemical engineering curriculum**

*K Novakovic<sup>a</sup>, M Parr<sup>b</sup> and J Glassey<sup>a</sup>*

<sup>a</sup> *School of Chemical Engineering and Advanced Materials, Newcastle University, UK*

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**Development of a safety education system for SMB operation**

*H Kwon<sup>a</sup>, J Lee<sup>b</sup> and I Moon<sup>a</sup>*

<sup>a</sup> *Department of Chemical and Biomolecular Engineering Yonsei University, KOR*

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**Performance indicators for the training assessment of industrial operators**

*D Manca, S Nazir, F Lucernoni, V Pras and S Colombo*

*Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta" Politecnico di Milano, Italy*

Wednesday 20 June, 2012

**Theme: Multi scale modelling and simulation**

**Simulation of bioethanol production process from residual microalgae biomass**

*Y Peralta-Ruíz, Y Pardo, Á González-Delgado and V Kafarov*

*Industrial University of Santander, Chemical Engineering Department, COL*

**Hydrodynamic and heat transfer modeling of polydisperse fluidised bed olefin polymerisation reactors**

*R Marandi<sup>a</sup>, S Hashim<sup>a</sup> and G Zahedi<sup>b</sup>*

<sup>a</sup> *Polymer Engineering Department, Faculty of Chemical Engineering, University Technology Malaysia, MAL*

<sup>b</sup> *Process Systems Engineering Centre, Faculty of Chemical Engineering, University Technology Malaysia, MAL*

**Modelling, validation and control of an evaporative cooling system for scraped surface heat exchangers**

*Peter Bongers<sup>ab</sup>, Cristhian Almeida<sup>a</sup> and Hans Hoogland<sup>a</sup>*

<sup>a</sup> *Structured Materials & Process Science, Unilever Research, NL*

<sup>b</sup> *Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, NL*

**Automated optimisation model to perform sensitivity analysis on cost of investment required to upgrade treatment plants in water networks.**

*E Arzate<sup>a</sup>, P Huitzil<sup>a</sup>, A González<sup>a</sup>, B E Martínez<sup>a</sup> and I E Grossmann<sup>b</sup>*

<sup>a</sup> *Instituto Mexicano del Petróleo MEX*

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**Mathematical investigation of the case hardening phenomenon explained by shrinkage and collapse mechanisms occurring during drying processes**

*Seddik Khalloufi<sup>a</sup> and Peter Bongers<sup>ab</sup>*

<sup>a</sup> *Structured Materials and Process Science Department, Unilever Research Vlaardingen, NL*

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**Dynamic modelling and simulation of Kühni extraction columns**

*M Jaradat<sup>ab</sup>, H Allaboun<sup>c</sup>, H J Bart<sup>ab</sup> and M Attarakih<sup>d</sup>*

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**Reynolds-averaged navier-stokes modelling of the near-field structure of accidental releases of carbon dioxide from pipelines**

*M Fairweather<sup>a</sup>, S A E G Falle<sup>b</sup>, J Hebrard<sup>c</sup>, D Jamois<sup>c</sup>, C Proust<sup>cd</sup>, C J Wareing<sup>a</sup> and R M Woolley<sup>a</sup>*

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**Large eddy simulation and particle impact kinetics for bend erosion prediction**

*D O Njobuenwu and M Fairweather*

*School of Process, Environmental and Materials Engineering, University of Leeds, UK*

**Prediction of the permeability of packed beds of non-spherical particles**

*M S Islam, R Caulkin, X Jia, M Fairweather and R A Williams*

*School of Process, Environmental and Materials Engineering, University of Leeds, UK*

**Syngas production from sugar cane bagasse in a circulating fluidised bed gasifier using Aspen Plus™: Modelling and simulation**

*Y O Ardila, J E J Figueroa, B H Lunelli, R M Filho and M R Wolf Maciel*

*Laboratory of Optimization, Design and Advanced Control. Department of Process and*

*Product Development, School of Chemical Engineering, State University of Campinas, BRA*

**Novel adiabatic reactor design for supercritical Fischer-Tropsch synthesis**

*E Durham, S Zhang, R Xu, M R Eden and C B Roberts*

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**Process analysis of rotary-type solar reactor for hydrogen production systems**

*H Matsumoto, H Mashimo and C Kuroda*

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**Modeling and simulation of suspension polymerisation of vinyl chloride via population balance model**

*Á Bárkányi, S Németh, and B G Lakatos*

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**Computational study of a rotating packed bed distillation column**

*R J Prada, E L Martínez and M R Wolf Maciel*

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**Sugarcane bagasse as raw material to syngas production: 3D simulation of gasification process**

