

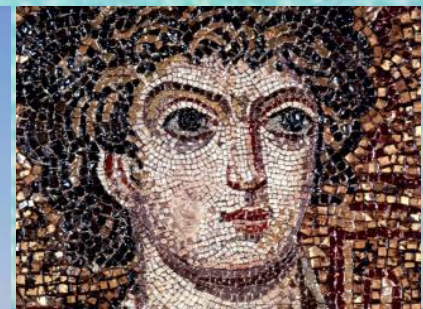


ESCAPE-21

An Event of the CAPE Working Party of EFCE –
Event Number: 690



PROGRAMME BOOK



21st European Symposium on Computer-Aided Process Engineering

Symposium Theme

“Process Systems Approaches for Addressing Grand Challenges in
Energy, Environment, Health, Bioprocessing & Nanotechnologies”

May 29 – June 1, 2011

Porto Carras Resort, Chalkidiki, Thessaloniki, Greece



SUNDAY, 29 MAY 2011

12:30 – 16:30 CAPE WP Meeting (by invitation only)

15:00 – 17:30 Registration

20:30 – 22:30 Opening Reception

MONDAY, 30 MAY 2011

08:30 – 09:00 Welcome & Opening Remarks – OLYMPIC HALL

09:00 – 10:30 Plenary Session 1 – OLYMPIC HALL

Chairs: Rafiqul Gani (DTU, Denmark)
Stratos Pistikopoulos (Imperial, UK)

09:00 – 09:40 **Innovation at Bayer CropScience**
Achim Noack (BAYER CropScience AG, Germany)

09:40 – 10:30 **Nanoscale process systems engineering: Design, fabrication, monitoring and control**
George Stephanopoulos (MIT, USA)

10:30 – 10:50 Coffee Break

10:50 – 12:40 Oral Presentations – 5 Parallel Sessions

Synthesis/Design I – TERPSIHORI HALL

Chair: Zdravko Kravanja (University of Maribor, Slovenia)

10:50 – 11:20 Development of a synthesis tool for Gas-To-Liquid complexes
Keynote **Jan van Schijndel^a, Nort Thijssen^a, Govert Baak^a, Abhijeet Avhale^a, Jerome Ellepola^a, Johan Grievink^b**
Presentation ^aShell Global Solutions International BV, P.O.Box 38000, Amsterdam, 1030 BN, The Netherlands
^bDelft University of Technology, Julianalaan 136, Delft, 2628 BL, The Netherlands

11:20 – 11:40 A novel design concept for the oxidative coupling of methane using hybrid reactors
Stanislav Jašo, Harvey Arellano-Garcia, Günter Wozny
Chair of Process Dynamics and Operation, Berlin Institute of Technology, Str. des 17. Juni 135, Sekr. KWT-9, D-10618 Berlin, Germany

11:40 – 12:00 Integrated design of a reactor and a gas-expanded solvent
Eirini Sioukrou, Amparo Galindo and Claire S. Adjiman
Department of Chemical Engineering, Centre for Process Systems Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

12:00 – 12:20 Modeling and design of reacting systems with phase transfer catalysis
Chiara Piccolo^a, George Hodges^b, Patrick M. Piccione^b, Rafiqul Gani^a
^a CAPEC-Department of Chemical and Biochemical Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
^b Process Studies Group, Syngenta, Jealott's Hill International Research Center, Bracknell, Berkshire RG42 6EY, UK

- 12:20 – 12:40 A strategy to extend reactive distillation column performance under catalyst deactivation
Rui M. Filipe^{a,b}, Henrique A. Matos^{b,c}, Augusto Q. Novais^d
^a *Área Departamental de Engenharia Química, Instituto Superior de Engenharia de Lisboa, R. Conselheiro Emídio Navarro, 1, 1959-007 Lisboa, Portugal*
^b *Centro de Processos Químicos, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*
^c *Departamento de Engenharia Química e Biológica, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*
^d *Unidade de Modelação e Optimização de Sistemas e Energia, Laboratório Nacional de Energia e Geologia, Est. do Paço do Lumiar, 1649-038 Lisboa, Portugal*

Optimization I – ERATO HALL

Chair: **Marianthi Ierapetritou** (Rutgers University, USA)

- 10:50 – 11:20 High-throughput methods for in silico discovery of peptides, proteins, and post-translational modifications in proteomics
Keynote
Presentation **Chris Floudas, Richard C. Baliban**
Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, 08540, USA
- 11:20 – 11:40 Tight convex and concave relaxations via Taylor models for global dynamic optimization
Ali M. Sahlodin^a and Benoît Chachuat^{a,b}
^a *Department of Chemical Engineering, McMaster University, Hamilton, ON L8S 4L7, Canada*
^b *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK*
- 11:40 – 12:00 Parallel solution of large-scale dynamic optimization problems
Carl D. Laird^a, Angelica V. Wong^a, Johan Akesson^b
^a *Artie McFerrin Department of Chemical Engineering, Texas A&M University, TX, USA*
^b *Department of Automatic Control, Lund University, Sweden*
- 12:00 – 12:20 Multiobjective optimization for plastic sheet production
M. Rivera-Toledo, G. Meneses-Castellanos, A. Flores-Tlacuahuac
Depto. Ing. y Ciencias Químicas, Universidad Iberoamericana, México D.F., México
- 12:20 – 12:40 A semidefinite programming approach to portfolio optimization
Raquel J. Fonseca, Wolfram Wiesemann, Berç Rustem
Department of Computing, Imperial College, London, UK

Molecular/Material Systems Engineering I – CHLOE HALL

Chair: **Claire Adjiman** (Imperial, UK)

- 10:50 – 11:20 PSE in pharmaceutical process development
Keynote **Krist V. Gernaey, Albert E. Cervera and John M. Woodley**
Presentation *Center for Process Engineering and Technology (PROCESS), Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, 2800 Kgs. Lyngby, Denmark*
- 11:20 – 11:40 Molecular design of biofuel additives for optimization of fuel characteristics
Subin Hada, Charles C. Solvason, Mario R. Eden
Department of Chemical Engineering, Auburn University, Auburn, AL 36849, USA
- 11:40 – 12:00 Online estimation of crystal size distribution (CSD) within industrial gibbsite precipitation plants
Jan K. Hurst^a, Parisa A. Bahri^a, Ali Noorai^b
^a *School of Engineering & Energy, Murdoch University, Perth 6150, Australia*
^b *Alcoa World Alumina & Chemicals, Perth 6953, Australia*
- 12:00 – 12:20 Convex optimization for shape manipulation of multidimensional crystal particles
Naim Bajcinca^{a,b}, Ricardo Per^a, Kai Sundmacher^{a,c}
^a *Max-Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr.1, 39106 Magdeburg, Germany*
^b *Technische Universität Berlin, Einsteinufer 17, 10857 Berlin, Germany*
^c *Otto-von-Guericke Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany*

12:20 – 12:40 Towards robust fabrication of non-periodic nanoscale systems via directed self assembly
Richard Lakerveld, George Stephanopoulos, Paul I. Barton
Process Systems Engineering Laboratory, Department of Chemical Engineering Massachusetts Institute of Technology, 77 Massachusetts Av, Cambridge 02139, USA

Biomedical Systems Engineering I – MARINA I

Chair: Athanasios Mantalaris (Imperial, UK)

10:50 – 11:20 Systems engineers' role in biomedical research

Keynote **Andreas A. Linninger**

Presentation *University of Illinois at Chicago, Laboratory for Product and Process Design, M/C 063, 851 S. Morgan St. - 218 SEO, Chicago 60607-7000, Illinois, USA*

11:20 – 11:40 Computational molecular design of drug delivery vehicles for Anti-HIV microbicides

Taylor Wilson^a, Amber Markey^b, Kyle V. Camarda^a, Sarah Kieweg^{c,d}

^a *Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS 66049 USA*

^b *Bioengineering Graduate Program, University of Kansas, Lawrence, KS 66049 USA*

^c *Department of Mechanical Engineering, University of Kansas, Lawrence, KS 66049 USA*

^d *Department of Obstetrics and Gynecology, University of Kansas, Lawrence, KS 66049 USA*

11:40 – 12:00 A minimal exercise extension for models of the glucoregulatory system

Alain Bock^a, Grégory François^a, Thierry Prud'homme^b, Denis Gillet^a

^a *School of Engineering, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH 1015 Lausanne, Switzerland*

^b *Lucerne University of Applied Sciences and Arts, CH 6048 Horw, Switzerland*

12:00 – 12:20 Insulin administration for people with type 1 diabetes

Dimitri Boiroux, Daniel Aaron Finan, Niels Kjølstad Poulsen, Henrik Madsen, John Bagterp Jørgensen

Department of Informatics and Mathematical Modeling, Technical University of Denmark, DK - 2800 Kgs. Lyngby, Denmark

12:20 – 12:40 Development of a fuzzy expert system for the control of glycemia in type 1 diabetic patients

Leonardo Nobile^a, Bartolomeo Cosenza^a, Marco Amato^b, Valentina Guarnotta^b, Carla Giordano^b, Aldo Galluzz^b, Mosè Galluzzo^a

^a *Dipartimento di Ingegneria Industriale, Università degli Studi di Palermo, Viale delle Scienze ed. 6, 90128, Palermo Italy*

^b *Dipartimento di Oncologia Sperimentale ed Applicazioni Cliniche, Sezione di Endocrinologia, Università degli Studi di Palermo, Piazza delle Cliniche 2, 90127 Palermo Italy*

Energy Systems Engineering I – MARINA II

Chair: Jiri Klemes (University of Pannonia, Hungary)

10:50 – 11:20 The role of supply chain analysis in market- driven product portfolio selection for the forest biorefinery

Keynote *Virginie Chambost, Behrang Mansoornejad, Paul Stuart*

Presentation *NSERC Environmental Design Engineering Chair Department of Chemical Engineering, École Polytechnique, 2920 Chemin de la Tour, Pavillon Aisenstadt, Montreal H3C 3A7, Canada*

11:20 – 11:40 A novel catalytic strategy for the production of liquid fuels from ligno-cellulosic biomass

Carlos A. Henao, Drew J. Braden, Christos T. Maravelias, James A. Dumesic

University of Wisconsin-Madison, 1415 Engineering Drive, Madison - Wisconsin, USA

11:40 – 12:00 Optimal operation of a concentrated solar thermal cogeneration plant

Amin Ghobeity, Alexander Mitsos

Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

12:00 – 12:20 Detailed operation scheduling and control for renewable energy powered microgrids

Miguel Zamarripa^a, Juan C. Vasquez^b, Josep M. Guerrero^b, Moisès Graells^a

^a *Chemical Engineering Department, ^b Automatic Control Systems Department.*

Universitat Politècnica de Catalunya, UPC.

EUETIB, 08028 - Comte d'Urgell 187, Barcelona, Spain

- 12:20 – 12:40 Optimization of mixed-refrigerant system in LNG liquefaction process
Kyungjae Tak^a, Wonsub Lim^a, Kwangho Choi^b, Daeho Ko^b, Il Moon^a
^a Department of Chemical and Biomolecular Engineering, Yonsei University, 262 Seongsanno, Seodaemun-gu, Seoul 120-749, Korea
^b GS E&C, GS Yeokjeon Tower 537, Namdaemun-ro 5-ga, Joong-gu, Seoul, Korea

12:40 – 14:20 Lunch

12:40 – 14:20 IEA Annex I Luncheon Meeting (by invitation only)

14:20 – 15:40 Plenary Session 2 - OLYMPIC HALL

Chairs: Luis Puigjaner (UPC, Spain)
Michael Georgiadis (AUn, Greece)

- 14:20 – 15:00 **State-of-the-art and progress in discrete and continuous optimization for process systems engineering**
Ignacio Grossmann (Carnegie Mellon University, USA)

- 15:00 – 15:40 **Perspectives on the energy system of China**
Zheng Li (Tsinghua University, China)

15:40 – 16:00 Coffee Break

16:00 – 17:40 Oral Presentations – 5 Parallel Sessions

Multi-scale Modelling I – MARINA II

Chair: Ioannis Androulakis (Rutgers University, USA)

- 16:00 – 16:20 Multi-Scale modelling of a membrane reforming power cycle with CO₂ capture
Øivind Wilhelmsen, Rahul Anantharaman, David Berstad, Kristin Jordal
SINTEF Energy Research, Sem Sælands vei 11, 7034 Trondheim, Norway
- 16:20 – 16:40 Sensitivity of shrinkage and collapse functions involved in pore formation during drying
Seddik Khalloufi^a, Cristhian Almeida-Rivera^a, Jo Jansen^a, Marcel Van-Der-Vaart^a, Peter Bongers^{a,b}
^a Unilever R&D Vlaardingen, Structured Materials and Process Science Department, 3130 AT Vlaardingen. The Netherlands. Tel. +31 10 460 8501, Fax. +31 10 460 5025,
^b Chemical Engineering and Chemistry, Eindhoven University of Technology, Eindhoven, The Netherlands
- 16:40 – 17:00 A process unit modeling framework within a heterogeneous simulation environment
Ingo Thomas
Linde AG, Linde Engineering Division, Dr.-Carl-von-Linde-Str. 6,14, 82049 Pullach, Germany
- 17:00 – 17:20 Simulation of reactive absorption: Model validation for CO₂-MEA system
Chinmay Kale^a, Inga Tönnies^b, Hans Hasse^b, Andrzej Góral^a
^a Laboratory of Fluid Separations, Department of Biochemical and Chemical Engineering, TU Dortmund University, Emil Figge Strasse 70, Dortmund, D-44227, Germany
^b Laboratory of Engineering Thermodynamics, Department of Mechanical and Process Engineering, University of Kaiserslautern, P.O. Box 3049, Kaiserslautern, Germany
- 17:20 – 17:40 An efficient high resolution FEM for PDE systems
Duc Hoang Minh^a, Harvey Arellano-Garcia^a, Lorenz T. Biegler^b
^a Chair of Process Dynamics and Operation, Berlin Institute of Technology, KWT-9, Str. des 17. Juni 135, D-10623 Berlin, Germany
^b Dept. of Chemical Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213-3890, USA

