

18TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING



CAPE WP



Event n° 667

JUNE 1-4, 2008

CENTRE DE CONGRÈS DE LYON, FRANCE

Organised by:
IFP

Supported by:
LGC - ENSIACET

On behalf of:
Société de Chimie
Industrielle
Société Française de
Génie des Procédés

FINAL PROGRAMME

**An Event of the CAPE Working
Party of the European Federation
of Chemical Engineering**

www.escape18.org



CONTENTS

Introduction	1
General Information	2
Committees	3
Symposium Programme	4
Synopsis	4
Sunday 1 June	8
Monday 2 June	9
Tuesday 3 June	15
Wednesday 4 June	21
Thursday 5 June	26
List of Posters	27
Floor Plan, List of Exhibitors	47
List of Hotels	48
Access Maps	49

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Process Systems Enterprise



TOTAL



SYMPOSIUM SECRETARIAT AND ORGANISATION

ESCAPE 18 c/o COLLOQUIUM

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ESCAPE 18

WELCOME AT ESCAPE 18

The main theme for **ESCAPE 18** is **CAPE for the Users!** CAPE systems are to be put in the hands of end users who need functionality and assistance beyond the core scientific and technological capacities of the systems. User-friendliness, online or web-based advice, decision support, knowledge management and organisational issues are important points that must be taken into account when deploying a CAPE system. These issues will be addressed in a special track and industrial case studies illustrating CAPE methods and tools are encouraged.

The other six main topics cover the usual scope of **ESCAPE 18** conferences, from off-line design to on-line systems, including numerical and computational methods, integrated and multiscale modelling, societal aspects, and CAPE education.

ESCAPE 18 includes a rich programme of 5 plenary lectures and 6 keynote talks from leaders in science and industry, 101 contributions presented in 26 sessions and 2 poster sessions for other 247 contributions.



GENERAL INFORMATION

VENUE

From Sunday 1 to Wednesday 4, June, at the:

Centre de Congrès de Lyon
50 quai Charles de Gaulle
69006 Lyon – France

ACCESS

Metro and Bus:

- Metro line A – stop at Foch and connect with Bus # 4 (direction: Cité Internationale)
- Metro line D – stop at Saxe-Gambetta and connect with bus # 4 (direction: Cité Internationale)

Direct bus:

- Bus # 58 (departure from place Bellecour – on the side of rue Victor Hugo, stops at: Parc Tête d'Or/Churchill)

ON SITE REGISTRATION

(VAT included)

Delegates 820 €

Students* 600 €

*Copy of the student card and approval note from the manager required.

2

Registration fees include:

- Admission to all sessions
- Congress proceedings
- Lunches and coffee breaks
- Invitation to the welcome cocktail on 1 June.

Registration fees do not include:

- Accommodation
- Participation to the gala dinner on 3 June
- Visit of IFP-Lyon on 5 June am.

CERTIFICATE OF ATTENDANCE

Certificates of attendance will be given to all participants.

LANGUAGE

Symposium sessions will be held in English. No simultaneous translation will be provided.

PRESENTATIONS

The pdf presentation files of the talks will be available for download upon authors agreement, after the symposium, on www.escape18.org and www.ifp.com

PROCEEDINGS

The symposium proceedings will be distributed to all conference participants at the conference site. Extended versions of selected papers will also be published in a special issue of *Computers and Chemical Engineering* after the conference.

Wi-Fi

A wi-fi zone has been set up for ESCAPE 18 participants within the welcome desk area.

GALA DINNER

Tuesday 3 June

The ESCAPE 18 gala dinner will take place in the prestigious "Manoir de la Garde" located in the Pays Beaujolais, in a middle-aged village of the golden stones land.

A short artistic live show will also contribute to make this moment a unique one!!

Free bus transfers provided from the congress center and back to the hotels.

Price per person : 100 € (all incl.)

La Garde - 69640 Jarnioux

Tel.: +33 (0)4 74 02 87 91



IFP PILOT PLANT VISIT

Thursday 5 June - 9h-11h30

The number of participants to this interesting visit is limited. Identification badges will be required for security reasons.

Bus transfer provided at:

- 8h30, from the congress center to IFP-Lyon,
- 11h30, from IFP to Lyon-Perrache railway station and to Lyon-Saint Exupéry airport.

Price per person: 30 € (all incl.)

NATIONAL ORGANISING COMMITTEE

Chair

Bertrand Braunschweig, IFP

Members

Didier Caudron
Stéphane Déchelotte
Pascal Floquet
Arsène Isambert
Christian Jallut
Xavier Joulia
Christian Latgé
Frédérique Léandri
Francis Luck
Francis Nativel
Hervé Roustan
Philippe Vacher

INTERNATIONAL SCIENTIFIC COMMITTEE

Conference Chair

Bertrand Braunschweig, France
Xavier Joulia, France

Topic Chair

Off-line systems

Rafiqul Gani, Denmark
Jan van Schijndel, The Netherlands

On-line systems

Chonghun Han, South Korea
Martin Wolf, Germany

Computational and numerical solution strategies

Lorens Biegler, USA
Michel Pons, France

Integrated and multiscale modelling and simulation

Luis Puigjaner, Spain
Costas Pantelides, UK

CAPE for the users!

Tahir I. Malik, UK
Wolfgang Marquardt, Germany

CAPE and society

Peter Glavic, Slovenia
Sophie Jullian, France

CAPE in education

Ian Cameron, Australia
Georges Heyen, Belgium

Members

Off-line systems

Ana Barbosa-Póvoa, Portugal
David Bogle, UK
Michael Doherty, USA
Andrzej Gorak, Germany
Johan Grievink, The Netherlands
Ignacio Grossmann, USA
Ludovit Jelemensky, Slovakia
Zdravko Kravanja, Slovenia
Christian Latgé, France
Henrique Matos, Portugal
Xuan Meyer, France
Ka Ming Ng, China
Sauro Pierucci, Italy
Heinz Preisig, Norway
Eva Sorensen, UK
Petr Srehlik, Czech Republic

On-line systems

Dominique Bonvin, Switzerland
Didier Caudron, France
Yann Creff, France
Sebastian Engell, Germany
Antonio España, Spain
Sten Bay Jorgensen, Denmark
Marie-Véronique Le Lann, France
Iqbal Mujtaba, UK
Jose Pinto, Brazil
Sigurd Skogestad, Norway
Venkat Venkatasubramanian, USA
Günter Wozny, Germany
Toshko Zhelev, Ireland

Computational and numerical solution strategies

Guido Buzzi-Ferraris, Italy
Benoit Chachuau, Switzerland
Pascal Floquet, France
Christodoulos Floudas, USA
Jacek Jezowski, Poland
François Maréchal, Switzerland
Hervé Pingaud, France
Stratos Pistikopoulos, UK
Mordechai Shacham, Israel
Alain Vacher, France
Peter Verheijen, The Netherlands

Integrated and multiscale modelling and simulation

Claire Adjiman, UK
Ana Maria Eliceche, Argentina
Christian Jallut, France
Thokozani Majozi, South Africa
Fernando Martins, Portugal
Natalia Menshutina, Russia
Gintaras Reklaitis, USA
George Stephanopoulos, USA
Jan Thullie, Poland
Gilles Trystram, France

CAPE for the users!

Rafael Batres, Japan
Sylvie Cauvin, France
Gabriella Henning, Argentina
Andrzej Kraslawski, Finland
Jean-Marc Le Lann, France
Jack Ponton, UK
Rajagopalan Srinivasan, Singapore
Lars Von Wede, Germany

CAPE and society

Arsène Isambert, France
Emilia Kondili, Greece
Sandro Macchietto, UK
Peter Mizsey, Hungary
Yuji Naka, Japan
Claudio Oller do Nascimento, Brazil
Valentin Plesu, Romania
En Sup. Yoon, Korea

CAPE in education

David Bogle, UK
Marie Debacq, France
Urban Gren, Sweden
Daniel Lewin, Israel

SYMPOSIUM PROGRAMME

ESCAPE 18

SYNOPSIS

SUNDAY 1 JUNE

9:30 Registration

Room Rhône 2

10:00

CAPE WP workshop
(members only)

Information session

Room Rhône 3

12:40 Lunch

Room Rhône 2

14:00

CAPE WP meeting
(members only)

Business meeting

17:20

17:40 ESCAPE 18
registration opening

18:00 Welcome cocktail

MONDAY 2 JUNE

8:30

Registration

Audit. Lumière

9:00 Opening ceremony: CAPE-WP President, Conference Presidents, IFP Director, IEP President

9:20

EFCE PhD award in CAPE
Harvey Arellano-Garcia (Technische Universität Berlin)

9:40

Plenary lecture - Topic 5 - PL 5.1
René Bañares-Alcantara (Oxford Univ, UK)
Chair: T. Malik, W. Marquardt

10:20

Coffee break

Room Rhône 3

Audit. Pasteur

Room Rhône 2

10:40

Keynote lectures

Topic 4 - KL 4.1
Philippe Sautet
(ENS Lyon, France)
Chair: T. Majoz, S. Pierucci

Topic 1 - KL1.1
Michael Hill
(M. Hill & Associates, USA)
Chair: R. Gani, C. Adjiman

Topic 3 - KL3.1
Ray Dickinson
(Shell Global Solution Intl., CO-LaN, The Netherlands)
Chair: B. Braunschweig, E. Fraga

11:20

Oral sessions

Topic 4 - Session 4.1 - Process Modelling & Simulation
Chair: T. Majoz, S. Pierucci

Topic 1 - Session 1.1 - Integrated Product / Process Design
Chair: R. Gani, C. Adjiman

Topic 3 - Session 3.1 - New IT Approaches
Chair: B. Braunschweig, E. Fraga

12:40

Lunch

14:00

Oral sessions

Topic 2 - Session 2.1 - Real Time Optimisation
Chair: D. Bonvin, D. Caudron

Topic 1 - Session 1.2 - Separation Process Synthesis & Design
Chair: X. Meyer, A. Barbosa Povo

Topic 3 - Session 3.2 - Large Scale Systems
Chair: G. Buzzi-Ferraris, M. Shacham

15:20

Poster session 1 & coffee break

16:40

Oral sessions

Topic 2 - Session 2.2 - Model Predictive and Intelligent Control
Chair: M.V. le Lann, S. Engell

Topic 5 - Session 5.1 - Decision & Management Support
Chair: S. Cauvin, R. Batres

Topic 6 - Session 6.1 - Environmentally Conscious Design
Chair: A. Isambert, P.S. Agachi

18:00

SYNOPSIS

TUESDAY 3 JUNE

8:30 Registration

Audit. Pasteur

9:00 **Plenary lecture - Topic 7 - PL 7.1**
Ian Cameron (Queensland Univ, Australia), Daniel Lewin (Technion Univ, Israel)
 Chair: G. Heyen, C. Han

9:40 **Plenary lecture - Topic 2 - PL 2.1**
*Benoît Chachuat (EPFL, Switzerland), Bala Srinivasan (Ecole Polytechnique de Montréal, Canada),
 Dominique Bonvin (EPFL, Switzerland)*
 Chair: G. Heyen, C. Han

10:20 Coffee break

Room Rhône 3

Audit. Pasteur

Room Rhône 2

10:40 **Keynote lectures**

Topic 4 - KL 4.2
Maurizio Fermeglia
 (Trieste Univ, Italy)
 Chair: C. Pantelides, I. Cameron

Topic 1 - KL1.2
Christian Latgé
 (CEA, France)
 Chair: J. Grievink, P. Vacher

Topic 6 - KL 6.1
Sandro Macchietto
 (Imperial College, UK)
 Chair: E. Kondili (tbc), S. Jullian

11:20 **Oral sessions**

Topic 4 - Session 4.2 - Multiscale Modelling
 Chair: C. Pantelides, I. Cameron

Topic 1 - Session 1.3 - New Approaches in Process Synthesis & Design
 Chair: J. Grievink, P. Vacher

Topic 6 - Session 6.2 - New Energy Sources and Systems
 Chair: E. Kondili (tbc), S. Jullian

12:40 Lunch

Room Rhône 1

CACE editorial board meeting

Room Rhône 3

Audit. Pasteur

Room Rhône 2

14:00 **Oral sessions**

Topic 2 - Session 2.3 - Online Application of Process Models
 Chair: Y. Creff, S.B. Jorgensen

Topic 5 - Session 5.2 - Quality Assurance & Agile Process Operation
 Chair: G. Henning, A. Kraslawski

Topic 3 - Session 3.3 - NLP, MILP, MINLP Optimisation
 Chair: P. Floquet, J. Jezowski

EURECHA

15:20 **Poster session 2 & coffee break**

IEP group meeting

16:40 **Oral sessions**

Topic 7 - Session 7.1 - CAPE in Education
 Chair: X. Joulia, H. Matos

Topic 1 - Session 1.4 - Plantwide & Network Synthesis
 Chair: E.S. Yoon (tbc), Z. Kravanja

Topic 6 - Session 3.4 - New Computational and Numerical Strategies
 Chair: S. Pistikopoulos, P. Verheijen

18:00
 19:00 Bus departure to the Manoir de la Garde

20:00
 23:00 Gala dinner

23:00 Bus departure to Lyon

WEDNESDAY 4 JUNE

8:30

Registration

Audit. Pasteur

9:00

Plenary lecture - Topic 6 - PL 6.1*Luc Nougier (IFP, France)*

Chair: C. Oller do Nascimento, G. Reklaitis

9:40

Plenary lecture - Topic 4 - PL 4.1*Jürgen Auersperg (Micromaterials Center Berlin Fraunhofer Institute IZM, Germany)*

Chair: C. Oller do Nascimento, G. Reklaitis

10:20

Coffee break

Room Rhône 3

Audit. Pasteur

Room Rhône 2

10:40

Oral sessions

Topic 2 - Session 2.4 - Fault Detection and Loss Prevention

Chair: S-H. Hsu, A. Espuna

Topic 4 - Session 4.3 - Physical Property Modelling

Chair: C. Jallut, A. Gorak

Topic 5 - Session 5.3 - Information Technologies for Supporting Engineering Design