*J E J Figueroa, Y C Ardila, B H Lunelli, R M Filho and M R Wolf Maciel*

*Laboratory of Optimization, Design and Advanced Control. Department of Process and Product Development, School of Chemical Engineering. State University of Campinas, BRA*

**CFD modelling and video analysis based model validation for a stirred reactor**

*A Egedy, T Varga and T Chován*

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**Dynamic modelling of a polypropylene production plant**

*F Lesage<sup>a</sup>, D Nedelec<sup>a</sup>, B Descales<sup>b</sup> and W D Stephens<sup>c</sup>*

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**Multi-scale modelling of biomass pyrolysis processes**

*Abhishek Sharma<sup>a</sup>, Vishnu Pareek<sup>a</sup>, and Dongke Zhang<sup>b</sup>*

<sup>a</sup> Department of Chemical Engineering, Curtin University, AUS

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**Information integration: Generating functional models from structural ones**

*M Rodríguez, J L De la Mata and M Eugenia Alvarez*

*Autonomous System Laboratory, Universidad Politécnica de Madrid, ESP*

**CFD study of liquid drainage in flotation foams**

*P R Brito-Parada, S J Neethling and J J Cilliers*

*Rio Tinto Centre for Advanced Mineral Recovery, Department of Earth Science and Engineering, Imperial College London, UK*

**Estimation of kinetic parameters and mathematic model validation for nylon-6 process**

*V I Funai, D N C Melo, N M N Lima, A F Pattaro, L Z Liñan, A J Bonon and R M Filho*

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**CPFD simulation of fluidised bed flow in FCC regenerator**

*B Cha<sup>a</sup>, J Kim<sup>a</sup>, S R Son<sup>b</sup>, D S Park<sup>b</sup> and M Il<sup>a</sup>*

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<sup>b</sup> SK Innovation Global Technology, KOR

**CFD simulation of three-dimensional multiphase flow in a rotating packed bed**

*E L Martínez, R Jaimes, J L Gomez and R M Filho*

*School of Chemical Engineering, University of Campinas, BRA*

**Monte Carlo simulation of shape evolution in solutions - A model study of BaSO<sub>4</sub> precipitation**

*A Voigt<sup>a</sup> and K Sundmacher<sup>ab</sup>*

<sup>a</sup> Process Systems Engineering, Otto-von-Guericke University Magdeburg, DEU

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**Using CAPE to enhance the sustainability of utilising natural gas in ammonia production**

*L Lewis<sup>a</sup>, E John<sup>a</sup>, A Albert<sup>a</sup>, C Koongeberry<sup>a</sup>, A Kisson<sup>b</sup>, and B Aufderheide<sup>ac</sup>*

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**Food supply chain planning and quality optimisation approach**

*A Mehdizadeh<sup>a</sup>, N Shah<sup>a</sup>, N Raikar<sup>b</sup> and P M M Bongers<sup>b</sup>*

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**Towards a generic tool to support multiscale modelling of discrete event systems**

*Y Zhao and A Yang*

Division of Civil, Chemical and Environmental Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, UK

**Extended rate-based model validation for polyester synthesis by reactive distillation**

*M Shah<sup>ab</sup>, A A Kiss<sup>b</sup>, E Zondervan<sup>a</sup>, and A B de Haan<sup>a</sup>*

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**Prediction of physical properties of non-electrolyte organic compounds by distance weighted group contribution methods**

*Juha-Pekka Pokki and V Alopaeus*

Aalto University, School of Chemical Technology, Department of Biotechnology and Chemical Technology, FIN

**Model based analysis of different apparent porosities in preparative protein chromatography**

*N Borga and B Nilsson*

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**Dynamic multiscale-modelling of microbial biopolymer production processes**

*C Chatzidoukas<sup>a</sup>, G Penloglou<sup>b</sup>, A Roussos<sup>b</sup>, C Kiparissides<sup>ab</sup>*

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**2D analysis of fixed bed reactor using CFD models**

*G Rádi, T Varga and T Chován*

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**Modeling of thermodynamic equilibrium in high temperature synthesis of ultrapure nanomaterials**

*A Bessarabova, I Bulatov<sup>b</sup>, A Kvasyuk<sup>a</sup> and A Kochetygov<sup>a</sup>*

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**A systematic experiment-based approach to modeling foam in packed columns**

*R Kraus, G Senger, Harvey Arellano-Garcia and Günter Wozny*

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**Simulation tools for the design of optimised membrane modules and processes**

*P Schiffmann, P Golubovskiy and J U Repke*

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**Theme: Tools for energy management**