Synthesis/Design II – CHLOE HALL

Chair: Benoit Chachuat (Imperial, UK)

- 16:00 – 16:20 Design and control of an energy integrated biodiesel process
Anton A. Kiss^a, Costin Sorin Bildea^b
^a AkzoNobel – Research, Development and Innovation, Velperweg 76, 6824 BM, Arnhem, The Netherlands
^b University “Politehnica” of Bucharest, Centre for Technology Transfer in Process Industries, Polizu 1-7, 011061 Bucharest, Romania
- 16:20 – 16:40 Logic-sequential approach to the synthesis of complex thermally coupled distillation systems
José A. Caballero^a, Ignacio E. Grossmann^b
^a Department of Chemical Engineering, University of Alicante., Ap Correos 99, 03080, Alicante, Spain
^b Department of Chemical Engineering, Carnegie Mellon University, 5000 Forbes Av. 15213. Pittsburgh, PA USA
- 16:40 – 17:00 Flowsheet optimization by memetic algorithms
Maren Urselmann, Sebastian Engell
 Process Dynamics and Operations Group, TU Dortmund, Emil-Figge-Str. 70, 44227 Dortmund, Germany
- 17:00 – 17:20 Computer aided design and analysis of continuous pharmaceutical manufacturing processes
Fani Boukouvala, Rohit Ramachandran, Aditya Vanarase, Fernando J. Muzzio, Marianthi G. Ierapetritou
 Dept. Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ USA
- 17:20 – 17:40 Biomass to chemicals: Design of an extractive reaction process for the production of 5-hydroxymethylfurfural
Ana I. Torres, Prodromos Daoutidis, Michael Tsapatsis
 Department of Chemical Engineering and Materials Science; University of Minnesota, Minneapolis, MN USA

Optimization II – ERATO HALL

Chair: Alexander Mitsos (MIT, USA)

- 16:00 – 16:20 Integrating graph-based representation and genetic algorithm for large-scale optimization: Refinery crude oil scheduling
Manojkumar Ramteke^a, Rajagopalan Srinivasan^{a,b}
^a Institute of Chemical and Engineering Sciences, A*STAR (Agency for Science, Technology & Research), 1 Pesek Road, Jurong Island, Singapore 627833
^b Department of Chemical & Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117576
- 16:20 – 16:40 Towards global optimization of combined distillation-crystallization processes for the separation of closely boiling mixtures
Martin Ballerstein^a, Achim Kienle^{b,c}, Christian Kunde^b, Dennis Michaels^a, Robert Weismantel^a
^a Eidgenössische Technische Hochschule Zürich, Institut für Operations Research, Rämistrasse 101, 8092 Zürich, Switzerland
^b Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany
^c Max-Planck-Institut für Dynamik komplexer technischer Systeme, Sandtorstraße 1, 39106 Magdeburg, Germany
- 16:40 – 17:00 Branch-and-Sandwich: An algorithm for optimistic bi-level programming problems
Polyxeni M. Kleniati, Claire S. Adjiman
 Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, United Kingdom
- 17:00 – 17:20 Efficient computation of first- and second-order sensitivities using an internal forward differentiation scheme
T. Barz, L. Zhu, G. Wozny, H. Arellano-Garcia
 Chair of Process Dynamics and Operation, Sekr. KWT-9, Berlin Institute of Technology, D-10623 Berlin, Germany
- 17:20 – 17:40 Approximate multi-parametric programming based B&B algorithm for MINLPs

Taoufiq Gueddar and Vivek Dua

Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, London WC1E 7JE, UK

Process Operations I – TERPSIHORI HALL

Chair: *Ana Barbosa (IST, UTL, Portugal)*

- 16:00 – 16:20 Optimal run length in factory operations to reduce overall costs
Peter Bongers^{a,b}, Cristhian Almeida-Rivera^a
^a *Structured Materials & Process Science, Unilever Research, Olivier van Noortlaan 120, 1330AC, Vlaardingen, The Netherlands.*
^b *Technical University of Eindhoven, Department of Chemical Engineering and Chemistry, PO Box 513, 5600 MB Eindhoven, The Netherlands*
- 16:20 – 16:40 Production optimization and scheduling across a steel plant
Iiro Harjunkoski^a, Sleman Saliba^a, Matteo Biondi^b
^a *ABB Corporate Research, Wallstadter Str. 59, 68526 Ladenburg, Germany*
^b *ABB S.p.A, Via Albareto 35, 16153 Genova, Italy*
- 16:40 – 17:00 New scheduling approach for shared resources and mixed storage policies
Pedro M. Castro^a, Luis J. Zeballos^{a,b}, Carlos A. Méndez^c
^a *UMOSE, Laboratório Nacional de Energia e Geologia, 1649-038 Lisboa, Portugal*
^b *Universidad Nacional del Litoral, Facultad Ingeniería Química, Santa Fe, Argentina*
^c *INTEC (Universidad Nacional del Litoral – CONICET), Santa Fe, Argentina*
- 17:00 – 17:20 Robust logistics network modeling and design against uncertainties
Yoshiaki Shimizu^a, Hideaki Fushimi^a, Takeshi Wada^b
^a *Toyohashi University of Technology, Toyohashi, Aichi 441-8580, Japan*
^b *Osaka Prefectural College of Technology, Neyagawa, Osaka 572-8572, Japan*
- 17:20 – 17:40 Freshwater production by MSF desalination process: Coping with variable demand by flexible design and operation
Ebrahim A. Hawaidi, Iqbal M. Mujtaba
School of Engineering Design & Technology, University of Bradford, West Yorkshire BD7 1DP, UK

Training and EURECHA – MARINA I

Chair: *Antonio Espuna (UPC, Spain)*

- 16:00 – 16:20 Integrating alternate reality games and social media in engineering education
Sonia Zheleva^a, Toshko Zhelev^b
^a *Faculty of Engineering & IT, Griffith College Limerick, Limerick, Ireland*
^b *Department of Chemical & Environmental Sciences, University of Limerick, Limerick, Ireland*
- 16:20 – 16:40 Modularization within the framework of the course Computer-Aided Plant Design
Lukasz Hady, Günter Wozny
Berlin Institute of Technology, Chair of Process Dynamics and Operation, Sekr. KWT 9, Str. des 17. Juni 135, D-10623 Berlin, Germany
- 16:40 – 17:00 Addressing interdisciplinary process engineering design, construction and operations through 4D virtual environments
Ian Cameron^a, Caroline Crosthwaite^a, David Shallcross^b, Roger Hadgraft^b, Jo Dalvean^b, Nicoleta Maynard^c, Moses Tade^c, John Kavanagh^d, Grant Lukey^e
^a *University of Queensland, Brisbane, Queensland, Australia 4072*
^b *University of Melbourne, Melbourne, Victoria, Australia 3010*
^c *Curtin University, Perth, Western Australia, Australia 6102*
^d *University of Sydney, Sydney, NSW, Australia 2006*
^e *Coogee Energy, Laverton North, Victoria, Australia 3026*
- 17:00 – 17:20 Is it possible to improve creativity? If yes, how do we do it?

Seungnam Kim, Woorim Moon, Woosik Kim, Seonjoo Park and Il Moon
Department of Chemical and Biomolecular Engineering Yonsei University, Seoul 120-749, Rep. of Korea

17:20 – 17:40 Use of advanced educational technologies in a process simulation course
Mordechai Shacham
Dept. Chem. Engng, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

17:40 – 19:40 Poster Presentations – 5 Parallel Sessions (3min per Poster)

Poster Session 1 – CHLOE HALL

Chair: Heinz Preisig (NTNU, Norway)

Synthesis/Design

- Optimal design of multiple dividing wall columns based on genetic programming
F.I. Gómez-Castro^{a,b}, M.A. Rodríguez-Ángeles^b, J.G. Segovia-Hernández^b, C. Gutiérrez-Antonio^c, A. Briones-Ramírez^d
^a Instituto Tecnológico de Celaya, Departamento de Ingeniería Química, Av. Tecnológico y García Cubas S/N, Celaya, Guanajuato, 38010, México
^b Universidad de Guanajuato, Campus Guanajuato, División de Ciencias Naturales y Exactas, Departamento de Ingeniería Química, Noria Alta S/N, Guanajuato, Guanajuato, 36050, México
^c CIATEQ, A.C., Av. del Retablo 150 Col. Fovissste, Querétaro, Querétaro, 76150, México
^d Exxerpro Solutions, Av. del Sol 1B Interior 4B, Plaza Comercial El Sol, El Tintero, Querétaro, Querétaro, 76134, México
- Retrofit design of a pharmaceutical batch process considering green chemistry and engineering principles
A. Banimostafa, S. Papadokostantakis, K. Hungerbühler
Swiss federal institute of technology (ETH), Zurich 8093, Switzerland
- A systematic approach towards applicability of reactive distillation
A.A. Kiss^a, P. Singh^b, C.J.G. van Strien^a
^a AkzoNobel – Research, Development and Innovation, Velperweg 76, 6824 BM, Arnhem, The Netherlands
^b Dutch Separation Technology Institute (DSTI), Stationsstraat 77, 3811MH, Amersfoort, The Netherlands
- Strategies for the robust simulation of thermally coupled distillation sequences
M.A. Navarro^a, J.A. Caballero^a, I.E. Grossmann^b
^a Department of Chemical Engineering, University of Alicante., Ap Correos 99, 03080, Alicante, Spain
^b Department of Chemical Engineering, Carnegie Mellon University, 5000 Forbes Av. 15213. Pittsburgh, PA USA
- Spatiotemporal pattern formation in an electrochemical membrane reactor during deep CO removal from reformat gas
R. Hanke-Rauschenbach^a, S. Kirsch^a, K. Sundmacher^{a,b}
^a Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany
^b Process Systems Engineering, Otto-von-Guericke University, Universitätsplatz 2, 39106 Magdeburg, Germany
- Optimization of design and operation of reverse osmosis based desalination process using MINLP approach incorporating fouling effect
K.M. Sassi, I.M. Mujtaba
School of Engineering Design and Technology, University of Bradford, Bradford, West Yorkshir, BD7 1DP, UK
- Phenomena-based process synthesis and design to achieve process intensification
P. Lutze^a, R. Gani^b, J.M. Woodley^{a,b}
^a PROCESS, Department of chemical and Biochemical Engineering, Technical University of Denmark, Soltofts Plads, DK-2800 Lyngby, Denmark
^b CAPEC, Department of chemical and Biochemical Engineering, Technical University of Denmark, Soltofts Plads, DK-2800 Lyngby, Denmark
- A novel process design for the hydroformylation of higher alkenes
M. Müller^{a,c}, V.A. Merchan^{a,c}, H. Arellano-García^{a,c}, R. Schomäcker^{b,c}, G. Wozny^{a,c}
^a Chair of Process Dynamics and Operation, Sekr. KWT-9
^b Dept. of Chemistry, Sekr. TC3
^c Technische Universität Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany
- Feasibility of reactive pressure swing batch distillation in a double column configuration
G. Modla

Budapest University of Technology and Economics, Department of Building Services and Process Engineering, H-1521 Budapest, Hungary