Chair: S. Déchelotte, R. Srinivasan

11:40

Ideas - Brainstorming Session

A. Kraslawski, R. Gani

Oral sessions

Topic 4- Session 4.4 - Dynamic Simulation

Chair: J.M. Le Lann, S. Macchietto

Topic 1 - Session 1.5 - Pharmaceutical & Bio Products

Chair: D. Bogle, F. Maréchal

12:40

Lunch

14:00

Oral sessions

Topic 2 - Session 2.5 - Process Monitoring & Data Validation

Chair: H. Preisig, H. Arellano-García

Topic 4 - Session 4.5 - Computational Fluid Dynamics

Chair: I. Mujtaba, N. Menshutina

Topic 1 - Session 1.6 - Process Scheduling

Chair: L. Puigjaner, T. Zhelev

Audit. Lumière

15:00

Best paper & best poster awards - Long term achievement award by A. Kraslawski

15:40

ESCAPE 18 assessment by W. Marquardt

16:00

ESCAPE 19 and PSE 2009 presentations by J. Thullie

16:20

Closing ceremony by B. Braunschweig and X. Joulia

16:30

THURSDAY 5 JUNE

9:00

IFP pilot plants visits

IFP-Lyon
Rond-point de l'échangeur de Solaize (Solaize)

11:30

PROGRAMME

SUNDAY 1 JUNE

09:30 Registration

10:00 **CAPE WP workshop** (members only) Room Rhône 2
Information session, part 1

11:00 Break

11:15 **CAPE WP workshop** (members only) Room Rhône 2
Information session, part 2

12:30 Lunch Room Rhône 3

14:00 **CAPE WP meeting** (members only) Room Rhône 2
Business meeting

17:00

17:40 ESCAPE 18 registration opening

18:00 Welcome Cocktail

ROOM RHÔNE 2

MONDAY 2 JUNE

08:30 Registration

09:00 **Opening Ceremony**

Auditorium Lumière

Sophie Jullian, IFP Director
Didier Caudron, IEP President
Andrzej Kraslawski, CAPE-WP President
Bertrand Braunschweig and Xavier Joulia, ESCAPE 18 Co-chairmen

09:20 **EFCE PhD Award in CAPE**

Auditorium Lumière

Chance Constrained Optimization of Process Systems under Uncertainty
Harvey Arellano-Garcia (Berlin Institute of Technology, Germany)

EFCE.1

09:40 **Plenary Lecture - Topic 5 - Cape for the users**

Auditorium Lumière

Chair: Tahir I. Malik (United Kingdom),
Wolfgang Marquardt (Germany)

Design and Integration of Policies to Achieve Environmental Targets
Rene Banares-Alcantara (University of Oxford, United-Kingdom)

PL5.1

10:20 Coffee Break

10:40 **Keynote Lecture - Topic 1 - Off-Line Systems**

Auditorium Pasteur

Chair: Rafiqul Gani (Denmark),
Claire Adjiman (United Kingdom)

Chemical Product Engineering - The Third Paradigm
Michael Hill (M Hill & Associates, LLC Mahwah, USA)

KL1.1

11:20 **Session 1.1 - Topic 1 - Off-Line Systems**

Auditorium Pasteur

Integrated Product / Process Design

Chair: Rafiqul Gani (Denmark),
Claire Adjiman (United Kingdom)

S1.1

11:20 *Expicient Interaction Prediction: Application of the Purdue Ontology for Pharmaceutical Engineering (POPE)*

M Hailemariam*, B Suresh, S Akkisetty, S Joglekar, S-H Hsu, R Morris, V Reklaitis, K Basu,
V Venkatasubramanian (Purdue University, USA)

11:40 *Integrated Design of Solvent-Based Extractive Separation Processes*

P Lek-Utaiwan*, B Suphanit¹, N Mongkolsiri², R Gani³

1 : King Mongkut's University of Technology, Thailand | 2 : SCG Chemicals Co., Ltd., Thailand | 3 : Technical University of Denmark

10:00

AUDIT. PASTEUR

Model of the Product Properties for Process Synthesis

P Bongers (Unilever R&D, The Netherlands)

12:20

A Population Balance Model Approach for Crystallization Product Engineering via Distribution Shaping Control

ZK Nagy (Loughborough University, United-Kingdom)

10:40

Keynote Lecture - Topic 4 - Integrated and multiscale modelling and simulation

Room Rhône 3

Chair: Thokozani Majози (South Africa),
Sauro Pierucci (Italy)

Modelling Reactions in Heterogeneous Catalysis from a Quantum Chemical Approach

Philippe Sautet (ENS Lyon, France)

KL4.1

11:20

Session 4.1 - Topic 4 - Integrated and multiscale modelling and simulation - Process Modelling & Simulation

Room Rhône 3

Chair: Thokozani Majози (South Africa),
Sauro Pierucci (Italy)

S4.1

ROOM RHÔNE 3

11:20

Biodiesel Production by Heat-Integrated Reactive Distillation

A Kiss (Akzo Nobel Chemicals, The Netherlands)

11:40

Absorption of Aromatic Hydrocarbons in Multicomponent Mixtures: a Comparison of Simulations and Measurements in a Pilot Plant

*D Richter^{*1}, H Thielert², G Wozny¹*

1 : Berlin University of Technology, Germany | 2 : UHDE GmbH, Germany

12:00

Energy-Preserving Method for Spatial Discretization: Application to an Adsorption Column

A Baaiu^{}, F Couenne, L Lefevre, Y Le Gorrec (University of Lyon 1, France)*

12:20

Enhanced Modelling and Integrated Simulation of Gasification and Purification Gas Units Targeted to Clean Power Production

M Perez-Fortes^{}, A Bojarski, S Ferrer-Nadal, G Kopanos, JM Nougues, E Velo, L Puigjaner (Technical University of Catalonia, Spain)*

10:40

Keynote Lectures - Topic 3 - Computational & numerical solutions strategies

Room Rhône 2

Chair: Bertand Braunschweig (France),
Eric Fraga (United-Kingdom)

Expanding Process Modelling Capability through Software Interoperability Standards: Application, Extension and Maintenance of CAPE OPEN standards

Ray Dickinson (Shell Global Solutions International, The Netherlands)

KL3.1

ROOM RHÔNE 2

11:20 Session 3.1 - Topic 3 - Computational & numerical solutions strategies - New IT Approaches Room Rhône 2

 Chair: Bertrand Braunschweig (France),
Eric Fraga (United-Kingdom)

S3.1

11:20 *Benchmarking Numerical and Agent-Based Models of an Oil Refinery Supply Chain*
*K Van Dam*¹, A Adhitya², R Srinivasan², R Srinivasan², Z Lukszo¹*
1 : Delft University of Technology, The Netherlands | 2 : National University of Singapore
11:40 *A Framework for Analysis of Computational Load of CAPE Tools*
P Rolandi, A Cano (Process Systems Enterprise Ltd, United-Kingdom)*
12:00 *Using Grid Computing to Solve Hard Planning and Scheduling Problems*
A Sundaramoorthy, C Maravelias, MC Ferris (University of Wisconsin, USA)*
12:20 *Service-Oriented CAPE: A New Direction for Software Applications*
*I Stalker*¹, E Fraga², A Yang³, N Mehandjiev¹*
1 : University of Manchester, United-Kingdom | 2 : University College London, United-Kingdom | 3 : University of Newcastle, United-Kingdom
12:40 Lunch
14:00 Session 1.2 - Topic 1 - Off-Line Systems - Separation Process Synthesis & Design Auditorium Pasteur

 Chair: Xuan Meyer (France),
Ana Barbosa-Povoa (Brazil)

S1.2

14:00 *Optimal Column Sequencing Multicomponent Mixtures*
A Harwardt, S Kossack, W Marquardt (Aachen Univ, Germany)*
14:20 *New Configuration for Heteroazeotropic Batch Distillation: I. Feasibility Studies*
*P Lang¹, F Denes*¹, X Joulia²*
1 : BUTE, Hungary | 2 : Ensicet LGC, France
14:40 *Study of a Novel Heat Integrated Hybrid Pervaporation Distillation Process: Simulation and Experiments*
MT Del Pozo Gomez, P Ruiz Carreira, JU Repke, A Klein, G Wozny (Technical University of Berlin, Germany)*
15:00 *Performance Analysis and Optimization of Enantioselective Fractional Extraction with a Multistage Equilibrium Model*
*AB De Haan*¹, Nj Kuipers², M Steensma³*
1 : Eindhoven University of Technology, The Netherlands | 2 : University Twente Enschede, The Netherlands | 3 : Akzo Nobel Salt Bv, The Netherlands

ROOM RHÔNE 2

AUDIT. PASTEUR

ROOM RHÔNE 3	14:00	Session 2.1 - Topic 2 - On-Line Systems - Real Time Optimisation	Room Rhône 3
		Chair: Dominique Bonvin (Switzerland), Didier Caudron (France)	S2.1
	14:00	<i>Computer Aided Operation of Pipeless Plants</i> S Piana*, S Engell (Universität Dortmund, Germany)	
	14:20	<i>Real-Time Optimization via Adaptation and Control of the Constraints</i> A Marchetti, B Chachuat*, D Bonvin (EPFL, Switzerland)	
	14:40	<i>Predictive Optimal Management Method for the control of polygeneration systems</i> A Collazos, F Maréchal* (EPFL, Switzerland)	
15:00	<i>Using Kriging Models for Real-Time Process Optimization</i> MVC Gomes* ¹ , IDL Bogle ² , EC Biscaia Jr. ³ , D Odloak ⁴ 1 : Petróleo Brasileiro S.A., Brazil 2 : University College London, United-Kingdom 3 : Universidade Federal do Rio de Janeiro, Brazil 4 : Universidade de São Paulo, Brazil		

ROOM RHÔNE 2	14:00	Session 3.2 - Topic 3 - Computational and numerical solution strategies - Large Scale Systems	Room Rhône 2
		Chair: Guido Buzzi-Ferraris (Italy), Mordechai Shacham (Israel)	S3.2
	14:00	<i>An Implementation of Parallel Computing for Hierarchical Logistic Network Design Optimization Using PSO</i> Y Shimizu*, H Kawamoto (Toyohashi Univ. of Technology, Japan)	
	14:20	<i>Large-Scale Nonlinear Programming Strategies for the Operation of LDPE Tubular Reactors</i> V Zavala*, L Biegler (Carnegie Mellon University, USA)	
	14:40	<i>A Model Reduction-Based Optimisation Framework for Large-Scale Simulators Using Iterative Solvers</i> I Bonis*, C Theodoropoulos (University of Manchester, United-Kingdom)	
15:00	<i>The Solution of Very Large Non-Linear Algebraic Systems</i> D Manca*, G Buzzi-Ferraris (Politecnico di Milano, Italy)		

15:20	Poster Session 1 & Coffee break	Poster Exhibition Area
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16:40

Session 5.1 - Topic 5 - Cape for the users - Decision & Management Support

Auditorium Pasteur

Chair: Sylvie Cauvin (France),
Rafael Batres (Japan)

S5.1

16:40

Support of Strategic Business Decisions at BASF's Largest Integrated Production Site Based On Site-Wide Verbund Simulation

S Brüggemann*¹, N Bauer¹, E Fuchs¹, A Polt¹, B Wagner¹, M Wulkow²
1 : BASF AG, Germany | 2 : CIT GmbH, Germany

17:00

A Compliance Management System for the Pharmaceutical Industry

J Fisher¹, A Aldea¹, R Banares-Alcantara*²
1 : Oxford Brookes University, United-Kingdom | 2 : University of Oxford, United-Kingdom

17:20

Business Process Model for Knowledge Management in Plant Maintenance

T Fuchino*¹, Y Shimada², M Miyazawa³, Y Naka¹
1 : Tokyo Institute of Technology, Japan | 2 : National Institute of Occupational Safety and Health, Japan | 3 : Mitsubishi Chemical Corporation, Japan |

17:40

Decision Support for Control Structure Selection During Plant Design

J Oldenburg*¹, Hj Pallasch¹, C Carroll², V Hagenmeyer¹, S Arora¹, K Jacobsen¹, J Birk¹, A Polt¹, P Van Den Abeel³
1 : BASF, Germany | 2 : Cornell University, USA | 3 : BASF, Belgium

AUDIT. PASTEUR

ROOM RHÔNE 3

16:40

Session 2.2 - Topic 2 - On-Line Systems - Model Predictive & Intelligent Control

Room Rhône 3

Chair: Marie-Véronique Le Lann (France),
Sébastien Engell (Germany)

S2.2

16:40

A combined Balanced Truncation and Multi-Parametric Programming approach for Linear Model Predictive Control

D Narciso*, E Pistikopoulos (Imperial College London, United-Kingdom)

17:00

Comparison of Model Predictive Control Strategies for the Simulated Moving Bed

A Dietz, JP Corriou* (ENSIC, France)

17:20

Analysis Of The Constraint Characteristics Of A Sheet Forming Control Problem Using Interval Operability Concepts

F Lima¹, C Georgakis*¹, J Smith², P Schnelle²
1 : Tufts University, USA | 2 : Dupont Engineering Research and Technology, USA

17:40

Optimal Control of Batch Processes Using Particle Swam Optimisation with Stacked Neural Network Models

F Herrera, J Zhang* (Newcastle University, United-Kingdom)

13

16:40

Session 6.1 - Topic 6 - CAPE and Society - Environmentally Conscious Design

Room Rhône 2

Chair: Arsène Isambert (France),
Paul Serban Agachi (Romania)

S6.1

16:40

Economic Analysis and Process Integration of Hydrogen Production Strategies
W Yuan*, N Sammons Jr, K Mcglocklin, M Eden (Auburn University, USA)

17:00

Integrated Gasification Combined Cycle (IGCC) Process Simulation and Optimization
F Emun*, M Gadalla, L Jiménez Esteller (University Rovira I Virgili, Spain)

17:20

Design of Sustainable Processes: Systematic Generation & Evaluation of Alternatives
A Carvalho*, A Carvalho², R Gani², H Matos¹
1 : Instituto Superior Técnico de Lisboa, Portugal | 2 : Tech. Univ. of Denmark

17:40

IDEF0 Activity Modeling for Integrated Process Design Considering Environmental, Health and Safety (EHS) Aspects
M Hirao*¹, H Sugiyama², U Fischer², K Hungerbuehler²
1 : University of Tokyo, Japan | 2 : ETH, Switzerland

18:00

End of the sessions

ROOM RHÔNE 2

08:30 Registration

09:00 **Plenary Lecture - Topic 7 - Cape in education**

Auditorium Pasteur

Chair: Chunghun Han (Republic of Korea),
Georges Heyen (Belgium)

Innovative Pedagogies for Enhanced Graduate Attributes in CAPE

Ian Cameron (University of Queensland, Australia) and Daniel Lewin (Tech. Univ, Israel)

PL7.1

09:40 **Plenary Lecture - Topic 2 - On-Line Systems**

Auditorium Pasteur

Chair: Chunghun Han (Republic of Korea),
Georges Heyen (Belgium)