**A prototype simulation-based optimisation approach to model feedstock development for chemical process industry**

*I Fahmi and S Cremaschi*

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**Multi-objective optimisation of coal-fired electricity production with CO<sub>2</sub> capture**

*J Cristóbal<sup>a</sup>, G Guillén-Gosálbez<sup>b</sup>, L Jiménez<sup>b</sup> and A Irabien<sup>a</sup>*

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**Multi-objective optimisation of absorption refrigeration systems involving renewable energy**

*José Ezequiel Santibañez-Aguilar<sup>a</sup>, J B González-Campos<sup>a</sup>, J M Ponce-Ortega<sup>a</sup>, M Serna-González<sup>a</sup> and M M El-Halwagi<sup>b</sup>*

<sup>a</sup> Universidad Michoacana de San Nicolás de Hidalgo, MEX

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**Design and thermal analysis of a solid oxide fuel cell system integrated with ethanol steam reforming**  
*C Thanomjit<sup>a</sup>, Y Patcharavorachot<sup>b</sup> and A Arpornwichanop<sup>a</sup>*

<sup>a</sup> Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, THA

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**Design of a hydrogen supply chain using multiobjective optimisation**

*S De-Leon Almaraz<sup>a</sup>, C Azzaro-Pantel<sup>a</sup>, L Montastruc<sup>a</sup>, L Pibouleau<sup>a</sup> and O B Senties<sup>b</sup>*

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**Numerical optimisation of steam cycles and steam generators designs for a coal-to-FT plant**

*E Martelli<sup>a</sup>, T G Kreutz<sup>b</sup>, M Gatti<sup>a</sup>, P Chiesa<sup>a</sup>, and S Consonni<sup>a</sup>*

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**Proposition of methodology for optimization of energy system design under uncertainty**

*M Dubuisa and F Maréchal*

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**Investigation of a proton-conducting SOFC with internal autothermal reforming of methane**

*Y Patcharavorachot<sup>a</sup> and A Arpornwichanop<sup>b,c</sup>*

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**Optimisation-based analysis of a dwelling with an air source heat pump**

*D Zhang, L G Papageorgiou and E S Fraga*

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**Development an optimization model for green supply chains: integration of CO<sub>2</sub> disposal and renewable energy supply**

*J Ryu<sup>a</sup>, J H Han<sup>b</sup> and I B Lee<sup>b</sup>*

<sup>a</sup> Department of Nuclear and Energy System, Dongguk University, KOR

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**Optimisation of a distributed small scale biodiesel production system in Greater London**

*A Kelloway, W A Marvin and P Daoutidis*

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**A model predictive control framework for residential microgrids**

*E D Mehleri<sup>a,b</sup>, L G Papageorgiou<sup>b</sup>, N C Markatos<sup>a</sup> and H Sarimveis<sup>a</sup>*

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**Optimal energy management and production scheduling**

*I Harjunkoski<sup>a</sup>, M Bauer<sup>a,c</sup> and T Kymäläinen<sup>b</sup>*

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**Improvements on hydrogen production efficiency based on switching multiple renewable power sources**

*L N Degliuomini<sup>a</sup>, D Feroldi<sup>a,b</sup>, P Luppi<sup>a,b</sup> and M Basualdo<sup>a,b,c</sup>*

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**Optimal planning of energy management system under demand uncertainty**

*G B Choi, S G Lee and J M Lee*

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**Energy management strategies for process site CO<sub>2</sub> emissions reduction**

*M Gharaie<sup>a</sup>, M Jobson<sup>a</sup>, M H Panjeshahi<sup>b</sup> and N Zhang<sup>a</sup>*

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**Optimal residential solar photovoltaic capacity in grid connected applications**

*S Huang<sup>a</sup>, J Xiao<sup>b</sup>, J F Pekny<sup>c</sup> and G V Reklaitis<sup>c</sup>*

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**Thermodynamic efficiency and cost-effective optimization of heterogeneous batch distillation**

*I Rodriguez-Donis<sup>a</sup>, N Hernandez-Gonzalez<sup>b</sup>, V Gerbaud<sup>c</sup>, and X Joulia<sup>c</sup>*

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**An alternative real-time optimisation algorithm with modifier adaptation: application to heat and power systems**

*F Serrallunga, M C Mussati and P A Aguirre*

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**Comparison of pervaporation models in flowsheeting environment**

*N Valentiny<sup>a</sup> and P Mizsey<sup>ab</sup>*

<sup>a</sup> Department of Chemical and Environmental Process Engineering, Budapest University of Technology and Economics, HUN

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**Constrained thermohydraulic optimisation of the flowrate distribution in crude preheat trains**

*B C G de Assis<sup>a</sup>, C O Gonçalves<sup>a</sup>, J L Borges<sup>b</sup>, V B G Tavares<sup>b</sup>, F S Liporace<sup>c</sup>, S G Oliveira<sup>c</sup>,*

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**Comparison of MEA and ammonia for heat-integrated coal-fired power plants with PCC processes**

*R Khalilpour and A Abbas*

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## Travelling to London

London is one of the world's best-connected cities, with five international airports serving 273 destinations, high-speed rail links to continental Europe and an extensive public transport network.