10. Enhancement of productivity of distillate fractions by crude oil hydrotreatment: development of kinetic model for the hydrotreating process
A.T. Jarullah, I.M. Mujtaba, A.S. Wood
School of Engineering, Design and Technology, University of Bradford, Bradford BD7 1DP, UK
11. A systematic methodology for the design of continuous active pharmaceutical ingredient production processes
A.E. Cervera^a, R. Gani^b, S. Kii^c, T. Skovby^d, K.V. Gernaey^a
^a *Center for Process Engineering and Technology (PROCESS), Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, 2800 Kgs. Lyngby, Denmark*
^b *CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, 2800 Kgs. Lyngby, Denmark*
^c *CHEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, 2800 Kgs. Lyngby, Denmark*
^d *H. Lundbeck A/S, Oddenvej 182, Lumsås, 4500 Nykøbing Sj, Denmark*
12. New algorithm for the determination of product sequences in azeotropic batch distillation
L. Hegely, P. Lang
Budapest University of Technology and Economics, Dept. of Building Services and Process Engineering, H-1521 Budapest, Muegyetem rkp. 3-5, Hungary
13. A retrofit strategy to achieve “Fast, Flexible, Future (F³)” pharmaceutical production processes
R. Singh^a, R. Rozada-Sanchez^b, T. Wrate^b, F. Muller^b, K.V. Gernaey^a, R. Gani^a, J.M. Woodley^a
^a *Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark*
^b *AstraZeneca Limited, Charter Way, Silk Road Business Park, Macclesfield, Cheshire SK10 2NA, UK*
14. Integrating process simulation and MINLP methods for the optimal design of absorption cooling systems
J.A. Reyes-Labarta^a, R. Brunet^b, J.A. Caballero^a, D. Boer^c, L. Jiménez^b
^a *Department of Chemical Engineering, University of Alicante, Ap. Correos 99, 03080. Alicante, Spain*
^b *Departament d’Enginyeria Química, Universitat Rovira i Virgili, Av. Paisos Catalans, 26, 43007, Tarragona, Spain*
^c *Departament d’Enginyeria Mecànica, Universitat Rovira i Virgili, Av. Paisos Catalans, 26, 43007, Tarragona, Spain*
15. A method for the design and planning operations of heap leaching circuits
J.Y. Trujillo^a, M.E. Mellado^b, E.D. Gálvez^{b,c}, L.A. Cisternas^{a,b}
^a *Departamento de Ingeniería Química, Universidad de Antofagasta, Chile*
^b *Centro de Investigación Científico Tecnológico para la Minería, CICITEM, Chile*
^c *Departamento de Ingeniería Metalúrgica, Universidad Católica del Norte, Chile*
16. A data mining approach for efficient systems optimization under uncertainty using stochastic search methods
G. Giannakoudis^a, A.I. Papadopoulos^a, P. Seferlis^{a,b}, S. Voutetakis^a
^a *Chemical Process Engineering Research Institute, Centre for Research and Technology-Hellas, 6th km Harilaou Thermi Road, 57001, Thessaloniki, Greece*
^b *Department of Mechanical Engineering, Aristotle University of Thessaloniki, 54124, Thessaloniki, Greece*
17. A business process model for process design that incorporates independent protection layer considerations
T. Fuchino^a, Y. Shimada^b, T. Kitajima^c, K. Takeda^d, R. Batres^e, Y. Naka^f
^a *Chemical Engineering Department, Tokyo Institute of Technology, 2-12-1, O-okayama, Meguro-ku, Tokyo, 152-8552, Japan*
^b *Chemical Safety Research Group, National Institute of Occupational Safety and Health, 1-4-6, Umezono, Kiyose, Tokyo, 204-0024, Japan*
^c *Institute of Technology, Tokyo University of Agriculture and Technology, 2-24-16, Naka-cho, Koganei, Tokyo, 184-8588, Japan*
^d *Department of Materials Science and Chemical Engineering, Shizuoka University, 3-5-1, Johoku, Naka-ku, Hamamatsu, 432-8011, Japan*
^e *Industrial Systems Engineering Group, Toyohashi University of Technology, Hibi-rigaoka 1-1, Tempaku-cho, Toyohashi, 441-8580, Japan*
^f *Chemical Resources Laboratory, Tokyo Institute of Technology, 4259, Nagatsuda, Midori-ku, Yokohama, 226-8503, Japan*
18. Conceptual design of glycerol etherification processes
E. Vlad, C.S. Bildea, E. Zaharia, G. Bozga
University Politehnica Bucharest, Department of Chemical Engineering, Polizu 1-7, 011061-Bucharest, Romania
19. Dynamic conceptual design under market uncertainty and price volatility
D. Manca, A. Fini, M. Oliosi
CMIC Department, Politecnico di Milano, 20133 Milano, Italy
20. Analysis of separation possibilities of multicomponent mixtures
L. Szabo, S. Nemeth, F. Szeifert
University of Pannonia, Department of Process Engineering, Egyetem Str. 10, H-8200 Veszprém, Hungary

21. Robust optimisation methodology for the process synthesis of continuous technologies
M.P. Patel^a, N. Shah^a, R. Ashe^b
^a CPSE, Dept. Chemical Engineering, Imperial College, London, SW7 2AZ, UK
^b AM Technology, The Heath Bus. & Tech. Park, Runcorn, Cheshire, WA7 4QX, UK
22. A shortcut design for Kaibel columns based on minimum energy diagrams
M. Ghadrani^a, I.J. Halvorsen^b, S. Skogestad^a
^a Norwegian University of Science and Technology, Chemical Engineering Department, 7491, Trondheim, Norway
^b SINTEF ICT, Applied Cybernetics, N-7465 Trondheim, Norway
23. New generalised double-column system for batch heteroazeotropic distillation
F. Denes^{a,b}, P. Lang^a, X. Joulia^b
^a BME Dept. of Process Engineering, Muegyetem rkp. 3-5, H-1521 Budapest, Hungary
^b University of Toulouse, INP-ENSIACET-LGC, 4, allée Emile Monso, 31432 Toulouse Cedex 4, France
24. Comparison of extractive and pressure-swing batch distillation for acetone-methanol separation
G. Modla, P. Lang
Budapest University of Technology and Economics, Department of Building Services and Process Engineering, H-1521 Budapest, Hungary
25. Systems analysis of benign hydrogen peroxide synthesis in supercritical CO₂
D.B. Bacik, W. Yuan, C.B. Roberts, M.R. Eden
Department of Chemical Engineering, Auburn University, AL 36849, USA
26. Design of pervaporation modules based on computational process modelling
P. Schiffmann, J.U. Repke
Institute of Thermal, Environmental and Natural Products Process Engineering Technische Universität Bergakademie Freiberg, Germany
27. Surrogate-based VSA process optimization for post-combustion CO₂ capture
M.M. Faruque Hasan^a, I.A. Karimi^a, S. Farooq^a, A. Rajendran^b, M. Amanullah^b
^a Department of Chemical & Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117576
^b School of Chemical and Biomedical Engineering, Nanyang Technological University 62 Nanyang Drive, Singapore 637459
28. A design methodology for internally heat-integrated distillation columns (IHIDIC) with side condensers and side reboilers (SCSR)
S. Maddu, R.K. Malik
Department of Chemical Engineering, Indian Institute of Technology – Bombay, Powai, Mumbai, Maharashtra 400076, India
29. A computer tool for the development of poly(lactic acid) synthesis process from renewable feedstock for biomanufacturing
G.A.R. Martinez^{a,b}, A.J.R. Lasprilla^{a,b}, B.H. Lunelli^{a,b}, A.L. Jardim^{a,b}, R.M. Filho^{a,b}
^a Laboratory of Optimization, Design and Advanced Control (LOPCA), School of Chemical Engineering, State University of Campinas (UNICAMP), Campinas (SP) 13083-852, Brazil
^b Institute of Biofabrication, State University of Campinas (UNICAMP), Campinas (SP) 13083-852, Brazil
30. Modified case based reasoning cycle for expert knowledge acquisition during process design
E. Roldán^a, S. Negny^a, J.M. Le Lann^a, G. Cortés^b
^a Laboratoire de Genie Chimique UMR 5503, INPT-ENSIACET, 4 allée Emile Monso, BP 44362 – 31 030 Toulouse, France.
^b Postgrade Department, ITO, Orizaba, Ver, 31400, México
31. Process intensification on membrane-based process for Blackcurrant Juice Concentration
Lene Fjerbaek Sotoft, Ben-Guang Rong, Knud V. Christensen, Birgir Norddahl
Institute of Chemical Engineering, Biotechnology and Environmental Technology, University of Southern Denmark, Niels Bohrs Alle 1, 5230 Odense, Denmark.

Molecular/Material Systems Engineering

32. GPU based parallel computing method for molecular weight distribution of batch free radical polymerization
Zhiqiang Chen^a, Xi Chen^{a}, Zhen Yao^b, Zhijiang Shao^a*
^a Department of Control Science and Engineering, Zhejiang University, Hangzhou 310027, China
^b Department of Chemical Engineering, Zhejiang University, Hangzhou 310027, China.
33. Models driven conception of an inverse formulation software tool
Juliette Heintz^{a,b}, Vincent Gerbaud^{a,b}, Jean-Pierre Belaud^{a,b}
^a Université de Toulouse, INP, UPS, LGC (Laboratoire de Génie Chimique), 4 allée Emile Monso, F-31030 Toulouse Cedex 04 – France. vincent.gerbaud@ensiacet.fr
^b CNRS, LGC (Laboratoire de Génie Chimique), F-31030 Toulouse Cedex 04– France

34. Iterative learning control of a reactive polymer composite moulding process using batch wise updated linearised models
Jie Zhang^a, Nikos G. Pantelidis^b
^a *School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU, UK*
^b *Mechanical Engineering Department, National Technical University of Athens, Greece*
35. Predicting a wide variety of constant pure compound properties by the targeted QSPR method
Mordechai Shacham^a, Neima Brauner^b
^a *Dept. Chem. Engng, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel*
^b *School of Engineering, Tel-Aviv University, Tel-Aviv 69978, Israel*

Biomedical Systems Engineering

36. A novel physiological based compartmental model for volatile anaesthesia
Alexandra Krieger^a, Nicki Panoskaltis^b, Athanasios Mantalaris^c, Michael C. Georgiadis^a, Efstratios N. Pistikopoulos^a
^a *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London, SW7 2AZ, UK*
^b *Department of Haematology, Imperial College London, Northwick Park & St. Mark's Campus, London, HA1 3UJ, UK*
^c *Biological Systems Engineering Laboratory, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London, SW7 2AZ, UK*
37. Modelling of the insulin delivery system for patients with type 1 diabetes Mellitus
Stamatina Zavitsanou^a, Nicki Panoskaltis^b, Athanasios Mantalaris^a, Michael C. Georgiadis^a, Efstratios N. Pistikopoulos^a
^a *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK*
^b *Department of Haematology, Imperial College London, Northwick Park & St. Mark's Campus, London, HA1 3UJ, UK*
38. Towards a high-fidelity model for model based optimisation of drug delivery systems in acute myeloid leukemia
Eleni Pefani^a, Nicki Panoskaltis^b, Athanasios Mantalaris^a, Michael C. Georgiadis^a, Efstratios N. Pistikopoulos^a
^a *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK*
^b *Department of Haematology, Imperial College London, Northwick Park & St. Mark's Campus, London, HA1 3UJ, UK*
39. Computational investigation of vascular surgical interventions on popliteal artery aneurysms
D. Papadimitriou^c, A.H. Alexopoulos^b, T. Gerasimidis^c and C. Kiparissides^{a,b}
^a *Department of Chemical Engineering, Aristotle University of Thessaloniki, P.O. Box 472, 541 24, Thessaloniki, Greece,*
^b *Chemical Process Engineering Research Institute, P.O. Box 60361, 57001, Greece,*
^c *5th Surgical Department, Aristotle University, Thessaloniky, Greece.*
40. Three dimensional simulation and experimental investigation of intrathecal drug delivery in the spinal canal and the brain
Ying Hsu, Timothy J. Harris Jr, H.D.M. Hettiarachchi, Richard Penn, Andreas A. Linninger
Laboratory for Product and Process Design (LPPD), Department of Bioengineering, University of Illinois at Chicago 851 S. Morgan St., 218 SEO, Chicago, Illinois 60607, USA
41. A computational model of cerebral vasculature, brain tissue, and cerebrospinal fluid
Nicholas M. Vaičaitis, Brian J. Sweetman, Andreas A. Linninger
Department of Bioengineering, University of Illinois at Chicago, 851 S. Morgan St, SEO 218, Chicago, IL 60607, USA
42. Physiologically-based pharmacokinetic modeling: Parameter estimation for Cyclosporin A
Eric Lueshen, Cierra Hall, Andrej Mošat and Andreas Linninger
University of Illinois at Chicago, Laboratory for Product and Process Design, M/C 063, 851 S. Morgan St. - 218 SEO, Chicago 60607-7000, Illinois, USA
43. Optimal design of chitosan-based scaffolds for controlled drug release using dynamic optimization
Belmiro P.M. Duarte^{a,b}, Nuno M.C. Oliveira^b, Maria J.C. Moura^a
^a *Dep. Chemical and Biological Engineering, Polytechnic Institute of Coimbra, R. Pedro Nunes, 3030-190 Coimbra, Portugal.*
^b *GEPSI-PSE Group, CIEPQPF, Dep. Chemical Engineering, University of Coimbra, R. Sílvio Lima — Pólo II; 3030-790 Coimbra, Portugal.*

Poster Session 2 – ERATO HALL

Chair: M. Nazmul Karim (Texas Tech, USA)