Model Parameterization Tailored to Real-time Optimization

Benoit Chachuat¹, Bala Srinivasan², Dominique Bonvin¹

1 : Ecole Polytechnique Fédérale de Lausanne, Switzerland | 2 : Ecole Polytechnique de Montréal, Canada

PL2.1

10:20 Coffee Break

10:40 **Keynote Lecture - Topic 1 - Off-Line Systems**

Auditorium Pasteur

Chair: Johan Grievink (The Netherlands),
Philippe Vacher (France)

Simulation in nuclear engineering design

Christian Latgé (CEA, France)

KL1.2

11:20 **Session 1.3 - Topic 1 - Off-Line Systems - New Approaches in Process Synthesis & Design**

Auditorium Pasteur

Chair: Johan Grievink (The Netherlands),
Philippe Vacher (France)

S1.3

11:20 ***Development of a Novel Petri Net Tool for Selection of Process Design Based on Inherent Safety Assessment Method***

F Moradi, PA Bahri (Murdoch University, Australia)*

11:40 ***Uncertainty Patterns and Sensitivity Analysis of an Indicator Based Process Design Framework***

S Papadokostantakis, S Agarwal^R, H Sugiyama¹, K Hungerbühler¹*

1 : Swiss Federal Institute of Technology, Switzerland | 2 : Indian Institute of Technology, India

12:00 ***The Application of a Task-Based Concept for the Design of Innovative Industrial Crystallizers***

R Lakerveld, HJM Kramer, PJ Jansens, J Grievink (Delft University of Technology, The Netherlands)*

12:20

AUDIT. PASTEUR

Systematic Design of Production Processes for Enantiomers with Integration of Chromatography and Racemisation Reactions*M Kaspereit*, J Garcia Palacios, T Meixús Fernández, A Kienle**1 : Max Planck Institute for Dynamics of Complex Technical Systems, Germany | 2 : Otto Von Guericke University, Germany*

10:40

Keynote Lecture - Topic 4 - Integrated and multiscale modelling and simulation

Room Rhône 3

Chair: Costas Pantelides (United Kingdom),
Ian Cameron (Australia)**Multiscale Molecular Modeling: a Tool for the Design of Nano Structured Materials***Maurizio Fermeglia (Universita Degli Studi Trieste, Italy)*

KL4.2

11:20

ROOM RHÔNE 3

Session 4.2 - Topic 4 - Integrated and multiscale modelling and simulation - Multiscale Modelling

Room Rhône 3

Chair: Costas Pantelides (United Kingdom),
Ian Cameron (Australia)

S4.2

11:20

Brownian Dynamics and Kinetic Monte Carlo Simulation in Emulsion Polymerization*HF Hernandez*, K Tauer (Max Planck Institute of Colloids and Interfaces, Germany)*

11:40

A Comprehensive Population Balance Model of Emulsion Polymerisation for PSD & MWD: Comparison to Experimental data*SJ Sweetman*, CD Immanuel¹, TI Malik², S Emmett², N Williams²**1 : Imperial College London, United-Kingdom | 2 : ICI Wilton Applied Research, United-Kingdom*

12:00

Rapid Process Design and Development of Complex Solution Copolymers*Y Dar*, TI Malik (ICI Wilton Applied Research, United-Kingdom)*

12:20

Shape – The Final Frontier*X Wang, C Ma, K Roberts (University of Leeds, United-Kingdom)*

10:40

ROOM RHÔNE 2

Keynote Lectures - Topic 6 - CAPE and Society

Room Rhône 2

Chair: Emilia Kondili (Greece) (tbc),
Sophie Jullian (France)**Sustainable Energy Futures, and what we can do about it***Sandro Macchietto (Imperial College, London, United-Kingdom)*

KL6.1

11:20 Session 6.2 - Topic 6 - CAPE and Society - New Energy Sources & Systems Room Rhône 2

Chair: Emilia Kondili (Greece) (tbc),
Sophie Jullian (France)

S6.2

11:20 A Prototype Agent-Based Modeling Approach for Energy System Analysis
*B-M Hodge**, *S Aydogan-Cremaschi*, *G Blau*, *J Pekny*, *GV Reklaitis* (Purdue University, USA)**11:40 Design of Heat-integrated Power Systems with Decarbonisation**
X Zheng, *F Kim**, *J Smith* (University of Manchester, United-Kingdom)**12:00 A Methodology for Designing and Evaluating Biomass Utilization Networks**
*N Ayoub**, *H Seki*, *Y Naka* (Tokyo Institute of Technology, Japan)**12:20 A Systematic Framework for Biorefinery Production Optimization**
*N Sammons**¹, *W Yuan*¹, *M Eden*¹, *B Aksoy*², *H Cullinan*²
1 : Auburn University, USA | 2 : Alabama Center for Paper and Bioresource Engineering, USA**12:40 Lunch****14:00 Session 5.2 - Topic 5 - CAPE for the users - Quality Assurance & Agile Process Operation** Auditorium Pasteur

Chair: Gabriela Henning (Argentina),
Andrzej Kraslawski (Finland)

S5.2

14:00 Process Analytical Technologies (PAT) - the Impact for Process Systems Engineering
*Z Chen*¹, *D Lovett*², *J Morris*^{3*}
1 : University Glasgow, United-Kingdom | 2 : Daresbury Innovation Centre, United-Kingdom | 3 : Newcastle University, United-Kingdom**14:20 Practical Challenges In Developing Data-Driven Soft Sensors For Quality Prediction**
J Liu^{1*}, *R Srinivasan*¹, *R Srinivasan*², *PN Selvaguru*³
1 : Institute of Chemical and Engineering Sciences, Singapore | 2 : National University of Singapore | 3 : Singapore Refining Company**14:40 Troubleshooting and Process Optimisation by Integrating CAPE Tools and Six Sigma Methodology**
G Dünnebieer (Bayer Technology Services, Germany)**15:00 Production-Line Wide Dynamic Bayesian Network Model for Quality Management in Papermaking**
*A Ropponen**, *R Ritala* (Tampere University of Technology, Finland)

ROOM RHÔNE 2

AUDIT. PASTEUR

14:00 **Session 2.3 - Topic 2 - On-Line Systems - Online Application of Process Models** Room Rhône 3

Chair: Yann Creff (France),
Sten Bay Jorgensen (Denmark)

S2.3

14:00 *Towards On-Line Model-Based Design of Experiments*

F Galvanin, M Barolo, F Bezzo (University of Padova, Italy)*

14:20 *Model Reduction Techniques for Dynamic Optimization of Chemical Plants Operation*

B Dorneanu, CS Bildea, J Grievink (Delft University of Technology, The Netherlands)*

14:40 *Fault Diagnosis and Identification System Applied to a Non-invasive Biosensor of Blood Glucose*

*M Basualdo*¹, Z. David², A. Rigalli²*

1 : UIIN-FRRO, Rosario, Argentina | 2 : UNR, Rosario, Argentina

15:00 *Online LQG Stabilization of Unstable Gas-Lifted Oil Wells*

E Jahanshahi, K Salahshoor, R Kharrat (Petroleum University of Technology, Iran)*

ROOM RHÔNE 3

14:00 **Session 3.3 - Topic 3 - Computational and numerical solution strategies - NLP, MILP, MINLP Optimisation** Room Rhône 2

Chair: Pascal Floquet (France),
Jacek Jezowski (Poland)

S3.3

14:00 *MILP-based Decomposition Method for the Optimal Scheduling of an Industrial Batch Plant*

*P Castro*¹, A Novais¹, A Carvalho²*

1 : DMS/INETI, Portugal | 2 : Hovione Loures, Portugal

14:20 *Rigorous Flowsheet Optimization using Process Simulators and Surrogate Models*

*J Caballero*¹, I Grossmann²*

1 : University of Alicante, Spain | 2 : Carnegie Mellon University, USA

14:40 *Multi-Operations Time-Slots Model for Crude-Oil Operations Scheduling*

*S Mouret*¹, IE Grossmann¹, P Pestiaux²*

1 : Carnegie Mellon University, USA | 2 : Total, France

15:00 *Optimum Experimental Design for Key Performance Indicators*

*S Körkel*¹, H Arellano-García², J Schöneberger², G Wozny²*

1 : Humboldt-Universität, Germany | 2 : Berlin Technische Universität, Germany

ROOM RHÔNE 2

15:20 **Poster Session 2 & Coffee break** Poster Exhibition Area

16:40	Session 1.4 - Topic 1 - Off-Line Systems - Plantwide & Network Synthesis	Auditorium Pasteur
	Chair: En Sup Yoon (Republic of Korea) (tbc), Zdravko Kravanja (Slovenia)	S1.4
16:40	Supply Chain Risk Management through HAZOP and Dynamic Simulation <i>A Adhitya*¹, R Srinivasan¹, I Karim²</i> <i>1 : Institute of Chemical and Engineering Sciences, Singapore 2 : National University of Singapore</i>	
17:00	A New Approach to the Design of Multicomponent Water/ Wastewater Networks <i>D Faria, M Bagajewicz* (University of Oklahoma, USA)</i>	
17:20	Synthesis of Cryogenic Energy Systems <i>X Del Nogal, J Kim*, R Perry, Smith (University of Manchester, United-Kingdom)</i>	
17:40	Effect of Catalytic Reactor Design on Plantwide Control Strategy: Application to Vam Plant CS Bildea*¹, A Dimian² <i>1 : Delft University of Technology, The Netherlands 2 : University of Amsterdam, The Netherlands</i>	
16:40	Session 7.1 - Topic 7 - CAPE in education	Room Rhône 3
	Chair: Xavier Joulia (France), Henrique Matos (Portugal)	S7.1
16:40	What is "IN" and What is "OUT" in Engineering Problem Solving <i>M Shacham*¹, M Cutlip², N Brauner³</i> <i>1 : Ben-Gurion University of the Negev, Israel 2 : University of Connecticut, USA 3 : Tel-Aviv University, Israel</i>	
17:00	CAPE Tools in Biotechnology: Why, When, What, Who. Which Ones and Where? <i>L Jiménez Esteller*, I Katakis, A Fabregat, T Schafer, S Rodriguez, JM Mateo, M Giamberini, B Rivera, P Argüeso, E Calero, L Vico, F Hernandez, R Genc, M Medir, JR Alabart, G Guillén-Gosálbez (University Rovira I Virgili, Spain)</i>	
17:20	Development of Sustainable Energy Systems: A New Challenge for Process Systems Engineering Education <i>C Azzaro-Pantel*¹, C Gourdon¹, X Joulia¹, JM Le Lann¹, S Astier², G Fontes², M David², A Ayache²</i> <i>1 : ENSIACET INPT-LGC, France 2 : ENSEIHT INPT, France</i>	
17:40	Enhancing the Understanding and Insights of Students and Industry Operators in Process Engineering Principles via Immersive 3D Environments <i>C Norton¹, I Cameron*¹, C Crosthwaite¹, N Balliu², M Tade², D Shallcross³, A Hoadley⁵, G Barton⁴, J Kavanagh⁴</i> <i>1 : University of Queensland, Australia 2 : Curtin University of Technology, Australia 3 : University of Melbourne, Australia 4 : University of Sydney, Australia 5 : Monash University, Australia</i>	

16:40

**Session 3.4 - Topic 3 - Computational and numerical solution strategies -
New Computational & Numerical Strategies**

Room Rhône 2

Chair: Stratos Pistikopoulos (United Kingdom),
Peter Verheijen (The Netherlands)

S3.4

16:40

Biclustering of Data Matrices in Systems Biology via Optimal Re-Ordering

*P Dimaggio¹, S McAllister¹, C Floudas^{*1}, XJ Feng², J Rabinowitz², H Rabitz² (Princeton University, USA)*

17:00

*Inductive Data Mining: Automatic Generation of Decision Trees from Data for QSAR
Modelling and Process Historical Data Analysis*

FC Ma, F Buontempo, X Wang (University of Leeds, United-Kingdom)*

17:20

*Optimization of WWTP Control by Means of Multi-Objective Genetic Algorithms and
Sensitivity Analysis*

*B Beraud^{*1}, C Lemoine¹, E Latrille², JP Steyer²*

1 : Veolia Environnement, France | 2 : INRA, France

17:40

Design of Constrained Nonlinear Model Predictive Control Based on Global Optimisation

*M Cizniar^{*1}, M Cizniar², M Fikar², MA Latif¹*

1 : CNRS – ENSIC Nancy, France | 2 : Slovak University of Technology, Slovakia

ROOM RHÔNE 2

18:00

End of the sessions

19:00

Bus departure to the Manoir de la Garde

20:00

Gala Dinner

23:00

Return by bus to the hotels around the Centre de Congrès de Lyon

08:30 Registration

09:00 **Plenary Lecture - Topic 6 - Cape and Society** Auditorium Pasteur

Chair: Claudio Oller Do Nascimento (Brazil),
Gintaras Reklais (USA)

Computational Chemical Engineering Modeling Applied to Energy and Reactor Design

Luc Nougier (IFP, France)

PL6.1

09:40 **Plenary Lecture - Topic 4 - Integrated and multiscale modelling and simulation** Auditorium Pasteur

Chair: Claudio Oller Do Nascimento (Brazil),
Gintaras Reklais (USA)

Challenges for multi-scale modeling of multiple failure modes in microelectronics

Jürgen Auersperg (Micromaterials Center, Germany)

PL4.1

10:20 Coffee Break

10:40 **Session 4.3 - Topic 4 - Integrated and multiscale modelling and simulation - Physical Property Modelling** Auditorium Pasteur

Chair: Christian Jallut (France),
Andrzej Gorak (Germany)

S4.3

10:40 *Modeling the Phase Equilibria of Nitriles by the soft-SAFT Equation of State*
*A Belkadi*¹, MK Hadj-Kali¹, V Gerbaud¹, X Joulia¹, F Llovel², L F Vega²*

1 : Université de Toulouse, France | 2 : Institut de Ciència de Materials de Barcelona, Spain

11:00 *Prediction of Partition Coefficients Between Food Simulants and Packaging Materials Using Molecular Simulation and a Generalized Flory Huggins Approach*

O Vitrac, G Gillet (INRA, France)*

11:20 *MEXA Goes CAMD - Computer-Aided Molecular Design for Physical Property Model Building*

*A Bardow*², S Kossack¹, E Kriesten¹, W Marquardt¹*

1 : Aachen University, Germany | 2 : Delft University, The Netherlands

10:40 **Session 2.4 - Topic 2 - On-Line Systems - Fault Detection & Loss Prevention** Room Rhône 3

Chair: S-H. Hsu (USA),
Antonio Espuña (Spain)