## Destination

London is roughly bounded by the M25 motorway and split north to south by the river Thames. The city can be broadly divided into five areas: North, South, East, West and Central.

The City of London is an extraordinary place. Established soon after the Romans invaded Britain in AD43, the City is where London began – the 'original' London – the place from which today's thriving metropolis grew.

Such history and its position as a world leader in international finance and business, has imbued the City of London with a unique character and a distinct identity. Pass between the dragons that mark its entrances and exits and you'll recognise a difference. This is where ancient and modern sit side by side; where medieval alleyways open out onto major streets; where historic churches snuggle up to soaring glass neighbours; where the past embraces the future.

Over 2,000 years of history are told through London's buildings – from the remains of its Roman walls to modern icons such as the Lloyd's Building. Old or new, there is much to marvel at – the mighty dome of St Paul's Cathedral, Tower Bridge and 30 St Mary Axe (the 'Gherkin') are just some of the landmarks that punctuate the City skyline.

The venue for *ESCAPE 22* is the University College London (UCL) in the Bloomsbury area of London. Bloomsbury is known as the home of British Museum, the British Library and the University College London. Historically, Britain's writers and intellectuals have favoured this area.

## Conference venue

UCL is located at the very centre of London and is well served by transport links from all over the UK and abroad. UCL was established in 1826 but is a modern, outward-looking institution, committed to engaging with the major issues of our times. One of the world's leading multidisciplinary universities, UCL today is a true academic powerhouse.

UCL is among the world's top universities, as reflected in performance in a range of rankings and tables. 21 Nobel prizewinners have come from the UCL community.

Visit our web-site to download location map and directions.

## Social programme

Welcome reception: A welcome reception will take place in the cloisters at UCL on the evening of Sunday 17 June. This will provide delegates with the opportunity to register for the conference and collect their conference material prior to the main conference commencing on Monday 18 June. This reception will be free of charge.

Conference dinner: A conference dinner will be held at the Grand Connaght rooms, London on Tuesday 19 June, 2012. This is included in the registration cost. (Please note: The student registration does not include the conference dinner, tickets can be purchased separately).

There is a wide variety of accommodation available around the area of the university; an accommodation list is available at: [www.icheme.org/escape22](http://www.icheme.org/escape22)

## Documentation

All delegates who are fully registered to attend the conference will be issued with either a copy of the conference proceedings or, if you registered after 1 May 2012, a link to an electronic copy of the proceedings containing copies of the full manuscripts and posters. All presentations given at the conference will be available (subject to the author's permission) on the conference web site after the conference.

## Official language

The conference language is English.

## Things to do

Whilst in London why not take in some of the city's sights and attractions such as the London Eye, the Natural History Museum, the Tower of London, St Paul's Cathedral and Buckingham Palace. For a comprehensive list of attractions, eateries and much more visit: [www.visitlondon.com](http://www.visitlondon.com)

## Travel

Whilst in London why not invest in an Oyster Card, a plastic smartcard you can use instead of paper tickets. You can put Travelcards, Bus & Tram season tickets and pay-as-you-go credit on it.

Oyster is the cheapest way to pay for single journeys on bus, tube, tram, DLR, London Overground and most National Rail services in London. You'll find Oyster ticket stops in newsagents, garages, off-licences and hundreds of other shops in London. The nearest vendor is Normans at UCL Hospital: 235 Euston Road, Euston, London, NW1 2BU. For more information visit: <https://oyster.tfl.gov.uk>

## Insurance

Delegates are advised to arrange adequate insurance, as the conference organisers cannot cover persons against cancellation of the booking, or theft of possessions.

## Medical attention

If you require medical attention during your stay with us, basic first aid will be available at reception. In case of emergencies and more urgent medical conditions, University College Hospital Accident and Emergency department can be found opposite the Bloomsbury Campus where the conference is being held.

[www.ucl.ac.uk/locations/ucl-maps/ucl-bloomsbury-campus-map](http://www.ucl.ac.uk/locations/ucl-maps/ucl-bloomsbury-campus-map)

Please note that there may be a charge for some treatments administered by the NHS if you are not currently a UK resident.

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