Optimization and Control

1. Feasibility analysis of black-box processes using an adaptive sampling kriging based method
F. Boukouvala, F.J. Muzzio, M.G. Ierapetritou
Dept. Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, 08854, USA
2. Control and dynamic optimization of a BTX dividing-wall column
A.A. Kiss^a, R.R. Rewagad^b
^a AkzoNobel – Research, Development and Innovation, Velperweg 76, 6824 BM, Arnhem, The Netherlands
^b University of Twente, Faculty of Science and Technology, Enschede, The Netherlands
3. Process dynamic optimization using ROMeO
F. Manenti^a, G. Buzzi-Ferraris^a, S. Pierucci^a, M. Rovaglio^b, H. Gulati^b
^a Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta”, Piazza Leonardo da Vinci 32, 20133 Milano, ITALY
^b Invensys Operations Management, 26561 Rancho Parkway South Lake Forest, 92630, California, USA
4. Multi-objective optimisation approach to optimal experiment design in dynamic bioprocesses using ACADO toolkit
F. Logist, D. Telen, E. Van Derlinden, J.F. Van Impe
BioTeC & OPTeC - Chemical Engineering Dept., Katholieke Universiteit Leuven, W. de Croylaan 46, B-3001 Leuven, Belgium
5. Increase the catalytic cracking process efficiency by implementation an optimal control structure. Case study
C. Popa, C. Pătrăşcioiu
Control Engineering and Computers Department, Petroleum Gas University of Ploiesti, Bucuresti Blvd., 39, 1006800, Ploiesti, Romania
6. A hybrid Branch-and-Cut approach for the capacitated vehicle routing problem
C.E. Gounaris^a, P.P. Repoussis^b, C.D. Tarantilis^b, C.A. Floudas^a
^a Computer-Aided Systems Laboratory, Department of Chemical and Biological Engineering, Princeton University, NJ 08544, USA
^b Center for Operations Research & Decision Systems, Department of Management Science & Technology, Athens University of Economics & Business, Athens 11362, Greece
7. MPC vs. PID. The advanced control solution for an industrial heat integrated fluid catalytic cracking plant
M. Iancu, M.V. Cristea, P.S. Agachi
Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Chemical Engineering Department, Arany Janos St., No. 11, 400028, Cluj-Napoca, Romania
8. A robust optimization based approach to the general solution of mp-MILP problems
M. Wittmann-Hohlbein, E.N. Pistikopoulos
Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College, London SW7 2BY, UK
9. A deterministic optimization approach for the unit commitment problem
M.G. Marcovecchio^{a,b}, A.Q. Novais^a, I.E. Grossmann^c
^a UMOSE/LNEG, Estrada do Paço do Lumiar 22, 1649-038, Lisbon, Portugal
^b INGAR/CONICET, Instituto de Desarrollo y Diseño, Santa Fe, Argentina
^c UNL, Universidad Nacional del Litoral, Santa Fe, Argentina
^c Department of Chemical Engineering, Carnegie Mellon University, USA
10. Simulation-based dynamic optimization of discretely controlled continuous processes
M. De Paula, E. Martínez
INGAR (Conicet-UTN), Avellaneda 3657, Santa Fe, S3002 GJC, Argentina
11. Evaluation of steady state multiplicity for the anaerobic degradation of solid organic waste
M. Sbarciog, A. Donoso-Bravo, A. Vande Wouwer
UMONS, Automatic Control Laboratory, 31 Boulevard Dolez, Mons 7000, Belgium
12. Multi-objective optimization of three-phase batch extractive distillation
A.A. Barreto^a, I.R. Donis^a, V. Gerbaud^{b,c}, X. Joulia^{b,c}
^a Instituto Superior de Tecnologías y Ciencias Aplicadas (InSTEC). Ave Salvador Allende y Luaces. Ciudad Habana. AP 6163. Cuba
^b Université de Toulouse, INP, UPS, LGC (Laboratoire de Génie Chimique), 4 allée Emile Monso, F-31432 Toulouse Cedex 04 – France
^c CNRS, LGC (Laboratoire de Génie Chimique), F-31432 Toulouse Cedex 04 – France
13. Self-adaptive differential evolution with taboo list for constrained optimization problems and its application to pooling problems
H. Zhang, G.P. Rangaiah
Department of Chemical & Biomolecular Engineering, National University of Singapore, Singapore 117576, Singapore

14. Disturbance estimation via moving horizon estimation for in-flight model-based wind estimation
A. Voelker, K. Kouramas, C. Panos, E. Pistikopoulos
Centre for Process Systems Engineering, Chemical Engineering, Imperial College, London, SW7 2AZ, UK
15. Optimal grade transitions in an industrial slurry-phase catalytic olefin polymerization loop-reactor series
V. Touloupides^{a,b}, V. Kanellopoulos^b, C. Chatzidoukas^{a,b}, C. Kiparissides^{a,b}
^a *Department of Chemical Engineering, Aristotle University of Thessaloniki*
^b *Centre for Research and Technology Hellas, P.O. Box 60 361, Thessaloniki, Greece*
16. Combined nonlinear model reduction and multiparametric nonlinear programming for nonlinear model predictive control
P. Rivotti, R.S.C. Lambert, L. Dominguez, E.N. Pistikopoulos
Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, SW7 2AZ, UK
17. Integrated design and control of pressure swing adsorption systems
H. Khajuria, E.N. Pistikopoulos
Centre of Process System Engineering, Department of Chemical Engineering, Imperial College London, SW7 2AZ, UK
18. A robust MILP-based approach to vehicle routing problems with uncertain demands
A. Aguirre^b, M. Coccolà^b, M. Zamarripa^a, C. Méndez^b, A. Espuña^a
^a *Chemical Engineering Department, Universitat Politècnica de Catalunya (UPC), Barcelona, Spain*
^b *INTEC (UNL-CONICET), Santa Fe, Argentina*
19. Integration of a multilevel control system in an ontological information environment
E. Muñoz, A. Espuña, L. Puigjaner
Department of Chemical Engineering, Universitat Politècnica de Catalunya, ETSEIB, Avda. Diagonal, 647, E-08028 - Barcelona, Spain
20. Control structure selection with regard to stationary and dynamic performance with application to a ternary distillation column
L.C. Pham, S. Engell
Process Dynamics and Operations Group, Department of Biochemical and Chemical Engineering, Technische Universität Dortmund, Emil-Figge-Str. 70, 44221 Dortmund, Germany
21. Membrane process optimization for hydrogen peroxide ultrapurification
R. Abejón, A. Gareá, A. Irabien
Departamento de Ingeniería Química y Química Inorgánica, Universidad de Cantabria, Av. Los Castros, 39005 Santander, Spain
22. Dynamic optimization of porous media combustor using a greybox neural model and NMPC technique
L. Henríquez-Vargas, V. Bubnovich, F. Cubillos
Chemical Engineering Department, Universidad de Santiago de Chile, Casilla 10233, Santiago, Chile
23. Monte Carlo assessment of the arrival cost evaluation method in moving horizon estimation for chemical processes
F.D. Rincón Cuellar, W.H. Hirota, R. Giudici, G.A.C. Le Roux
Department of Chemical Engineering, Polytechnic School of the University of São Paulo, Av. Luciano Gualberto trav.3, 380, São Paulo, 05508-900 Brazil
24. Adaptive advanced control of a copolymerization system
N.M.N. Lima^a, L.Z. Liñan^a, F. Manenti^b, R.M. Filho^a, M. Embiruçu^c, M.R.W. Maciel^a
^a *University of Campinas (UNICAMP), Department of Chemical Processes, Barão Geraldo, 13083-970, Campinas-SP, Brazil*
^b *Politecnico di Milano, CMIC dept. "Giulio Natta", Piazza Leonardo da Vinci 32, 20133, Milano, Italy*
^c *Federal University of Bahia, Polytechnic Institute, Federação, 40210-630, Salvador-BA, Brazil*
25. Control of processes with multiple steady states using MPC and RBF neural networks
A. Alexandridis^a, H. Sarimveis^b
^a *Department of Electronics, Technological Educational Institute of Athens, Agiou Spyridonos, Aigaleo, 12210, Greece*
^b *School of Chemical Engineering, National Technical University of Athens, 9 Heroon Polytechniou street, Zografou campus, Athens, 15780, Greece*
26. Simulation optimization of cost, safety and displacements in a construction design
E.S. Telis^{a,b}, G. Besseris^{a,b}, C. Stergiou^{a,b}
^a *Department of Mechanical Engineering, Technological and Educational Institute of Piraeus, P. Ralli & Thivon Avenue 250, Aigaleo 12224, Athens, Greece*
^b *Kingston University, Faculty of Engineering, Penrhyn Road, Kingston upon Thames, KT1 2EE, London, England*
27. Methodologies for input-output data exchange between LabVIEW® and MATLAB®/Simulink® software for real time control of a pilot scale distillation process
A.J.S. Chambel, C.I.C. Pinheiro, J. Borges, J.M. Silva
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^c Instituto Superior de Engenharia de Lisboa, Rua Conselheiro Emídio Navarro, 1, 1950-062 Lisboa, Portugal

28. Dynamic modeling and optimization of flash separators for highly-viscous polymerization processes
P. Pladis^b, V. Kanellopoulos^b, A. Baltas^b, C. Kiparissides^{a,b}
^a Department of Chemical Engineering, AUTH, Thessaloniki, 541 24, Greece
^b Centre for Research and Technology Hellas, Thessaloniki, 570 01, Greece
29. A novel approximation technique for online and multi-parametric model predictive control
R.S.C. Lambert, P. Rivotti, E.N. Pistikopoulos
Centre for Process Systems Engineering, Imperial College, London, SW7 2AZ, UK
30. Use of commercial structured databases as innovative solution for FEED projects
F. Ferrari, L. Selmi
Foster Wheeler Italiana, via Caboto 1, Corsico 20094, Italy
31. Controlled variables from optimal operation data
J. Jäschke, S. Skogestad
Department of Chemical Engineering; NTNU; Trondheim, Norway
32. Robust reallocation and upgrade of sensor networks for fault diagnosis
S. Kolluri, M. Bhushan
Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai-400076, India
33. Explicit/Multi-parametric model predictive control of a solid oxide fuel cell
K. Kouramas^a, P.S. Varbanov^b, M.C. Georgiadis^c, J.J. Klemeš^b, E.N. Pistikopoulos^a
^a Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK
^b Centre for Process Integration and Intensification CPI2, Research Institute for Chemical and Process Engineering, Faculty of Information Technology, University of Pannonia, Egyetem u. 10, 8200 Veszprém, Hungary
^c Department of Engineering Informatics and Telecommunications, University of Western Macedonia, Kozani 50100, Greece
34. A theoretically rigorous approach to soft sensor development using Principal Components Analysis
C.K.N. Kartik, S. Narasimhan
Indian Institute of Technology Madras, Chennai, India
35. Experimental comparison of type-1 and type-2 fuzzy logic controllers for the control of level and temperature in a vessel
B. Cosenza, M. Galluzzo
Dipartimento di Ingegneria Industriale, Università degli Studi di Palermo, Viale delle Scienze, Ed. 6, 90128 Palermo, Italy
36. Tuning a distillation column simulator
K.E. Häggblom, R.K. Ghosh
Process Control Laboratory, Dept. of Chemical Engineering, Åbo Akademi University, Biskopsgatan 8, FIN-20500 Åbo, Finland
37. A comparative study of MPC-based control configurations of an industrial bioreactor to produce ethanol
A. Romo-Hernández^a, S. Hernández^a, A. Sánchez^b, H. Hernández-Escoto^a
^a Universidad de Guanajuato, Departamento de Ingeniería Química, Noria Alta s/n, Col. Noria Alta, Guanajuato, Guanajuato, 36050, México
^b Centro de Investigación y Estudios Avanzados, Unidad de Ingeniería Avanzada, Av. Científica 1145, Col. El Bajío, Zapopan, Jalisco, 45015, México
38. Optimal temperature tracking of a solid state fermentation reactor
C. González-Figueroa^a, O.R. Ayala^b, S. Aguilar^b, O. Aroche^b, A. Loukianov^b, A. Sánchez^b
^a Universidad Autónoma de Guadalajara, Departamento de Química, Av. Patria 1201, Col. Lomas del Valle, Zapopan 45129, México
^b Centro de Investigación y Estudios Avanzados, Unidad de Ingeniería Avanzada, Av. Científica, Col. El Bajío, Zapopan 45010, México
39. A Worst-Case observer for impurities in enantioseparation by preferential crystallization
S. Hofmann^a, M. Eicke^c, M.P. Elsner^c, A. Seidel-Morgenstern^{b,c}, J. Raisch^{a,c}
^a Technische Universität Berlin, Einsteinufer 17, 10587 Berlin, Germany
^b Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany
^c Max-Planck Institut für Dynamik Komplexer Technischer Systeme, Sandtorstr. 1, 39106 Magdeburg, Germany
40. Economic plantwide control of C₄ isomerization process
R. Jagtap, S. Goenka, N. Kaistha
Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India
41. Statistical process control of multivariate systems with autocorrelation
T.J. Rato, M.S. Reis

CIEPQPF, Department of Chemical Engineering, University of Coimbra, Rua Sívio Lima, 3030-790, Coimbra, Portugal

42. Free radicals copolymerization optimization, system: acrylonitrile-vinyl acetate in CSTR
S.V. Vallecillo-Gómez, J.C. Tapiá-Picazo, A. Bonilla-Petriciolet, G.G. De-Alba-Pérez-de-Gracia
Department of Chemical and Biochemical Engineering, Instituto Tecnológico de Aguascalientes. Adolfo López Mateos 1801, Bona Gens, Aguascalientes, Ags., 20256, México
43. Control of an azeotropic distillation process to acetonitrile production
A.R. Ruiz, N.B. Beltrán, A. Leguizamón R., J.R. Guevara L., I.D. Gil C.
Grupo de Ingeniería de Sistemas de Proceso- Departamento de Ingeniería Química y Ambiental, Universidad Nacional de Colombia – Sede Bogotá, Carrera 30 45-03, Bogotá, Colombia
44. Optimization of IMC-PID tuning parameters for adaptive control: Part 1
C.W. Chu, B.E. Ydstie, N.V. Sahinidis
Carnegie Mellon University, 5000 Forbes Ave., Pittsburgh, PA 15213, USA
45. Optimization of hybrid reactive distillation-pervaporation system
V. Amte
Department of Chemical Engineering, Indian Institute of Technology, Bombay 400076, India
46. Software application for intelligent control of a bioprocess. Case study
C. Tănase^a, M. Caramihai^a, C. Ungureanu^a, G. Sârbu^a, A.A. Chirvase^b, O. Muntean^a
a Politehnica University of Bucharest, 1, Polizu Street, district 1, CP 011061, Bucharest, Romania
b National Research & Development Institute for Chemistry and Petrochemistry ICECHIM, 202, Splaiul Independetei, district 6, CP 060021, Bucharest, Romania
47. Design of robust PID controller for processes with stochastic uncertainties
P.L.T. Duong, M. Lee
Yeungnam University, Gyeongsan 712-749, Rep. Korea
48. Towards benchmarking of multivariable controllers in chemical/biochemical industries: Plantwide control for ethylene glycol production
Jakob K. Huusom, Dawid J. Bialas, John B. Jørgensen, Gürkan Sin
DTU, Denmark

Poster Session 3 – TERPSIHORI HALL

Chair: Iqbal Mujtaba (University of Bradford, UK)