S2.4

10:40 *Sensor Placement for Fault Detection and Localization*

C Gerkens*, G Heyen (Université de Liege, Belgium)

11:00 *Fault Detection and Isolation Based on the Model-Based Approach : Application on Chemical Processes*

N Olivier-Maget*, G Hetreux, JM Le Lann, MV Le Lann (Université de Toulouse, France)

11:20 *Optimization of Preventive Maintenance Scheduling in Processing Plants*

D Nguyen, M Bagajewicz* (University of Oklahoma, USA)

ROOM RHÔNE 3

10:40 **Session 5.3 - Topic 5 - CAPE for the users - Information Technologies for Supporting Engineering Design** Room Rhône 2

Chair: Stéphane Déchelotte (France),
Rajagopalan Srinivasan (Singapore)

S5.3

10:40 *OntoCAPE 2.0 – a (Re-)Usable Ontology for Computer-Aided Process Engineering*

J Morbach, A Wiesner*, W Marquardt (Aachen University, Germany)

11:00 *A Generic Scientific Information Management System for Process Engineering*

S Cauvin*, M Barbieux, L Carrie, B Celse (IFP, France)

11:20 *OntoMODEL: Ontological Mathematical Modeling Knowledge Management*

P Suresh*¹, G Joglekar¹, S-H Hsu¹, P Akkisety¹, L Hailemariam¹, A Jain², G Reklaitis¹,
V Venkatsubramanian¹

1 : Purdue University, USA | 2 : United Airlines, USA

ROOM RHÔNE 2

11:40 **Session 4.4 - Topic 4 - Integrated and multiscale modelling and simulation - Dynamic Simulation** Auditorium Pasteur

Chair: Jean-Marc Le Lann (France),
Sandro Macchietto (United Kingdom)

S4.4

11:40 *Modeling of Catalytic Hydrogen Generation from Sodium Borohydride*

A Gonçalves*¹, P Castro¹, A Novais¹, C Rangel¹, H Matos²

1 : INETI Lisbon, Portugal | 2 : UTL/IST Lisbon, Portugal

12:00 *An Integrated Framework for Model-Based Flow Assurance in Deepwater Oil & Gas Production*

E Luna-Ortiz*¹, P Lawrence², CC Pantelides², CS Adjiman¹, CD Immanuel¹

1 : Imperial College London, United-Kingdom | 2 : Process Systems Enterprise Ltd., United-Kingdom

AUDIT. PASTEUR

12:20

PASTEUR

Towards a New Generation Heat Exchanger Models*G Haarlemmer*¹, J Pigourier²**1 : RSI, France | 2 : Axens, France*

11:40

Session 1.5 - Topic 1 - Off-Line Systems - Pharmaceutical & Bio Products Room Rhône 2Chair: David Bogle (United Kingdom),
François Maréchal (France)

S1.5

11:40

ROOM RHÔNE 2

Cell Cycle Modelling for Off-Line Dynamic Optimisation of Mammalian Cultures*CM Lam*, K Sriyudthsak, C Kontoravdi, K Kothari, HH Park, EN Pistikopoulos, A Mantalaris*
(Imperial College London, United-Kingdom)

12:00

Population Balance Modeling of Influenza Virus Replication in MDCK Cells During Vaccine Production*T Müller*¹, J Schulze-Horse², Y Sidorenko², U Reich², A Kienle¹**1 : Otto Von Guericke Universität, Germany | 2 : Max Planck Institut für Dynamik Komplexer Technischer Systeme, Germany*

11:40

RHÔNE 3

Ideas - Brainstorming Session

Room Rhône 3

Chair: Andrzej Kraslawski (Finland),
Rafiqul Gani (Denmark)

12:40

Lunch

14:00

Session 4.5 - Topic 4 - Integrated and multiscale modelling and simulation - Computational Fluid Dynamics

Auditorium Pasteur

Chair: Iqbal Mujtaba (United Kingdom),
Natalia Menshutina (Russia)

S4.5

14:00

AUDIT. PASTEUR

Modelling and Simulation of a Membrane Microreactor Using Computational Fluid Dynamics*P Chasanis*¹, EY Kenig¹, V Hesse², S Schmitt²**1 : University of Dortmund, Germany | 2 : Institut für Mikrotechnik Mainz GmbH, Germany*

14:20

Modelling Comparison of High Temperature Fuel Cell Performances: Electrochemical Behaviours of SOFC and PCFC*J-M Klein*, J Deseure (LEPMI, France)*

14:40

Application of a Digital Packing Algorithm to Cylindrical Pellet-Packed Beds*R Caulkin*, A Ahmad, M Fairweather, X Jia, R Williams (University of Leeds, United-Kingdom)*

23

14:00 **Session 2.5 - Topic 2 - On-Line Systems - Process Monitoring & Data Validation** Room Rhône 3

Chair: H. Preisig (Norway),
H. Arellano-Garcia (Germany)

S2.5

14:00 *Off-line design of PAT* systems for on-line applications*

R Singh, K Gernaey, R Gani (Technical University of Denmark)*

14:20 *Estimation of a Class of Stirred Tank Bioreactors with Discrete-Delayed Measurements*

H Hernández-Escoto, R Aguilar-López², MI Neria-González², AR Domínguez-Bocanegra²*

1 : Universidad de Guanajuato, Mexico | 2 : Instituto Politécnico Nacional, Mexico

14:40 *A Mathematical Programming Framework for Optimal Model Selection/Validation of Process Data*

BP Duarte, MJ Moura¹, FJ Neves², NM Oliveira³*

1 : Polytechnic School of Engineering, Portugal | 2 : CUF – Químicos Industriais S.A., Portugal | 3 : University of Coimbra, Portugal

ROOM RHÔNE 3

14:00 **Session 1.6 - Topic 1 - Off-Line Systems - Process Scheduling** Room Rhône 2

Chair: Luis Puigjaner (Spain),
Toshko Zhelev (Ireland)

S1.6

14:00 *A Novel Network-based Continuous-time Formulation for Process Scheduling*

D Gimenez¹, G Henning, C Maravelias²*

1 : Universidad Nacional del Litoral, Argentina | 2 : University of Wisconsin, USA

14:20 *Batch Scheduling with Intermediate Due Dates Using Timed Automata Models*

S Subbiah, T Tometzki, S Engell (Universität Dortmund, Germany)*

14:40 *A Decomposition Approach to Short-Term Scheduling of Multi-Purpose Batch Processes*

N Trautmann, R Fink², H Sagebieß², C Schwindt²*

1 : University of Bern, Switzerland | 2 : Clausthal University of Technology, Germany

ROOM RHÔNE 2

15:00	Best paper and best poster awards Long term achievement award	Auditorium Lumière
	Andrzej Kraslawski (Finland)	
15:40	ESCAPE 18 assessment	Auditorium Lumière
	Wolfgang Marquardt (Germany)	
16:00	ESCAPE 19 and PSE 2009 presentations	Auditorium Lumière
	Jan Thullie (Poland)	
16:20	Closing ceremony	Auditorium Lumière
	Bertrand Braunschweig and Xavier Joulia (France)	
16:30	End of the 18th European Symposium on Computer Aided Process Engineering	

THURSDAY 5 JUNE

- 08:30 Bus departure from the congress center to IFP-Lyon
-
- 09:00 **IFP pilot plants visit** (upon registration only)
IFP-Lyon - Rond-point de l'échangeur de Solaize (Solaize)
-
- 11:30 Bus to Lyon-Perrache railway station and to the airport
-

NOTES

LIST OF POSTERS

The posters will be displayed from 2 to 4 June.

Topic 1 - Off-Line Systems

- P001** *Combined Nitrogen and Phosphorus Removal: Model Based Process Optimization*
N Alasino*, M Mussati, N Scenna, P Aguirre (INGAR Instituto de Desarrollo y Diseño (CONICET-UTN), Argentina)
-
- P002** *A Systematic Procedure for Optimizing Crude Oil Distillation Systems*
H Alhammedi* (University of Bahrain)
-
- P003** *Integrated Design and Control of Processes Coupling Exothermic and Endothermic Reactions*
P Altimari, CS Bildea* (Delft University of Technology, the Netherlands)
-
- P004** *A Study on Naphtha Catalytic Reforming Reactor Simulation and Analysis*
R Alves*, F Menten, R Guardani, C Nascimento (University of São Paulo, Brazil)
-
- P005** *Computer Aided Modeling of an Extractive Fermentation Process for Bioethanol Production: Outlook for Development of Reaction-Separation Process*
RR Andrade*, EC Rivera, DIP Atala, R Maciel Filho, F Maugeri Filho, AC Costa (State University of Campinas, Brazil)
-
- P006** *Evaluation of Pervaporation Process for Recovering a Key Orange Juice Flavour Compound: Modeling and Simulation*
WA Araujo, MET Alvarez, EB Moraes*, MR Wolf Maciel (State University of Campinas, Brazil)
-
- P007** *A Microeconomics-Based Approach to Product Design under Uncertainty*
C Whitnack, A Heller, M Bagajewicz* (University of Oklahoma, USA)
-
- P008** *Model Predictive Control Based Planning in the Fruit Industry*
A Blanco¹, G Masini², N Petracci¹, A Bandoni*¹
1 : Plapiqui (UNS-CONICET), Argentina | 2 : Universidad Nacional del Comahue, Argentina
-
- P009** *Representation of Residue Curve Maps with Pinch Zones*
J Bone*¹, M-I Galan¹, J Costa¹, X-M Meyer², M Meyer², AE Plesu³
1 : University of Barcelona, Spain | 2 : INPT-ENSIACET, France | 3 : University Politehnica of Bucharest, Romania
-
- P010** *A Heat Transfer Model of an Ice Cream Single Screw Extruder*
P Bongers*¹, I Campbell²
1 : Unilever R&D, The Netherlands | 2 : Unilever R&D, United-Kingdom
-
- P011** *Compensation of Inlet Flowrate Fluctuations in Offshore Downstream Sections. Control Algorithm and Performance Evaluation*
G Bomard*¹, E Verbrugge³, H Khatib²
1 : CNRS, GIPSA Lab, France | 2 : RSI, France | 3 : Total, France

- P012** *Computer Aided Polymer Design using Group Contribution plus Property Models*
K Chelakara Satyanarayana*, J Abildskov, R Gani (Technical University of Denmark)
- P013** *Enhanced Algebraic Property Clustering Techniques for Molecular Synthesis*
N Chemmangattuvalappil*, C Solvason¹, F Eljack², M Eden¹
1 : Auburn University, USA | 2 : Qatar University, Qatar
- P014** *Optimize Process Condensate Reusing System for Ammonia Plant by the Synthesis of MEN*
L Chen*, J Du¹, Z Gao¹, P Yao¹, WD Seider²
1 : Dalian University of Technology, China | 2 : University of Pennsylvania, USA
- P015** *Supply Chain Design Considering Plants Performance*
G Corsano*, J Montagna (INGAR, CONICET, Argentina)
- P016** *A Reverse Engineering Approach to Design Oriented Properties Polymers*
MC Costa*, AL Jardini, AF Romão, MR Wolf Maciel, R Maciel Filho (State University of Campinas, Brazil)
- P017** *Entrainer-Based Reactive Distillation versus Conventional Reactive Distillation for the Synthesis of Fatty Acid Esters*
M de Jong*, A Dimian², A de Haan¹
1 : Eindhoven University of Technology, The Netherlands | 2 : University of Amsterdam, The Netherlands
- P018** *Mathematical Modeling for the Crystalization Process of Hydroxiapatite from Bera-Whitlockite*
VR Dejeu*, R Barabas, A Pop, E Bogya, A Imre, PS Agachi (University Babes-Bolyai, Romania)
- P019** *New Configuration for Heteroazeotropic Batch Distillation: II. Rigorous Simulation Results*
F Denes*, P Lang¹, G Modla¹, X Joulia²
1 : Bute, Hungary | 2 : ENSIACET LGC, France
- P020** *Studying Extractive Distillation Processes Using Optimization*
AM Emhamed, B Czuczai, E Rév, Z Lelkes* (Budapest University of Technology and Economics, Hungary)
- P021** *Optimization of Caustic Treatment Processes of Zeolite's Sorbents*
A Ermakov, D Dvoretzky*, S Dvoretzky (Tambov State Technical University, Russia)
- P022** *Supply Chain Optimization with Homogenous Product Transport Constraints*
T Farkas¹, Z Valentinyi*², E Rév³, Z Lelkes³
1 : Optasoft KFT, Hungary | 2 : Provimi Pet Food, Hungary | 3 : Bute, Hungary
- P023** *A Sensitivity Analysis on Optimal Solutions Obtained for a Reactive Distillation Column*
R Filipe*, S Hauan², H Matos³, A Novais⁴
1 : Instituto Superior de Engenharia de Lisboa, Portugal | 2 : Carnegie Mellon University, USA | 3 : Instituto Superior Técnico, Portugal | 4 : Instituto Nacional de Engenharia, Tecnologia e Inovação, Portugal
- P024** *Optimal CO Clean-up Reactors Design. Modeling and Optimization Aspects.*
J Francesconi*, D Oliva, M Mussati, P Aguirre (INGAR - Instituto de Desarrollo y Diseño (CONICET-UTN), Argentina)
- P025** *Synthesis of Zero Effluent Multipurpose Batch Processes using Effective Scheduling*
J Gouws*, T Majozi (University of Pretoria, South Africa)