Process Operations

1. A simulated annealing approach for the bi-objective design and scheduling of multipurpose batch plants
N. Chibeles-Martins^{a,c}, T. Pinto-Varela^{a,b}, A.P. Barbósa-Póvoa^b, A.Q. Novais^a
^a Unidade de Modelação e Optimização de Sistemas Energéticos (DMS- INETI), LNEG, Lisboa, Portugal
^b Centro de Estudos de Gestão, IST, UTL, Av. Rovisco Pais, 1049-101 Lisboa, Portugal
^c Centro de Matemática e Aplicações, CMA, FCT-UNL, Qta da Torre, 28259-516, Caparica, Portugal
2. Operating procedure synthesis subject to restricted state transition using differential evolution
Y. Shimizu
Toyohashi University of Technology, Toyohashi, Aichi 441-8580, Japan
3. MILP formulation for resource-constrained project scheduling problems
T.S. Kyriakidis^a, G.M. Kopanos^b, M.C. Georgiadis^{a,c}
^a Department of Engineering Informatics & Telecommunications, University of Western Macedonia, Karamanli and Lygeris Street, Kozani 50100, Greece
^b Department of Chemical Engineering, Universitat Politècnica de Catalunya, Av. Diagonal 647, Barcelona 08028, Spain
^c Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece
4. Self-learning of fault diagnosis identification
J.L. de la Mata, M. Rodríguez
Technical University of Madrid, José Gutiérrez Abascal 2, Madrid 28006, Spain
5. Decision support system for multiproduct pipeline and inventory management systems
S. Relvas^a, A.P. F.D. Barbosa-Póvoa^a, H.A. Matos^b, P. Pinto^a
^a CEG-IST, UTL, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
^b CPQ, IST, UTL, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

6. Ice cream scheduling: modeling the intermediate storage
M.A.H. van Elzaker^a, E. Zondervan^a, C. Almeida-Rivera^b, I.E. Grossmann^c, P.M.M. Bongers^{b,d}
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^d *Hoogewerff Chair for Product-driven Process Technology, Dep. Chem. And Chem. Eng., Eindhoven University of Technology*
7. Simultaneous optimization of planning and scheduling in an oil refinery
E. Zondervan, T.P.J. van Boekel, J.C. Fransoo, A.B. de Haan
Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands
8. Robust market launch planning for a multi-echelon pharmaceutical supply chain
K.R.N. Hansen^a, M. Grunow^b, R. Gani^a
^a *Technical University of Denmark, Kgs. Lyngby 2800, Denmark*
^b *Technische Universität München, München 80804, Germany*
9. Modelling and dynamic optimisation for optimal operation of industrial tubular reactor for propane cracking
M. Berreni, M. Wang
Process Systems Engineering Group, School of Engineering, Cranfield University, MK43 0AL, UK
10. An efficient mathematical framework for detailed production scheduling in food industries: The icecream production line
G.M. Kopanos^a, L. Puigjaner^a, M.C. Georgiadis^b, P.M.M. Bongers^c
^a *Universitat Politècnica de Catalunya-ETSEIB, Diagonal 647, Barcelona 08028, Spain*
^b *Aristotle University of Thessaloniki, Department of Chemical Engineering, Thessaloniki 54124, Greece*
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11. Corporate production planning for industrial gas supply chains under low-demand conditions
M. D'Isanto^a, F. Manenti^a, N.M.N. Lima^b, L.Z. Linan^b
^a *Politecnico di Milano, CMIC Dept. "Giulio Natta", Piazza Leonardo da Vinci 32, 20133 Milano, ITALY*
^b *University of Campinas (UNICAMP), Department of Chemical Processes, PO Box 6066, 13081-970, Campinas, São Paulo, BRAZIL*
12. Standards for continual scheduling of batch operations
C. Siletti^a, D. Petrides^b, D. Vardalis^c
^a *Intelligen, Inc. 700 Walton Ave., Mt. Laurel, NJ 08054 USA*
^b *Intelligen, Inc. 2326 Morse Ave, Scotch Plains, NJ 07076 USA*
^c *Intelligen Europe, Thessaloniki, Greece*
13. New tools for the detailed scheduling of refined products pipelines
V.G. Cafaro, D.C. Cafaro, C.A. Méndez, J. Cerdá
INTEC (UNL-CONICET), Güemes 3450, (3000) Santa Fe, Argentina
14. A MILP planning model for a real-world multiproduct pipeline network
S.N. Boschetto^a, L. Magatão^a, F. Neves-Jr^a, A.P.F.D. Barbosa-Póvoa^b
^a *CPGEI – Federal University of Technology – Paraná. Av. Sete de Setembro, n. 3165, 80230-901, Curitiba, Brazil*
^b *CEG-IST – Instituto Superior Técnico – UTL – Lisboa, Av. Rovisco Pais, 1049-001, Lisboa, Portugal*
15. Optimal scheduling of biodiesel plants through property-based integration with oil refineries
V. Kazantzi^a, S. Bezergianni^b, R. Elms^c, F. Eljack^d, M.M. El-Halwagi^e
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16. Integration of financial statement analysis in the optimal design and operation of supply chain networks
P. Longinidis^a, M.C. Georgiadis^{a,b}, P. Tsiakis^c
^a *Department of Engineering Informatics & Telecommunications, University of Western Macedonia, Karamanli & Lygeris Street, Kozani 50100, Greece*
^b *Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece*
^c *IBM UK Ltd, 76-78 Upper Ground, South Bank London SE1 9PZ, UK*
17. Integrated production planning and scheduling optimization of multi-site, multi-product process industry
N.K. Shah, M.G. Ierapetritou
Department of Chemical and Biochemical Engineering, Rutgers University, 98 Brett Road, Piscataway, New Jersey 08854, USA
18. Simulation-based reactive scheduling in tomato processing plant with raw material uncertainty
A. Koulouris, I. Kotelida

Alexandria Technological Educational Institute of Thessaloniki, 57400 Sindos, Greece

19. Modeling Next Generation Feedstock Development for Chemical Process Industry
S. Cremaschi
Department of Chemical Engineering, The University of Tulsa, 800 South Tucker Drive, Tulsa, Oklahoma 74104, USA
20. Study of closed operation modes of batch distillation columns
L. Hegely, P. Lang
Budapest University of Technology and Economics, Dept. of Building Services and Process Engineering, H-1521, Budapest, Hungary
21. Dynamic failure assessment of incidents reported in the Greek Petrochemical Industry
E.C. Marcoulaki, M. Konstandinidou, I.A. Papazoglou
Laboratory of System Reliability and Industrial Safety, National Centre for Scientific Research "Demokritos", PO Box 60228, Aghia Paraskevi, Athens 15310, Greece
22. An evaluation method for plant alarm system based on a Two-Layer Cause-Effect Model
N. Kimura^a, K. Takeda^b, M. Noda^c, T. Hamaguchi^d
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^d *Graduate School of Engineering, Nagoya Institute of Technology, Gokiso, Showa-ku, Nagoya 466-8555, Japan*
23. Generating cause-implication graphs for process systems via blended hazard identification methods
E. Németh^a, B.J. Seligmann^a, K. Hockings^b, J. Oakley^b, C. O'Brien^c, K.M. Hango^d, I.T. Cameron^a
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^b *BlueScope Steel Ltd, Port Kembla, Australia 2500*
^c *BP Refinery (Bulwer Island), Brisbane, Australia 4008*
^d *Process Control Research Group, HAS Computer and Automation Research Institute, Budapest 1111, Hungary*
24. Data mining and decision making tool development for an industrial dual sequential batch reactor
S. Gutiérrez, A. Ferrari, A. Benítez
IIQ - Department of Reactors Engineering, Engineering School - University of the Oriental Republic of Uruguay, Herrera y Reissig 565, CP 11300, Montevideo, Uruguay
25. Agent-based coordination framework for disruption management in a chemical supply chain
B. Behdani^a, Z. Lukszo^a, A. Adhitya^b, R. Srinivasan^{b,c}
^a *Faculty Technology, Policy and Management, TU Delft, the Netherlands*
^b *Institute of Chemical and Engineering Sciences, A*STAR, Singapore*
^c *National University of Singapore, Dept of Chemical and Biomolecular Eng, Singapore*
26. Recipe-driven dynamic hybrid simulation of batch processes: a combined optimization/simulation approach
G. Hétreux, A. Ramaroson, J.M. Le Lann
Laboratoire de Génie Chimique, UMR-CNRS 5503 / INPT-ENSIACET, 4, allée Emile Monso, 31030 Toulouse Cedex 4, France
27. Simulation-based dynamic optimization under uncertainty of a industrial biological process
Guillermo A. Durand^a, Anibal M. Blanco^a, Fernando D. Mele^b, J. Alberto Bandoni^a
^a *Planta Piloto de Ingeniería Química, PLAPIQUI (UNS – CONICET), Camino La Carrindanga Km7, (8000) Bahía Blanca, Argentina*
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28. Systematic synthesis of emergency response procedures for batch chemical processes
M.L. Yeh, C.T. Chang
Department of Chemical Engineering, National Cheng Kung University, 1 Ta-Hsueh Road, Tainan 70101, Taiwan (R.O.C.)

Multi-scale Modelling

29. Detailed mathematical modelling of Liquid-Liquid extraction columns
M. Jaradat^{a,c}, M. Attarakih^{b,c}, H.J. Bart^{a,c}
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^c *Centre of Mathematical and Computational Modelling, TU Kaiserslautern, Germany*
30. Modeling the liquid back mixing characteristics for a kinetically controlled reactive distillation process
M. Shah^a, E. Zondervan^a, A.A. Kiss^b, A.B. de Haan^a
^a *Process Systems Engineering, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, 5600 MB, The Netherlands*
^b *AkzoNobel – Research, Development & Innovation, Process Technology ECG, Velperweg 76, 6824 BM Arnhem, The Netherlands*
31. Application of computer-aided multi-scale modelling framework – Aerosol case study

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^b Firmenich Inc., 250 Plainsboro Road, Plainsboro, NJ, 08536, USA

32. Mathematical description of mass transfer in supercritical-carbon-dioxide-drying processes
C. Almeida-Rivera^a, S. Khalloufi^a, J. Jansen^a, P. Bongers^{a,b}
^a Unilever R&D Vlaardingen, Olivier van Noortlaan 120, 3130 AC, Vlaardingen, The Netherlands
^b Hoogwerff chair in Product-Driven Process Engineering, Eindhoven University of Technology, PO Box 513, 5600 MB, Eindhoven, The Netherlands
33. Three-moments conserving sectional techniques for the solution of coagulation and breakage population balances
M. Kostoglou^a, M.C. Georgiadis^b
^a Department of Chemistry, Aristotle University, Univ. Box 116, 54124 Thessaloniki, Greece
^b Department of Chemical Engineering, Aristotle University of Thessaloniki, 54124, Greece
34. Modelling and simulation of forced convection drying of electric insulators
C. Vasile-Mircea, G. Firuta, M.L. Mihai
Babes-Bolyai University, 11 Arany Janos Street, 400028 Cluj-Napoca, Romania
35. Comprehensive mathematical modeling of controlled radical copolymerization in tubular reactors
M. Asteasuain^a, D. Covan^a, C. Sarmoria^a, A. Brandolin^a, C.L. de Araujo^b, J.C. Pinto^b
^a PLAPIQUI (CONICET-UNS), Camino La Carrindanga km 7, Bahía Blanca 8000, Argentina
^b Programa de Engenharia Química da COPPE/UFRJ, Universidade Federal do Rio de Janeiro, Cidade Universitária, CP:68502, Rio de Janeiro, RJ 21945-970, Brazil
36. Multi-scale modeling of activated sludge floc structure formation in wastewater bioreactors
I.D. Ofițeru^{a,b}, M. Bellucci^b, V. Lavric^a, C. Picioreanu^c, T.P. Curtis^b
^a University Politehnica of Bucharest, Chemical Engineering Department Polizu 1-7, Bucharest 011061, Romania
^b Newcastle University, School of Civil Engineering and Geosciences, Cassie Building, Newcastle upon Tyne NE1 7RU, UK
^c Delft University of Technology, Department of Biotechnology, Julianalaan 67, 2628 BC Delft, The Netherlands
37. Modeling and simulation of a gas cleaning section in a Cu/Ni metallurgical plant
M. Alic^a, T.A. Hauge^{b,c}, B. Lie^a
^a Telemark University College, Porsgrun N-3918, Norway
^b Xstrata Nikkelverk, Kristiansand N-4606, Norway
^c Agder University, Grimstad N-4898, Norway
38. A novel approach to the biomass pyrolysis step and product lumping
D. Bernocco, P. Greppi, E. Arato
PERT - Process Engineering Research Team
Department of Construction, Environment and Land Engineering
UNIGE - Università degli Studi di Genova, Via Opera Pia 15, 16145 Genova, Italy
39. Stochastic Monte Carlo simulations as an efficient multi-scale modeling tool for the prediction of multi-variate distributions
D. Meimaroglou^{a,c}, C. Kiparissides^{a,b}
^a Chemical Process Engineering Research Institute, Centre for Research and Technology Hellas, 570 01, Thessaloniki, Greece
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^c Current Address: Laboratory of Reactions and Process Engineering, Nancy University, LRGP-ENSIC-INPL, 1 rue Grandville, BP 20451, 54000 Nancy, France
40. CFD modelling of the demister in the multi stage flash desalination plant
H. Al-Fulaij^a, A. Cipollina^b, G. Micale^b, D. Bogle^c, H. Ettouney^d
^a Department of Chemical Engineering, College of Engineering and Petroleum, Kuwait University, P.O. Box 5969, Safat 13060, Kuwait, engrhala@yahoo.com
^b Dipartimento di Ingegneria Chimica dei Processi e dei Materiali, Università di Palermo, Italy
^c Department of Chemical Engineering, University College London, London, UK
^d Department of Chemical Engineering, College of Engineering and Petroleum, Kuwait University, Kuwait
41. 3D Cellular automata for modeling of spray freeze drying process
S. Ivanov, A. Troyankin, P. Gurikov, A. Kolnoochenko, N. Menshutina
D. Mendeleev University of Chemical Technology of Russia (MUCTR), CAPE Department, Miusskaya sq. 9, Moscow, 125047, Russia
42. Spatially 3D simulation of a catalytic monolith by coupling of 1D channel model with CFD
J. Štěpánek^a, P. Kočí^a, M. Kubíček^b, F. Plát^a, M. Marek^a
^a Dept. of Chemical Engineering
^b Dept. of Mathematics, Institute of Chemical Technology, Prague, Czech Republic

43. A generic framework for stochastic dynamic simulation of chemical engineering systems using free/open source software
C. Sandrock, P. de Vaal
Department of Chemical Engineering; University of Pretoria; South Africa
44. Process modelling and model reduction for chemical engineering applications
B. Dorneanu^{a,b}, J. Grievink^a, C.S. Bildea^c
^a *Delft University of Technology, Dept. of Chemical Engineering, Julianalaan 136, 2628BL Delft, The Netherlands*
^b *Delft University of Technology, Process and Energy Dept., Leeghwaterstraat 44, 2628CA Delft, The Netherlands*
^c *University Politehnica of Bucharest, Dept. of Chemical Engineering, Str. Gh. Polizu 1- 7, 001061 Bucharest, Romania*
45. General-purpose graphics processing units application for diffusion simulation using cellular automata
A.Kolnoochenko, P. Gurikov, N. Menshutina
CAPE Department, MUCTR, Moscow, Russia
46. A reduced-order approach of distributed parameter models using proper orthogonal decomposition
M. Valbuena, D. Sarabia, C. de Prada
Department of Systems engineering and Automatic, C/Real de Burgos s/n, Valladolid, University of Valladolid, Spain
47. Prediction of the permeability and filtration - Performance of packed beds
Mishal Islam, Xiaodong Jia, Michael Fairweather, Richard Williams
School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT, UK
48. Modelling of pipe bend erosion by dilute particle suspensions
Derrick O. Njobuenwu and Michael Fairweather
Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT, UK
49. Integral formulation of the population balance equation using the cumulative QMOM
Menwer Attarakih^{a,b,c}, M. Jaradat^{b,c}, M. Hlawitschka^{b,c}, H.-J. Bart^{b,c}, J. Kuhnert^d
^a *Al-Balqa Applied University, Faculty of Eng. Tech, POB 15008, 11134 Amman, Jordan*
^b *TU Kaiserslautern, Lehrstuhl für Thermische Verfahrenstechnik, POB 3049, 67653 Kaiserslautern, Germany*
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Poster Session 4 – MARINA I

Chair: Mario Eden (Auburn University, USA)

Training and Education

1. Long distance operator training
Y. Bessiris^a, D. Kyriakopoulou^a, F. Ghajar^b, C. Steuckrath^b
^a *Hyperion Systems Engineering, 38 Strovolou Avenue, CY-2018 Nicosia, Cyprus*
^b *Saudi Aramco, Saudi Arabia*
2. Academic performance and success rate: A challenge problem for the PSE community
M. Graells, A. Espuña
Chemical Engineering Department, Universitat Politècnica de Catalunya (UPC). EUETIB, 08028 - Comte d'Urgell 187, Barcelona, Spain
3. MOSAIC, an environment for web-based modelling in the documentation level
S. Kuntsche, H. Arellano-Garica, G. Wozny
TU Berlin, KWT-9, Straße des 17. Juni 135, D-10623 Berlin, Germany
4. The TriLab and ilough-Lab portal – Systematic evaluation of the use of remote and virtual laboratories in engineering education
M. Abdulwahed, Z.K. Nagy
Chemical Engineering Department, Loughborough University, Loughborough, LE11 3TU, UK

Environmental Systems Engineering

5. Supply chain design and planning with environmental impacts: An RTN approach
T. Pinto-Varela^{a,b}, A.P.F.D. Barbosa-Póvoa^b, A.Q. Novais^a
^a *UMOSE/LNEG, Estrada da Portela, Bairro do Zambujal, 2720-866 Amadora, Portugal*

^b Centro de Estudos de Gestão, IST- UTL, Av. Rovisco Pais, 1049 –001 Lisboa, Portugal

6. Modelling the natural gas pipeline internal corrosion rate resulting from hydrate formation
E.O. Obanijesu, M.K. Akindeju, P. Vishnu, M.O. Tade
Department of Chemical Engineering, Curtin University, Perth, WA 6102, Australia
7. Multilevel strategies for the retrofit of a large industrial water system
H. Tokos^a, Z.N. Pintarić^b, Y. Yang^a, Z. Kravanja^b
^a State Key Laboratory of Chemical Engineering, Zhejiang University, Department of Chemical and Biochemical Engineering, Hangzhou, 310027, P. R. China
^b University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova 17, SI-2000 Maribor, Slovenia
8. Synthesis of water integration networks in eco-industrial parks
E. Rubio-Castro^a, J.M. Ponce-Ortega^a, M.M. El-Halwagi^b, M. Serna-González^a, A. Jiménez-Gutiérrez^c
^a Chemical Engineering Department, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán, 58060, México
^b Chemical Engineering Department, Texas A&M University, College Station, TX, 77843, USA
^c Chemical Engineering Department, Instituto Tecnológico de Celaya, Celaya, Guanajuato, 38010, México
9. Eco industrial parks for water and heat management
M. Boix, L. Montastruc, L. Pibouleau, C. Azzaro-Pantel, S. Domenech
LGC-CNRS-INPT, Université de Toulouse, 4, Allée Emile Monso, BP 84234, 31432 Toulouse, France
10. Effect of demister separation efficiency on the freshwater purity in MSF desalination process
E.A. Hawaidi, I.M. Mujtaba
School of Engineering Design & Technology, University of Bradford, West Yorkshire BD7 1DP, UK
11. Design of an electric and electronic equipment recovery network in Portugal – Costs vs. Sustainability
P. Furtado^a, M.I. Gomes^b, A.P. Barbosa-Povoa^a
^a CEG, IST-UTL, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
^b CMA, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal
12. On the model based optimization of secreting mammalian cell cultures via minimal glucose provision
A. Kiparissides, E.N. Pistikopoulos, A. Mantalaris
Biological Systems Engineering Laboratory, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College, London, UK
13. Evaluating the reactivity of limestone utilized in Flue Gas Desulfurization. An application of the Danckwerts theory for particles reacting in acidic environments and agitated vessels with Archimedes number less than 40.
C. De Blasio^a, C. Carletti^{a,b}, L. Järvinen^c, T. Westerlund^a
^a Department of Chemical Engineering, Åbo Akademi University, Åbo, Finland
^b Universidad Simón Bolívar, Caracas, Venezuela
^c Department of Physics and Astronomy, University of Turku, Turku, Finland
14. Sustainability in chemical processes: Application of different environmental methodologies to evaluate process alternatives
A.N. Mendes^a, A. Carvalho^b, H.A. Matos^a
^a CPQ/DEQB-IST, UTL, Av. Rovisco Pais, 1049-001, Lisboa, Portugal
^b CEG-IST, UTL, Av. Rovisco Pais, 1049-001, Lisboa, Portugal
15. Design and simulation of eco-efficient biodiesel manufacture
S. Couto^{1,a}, T.M. Mata^{1,a}, A.A. Martins^{1,b}, B. Moura¹, J. Magalhães¹, N.S. Caetano^{2,a}
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¹ Faculty of Engineering, University of Porto (FEUP), R. Dr. Roberto Frias S/N, 4200-465 Porto, Portugal
² School of Engineering (ISEP), Polytechnic Institute of Porto (IPP), R. Dr. António Bernardino de Almeida, 4200-072 Porto, Portugal
16. New environmentally-conscious design approach and evaluation tool for chemical processes
C.M. Torres, M. Gadalla, J.M. Mateo, L. Jiménez
Departament d'Enginyeria Química, Universitat Rovira i Virgili, Av. Països Catalans 26, Tarragona 43007, Spain
17. Optimal reactor design for the hydroformylation of long chain alkenes in biphasic liquid systems
A. Peschel^a, B. Hentschel^b, H. Freund^a, K. Sundmacher^{a,b}
^a Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstrasse 1, 39106 Magdeburg, Germany
^b Otto-von-Guericke University, Universitätsplatz 2, 39106 Magdeburg, Germany
18. Optimal design of real world industrial wastewater treatment networks
B. Galán^a, I.E. Grossmann^b
^a Department of Chemical Engineering, University of Cantabria, Avda. De los Castros, s/n 39005, Santander, Spain

^b Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, United States

19. Integrating process simulation, multi-objective optimization and LCA for the development of sustainable processes: application to biotechnological plants

R. Brunet^a, K.S. Kumar^b, G. Guillén-Gosálbez^a, L. Jiménez^a

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^b Department of Chemical Engineering, National Institute of Technology, Mahatma Gandhi Avenue, Durgapur 713 209, West Bengal, India

20. Multi-objective optimization of integrated bioethanol-sugar supply chains considering different LCA metrics simultaneously

A. Kostin^a, F.D. Mele^b, G. Guillén-Gosálbez^a

^a Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona, Spain

^b Ingeniería de Procesos y Gestión Industrial, Universidad Nacional de Tucumán, Tucumán, Argentina

21. Optimization of solar assisted reverse osmosis plants considering economic and environmental concerns

R. Salcedo-Díaz^a, G. Guillén-Gosálbez^b, L. Jiménez^b, E. Antipova^b

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^b Department of Chemical Engineering, University Rovira i Virgili, Av. Països Catalans, 26, 43007, Tarragona, Spain

22. A mixed-integer programming model for pollution trading

V. Rico-Ramirez^a, F. Lopez-Villarreal^a, S. Hernandez-Castro^b, U.M. Diwekar^c

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^c Vishwamitra Research Institute, 368 56-th Street, Clarendon Hills, IL, 60514, USA

23. IMP generalized software to evaluate the minimum water consumption from various objective functions, for use both in refineries, gas and petrochemical complex

E. Arzate, P. Huitzil, B.E. Martínez, A. González, M.T. Sanchezllanes, I. E. Grossmann

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^b Department of Chemical Engineering Carnegie Mellon University, Pittsburg, PA, USA

Bioprocess Systems Engineering

24. Dynamic modelling of the margarine production process

Peter Bongers^{a,b}, Cristhian Almeida-Rivera^a

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120, 1330AC, Vlaardingen, The Netherlands

^b Technical University of Eindhoven, Department of Chemical Engineering and Chemistry, PO Box 513, 5600 MB Eindhoven, The Netherlands

25. Predicting microbial growth kinetics with the use of genetic circuit models

Michalis Koutinas^a, Alexandros Kiparissides^a, Victor de Lorenzo^b, Vitor A.P. Martins dos Santos^c, Efstratios N. Pistikopoulos^a, Athanasios Mantalaris^a

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^c Chair for Systems and Synthetic Biology, Wageningen University, Dreijenplein 310, 6703 HB Wageningen, The Netherlands

26. Assessment of Jatropha Curcas bioprocess for fuel production using LCA and CAPE

Sayed Gillani^{abc}, Caroline Sablayrolles^{bc}, Jean-Pierre Belaud^{ab}, Mireille Montrejaud-Vignoles^{bc}, Jean Marc Le Lann^{ab}

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^c INRA; LCA (Laboratoire de Chimie Agro-Industrielle); 31029 Toulouse, France.

27. Integration of stochastic simulation with advanced multivariate and visualisation analyses for rapid prediction of facility fit issues in biopharmaceutical processes

Adam Stonier^b, Dave Pain^b, Ashley Westlake^b, Nicholas Hutchinson^c, Nina F Thornhill^d, Suzanne S. Farid^a

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^c Parker Hannifin Ltd, Parker Domnick Hunter, Process Division, Durham Road, Durham DH3 2SF, UK