- P026** *Modeling Phase Change in Heat Exchanger Network Synthesis*
MMF Hasan^{*1}, IA Karimi¹, H Alfadala²
1 : National University of Singapore | 2 : Qatar University, Qatar
-
- P027** *Design of a Syngas Infrastructure*
PM Herder^{*}, RM Stikkelman, GPJ Dijkema, AF Correlje (Delft University of Technology, The Netherlands)
-
- P028** *Implementation of a Reactive Dividing Wall Distillation Column in a Pilot Plant*
R Sandoval-Vergara¹, of Barroso-Muñoz¹, H Hernandez-Escoto¹, JG Segovia-Hernandez¹, S Hernandez^{*1}, V Rico-Ramírez²
1 : Universidad de Guanajuato, Mexico | 2 : Instituto Tecnológico de Celaya, Mexico
-
- P029** *Systematic Design of Chemical Conversion Processes*
M Hillestad^{*} (NTNU, Norway)
-
- P030** *Optimization of a Bio-ethanol Purification Process Using Conceptual Design and Simulation Tools*
P Hoch¹, J Espinosa^{*2}
1 : Plapiqui-UNS-CONICET, Argentina | 2 : INGAR-CONICET, Argentina
-
- P031** *Improvement of Operating Procedures through the Reconfiguration of a Plant Structure*
S Hoshino^{*}, H Seki, T Sugimoto, Y Naka (Tokyo Institute of Technology, Japan)
-
- P032** *Energy-Efficient Synthesis of Distillation Sequences*
S Jain, J Kim^{*}, R Smith (University of Manchester, United-Kingdom)
-
- P033** *Superstructure Optimization for the Optimal Design of Petroleum Refinery Topology with Environmental Considerations*
CS Khor^{*1}, A Loh¹, TA Elkamel², Albahri³
1 : Universiti Teknologi Petronas, Malaysia | 2 : University of Waterloo, Canada | 3 : Kuwait University
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- P034** *Graph-theoretic Approach to Optimal Synthesis of Supply Networks: Distribution of Gasoline from a Refinery*
Y Kim¹, LT Fan², C Yun¹, SB Park¹, S Park^{*1}, B Bertok³, F Friedler³
1 : KAIST, Republic of Korea | 2 : Kansas State University, USA | 3 : University of Pannonia, Hungary
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- P035** *Addressing Robustness for Crude Oil Scheduling under Uncertainty*
J Li, Ia Karimi^{*}, R Srinivasan (National University of Singapore)
-
- P036** *Feasibility Study of Diethyl Carbonate Synthesis by Equilibrium Limited Consecutive Reactions in Batch Reactive Distillation*
T Lukacs^{*1}, C Steger¹, M Meyer², E Rev¹, Z Lelkes¹
1 : BME, Hungary | 2 : INPT-ENSIACET LGC, France
-
- P037** *Optimal Design and Operation of Multivessel Batch Distillation Column with Fixed Product Demand and Strict Product Specifications*
M Mahmud¹, I Mujtaba¹, M Emtir^{*2}
1 : University of Bradford, United-Kingdom | 2 : Libyan Petroleum Institute, Libya

- P038** *Interfacial and Bulk Thermal Conductivity from Dynamic Temperature Profiles on One Side of Sample*
Z Zeng*, T Malik (ICI Wilton Applied Research Group, United-Kingdom)
- P039** *Enterprise-Wide Optimization under Tight Supply Contracts and Purchase Agreements*
F Manenti, D Manca (Politecnico di Milano, Italy)
- P040** *Entrainer Selection for Pressure Swing Batch Distillation*
G Modla*, P Lang, Kopasz (Bute, Hungary)
- P041** *Heterogeneous Kinetics and Residue Curve Map Determination for Ethyl tert-Butyl Ether Synthesis via Reactive Distillation Using Ion Exchange Resin Catalysts*
U Muhammad*, AR Saleemi, M Faheem, S Qaiser (University of Engineering & Technology, Pakistan)
- P042** *Optimizing FCC Units to Get Maximum Benefits via Metamodeling Approach*
G Navas, A Uribe*, O Guerra, S Montagut (Instituto Colombiano del Petroleo, Colombia)
- P043** *An Integrated Framework for Operational Scheduling of a Real-World Pipeline Network*
S Boschetto*, L Felizani¹, L Yamamoto¹, L Magatão¹, S Stebel¹, F Neves-Jr¹, L Arruda¹, R Lüders¹, P Ribas², L Bernardo²
1 : Federal University of Technology, Brazil | 2 : Petrobras – CENPES, Brazil
- P044** *An Optimization Framework of Multibed Pressure Swing Adsorption Systems*
D Nikolic*, M Georgiadis, E Kikkinides (University of Western Macedonia, Greece)
- P045** *Product Portfolio Management with Discrete-Event Simulation and Genetic Algorithms*
JL Perez-Escobedo*, A Aguilar-Lasserre², C Azzaro-Pantel¹, L Pibouleau¹, S Domenech¹
1 : ENSIACET INPT, France | 2 : Instituto Tecnológico de Orizaba, Mexico
- P046** *Numerical Analysis and Measurements Comparison of Flow Distribution Impact on a Plate-Fin Heat Exchanger Performance.*
F Picard*(1, 2), G Bergin¹, G Temoin¹, D Averous¹
1 : Nordon Cryogenie SA, France | 2 : Laboratoire de Genie Chimique - UMR 5503, France
- P047** *Multi-Objective Design of Multipurpose Batch Facilities Using Economic Assessments*
TR Pinto*, AP Barbósa-Póvoa², AQ Novais¹
1 : INETI, Portugal | 2 : CEG – IST, Portugal
- P048** *Oil Products Pipeline Scheduling with Tank Farm Inventory Management*
S Relvas*, HA Matos², AP Barbosa-Póvoa¹, J Fialho³
1 : CEG – IST, Portugal | 2 : CPQ – IST, Portugal | 3 : CLC, Portugal
- P049** *Role of Discrete Simulation in Refinery Offsites Design*
RR Rieubon* (TECHNIP, France)
- P050** *Finding Batch Extractive Distillation Product Sequence from Thermodynamic Insight*
I Rodriguez-Donis*, V Gerbaud, X Joullia (Laboratoire de Génie Chimique - UMR 5503, France)
- P051** *Methodology of Conceptual Process Synthesis for Process Intensification*
BG Rong*, E Kolehmainen, I Turunen (Lappeenranta University of Technology, Finland)

- P052** *Chemical Unit Start-up: from control strategy design to operators training*
A Roussillon* (Rhodia, France)
-
- P053** *Process Plant Knowledge Based Simulation and Design*
JB Savkovic-Stevanovic*, SB Krstic¹, MG Milivojevic¹, MB Perunicic²
1 : University of Belgrade, Serbia and Montenegro | 2 : University of Novi Sad, Serbia and Montenegro
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- P054** *Optimal Experimental Design of a Catalytic Fixed Bed Reactor*
J Schoeneberger¹, H Arellano-Garcia¹, H Thielert*², S Koerke³, G Wozny¹
1 : Berlin University of Technology, Germany | 2 : UHDE GMBH, Germany | 3 : Humboldt Universitaet, Germany
-
- P055** *Integrating Laboratory Experiments with Process Simulation for Reactor Optimization*
J Seay*¹, H Werhan¹, M Eden², R D'alexandro¹, T Thomas⁴, H Redlingshoefer³, C Weckbecker³, K Huthmacher³
1 : Degussa Corporation, USA | 2 : Auburn University, USA | 3 : Degussa GmbH, Germany | 4 : University of South Alabama, USA
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- P056** *Study of Arrangements for Distillation of Quaternary Mixtures Using Less than N- 1 Columns*
D.M Méndez-Valencia¹, M Vázquez-Ojeda¹, J.G Segovia-Hernández*¹, H Hernández Escoto¹, A Bonilla-Petriciolet²
1 : Universidad de Guanajuato, Mexico | 2 : Instituto Tecnológico de Aguascalientes, Mexico
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- P057** *A Hybrid Meta-heuristic Method for Logistics Optimization Associated with Production Planning*
Y Shimizu*, Y Yamazaki, T Wada (Toyohashi Univ. of Technology, Japan)
-
- P058** *Visual Mixture Design Using Property Clustering*
C Solvason*¹, FT Eljack(1, 2), N Chemmangattuvalappil¹, M Eden¹
1 : Auburn University, USA | 2 : Qatar University, Qatar
-
- P059** *Generalization of Feasibility Analysis and Conceptual Design Methods for Reactive Distillation to the Case of Multireaction Systems*
CS Steger*, R Thery, D Rouzineau, X Meyer, M Meyer (CNRS LGC, France)
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- P060** *Development Planning for Offshore Oilfield Infrastructure Under Gradual Uncertainty Resolution*
B Tarhan*, I Grossmann (Carnegie Mellon University, USA)
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- P061** *Model Based Scale-Up of Affinity Membrane Adsorbers*
P Van Beijeren*¹, P Kreis¹, M Mutter², S Sommerfeld², W Bäcker², A Górák¹
1 : Universität Dortmund, Germany | 2 : Bayer Technology Services, Germany
-
- P062** *The Role of Financial Engineering Techniques in Supply Chain Risk Management – Emerging Opportunities*
V Varma¹, G Reklaitis*²
1 : Air Products & Chemicals Inc, USA | 2 : Purdue University, USA
-
- P063** *An Investment Planning Model for Stepwise Capacity Expansions of Chemical Plants*
A Wiesner*¹, M Schlege¹, J Oldenburg², L Würth¹, R Hannemann¹, A Polt²
1 : Aachen University, Germany | 2 : BASF, Germany

P064 *Divided Wall Distillation Column Dynamic Modelling and Control*
A Woinaroschy*, R Isopescu (University Politehnica of Bucharest, Romania)

Topic 2 - On-Line Systems

P065 *Process Monitoring in Chemical Industries - A Hidden Markov Model Approach*
G Almeida*, S Park (University of Sao Paulo, Brazil)

P066 *Nonlinear Dynamics and Control of the Monolithic Loop Reactor for Fischer-Tropsch Synthesis*
P Altimari*, CS Bildea, J Van Ommen, J Grievink (Delft University of Technology, The Netherlands)

P067 *Monitoring Batch Polymerization Using Cumulative Amount Changes*
C Alvarez*, A Brandolín¹, M Sánchez¹, L Puigjaner²
1 : Plapiqui, Argentina | 2 : Universitat Politècnica de Catalunya, Spain

P068 *Robust (Adaptative) Dynamic Data Reconciliation and Gross Error Estimation for Unknown Error Distribution Based on the Generalized T Distribution*
D Aragón*, P.A Roland², J.A Romagnoli¹
1 : Louisiana State University, USA | 2 : Process Systems Enterprise Ltd, United-Kingdom

P069 *New Method for Sensor Network Design and Upgrade for Optimal Process Monitoring*
M Bagajewicz*, D Nguyen, S Kumar Sugumar (University of Oklahoma, USA)

P070 *Fault Diagnosis and Identification System Applied to a Non- invasive Biosensor of Blood Glucose*
M Basualdo*, D Zumoffen², A Rigallí³
1 : UTN-FRRO, Argentina | 2 : CIFASIS-CONICET-UNR, Argentina | 3 : Facultad de CS. Médicas- CONICET-UNR, Argentina

P071 *Validation of an Ice Cream Factory Operations Model*
P Bongers*, B Bakker (Unilever R&D, The Netherlands)

P072 *A Functional Systems Approach To the Development of Improved Hazard Identification for Advanced Diagnostic Systems*
I Cameron*, B Seligmann¹, K Hangos², E Nemeth², R Lakner³
1 : University of Queensland, Australia | 2 : Hungarian Academy of Sciences, Hungary | 3 : University of Pannonia, Hungary

P073 *A Novel Proactive-Reactive Scheduling Approach in Chemical Multiproduct Batch Plants*
E Capon*, G Kopanos, A Bonfill, A Espuna, L Puigjaner (Politechnic University of Cataluña, Spain)

P074 *Model Predictive Control of the Waste Water Treatment Plant Based on the Benchmark Simulation Model No.1 - BSM1*
VM Cristea*, C Pop, PS Agachi (Babes-Bolyai University, Romania)

P075 *Load Balancing Control System of a Furnace from Atmospheric Distillation Unit*
P Cristian*, M Sanda (Petroleum-Gas University of Ploiesti, Romania)

- P076** *Optimal Operation of Sublimation Time of the Freeze Drying Process by Predictive Control: Application of the MPC@CB Software*
N Daraoui*, P Dufour, H Hammouri, A Hottot (Université Lyon 1, France)
- P077** *Novel Parametric and Non-Parametric Approach for the Online and Real-Time Evaluation of the Variability of an Effluent (EVE)*
O Daniel*, MP Denieul, C Lemoine, M Coste (Veolia Environnement R&D, France)
- P078** *Improving Steady-State Identification*
G Le Roux*, B Faccini Santoro¹, F Falla Sotelo¹, M Teissier², X Joulia²
1 : Universidade de Sao Paulo, Brazil | 2 : Ecole Nationale Supérieure d'Ingenieurs en Arts Chimiques et Technologiques, France
- P079** *Dynamic Behaviour of the CSTR: A Thermodynamic Point of View*
A Favache*, D Dochain¹, B Maschke²
1 : Université Catholique de Louvain, Belgium | 2 : Université Lyon 1, France
- P080** *Application of Adaptive Neurofuzzy Control Using Software Sensors to Continuous Distillation*
J Fernandez de Canete*, P del Saz, S Gonzalez-Perez (University of Malaga, Spain)
- P081** *Correlation-Based Just-in-Time Modeling for Soft-Sensor Design*
K Fujiwara*, M Kano, S Hasebe (Kyoto University, Japan)
- P082** *Closed-Loop Control of Restart-up of Anaerobic USBF Reactors after Short Stops*
C García, F Molina, EF Carrasco*, JM Lema, E Roca (University of Santiago de Compostela, Spain)
- P083** *Grey-Box Modelling of an Industrial Hydrodesulphurization Process*
E Gomez¹, C de Prada*, D Sarabia¹, C Mendez², S Cristea¹, JM Sola³, E Unzueta³
1 : University of Valladolid, Spain | 2 : INTEC, Argentina | 3 : Petronor, Spain
- P084** *Optimal Management of Hydrogen Supply and Consumption Networks of Refinery Operations*
C Méndez*, E Gómez¹, D Sarabia¹, J Cerdá², C de Prada¹, J Sola³, E Unzueta³
1 : Universidad de Valladolid, Spain | 2 : INTEC, Argentina | 3 : Petronor, Spain
- P085** *Output-Feedback Control of a High Temperature Homopolymerization Reactor*
H Hernández-Escoto*, S Hernández-Castro, JG Segovia-Hernández (Universidad de Guanajuato, Mexico)
- P086** *Multi-Agent Control System of a Kraft Recovery Boiler*
I Herrera*, S Park (University of São Paulo, Brazil)
- P087** *A Heuristic for the Short-Term Planning of Multi-Purpose Continuous Plants*
S Hermann*, C Schwindt (Clausthal University of Technology, Germany)
- P088** *Diagnosis of Chemical Processes by Fuzzy Clustering Methods: New Optimisation Method of Fuzzy Partitions*
C Isaza, MV Le Lann*, J Aguilar-Martín (University of Toulouse, France)