^d Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

28. Optimizing cyanobacteria metabolic network for ethanol production
Cecilia Paulo^a, Jimena Di Maggio^a, Vanina Estrada^{a,c}, M. Soledad Diaz^{a,b}
^a *Planta Piloto de Ingenieria Química PLAPIQUI (UNS-CONICET)*
^b *Department of Chemical Engineering, Universidad Nacional del Sur*
^c *Department of Biology, Biochemistry and Pharmacy, Universidad Nacional del Sur Camino La Carrindanga Km 7, 8000 Bahía Blanca, Argentina*
29. Techno-economic analysis under uncertainty for early stage design of the forest biorefinery
Eemeli Hytönen, Paul Stuart
NSERC Environmental Design Engineering Chair, Department of Chemical Engineering, École Polytechnique, 2920 Chemin de la Tour, Pavillon Aisenstadt, Montreal H3C 3A7, Canada
30. BIOCORE– A systems integration paradigm in the real-life development of a lignocellulosic biorefinery
Aikaterini D. Mountraki^a, Athanassios Nikolakopoulos^a, Bouchra Benjelloun Mlayah^b, Antonis C. Kokossis^a
^a *School of Chemical Engineering, National Technical University of Athens, Greece*
^b *Compagnie Industrielle de la Matière Végétale, France*
31. Non linear identification of Spirulina maxima growth and characteristics
Márcia P. Vega, José W. Silva, Maria A.C.L. Oliveira
Departamento de Engenharia Química, Universidade Federal Rural do Rio de Janeiro, BR465, km7, Seropédica - RJ, 23890-000, phone/fax: +55-21-5521-3787-3742, Brazil
32. Real-time optimization for lactic acid production from sucrose fermentation by Lactobacillus plantarum
Betânia H. Lunelli^a, Delba N. C. Melo^a, Edvaldo R. de Moraes^a, Igor R. S. Victorino^a, Eduardo C. Vasco de Toledo^b, Maria Regina Wolf Maciel^a, Rubens Maciel Filho^a
^a *Laboratory of Optimization, Design and Advanced Control, School of Chemical Engineering, State University of Campinas, University City “Zeferino Vaz”, 13083-852, Campinas, Brazil*
^b *Petrobras SA, Paulínia Refinery (REPLAN), Paulínia, São Paulo, Brazil*
33. Model-based dynamic optimisation of microbial processes for the high-yield production of biopolymers with tailored-made molecular properties
Giannis Penloglou^{a,b}, Christos Chatzidoukas^a, Avraam Roussos^b, Costas Kiparissides^{a,b}
^a *Department of Chemical Engineering, Aristotle University of Thessaloniki, P.O. Box 472, 54124, Thessaloniki, Greece*
^b *Chemical Process Engineering Research Institute, Centre for Research and Technology Hellas, P.O. Box 60361, 57001, Thessaloniki, Greece*
34. Systematic procedure for integrated process operation: Reverse electro-enhanced dialysis during lactic acid fermentation
Oscar Andrés Prado-Rubio, Sten Bay Jørgensen, Gunnar Jonsson
Department of Chemical and Biochemical Engineering, Technical University of Denmark (DTU), DK-2800 Lyngby, Denmark
35. Bioprocessing of exopolysaccharides (EPS): CFD characterization of bioreactor conditions
Serafim Vlaev^a, Konstantza Tonova^a, Kostantsa Pavlova^b, Mohammed Elqotbi^c
^a *Institute of Chemical Engineering*
^b *Institute of Microbiology, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., Bl. 103 and Bl. 25, 1113 Sofia, Bulgaria*
^c *Polytech’Lille, Avenue Paul Langevin, 59655 Villeneuve d’Ascq, France*
36. Simultaneous design and scheduling of a plant for producing ethanol and derivatives
Yanina Fumero, Gabriela Corsano, Jorge M. Montagna
I_GAR - Instituto de Desarrollo y Diseño – CO_ICET. Avellaneda 3657, (S3002GJC) Santa Fe, Argentina
37. Glycerol metabolic conversion to succinic acid using Actinobacillus succinogenes: A metabolic network-based analysis
Michael Binns^a, Anestis Vlysidis^a, Colin Webb^a, Constantinos Theodoropoulos^a, Pedro de Auri^b, Marta Cascante^b
^a *School of Chemical Engineering and Analytical Science, University of Manchester, Manchester, M13 9PL, UK*
^b *Department of Biochemistry and Molecular Biology, Faculty of Biology, University of Barcelona, 08028 Barcelona, Catalunya, Spain*
38. Design and operation of a continuous reactor for acid pretreatment of lignocellulosic biomass
Mauricio Sales-Cruz^a, Edgar Ramírez-Jiménez^b, Teresa López-Arenas^a
^a *Departamento de Procesos y Tecnología, Universidad Autónoma Metropolitana-Cuajimalapa, Artificios 40, 01120 Mexico D.F., Mexico*
^b *Departamento de Ingeniería Química Petrolera, ESIQIE-Instituto Politécnico Nacional, Zacatenco, 07738 Mexico D.F., Mexico*
39. Viscosity prediction of compounds derived from castor oil: parameter optimization
Teresa López-Arenas^a, Gloria Aca-Aca^b, Oscar Sánchez-Daza^b, Mauricio Sales-Cruz^a
^a *Departamento de Procesos y Tecnología, Universidad Autónoma Metropolitana-Cuajimalapa, Artificios 40, 01120 Mexico D.F., Mexico*
^b *Facultad de Ingeniería Química, Benemérita Universidad Autónoma de Puebla, Ciudad Universitaria, 72570 Puebla Pue., México*

40. Simulations of hydrodynamical stress in stirred-tank bioreactors using CFD technology
Y. Verkhola^a, P. Lavrov^a, E. Guseva^a, N. Menshutina^a, J. Boudrant^b
^a *Mendeleev University of Chemical Technology of Russia High Technology Department Building 9, Miusskaya square, 125047, Moscow, Russian Federation*
^b *Inpl-Ensaia Laboratory of Chemical Engineering Science Building 2, avenue de la foret de Hayer, PB 172, 54505, Vandoeuvre-les-Nancy, France*
41. System inversion of multidimensional population balance systems
Henrique Menarin^a and Naim Bajcinca^{a,b}
^a *Max-Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr.1, 39106 Magdeburg, Germany*
^b *Technische Universität Berlin, Einsteinufer 17, 10857 Berlin, Germany*
42. Implementation and initial evaluation of a decision support platform for selecting production routes of biomass-derived chemicals
Marinella Tsakalova^a, Ta-Chen Lin^b, Aidong Yang^b, Antonis C. Kokkosis^a
^a *School of Chemical Engineering, National Technical University of Athens, Greece*
^b *Faculty of Engineering and Physical Sciences, University of Surrey, UK*
43. Dynamic process monitoring and fault detection in a batch fermentation process: comparative performance assessment between MPCA and BDPCA
Isaac Monroy^a, Kris Villez^b, Moisès Graells^a, Venkat Venkatasubramanian^b
^a *Chemical Engineering Department, Universitat Politècnica de Catalunya, EUETIB. Comte d'Urgell 187, 08036, Barcelona, Spain*
^b *Laboratory for Intelligent Process Systems, School of Chemical Engineering, Purdue University, 480 Stadium Mall Drive, 47907, West Lafayette, IN, USA.*
44. Standards for continual scheduling of batch operations
Charles Siletti^a, Demetri Petrides^b, Dimitri Vardalis^c
^a *Intelligen, Inc. 700 Walton Ave., Mt. Laurel, NJ 08054 USA*
^b *Intelligen, Inc. 2326 Morse Ave, Scotch Plains, NJ 07076 USA*
^c *Intelligen Europe, Thessaloniki, Greece*
45. Kinetic modelling of cytosolic glucose metabolism
Ning Chen^{a,b}, Karen Polizzi^c, Cleo Kontoravdi^{a,b}
^a *Centre for Process System Engineering,*
^b *Department of Chemical Engineering and Chemical Technology,*
^c *Division of Molecular Biosciences, Department of Life Sciences, Imperial College London, South Kensington Campus, London SW7 2AZ, U.K.*

Poster Session 5 – MARINA II

Chair: Jiri Klemes (University of Pannonia, Hungary)

Energy Systems Engineering

1. Simulation of membrane water gas shift reactors by a two-dimensional model
M. De Falco^a, V. Piemonte^b, A. Basile^c
^a *Faculty of Engineering, University Campus Bio-Medico of Rome, via Alvaro del Portillo 21, 00128 Rome, Italy*
^b *Department of Chemical Engineering Materials & Environment, University of Rome "La Sapienza", via Eudossiana 18, 00184 Rome, Italy.*
^c *CNR-ITM, c/o University of Calabria, Via Pietro Bucci, Cubo 17/C, 87030 Rende (CS), Italy.*
2. Optimal biorefinery planning considering simultaneously economic and environmental objectives
José Ezequiel Santibáñez-Aguilar, J. Betzabe González-Campos, José María Ponce-Ortega, Medardo Serna-González
Chemical Engineering Department, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Mich., 58060, México
3. Techno-economical and environmental evaluations of igcc power generation process with carbon capture and storage (CCS)
Calin-Cristian Cormos, Ana-Maria Cormos, Paul Serban Agachi
Babes – Bolyai University, Faculty of Chemistry and Chemical Engineering, Arany Janos Street, No. 11, RO-400028, Cluj – Napoca, Romania
4. Optimization of lignocellulosic based diesel
Mariano Martín, Ignacio E. Grossmann
Center for Advanced Process Decision-Making, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, 15213, USA

5. Using low-grade heat for solvent extraction based efficient water desalination
Kary Thanapalan, Vivek Dua
Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, London WC1E 7JE, UK
6. Impact of hydrogen injection in natural gas infrastructures
Guillermo Hernández-Rodríguez, Luc Pibouleau, Catherine Azzaro-Pantel, Serge Domenech
Université de Toulouse, Laboratoire de Génie Chimique, LGC UMR CNRS 5503 ENSIACET INPT- 4 allée Emile Monso – BP 44362 - 31432 TOULOUSE Cedex 4-France
7. Optimal design and operation of distributed energy systems
E. D. Mehleri^{a, b}, H. Sarimveis^a, N. C. Markatos^a, L. G. Papageorgiou^b
^a*School of Chemical Engineering, National Technical University of Athens, GR-157 80 Athens, Greece*
^b*Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, London WC1E 7JE, UK*
8. Optimizing the lignocellulosic biomass-to-ethanol supply chain: A Case Study for the Midwestern United States
W. Alex Marvin^a, Lanny D. Schmidt^a, Saif Benjaafar^b, Douglas G. Tiffany^c, Prodromos Daoutidis^a
^a*Chemical Engineering & Material Science, University of Minnesota, Minneapolis, MN, USA*
^b*Industrial & Systems Engineering, University of Minnesota, Minneapolis, MN, USA*
^c*Applied Economics, University of Minnesota, Saint Paul, MN, USA*
9. Modeling and simulation of the production of lead and elementary sulphur from lead sulphide concentrates
Giulia Bozzano^a, Mario Dente^a, Sauro Pierucci^a, Massimo Maccagni^b
^a*Politecnico di Milano, dept. CMIC, p.zza L. Da Vinci, 32, Milan, Italy*
^b*Engitec Technologies S.p.A., Via Borsellino e Falcone, 31, Novate Milanese – Italy*
10. Network generation and analysis of complex biomass conversion systems
Srinivas Rangarajan^a, Ted Kaminski^b, Eric Van Wyk^b, Aditya Bhan^a, Prodromos Daoutidis^a
^a*Department of Chemical Engineering and Materials Science, 421 Washington Ave. SE., Minneapolis, MN 55455, USA*
^b*Department of Computer Science and Engineering, 200 Union Street SE Minneapolis, MN 55455, USA*
11. Fractional-order transfer functions applied to the modelling of hydrogen PEM fuel cells
Vitor V. Lopes^a, Carmen M. Rangel^b, Augusto Q. Novais^a
^a*Energy Systems Modeling and Optimization Unit*
^b*Hydrogen and Fuel Cell Unit, National Laboratory for Energy and Geology (LNEG), 1649-038 Lisboa, Portugal*
12. Modeling post-combustion CO₂ capture with amine solvents
Grégoire Léonard, Georges Heyen
Laboratory for Analysis and Synthesis of Chemical Systems, University of Liège, Allée de la chimie 3, Bât. B6a, 4000 Liège, Belgium
13. Modelling biomass and biofuels supply chains
Christiana Papapostolou^a, Emilia Kondili^b, John K. Kaldellis^c
^{a, b}*Optimisation of Production Systems Lab., TEI of Piraeus, 250 P. Ralli and Thivon Av., Aegaleo 12244, Greece*
^c*Lab of Soft Energy Applications & Environmental Protection, TEI of Piraeus, P.O. Box 41046, Athens 12201, Greece*
14. Design and performance optimisation of hybrid energy systems
E. Kondili^a, J. K. Kaldellis^b
^a*Optimisation of Production Systems Lab.*
^b*Lab of Soft Energy Applications & Environmental Protection, TEI of Piraeus, P.O. Box 41046, Athens 12201, Greece*
15. Recurrent neural network prediction of steam production in a Kraft recovery boiler
Matthieu Sainlez^a, Georges Heyen^b
^a*CRISIA, Haute Ecole Robert Schuman, Belgium*
^b*LASSC, Université de Liège; Liège, Belgium*
16. Improved wind power forecasting with ARIMA models
Bri-Mathias Hodge, Austin Zeiler, Duncan Brooks, Gary Blau, Joseph Pekny, Gintaras Reklatis
Purdue University School of Chemical Engineering, 480 Stadium Mall Dr., West Lafayette, IN 47907, USA
17. Power reduction in air separation units for oxy-combustion processes based on exergy analysis
Chao Fu, Truls Gundersen
Department of Energy and Process Engineering, Norwegian University of Science and Technology, Kolbjoern Hejes vei 1.A, Trondheim, NO-7491, Norway
18. Multi-objective optimization of the electricity production from hard coal burning
Jorge Cristóbal^a, Gonzalo Guillén-Gosálbez^b, Laureano Jiménez^b, Angel Irabien^a
^a*Departamento de Ingeniería Química y Química Inorgánica, Universidad de Cantabria, Av. de los Castros s/n, Santander, 39005, Spain*
^b*Departamento de Ingeniería Química, Escuela Técnica Superior de Ingeniería Química, Universidad Rovira i Virgili, Av. Països Catalans 26, Tarragona, 43007, Spain*