- P089** *Near-Optimal Operation of an Evaporator using Self-Optimizing Control*
*V Kariwala¹, Y Cao^{*2}*
1 : Nanyang Technological University, Singapore | 2 : Cranfield University, United-Kingdom
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- P090** *Comparison of Features in Classifying Steel Surface Quality*
*D Kim^{*1}, JJ Liu², C Han¹*
1 : Seoul National University, Republic of Korea | 2 : Samsung Electronics Asan, Republic of Korea
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- P091** *Data Reconciliation for Industrial Processes*
L Krishnan-Dumitrescu^{}, W El Osta, C Laigneau (TECHNIP, France)*
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- P092** *Integrating Strategic, Tactical and Operational Supply Chain decision levels in a Model Predictive Control Framework*
JM Lainez^{}, GM Kopanos, M Badell, A España, L Puigjaner (Universitat Politècnica de Catalunya, Spain)*
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- P093** *Optimization and Control for Real Time Integration of the Biotechnological Process of Acrylic Acid Synthesis: A Two-Layer Approach Using Model Predictive Control Application*
*B.H Lunelli¹, D.N Melo¹, E.C Vasco de Toledo², MR Wolf Maciel¹, R. Maciel Filho^{*1}*
1 : State University of Campinas, Brazil | 2 : Petrobras SA, Paulínia Refinery, Brazil
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- P094** *Hybrid Strategy for Real Time Optimization with Feasibility Driven for a Large Scale Three Phase Catalytic Slurry Reactor*
*DNC Melo¹, A.P Mariano¹, E.C Vasco de Toledo², C.B Costa¹, R. Maciel Filho^{*1}*
1 : State University of Campinas (Unicamp), Brazil | 2 : Petrobras SA, Paulínia Refinery, Brazil
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- P095** *Diagnosis of Hybrid Systems Coupling Classification Method and Dynamic Hybrid Simulation*
A Mokhtari, MVLe Lann^{}, G Hétreux, JM Le Lann (University of Toulouse, France)*
-
- P096** *Determination of Apparent Kinetic Parameters by Simulation of Anaerobic Digestion Processes Using Pulse OLR Disturbances*
F Molina, C García, EF Carrasco^{}, E Roca, JM Lema (University of Santiago de Compostela, Spain)*
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- P097** *Improving the Representation of Process Information in Multi-Label Fault Diagnosis Systems*
I Monroy^{}, G Escudero, M Graells (Universitat Politècnica de Catalunya, Spain)*
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- P098** *Adaptive Control of Simultaneous Saccharification - Fermentation Process from Starch to Ethanol (SSFSE)*
*S Ochoa^{*1}, V Lyubenova², J-U Repke¹, M Ignatova², G Wozny¹*
1 : Technical University of Berlin, Germany | 2 : Bulgarian Academy of Sciences, Bulgaria
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- P099** *Advanced Control Monitoring in Petrobras' Refineries: Quantifying Economic Gains in a Real-Time Basis*
R Pinotti^{}, AC Zanin, LFL Moro (Petrobras, Brazil)*
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- P100** *Comparative Analysis of Robust Estimators on Nonlinear Dynamic Data Reconciliation*
DM Prata, JC Pinto, EL Lima^{} (Universidade Federal do Rio de Janeiro, Brazil)*
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- P101** *Model-Based Monitoring of a Non-Uniform Batch in a Freeze-Drying Process*
V Rasetto^{}, D Marchisio, D Fissore, A Barresi (Politecnico di Torino, Italy)*

- P102** *State Estimation for Dynamic Prediction of Hydrate Formation in Oil and Gas Production Systems*
J Rodriguez*, CS Adjiman, CD Immanuel (Imperial College London, United-Kingdom)
- P103** *RCS for Process Control: Is There Anything New Under the Sun?*
M Rodriguez*, R Sanz (ASLAB-UPM, Spain)
- P104** *A Real-Time Optimisation Engine for Nonlinear Model-Based Optimising Control of Large-Scale Systems*
P Rolandi*¹, J Romagnoli²
1 : Process Systems Enterprise Ltd, United-Kingdom | 2 : Louisiana State University,, USA
- P105** *Data Treatment and Analysis for On-Line Dynamic Process Optimization*
NPG Salau*, G Tonel, JO Trierweiler, AR Secchi (Federal University of Rio Grande do Sul, Brazil)
- P106** *On-Line System Identification and Control with the Extended Kalman Filter*
R Scheffer*¹, R Maciel²
1 : Huntsman, Belgium | 2 : UNICAMP, Brazil
- P107** *Process Real-Time Optimization using Evolutionary Improvement Algorithm*
K Seunghyok*, C Seungjune, Y En Sup (Seoul National University, Republic of Korea)
- P108** *Fault Isolation and Fault Intensity Estimation based on SDG, SVM and PCA*
BS Shin¹, G Lee*², CJ Lee¹, C Han¹, ES Yoon¹
1 : Seoul National University, Republic of Korea | 2 : Chungju National University, Republic of Korea
- P109** *Nonlinear Model Predictive Control of a Swelling Constrained Industrial Batch Reactor*
L Simon*¹, Z Nagy², K Hungerbuehler¹
1 : ETH Zurich, Switzerland | 2 : Loughborough University, United-Kingdom
- P110** *An adapted SLAB Model Using Sensor Data for the Prediction on the Dispersion of Hazardous Gas Releases*
W So*¹, D Shin², Es Yoon¹
1 : Seoul National University, Republic of Korea | 2 : Myongji University, Republic of Korea
- P111** *Real-Time Optimization for Large Scale Processes: Control of an Autorefrigerated CSTR Polymerization Reactor*
E.C Vasco de Toledo¹, DNC Melo², A.P Mariano², R. Maciel Filho*²
1 : Petrobras SA, Paulinia Refinery, Brazil | 2 : State University of Campinas, Brazil
- P112** *Nonlinear Identification and Model Based Control of An Oil Well Drilling Process*
M Vega*¹, C Sheid¹, L Caçada¹, M Mancini¹, A Martins²
1 : Universidade Federal Rural do Rio de Janeiro, Brazil | 2 : CENPES/Petrobras, Brazil
- P113** *Hybrid Fault Diagnosis for Large Chemical Plants Under Control*
D Zumoffen¹, M Basualdo*²
1 : CIFASIS-CONICET-UNR, Argentina | 2 : UTN-FRRO, Argentina

Topic 3 - Computational & Numerical Solutions Strategies

- P114** *Robust and Efficient Implementation of Strategies for Chemical Engineering Regression Problems*
V. Alvarez*, R. Maduro, M. Aznar (State University of Campinas, Brazil)
-
- P115** *Identifiability Analysis and Optimization-Based State and Parameter Estimation in Bioreactor*
H Arellano-García*, G Wozny (Berlin University of Technology, Germany)
-
- P116** *Process Simulation & Optimization Sequential modular approach or global approach? and why not both?*
P Baudet*, P Castelain, O Baudouin (Prosim SA, France)
-
- P117** *Simulis® Thermodynamics: an open framework for users and developers*
O Baudouin*, S Dechelotte, P Guittard, A Vacher (Prosim SA, France)
-
- P118** *New Approach for Chemical Transfer Reaction Model*
Z Benjelloun-Dabaghi*, R Cadours, S Cauvin-Delaide, P Mougín (IFP, France)
-
- P119** *Global Optimization of an Aggregated GDP Model for Distillation Sequences*
M Bergamini¹, P Aguirre²
1 : LPC - FI - UBA - CONICET, Argentina | 2 : INGAR - CONICET, Argentina
-
- P120** *Modeling and Simulation of the Particle Size Distribution for Emulsion Polymerization in a Tubular Reactor*
A Bouaswaig*, W Mauntz, S Engell (Universität Dortmund, Germany)
-
- P121** *Bidirectional Branch and Bound Approach for Controlled Variable Selection*
Y Cao*¹, V Kariwala²
1 : Cranfield University, United-Kingdom | 2 : Nanyang Technological University, Singapore
-
- P122** *Biofiltration of VOCS in the Natural Bed- Modelling Verification*
K Chmiel-Kurowska*, M Palica, L Kurowski, J Thullie (Silesian University of Technology, Poland)
-
- P123** *Composite Zeolite Membranes Characterization by Using a Transient State Experimental Technique and a Parameter Estimation Procedure*
L Courthial¹, A Baudot¹, M Tayakout-Fayolle¹, C Jallut²
1 : IFP-Lyon, France | 2 : Université Lyon 1, France
-
- P124** *Modified Outer Approximation Algorithm for Optimizing Complex Distillation Processes*
B Czuczaj*, T Farkas, E Rév, Z Lelkes (Budapest University of Technology and Economics, Hungary)
-
- P125** *MPC@CB Software : A Solution for Model Predictive Control*
B Da Silva*, P Dufour, N Sheiba Othman, S Othman (University Lyon 1, France)
-
- P126** *Reduction of Computational Load Associated with the Integration of Dae Systems*
SC de Graaf*¹, P Kittilsen¹, HA Preisig²
1 : Cybernetica As, Norway | 2 : Norwegian University of Science and Technology, Norway

- P127** *An Initialization Procedure for Steady-State Models. Example: Distillation Column*
I Dones*, H Preisig (NTNU, Norway)
-
- P128** *Parallel Simulation of Molten Carbonate Fuel Cells*
M Dosta*¹, M Mangold¹, A Kienle², V Svjatnyj³
1 : Max Planck Institute for Dynamics of Complex Technical Systems, Germany | 2 : Otto-Von-Guericke-University, Germany | 3 : National Technical University of Donetsk, Ukraina
-
- P129** *Detection of Multiple Structural Changes in Linear Processes Through Change Point Analysis and Bootstrapping*
B Duarte*¹, P Saraiva²
1 : Instituto Superior de Engenharia de Coimbra, Portugal | 2 : University of Coimbra, Portugal
-
- P130** *Improvement of the Computational Performance of STN/RTN Formulations for Short-Term Scheduling of Multipurpose Batch Plants*
GA Durand, JA Bandoni* (Plapiqui (UNS) – CONICET, Argentina)
-
- P131** *Development of Mechanistic Models for UASB and UAF Pulsed Anaerobic Digesters*
A Franco, C García, EF Carrasco*, E Roca (University of Santiago de Compostela, Spain)
-
- P132** *Modeling of Anaerobic Bioreactors Oriented to Optimization. Solutions for IPDAE Systems*
M Fuentes Mora*, MC Mussati, NJ Scenna, PA Aguirre (Ingar Instituto de Desarrollo Y Diseño - CONICET-UTN, Argentina)
-
- P133** *Applications of Grey Programming to Process Design*
E Galvez¹, E Galvez³, L Cisternas*(2, 3), PS Patino², KL Ossandon²
1 : Universidad Católica del Norte, Chile | 2 : Universidad de Antofagasta, Chile | 3 : Centro de Investigación Científica y Tecnológica para la Minería, Chile
-
- P134** *Algorithmic Methods for the Optimal Lumping of Analytical Data for Compositional Studies*
M Georgiadis*¹, L Papageorgiou²
1 : University of Western Macedonia, Greece | 2 : University College London, United-Kingdom
-
- P135** *Tearing for Parallelization and Control of Sparsity in Process Flowsheeting*
P Greppi* (Genova Università Degli Studi, Italy)
-
- P136** *Flexible and Configurable MILP-Models for Meltshop Scheduling Optimization*
I Harjunkoski*, G Sand (ABB Corporate Research, Germany)
-
- P137** *Novel Convex Underestimators and their Application to the Synthesis of Combined Reaction Distillation Processes*
M Jach¹, A Kienle*², D Michaels¹, R Weismantel¹
1 : Otto-Von-Guericke-Universität, Germany | 2 : Max-Planck-Institut für Dynamik Komplexer Technischer Systeme, Germany
-
- P138** *Multiobjective Optimization of a Liquid-Feed Direct Methanol Fuel Cell*
I Jeong*, J Kim, J Kim, I Moon (Yonsei University, Republic of Korea)
-
- P139** *Functional Data Analysis for the Development of a Calibration Model for Near-infrared Data*
C Jiang*, E Martin (Newcastle University, United-Kingdom)

- P140** *Optimization of Ideal Petlyuk Sequences Using a Multi Objective Genetic Algorithm with Constraints*
A Jiménez-Gutiérrez¹, C Gutiérrez-Antonio^{*1}, A Briones-Ramírez²
1 : Instituto Tecnológico de Celaya, Mexico | 2 : Innovación Integral de Sistemas S.A. de C.V., Mexico
-
- P141** *Application of Global Sensitivity Analysis to Biological Models*
A Kiparissides*, M Rodríguez-Fernandez, S Kucherenko, A Mantalaris, E.N Pistikopoulos (Imperial College London, United-Kingdom)
-
- P142** *Development of a Sophisticated Framework for Complex Single- and Multi-Objective Optimization Tasks*
M Leipold^{*1}, S Gruetzmann¹, G Fieg¹, D Maschmeyer², J Sauer³, H Wiederhold³
1 : Hamburg University of Technology, Germany | 2 : Oxeno GmbH, Germany | 3 : Degussa GmbH, Germany
-
- P143** *Towards Resilient Supply Chains: Uncertainty Analysis Using Fuzzy Mathematical Programming*
K Mitra¹, R Gudi^{*2}, S Patwardhan², G Sardar¹
1 : Tata Consultancy Services Limited, India | 2 : Indian Institute of Technology, India
-
- P144** *Product Data Quality in the Vaccine Industry, Model-Driven Architecture for Interoperability Between Information Systems*
N Moalla^{*(1, 2)}, A Bouras¹, Y Ouzrout¹, G Neubert¹
1 : LIESP Laboratory, France | 2 : Sanofi Pasteur, France
-
- P145** *IBM Global Engineering Solutions delivers collaborative innovation for competitive advantage*
O Multon*, L Nouzarede (IBM, France)
-
- P146** *Modelling of Optimal Investment Policies for the Multiperiod Retrofitting of Chemical Plants*
Z Novak Pintaric*, Z Kravanja (University of Maribor, Slovenia)
-
- P147** *Modelling and Identification of the Bio-Ethanol Production Process from Starch: Cybernetic vs Unstructured Modelling Approaches.*
S Ochoa^{*1}, A Yoo², J-U Repke¹, G Wozny¹, D.R Yang²
1 : Technical University of Berlin, Germany | 2 : University of Korea, Republic of Korea
-
- P148** *Multi-Objective Optimization of Polygeneration Systems Integrated in District Heating and Cooling Networks*
J Ortiga*, JC Bruno, A Coronas (Universitat Rovira I Virgili, Spain)
-
- P149** *New Method of Stochastic Optimization on Example of Cyclic Reactor of Thin Organic Synthesis*
D Dvoretzky*, S Dvoretzky¹, E Peshkova¹, G Ostrovsky²
1 : Tambov State Technical University, Russia | 2 : Karpov Institute of Physical Chemistry, Russia
-
- P150** *Upstream Simulation Lifecycle*
D Paen^{*1}, P Roux², A Ricordeau³, A Vacher⁴, M Gainville²
1 : RSJ, France | 2 : IFP, France | 3 : Total, France | 4 : PROSIM, France

- P151** *Calculation of Critical Points in Reactive Mixtures Using a Global Optimization Approach*
F Sánchez-Mares¹, A Bonilla-Petriciolet^{*1}, JG Segovia-Hernández², JC Tapia-Picazo¹, A Ponsich³
1 : Instituto Tecnológico de Aguascalientes, Mexico | 2 : Universidad de Guanajuato, Mexico | 3 : Instituto Tecnológico Autónomo de México
-
- P152** *Particle Swarm Optimisation in Heat Exchanger Network Synthesis Including Detailed Equipment Design*
A Silva¹, M Ravagnani¹, E Biscua Jr.^{*2}
1 : Universidade Estadual de Maringá, Brazil | 2 : PEQ/COPPE/UFRJ, Brazil
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- P153** *A Priori Regression Analysis for the Calibration of Complex Dynamic Models: Application to a Model of Antibiotic Production with S. Coelicolor*
G Sin^{*}, K Germaey (Technical University of Denmark)
-
- P154** *MILP-based Heuristic for the Optimal Design of Water Networks*
J Teles^{*}, P Castro, A Novais (DMS/INETI, Portugal)
-
- P155** *Comprehensive Evaluation of EKF, CEKF, and Moving Horizon Estimators for On-Line Processes Applications*
G Tonel, NP Salau^{*}, JO Trierweiler, AR Secchi (Federal University of Rio Grande do Sul, Brazil)
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- P156** *A Single Stage Approach for Designing Water Network with Multiple Contaminants*
K Walczyk, J Jezowski^{*} (Rzeszow University of Technology, Poland)
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- P157** *Modeling Piecewise Under- and Overestimators for Bilinear Process Network Synthesis via Mixed-integer Linear Programming*
DS Wicaksono^{*}, IA Karimi (National University of Singapore)

Topic 4 - Integrated and Multiscale Modelling and Simulation

- P158** *Dynamic Modelling of a Rotating Disk Contactor Using the Primary and Secondary Particle Method (PSPM)*
M Attarakih^{*1}, M Jarada², H Allaboun², HJ Bart³, N Faqir⁴
1 : Al-Balqa Applied University, Jordan | 2 : Jordan University of Science, Jordan | 3 : University of Kaiserslautern, Germany | 4 : University of Jordan
-
- P159** *Computational Fluid Dynamics : A tool to the formulation of therapeutic aerosols*
N Bardin-Monnier^{*}, V Falk, L Marchal-Heussler (LSGC - UPR CNRS 6811, France)
-
- P160** *Heat Exchanger Network (HEN) costs and performances estimation for multi-period operation*
R Bolliger, F Palazzi, F Marechal^{*} (Ecole Polytechnique Fédérale de Lausanne, Switzerland)
-
- P161** *A Study of Water Transport Phenomena in a Polymer Electrolyte Membrane Fuel Cell with 2D Steady-State Model*
H Chung^{*}, T Ha, S Cho, C Han (School of Chemical and Biological Engineering, Republic of Korea)

- P162** *A Stochastic Programming Approach for Clinical Trials Planning*
M Colvin, C Maravelias* (University of Wisconsin, USA)
-
- P163** *Modelling of Precipitation in Turbulent Flow via the Joint Species-Number Density PDF Method*
GY di Veroli*, S Rigopoulos (University of Manchester, United-Kingdom)
-
- P164** *Large Eddy Simulation of Particle Dispersion in a Straight, Square Duct Flow*
M Fairweather*, J Yao (University of Leeds, United-Kingdom)
-
- P165** *Test Bench Dimensioned by Specific Numerical Tool*
N Gascoin*, P Gillard¹, G Abraham¹, M Bouchez²
1 : LEES, France | 2 : MBDA-France
-
- P166** *Optimization of SOFC Interconnect Design Using Multiphysic Computation*
D Grondin*, J Deseure¹, M Zahid², M Jose Garcia², Y Bulte¹
1 : LEPMI, France | 2 : European Institute for Energy Research, Germany
-
- P167** *Multi-objective Scheduling for Environmentally-friendly Batch Operations*
I Halim*, R Srinivasan²
1 : Institute of Chemical and Engineering Sciences, Singapore | 2 : National University of Singapore
-
- P168** *Operability Analysis and Conception of Microreactor by Integration of Reverse Engineering and Rapid Manufacturing*
AL Jardim*, MC Costa, AR Bineli, AF Romão, R Maciel Filho (UNICAMP, Brazil)
-
- P169** *Use of a Heterogeneous Model for Hydrodynamic Simulation of Foam Monoliths*
J Jerez, L Duarte, I Ordóñez, R Martínez* (Universidad Industrial de Santander, Colombia)
-
- P170** *Modelling of Integrated Multiscale Process with Microdevices*
RV Tona Vásquez, L Jiménez Esteller* (University Rovira I Virgili, Spain)
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- P171** *Modeling of Honeycomb Monoliths by a Two-Dimensional and Multi-Channel Strategy*
J Jiménez, F Silva, I Ordóñez, R Martínez* (Universidad Industrial de Santander, Colombia)
-
- P172** *Multi-Scale Framework for Steam-Methane Reforming Reaction with in-Situ Adsorption*
A Kapil, S Bhat, J Sadhukhan, (Univ of Manchester, United-Kingdom)
-
- P173** *Optimisation with Energy Recovery for Oxidative Desulphurization of Heavy Gas Oil*
H Khalfalla¹, I Mujtaba*, M Elgarni², H Elakrami³
1 : University of Bradford, United-Kingdom | 2 : Libyan Petroleum Institute, Libya | 3 : Al-Fateh University, Libya
-
- P174** *Numerical Determination of Heat Transfer Coefficient for Nanofluids in Microchannels*
L Kurowski*, J Thullie, K Chmiel-Kurowska, G Dzido (Silesian University of Technology, Poland)
-
- P175** *Ion-Specific Potential of Mean Force Between Two Aqueous Proteins*
ERA Lima, FW Tavares, EC Biscaia Jr.* (UFRJ, Brazil)
-
- P176** *A Heteronuclear Group Contribution Method for Associating Chain Molecules (SAFT-Gamma)*
A Lympieriadis*, C.S Adjiman, A Galindo, G Jackson (Imperial College London, United-Kingdom)

- P177** *Morphological Population Balance for Modelling Shape Evolution of Crystals Grown From Solution*
C Ma, X Wang*, KJ Roberts (University of Leeds, United-Kingdom)
- P178** *An Analytical–Numerical Method for Solving a Heap Leaching Problem of One or More Solid Reactants from Porous Pellets*
M Mellado, L Cisternas* (CICITEM, Chile)
- P179** *Modeling of Polyvinyl Acetate Polymerization Process for Control Purposes*
T Miteva*¹, R Alvarez², N Hvala¹, D Kukanja³
1 : Jozef Stefan Institute, Slovenia | 2 : UPC, Spain | 3 : Mitol, Slovenia
- P180** *Image Based Characterization and Molecular Modeling of Line-Edge Roughness on Positive Resist*
R Mukherjee¹, A Palazoglu², J Romagnoli*¹
1 : Louisiana State University, USA | 2 : Davis Chemical Engineering & Materials Science, USA
- P181** *Thermodynamic Analysis and Properties Modeling of Thermochemical Processes for Massive Hydrogen Production*
J O'connell*¹, J Murphy¹, M Gorenssek², M Theis³
1 : University of Virginia, USA | 2 : Savannah River National Laboratory, USA | 3 : Clemson University, USA
- P182** *Thermochemical Multi-Phase Models Applying the Constrained Gibbs Energy Method*
R Pajarre*, P Blomberg, P Koukkari (VTT, Finland)
- P183** *Industrial Applications of the Multi-Phase Thermochemical Simulation*
R Pajarre*, P Koukkari, K Penttilä (VTT, Finland)
- P184** *Reactor Modeling for the Shenhua Direct Coal Liquefaction Project*
F Parmentier*¹, D de Gruy²
1 : RSI, France | 2 : Axens North America, USA
- P185** *Prediction of the Melting Point Temperature Using a Linear QSPR for Homologous Series*
I Paster¹, M Shacham*¹, N Brauner²
1 : Ben-Gurion University of the Negev, Israel | 2 : Tel-Aviv University, Israel
- P186** *A General Mathematical Model for a Moving Bed Gasifier*
S Pierucci*, E Ranzi (CMIC Politecnico di Milano, Italy)
- P187** *Modelling of an Hybrid Wastewater Treatment Plant*
MN Pons*¹, M Lourenco Da Silva¹, O Potier¹, E Arnos², P Battaglia²
1 : Nancy-University, France | 2 : GEMCEA, France
- P188** *Numerical Approach for the Enzymatic Elimination of Phenol in a Torus Reactor*
L Pramparo*¹, J Pruvost², F Stüber¹, J Font¹, A Fortuny³, A Fabregat¹, P Legentilhomme², J Legrand², C Bengoa¹
1 : University Rovira I Virgili, Spain | 2 : University Politècnica de Catalunya Vilanova I, Spain | 3 : Université de Nantes, France
- P189** *Three Principle Model Reductions Based on Time-Scale Considerations*
HA Preisig* (Norwegian University of Science and Technology, Norway)

- P190** *LNG Life Cycle Modelling*
R Coupier¹, F Rey^{*2}
1 : RSJ, France | 2 : TECHNIP, France
-
- P191** *Modelling Solids Transport in an Industrial Flighted Rotary Dryer*
M Sheehan*, O Ajayi, A Lee (James Cook University, Australia)
-
- P192** *Excipient Design for Protein Drug Formulation via Molecular Simulation and Computational Molecular Design*
S Shulda*, J Ashley, Y Li, E Topp, K Camarda (University of Kansas, USA)
-
- P193** *Dimension Reduction of Two-Dimensional Population Balances Based on the Quadrature Method of Moments*
A Voigt*, W Heineken², D Flockerk², K Sundmacher¹
1 : Ovg-University Magdeburg, Germany | 2 : Max-Planck-Institute for Dynamics of Complex Technical Systems, Germany
-
- P194** *Predictions of the Consequences of Natural Gas-Hydrogen Explosions Using a Novel CFD Approach*
RM Woolley¹, M Fairweather^{*1}, SAE Falle¹, JR Giddings²
1 : University of Leeds, United-Kingdom | 2 : Mantis Numerics Ltd, United-Kingdom
-
- P195** *Three Dimensional Multiphase Computations for the Characterizing the Counter-Current Flow Behavior*
Y Xu^{*1}, S Yuan², Ju Paschke¹, G Repke¹, J Wozny¹
1 : Technical University Berlin, Germany | 2 : Shanghai Jiao Tong University, China

Topic 5 - CAPE for the users!

- P196** *CAPE Methods and Tools for Systematic Analysis of New Chemical Product Design and Development*
R Alvarado-Morales*, N Al-Haque, KV Gernaey, JM Woodley, R Gani (Technical University of Denmark)
-
- P197** *A Graphical Approach for Hazard Identification*
R Batres^{*1}, T Suzuki¹, Y Shimada², T Tetsuo³
1 : Toyohashi University of Technology, Japan | 2 : National Institute of Occupational Safety and Health, Japan | 3 : Tokyo Institute of Technology, Japan
-
- P198** *Multi-agent Service Composition for Technology Selection*
R Batres*, H Takashima, S Yoshiaki (Toyohashi University of Technology, Japan)
-
- P199** *Introduction of CAPE into an Active Pharmaceuticals Ingredients Company*
M. Ben Tollia, R. Novoa*, M. Hasson, E. Manoff (Chemagis A Subsidiary of Perigo, Israel)
-
- P200** *Formal Modeling of a Project-Oriented Fractal Company for Process Development in the Pharmaceutical Sector*
M Canavesio, E Martínez* (UTN, Argentina)

- P201** *A VR System to Enable the Capture and Verification of Operating Instructions*
C Palmer¹, W Liu², PWH Chung^{*1}
1 : Loughborough University, United-Kingdom | 2 : Beijing University of Petroleum, China
- P202** *Development of a CAPE-Open Simulation Component for a GAMS-modeled Process Unit*
A Domancich^{*}, V Perez, P Hoch, N Brignole (UNS, Argentina)
- P203** *Integrated Decision Support Tool for Pharmaceutical Product Development*
A Jain^{*1}, P Kumar², G Joglekar², L Hailemariam², P Suresh², C Zhao², K Morris², G Reklaitis², V Venkatasubramanian²
1 : United Airlines, USA | 2 : Purdue University, USA
- P204** *Problems Mapping with Social Networks. Example of Ceramic Membranes*
A Kraslawski^{*}, M Mänttärä, A Fiola (Lappeenranta Univ. of Technology, Finland)
- P205** *Hazop Support System and its Use for Operation*
K Kwamura^{*1}, Y Naka², T Fuchino³, A Aoyama⁴, N Takagi⁵
1 : Techno Management Solutions Ltd., Japan | 2 : Tokyo Inst of Tech., Japan | 3 : Tokyo Inst of Tech., Japan | 4 : Ritsumei Univ., Japan | 5 : Systems Safety Consulting Ltd., Japan
- P206** *Acceleration of the Retrieval of Past Experiences in Case Based Reasoning: Application for Preliminary Design in Chemical Engineering*
S Negny^{*}, JM Le Lann (INPT-ENSIACET-LGC, France)
- P207** *Visual Exploration of Multi-State Process Operations Using Self-Organizing Maps*
YS Ng¹, R Srinivasan^{*2} (National University of Singapore)
- P208** *Ontological Framework for the Implementation of Waste Minimisation Methodologies into Process Industries*
A Reyes-Cordoba^{*}, P Sharratt, J Arizmendi-Sanchez (University of Manchester, United-Kingdom)
- P209** *Multi-Criteria Decision Making in Product-driven Process Synthesis*
K Ridder¹, C Almeida-Rivera^{*2}, P Bongers², S Bruin¹, SD Flapper¹
1 : Eindhoven University of Technology, The Netherlands | 2 : Unilever Food and Health Research Institute, The Netherlands
- P210** *Towards an Interface Standard for Automated Design: a Proposal*
I Stalker^{*1}, E Fraga²
1 : University of Manchester, United-Kingdom | 2 : University College London, United-Kingdom
- P211** *Improvement of the Production Process of Leached Optical Fibers in a Technological and Organizational Context*
D Stekelenburg¹, Z Lukszo^{*1}, J Lowe²
1 : Delft University of Technology, The Netherlands | 2 : Schott North America Inc, USA
- P212** *Quality Assurance of Simulation Results*
L Testard^{*} (Halias, France)

P213 *Decision Tree Based Qualitative Analysis of Operating Regimes in Industrial Production Process**T Varga*¹, F Szeifert¹, J Réti², J Abonyi¹**1 : University of Pannonia, Hungary | 2 : Borsodchem Ltd, Hungary***P214** *Management and Reuse of Mathematical Models in Chemical Industries with MOVE**L Von Wedel* (Aixcape, Germany)***P215** *Mobatec ModellerA flexible and transparent tool for building dynamic process models.**M Westerweele*, J Laurens (Mobatec, The Netherlands)***Topic 6 - CAPE and Society****P216** *Collaboration Among Companies or Better Energy Management**MH Agha*, R Thery, G Hetreux, A Hait, JM Le Lann (INPT - ENSIACET - LGC, France)***P217** *Process Dynamic and Industrial Accident Simulators: Coupling two Different Worlds into an Integrated Platform**S Brambilla*, F Manenti, D Manca (Politecnico di Milano, Italy)***P218** *Optimization of Synthesis Gas Production Plant Using Recycled Carbon Dioxide**S Choi*, S Kim, C Han, ES Yoon (Seoul National University, Republic of Korea)***P219** *Mathematical Modeling of Limestone Dissolution in Batch Stirred Tank Reactors in Presence of Diluted Strong Acid**C de Blasio*, J Ahlbeck, F Bjondahl (Åbo Akademi University, Finland)***P220** *Biodiesel Production from Vegetable Oils: Operational Strategies for Large Scale Systems**N de Lima Da Silva, E.C Rivera, C Benedito Batistella, D.R Lima, R Maciel Filho*, M.R Wolf Maciel (State University of Campinas, Brazil)***P221** *Simulation of Process Related Safety Limit of Alkoxylation Reactors**S Degenkolbe*, M Süßmuth, W Witt (Brandenburgische Technische Universität, Germany)***P222** *Anhydrous Bioethanol for Fuels and Chemicals – Evaluations of Alternative Distillations and Solvents**MOS Dias, FAD Mateus, R Maciel Filho*, MR Wolf Maciel, CEV Rossell (State University of Campinas, Brazil)***P223** *Evaluation of Energy Demand during Bioethanol Production from Sugarcane and Sugarcane Bagasse - Computer Based Scenario Approach**MOS Dias, R Maciel Filho*, MR Wolf Maciel, CEV Rossell (State University of Campinas, Brazil)***P224** *An Optimization Model for the Design of Closed Loop Supply Chains with Minimum Environmental Impacts**A Diniz Cunha*, MI Gomes Salema³, AP Barbosa Póvoa², A Q. Novais¹**1 : DMS, INETI, Portugal | 2 : CEG-IST, Portugal | 3 : CMA, FCT, Portugal*

- P225** *Minimization of Life Cycle Greenhouse Emissions and Cost in the Operation of Steam and Power Plants*
P Martinez, AM Eliceche* (Universidad Nacional del Sur, Argentina)
- P226** *Developing a Lake Eutrophication Model and Determining Biogeochemical Parameters: A Large Scale Parameter Estimation Problem*
V Estrada, E Parodi, S Diaz* (Universidad Nacional del Sur, Argentina)
- P227** *Structural Optimisation of Sustainable Chemical Process Flowsheets under Uncertainty*
G Guillén-Gosálbez*, JA Caballero², L Jiménez Esteller¹
1 : Universidad Rovira I Virgili, Spain | 2 : University of Alicante, Spain
- P228** *A New Model for Phase Equilibria of the Ternary System (H₂O – HI – I₂)*
MK Hadj-Kali*, V Gerbaud¹, JM Borgard², P Floquet¹, X Joulia¹, P Carles²
1 : LGC - CNRS - ENSIACET – INPT, France | 2 : CEA, France
- P229** *Computer Aided Design of Occupationally Healthier Processes*
M Hassim, M Hurme* (Helsinki University of Technology, Finland)
- P230** *Energy Management in a Stand-Alone Power System for the Production of Electrical Energy with Long Term Hydrogen Storage*
D Ipsakis*, D Ipsakis², S Voutetakis¹, P Seferlis¹, P Seferlis³, F Stergiopoulos¹, S Papadopoulou⁴, C Elmasides⁵, C Keivanidis⁵
1 : C.P.E.R.I., Greece | 2 : Aristotle University of Thessaloniki, Greece | 3 : Aristotle University of Thessaloniki, Greece | 4 : Alexander Technological Educational Institute of Thessaloniki, Greece | 5 : Systems Sunlight SA, Greece
- P231** *Mapping Environmental Issues Within Supply Chains: an LCA Based Approach*
JM Lainez*, AD Bojarski, A Espuña, L Puigjaner (Universitat Politècnica de Catalunya, Spain)
- P232** *Exergy Analysis of Biological Hydrogen Production*
A Modarresi, W Wukovits*, A Friedl (Vienna University of Technology, Austria)
- P233** *Sensitivity Analysis of a Model for Atmospheric Dispersion of Toxic Gases*
N Pandya*, E Marsden¹, P Floquet², N Gabas²
1 : ICSI, France | 2 : ENSIACET, France
- P234** *A Generic Framework for Modeling, Design and Optimization of Industrial Phosphoric Acid Production Processes*
A Papadopoulos*, K Seferlis²
1 : Chemical Process Engineering Research Institute, Greece | 2 : Aristotle University of Thessaloniki, Greece
- P235** *Sensitivity Analysis of the Benchmark Simulation Model N° 1*
MN Pons*, U Jeppsson², X Flores Alsina³, L Benedetti⁴, M Lourenco Da Silva¹, I Nopens⁴, J Alex⁵, J Copp⁶, K Gernaey⁷, C Rosen⁸, JP Steyer⁹, P Vanrolleghem¹⁰
1 : Nancy-University, France | 2 : Lund University, Sweden | 3 : University of Girona, Spain | 4 : Ghent University, Belgium | 5 : IFAK E.V., Germany | 6 : Primodal Inc., Canada | 7 : DTU, Denmark | 8 : Veolia Water, Sweden | 9 : LBE-INRA, France | 10 : Univ. of Laval, Canada
- P236** *Fundamental Aspects to Improve Risk Potential Assessment of Chemical Process Industry*
N Ramzan*, W Witt (Brandenburgische Technische Universität, Germany)

- P237** *Fisher Information: A Generalized Sustainability Index?*
V Rico-Ramirez^{*1}, PA Quintana-Hernandez¹, JA Ortiz-Cruz¹, S Hernandez-Castro²
1 : Instituto Tecnológico de Celaya, Mexico | 2 : Universidad de Guanajuato, Mexico
- P238** *Simulation of PEMFC Super Capacitor Hybrid System*
S Sailer^{*(1, 2)}, F Druart¹, D Riu², P Ozil¹
1 : LEPMI, France | 2 : G2ELAB, France
- P239** *Modeling and Optimizaion of the Steam Consumption in the Specialty Chemicals Industry*
A Szijarto^{*}, C Rerat, S Papadokonstantakis, K Hungerbuehler (ETH, Switzerland)
- P240** *Reduction of Polluting Effluents in a Polymerization Process using Simultaneous Mass and Heat Integration*
JC Tapia-Picazo^{*1}, A Jiménez², A Bonilla-Petriciolet¹, JG Segovia-Hernández³
1 : Instituto Tecnológico de Aguascalientes, Mexico | 2 : Instituto Tecnológico de Celaya, Mexico | 3 : Universidad de Guanajuato, Mexico
- P241** *Is Reactive Distillation a Sustainable PI Solution?*
M Van Der Heijden, J Grievink^{*} (Delft University of Technology, The Netherlands)
- P242** *Towards Improved Cleaning of FMCG Plants: a Model-based Approach*
A Yang^{*1}, EB Martin¹, GA Montague¹, P Fryer²
1 : Newcastle University, United-Kingdom | 2 : Birmingham University, United-Kingdom
- P243** *About Energy Efficiency Improvement of Auto-thermal Thermophilic Aerobic Digestion Processes*
T Zhelev^{*1}, N Vaklieva², D Jamniczky-Kaszás¹
1 : Univetsy of Limerick, Ireland | 2 : Institute of Chemical Engineering, Bulgaria

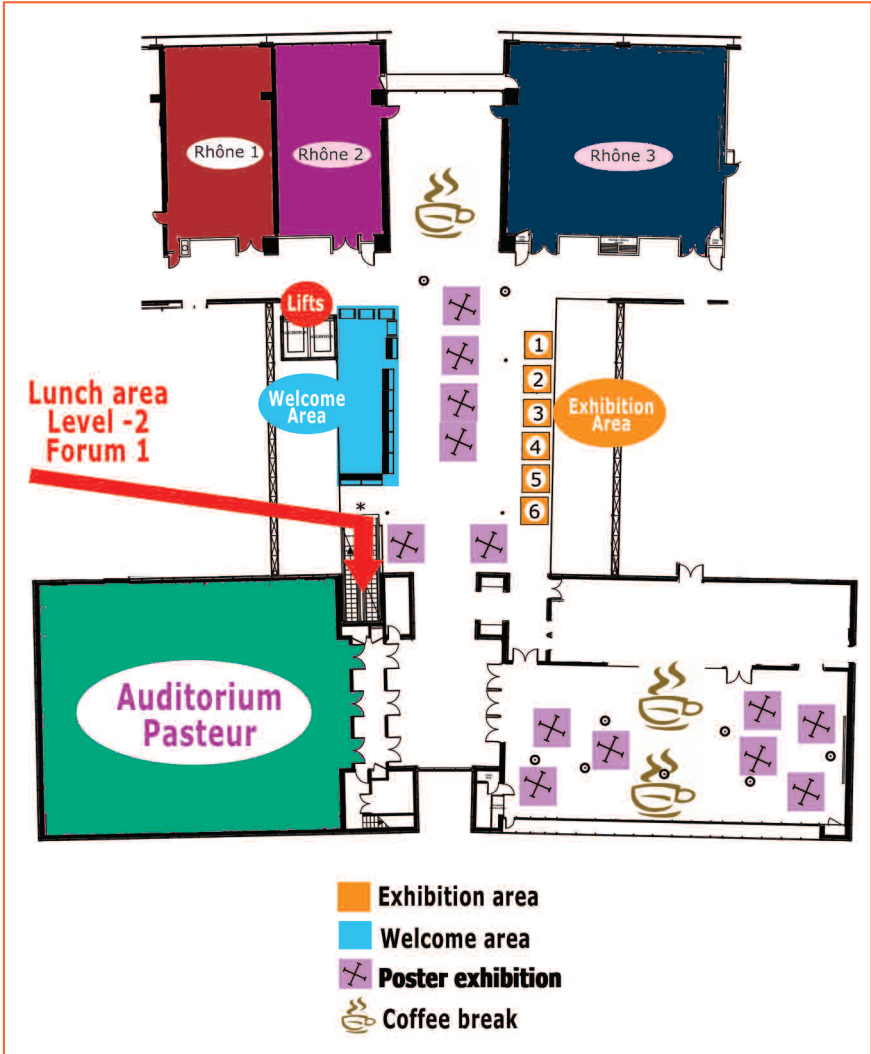
Topic 7 - CAPE in Education

- P244** *Teaching Mono and Multi-objective Genetic Algorithms in Process Systems Engineering : an illustration with the MULTIGEN environment*
A Gomez^{*}, C Azzaro-Pantel, L Pibouleau, S Domenech (ENSIACET INPT, France)
- P245** *Operator Training Simulator Development for Ethylene Plant Tertiary Refrigeration System*
HH Hashim^{*1}, LW Chong¹, AH M Jelani²
1 : Petronas Group Technology Solutions, Malaysia | 2 : Ethylene Malaysia SDN BHD, Malaysia
- P246** *Virtual and Remote Laboratory for Robotics E-Learning*
C Jara^{*}, F Candelas, F Torres (Universidad de Alicante, Spain)
- P247** *Virtual Reality Operator Education of a Hydrogen Fueling Station*
J Kim^{*}, E Kim, Y Lee, I Moon (Yonsei University, Republic of Korea)

EXHIBITORS

- Elsevier 1
- IBM 4
- Mobatec 5
- Paragon (AIMMS) 2
- Pro Sim 6
- PSE 3

FLOOR PLAN



LIST OF HOTELS

4 Stars Hotel

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22, quai Charles de Gaulle
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Tel : +33 (0)4 78 17 86 86

3 Stars Hotels

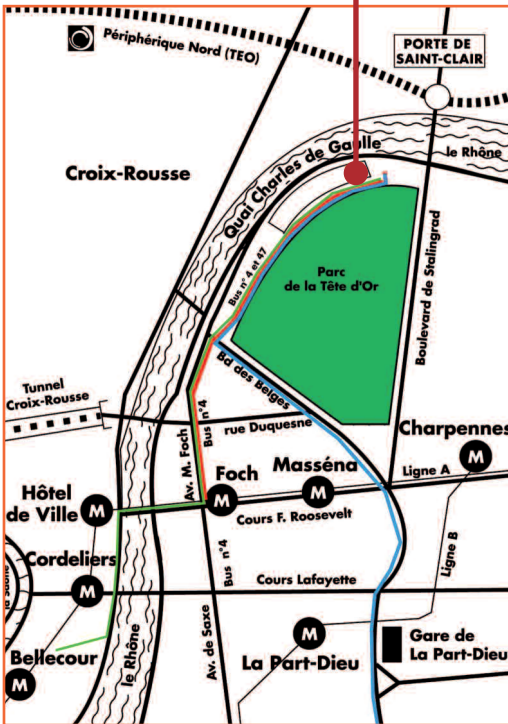
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 - **Carlton Lyon / Groupe Accor**
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 - **Best Western Charlemagne**
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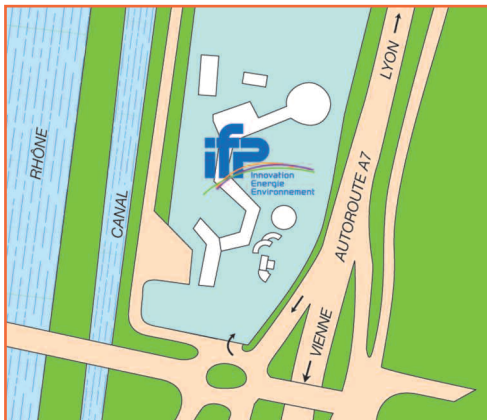
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-

ACCESS MAPS

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From Lyon to Solaize:
Take the A7 highway
(towards Vienne-Marseille)
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