19. Oil well drilling process - Simulation and experimental multi-objective studies
Márcia Peixoto Vega^a, Marcela Galdino de Freitas^a, Claudia Miriam Scheid^a and André Leibsohn Martins^b
^a DEQ -UFRRJ, BR 465, km7 – CEP: 23890-000 – Seropédica – RJ – Brasil
^b PETROBRAS S.A./CENPES, Av. Hum Quadra 07, Ilha do Fundão, Rio de Janeiro, 21494-900, Rio de Janeiro, RJ, Brasil
20. Fisher information based time-series segmentation of streaming process data for monitoring and supporting on-line parameter estimation in energetic systems
László Dobos, János Abonyi
Department of Process Engineering, University of Pannonia, Egyetem street 10, Veszprém, H-8200, Hungary
21. NMPC for oil reservoir production optimization
Carsten Völcker^a, John Bagterp Jørgensen^a, Per Grove Thomsen^a, Erling Halfdan Stenby^b
^a Department of Informatics and Mathematical Modeling, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
^b Department of Chemistry, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
22. Site-wide process integration for low grade heat recovery
Ankur Kapil^a, Igor Bulatov^a, Robin Smith^a, Jin-Kuk Kim^b
^a Centre for Process Integration, School of Chemical Engineering and Analytical Science, The University of Manchester, M13 9PL, Manchester, United Kingdom
^b Department of Chemical Engineering, Hanyang University, 17, Haengdang-dong, Seongdong-gu, Seoul, Republic of Korea
23. New optimization method for retrofitting heat exchanger networks with intensified heat transfer
Ming Pan^a, Igor Bulatov^a, Robin Smith^a, Jin-Kuk Kim^b
^a Centre for Process Integration, School of Chemical Engineering and Analytical Science, The University of Manchester, M13 9PL, Manchester, United Kingdom
^b Department of Chemical Engineering, Hanyang University, 17, Haengdang-dong, Seongdong-gu, Seoul, Republic of Korea
24. The effects of electricity storage on large scale wind integration
Shisheng Huang^a, Bri-Mathias S. Hodge^a, Jingjie Xiao^b, Gintaras V. Reklaitis^a, Joseph F. Pekny^a
^a School of Chemical Engineering, Purdue University, 480 Stadium Mall Dr., West Lafayette, IN 47907, USA
^b School of Industrial Engineering, Purdue University, 315 N. Grant Street, West Lafayette, IN 47907, USA
25. A discrete approach to model thermal conversion of beds of solid fuels by the Discrete Particle Method (DPM)
Bernhard Peters^a, Algis Dziugys^b
^a Université du Luxembourg, 6, rue Coudenhove-Calergi, L-1359 Luxembourg
^b Lithuanian Energy Institute, Breslaujos, 3, Kaunas, Lithuania
26. Monitor and diagnosis of LNG plant fractionation process using k-mean clustering and principal component analysis
Hahyung Pyun, Daeyoun Kim, Kyungjin Kim, Chonghun Han
School of Chemical and Biological Engineering, Seoul National University, Seoul 151-741, Republic of Korea
27. Design of integrated gasification combine cycle plant with carbon capture and storage based on co-gasification of coal and biomass
Victoria Maxim, Calin-Cristian Cormos, Paul Serban Agachi
Babes – Bolyai University, Faculty of Chemistry and Chemical Engineering 11 Arany Janos Street, RO-400028, Cluj – Napoca, Romania
28. Optimization of sustainable energy planning with consideration of uncertainties in learning rates and external cost factors
Seunghyok Kim, Jamin Koo, En Sup Yoon
School of Chemical and Biological Engineering, Seoul National University, Republic of Korea
29. SynFlex: A computational framework for synthesis of flexible heat exchanger networks
M. Escobar, J.O. Trierweiler^a, I.E. Grossmann^b
^a Federal University of Rio Grande do Sul, Brasil
^b Carnegie Mellon University Pittsburgh, PA 15231 USA
30. Modeling and optimization of supercritical phase fischer-tropsch synthesis
Wei Yuan, Gregory C. Vaughan, Christopher B. Roberts, Mario R. Eden
Department of Chemical Engineering, Auburn University, AL 36849, USA
31. Optimization of pipeline unloading operations in a LPG terminal
S.Arun Srikanth, Sridharakumar Narasimhan, Shankar Narasimhan
Department of Chemical Engineering, IIT Madras, Chennai, 600036, India
32. Improving energy efficiency of a dyes intermediates synthesis plant. A developing country specific Case Study
Zsófia Fodor^a, Paul Krajník^b, Petar Sabev Varbanov^a, Jiří Jaromír Klemesš^a
^a Centre for Process Integration and Intensification - CPI2, Research Institute of Chemical Technology and Process Engineering, FIT, University of Pannonia, Egyetem utca 10, 8200, Veszprém, Hungary

^b HUNTSMAN Global Head / Processing & Engineering, Textile Effects, Basel, Switzerland 4057

33. Evaluation of design issues and simulation studies in a solar based hydrogen production unit at CERTH in Thessaloniki
Chrysovalantou Ziogou^a, Dimitris Ipsakis^a, Fotis Stergiopoulos^{a,b}, Simira Papadopoulou^{a,b}, Stella Bezergianni^a, Spyros Voutetakis^a
^a Chemical Process Engineering Research Institute (C.P.E.R.I.), Centre for Research and Technology Hellas (CE.R.T.H.), P.O. Box 60361, 57001 Thessaloniki, Greece
^b Department of Automation, Alexander Technological Educational Institute of Thessaloniki, P.O. Box 141, 57400 Thessaloniki, Greece
34. The role of energy consumption in batch process scheduling and optimization
Mate Hegyhati, Ferenc Friedler
Department of Computer Science and Systems Technology, University of Pannonia, Veszprem, Egyetem u. i0, H-8200, Hungary
35. Energy water and process technologies integration for the simultaneous production of ethanol and food from the whole Corn Plant
Lidija Čuček^a, Mariano Martín^b, Ignacio E. Grossmann^b, Zdravko Kravanja^a
^a University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova ulica 17, Maribor 2000, Slovenia
^b Carnegie Mellon University, Department of Chemical Engineering, Pittsburgh, PA 15213, USA
36. Multiscale modelling of biorefineries
Seyed Ali Hosseini^{a,b}, Nilay Shah^b
^a Department of Chemical Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, GU2 7XH, UK
^b Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London Technology and Medicine, United Kingdom
37. Energy targeting in heat integrated water networks with isothermal mixing
Santanu Bandyopadhyay, Gopal Chandra Sahu
Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India
38. Design of renewable energy systems incorporating uncertainties through pinch analysis
Santanu Bandyopadhyay
Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India
39. Assessment for carbon capture and storage opportunities: Greek Case Study
Christos Ioakimidis^a, Nikolaos Koukouzas^c, Anna Chatzimichali^b, Sergio Casimiro^b, Grigorios Itskos^c
^a Deusto Institute of Technology – DeustoTech Energy, University of Deusto, Spain
^b Mechanical Engineering, Instituto Superior Técnico, (IN+,UTL) MIT Portugal, Sustainable Energy Systems, Av. Professor Anibal Cavaco Silva, 2744016 Porto Salvo, Lisbon, Portugal
^c Centre for Research & Technology Hellas / Institute for Solid Fuels Technology & Applications, (CERTH/ISFTA), Mesogeion Ave. 357359, GR15231 Halandri, Athens Greece
40. Exergy-based methods for computer-aided design of energy conversion systems
George Tsatsaronis, Tatiana Morosuk
Technische Universität Berlin Marchstr.18 10587 Berlin, Germany
41. Regional Optimiser (RegiOpt) - Sustainable energy technology network solutions for regions
K.H. Kettl^a, N. Niemetz^a, N. Sandor^a, M. Eder^a, I. Heckl^b, M. Narodslawsky^a
^a Institute for Process and Particle Engineering, Graz University of Technology, Inffeldgasse 21a, 8010 Graz, Austria
^b Centre for Advanced Process Optimization (CAPO), University of Pannonia, Egyetem út. 10, 8200 Veszprém, Hungary
42. Techno-economic analysis for ethylene and methanol production from the Oxidative Coupling of Methane Process
Daniel Salerno, Harvey Arellano-Garcia, Günter Wozny
Chair of Process Dynamics and Operations, Sekr, KWT-9 Berlin Institute of Technology, Strasse des 17 Juni135, D-10623, Berlin, Germany

19:40 – 21:30 Poster Session – with beer, snacks & music

08:30 – 09:50 Plenary Session 3 - OLYMPIC HALL

Chairs: David Bogle (UCL, UK)
Antonios Kokossis (NTUA, Greece)

08:30 – 09:10 Addressing key green engineering challenges - The role of process systems engineering
Conchita Jiménez-González (*GlaxoSmithKline, USA*)

09:10 – 09:50 Multi-scale models for the design of crystalline solids
Mike Doherty (*University of California Santa Barbara, USA*)

09:50 – 10:20 ESCAPE22 & PSE2012 presentations

10:20 – 10:50 Coffee Break

10:50 – 12:30 Oral Presentations – 5 Parallel Sessions

Multi-scale Modelling II – MARINA I

Chair: Kostas Theodopoulos (University of Manchester, UK)

10:50 – 11:10 A CFD-population balance model for the simulation of Kühni extraction column
Mark W. Hlawitschka^{a,b}, Moutasem Jaradat^{a,b}, Fang Chen^{a,b}, Menwer M. Attarakih^c, Jörg Kuhnert^{b,d}, Hans-Jörg Bart^{a,b}
^a TU Kaiserslautern, Kaiserslautern, Germany
^b Al-Balqa Applied University, Amman, Jordan
^c Centre of Mathematical and Computational Modelling, TU Kaiserslautern, Germany
^d Fraunhofer ITWM, 67663 Kaiserslautern, Germany

11:10 – 11:30 CFD study on the application of rotary kiln in pyrolysis
Ka-Leung Lam, Adetoyese O. Oyedun, Chi-Wai Hui
Department of Chemical and Biomolecular Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

11:30 – 11:50 A Multi-scale Systems Approach to Granulation Process Design
Rohit Ramachandran
Rutgers University, 98 Brett Road, Piscataway, NJ, USA

11:50 – 12:10 A multi-layered ontology for physical-chemical-biological processes
Heinz A Preisig
Department of Chemical Engineering, NTNU, Trondheim, Norway

12:10 – 12:30 Towards a rigorous model of electro dialysis processes
Matthias Johannink, Adel Mhamdi, Wolfgang Marquardt
Aachener Verfahrenstechnik, RWTH Aachen University, 52065 Aachen, Germany

Synthesis/Design III – CHLOE HALL

Chair: Georges Heyen (University of Liege, Belgium)

10:50 – 11:10 Computer aided flowsheet design using group contribution methods
Susilpa Bommarreddy^a, Mario R. Eden^a, Rafiqul Gani^b
^a Department of Chemical Engineering, Auburn University, AL 36849, USA
^b CAPEC, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

11:10 – 11:30 Constructive nonlinear dynamics for reactor network synthesis with guaranteed robust stability
Xiao Zhao, Wolfgang Marquardt
AVT-Lehrstuhl für Prozesstechnik, RWTH Aachen University, Templergraben 55, 52056 Aachen, Germany

- 11:30 – 11:50 Design of flexible process flow sheets with a large number of uncertain parameters
Mihael Kasaš, Zdravko Kravanja, Zorka Novak Pintarič
University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova 17, SI-2000 Maribor, Slovenia
- 11:50 – 12:10 A superstructure optimization approach for optimal refinery water network systems synthesis with membrane-based regenerators
Cheng Seong Khor, Nilay Shah
Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ UK
- 12:10 – 12:30 Synthesis tool for separation processes in the pharmaceutical industry
Ana I. C. Morão^{a,b}, Edwin Zondervan^b, Gerard Krooshof^c, Rob Geertman^d, André B. de Haan^b
^a *Institute for Sustainable Process Technology, P.O. Box 247, 3800 AE Amersfoort, The Netherlands*
^b *Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands*
^c *DSM Research, P.O. Box 18, 6160 MD Geleen, The Netherlands*
^d *MSD, Merck Manufacturing Division, API-PD, P.O. Box 20 5340 BH Oss, The Netherlands*

Control I – ERATO HALL

Chair: Sebastian Engell (TUD, Germany)

- 10:50 – 11:10 Multi-model MPC for nonlinear systems: Case study of a complex pH neutralization process
Weiting Tang, M. Nazmul Karim
Department of Chemical Engineering, Texas Tech University, 6th Street and Canton, Lubbock, TX 79409, USA
- 11:10 – 11:30 Systematic identification and robust control design for uncertain time delay processes
Jakob K. Huusom^a, Niels K. Poulsen^b, Sten B. Jørgensen^a, John B. Jørgensen^b
^a *CAPEC, Department of Chemical and Biochemical Engineering*
^b *Department of Informatics and Mathematical Modelling*
Technical University of Denmark, DK-2800 Lyngby, Denmark
- 11:30 – 11:50 Experimental evaluation of a robust NMPC strategy for an unstable nonlinear process
Udo Schubert, Andreas Lange, Harvey Arellano-Garcia, Günter Wozny
Chair of Process Dynamics and Operation; Berlin Institute of Technology, Sekr. KWT-9, Straße d. 17. Juni 135, D-10623 Berlin, Germany
- 11:50 – 12:10 Implementation of model predictive controller in a pharmaceutical development plant
Stéphane Hattou^a, Marie-Véronique Le Lann^{b,c}, Karlheinz Preuss^d, Boris Roussel^a, Michel Cabassud^{e,c}
^a *SANOFI-AVENTIS, 371, rue du Pr Joseph Blayac 34184 Montpellier cedex 4, France*
^b *CNRS ; LAAS ;7, avenue du Colonel Roche ;F-31077 Toulouse, France*
^c *Université de Toulouse ; UPS, INSA, INP, ISAE ; LAAS, LGC ;F-31077 Toulouse, France*
^d *engineo GmbH, Ginsheimer Str. 1, 65462 Gustavsburg (Mainz), Germany*
^e *LGC, BP 84234, Campus INP-ENSIACET 4 allée Emile Monso 31030 Toulouse cedex 4, France*
- 12:10 – 12:30 A disturbance estimation approach for online model-based redesign of experiments in the presence of systematic errors
F. Galvanin^a, M. Barolo^a, G. Pannocchia^b, F. Bezzo^a
^a *CAPE-Lab, Dipartimento di Principi e Impianti di Ingegneria Chimica, Università di Padova, via Marzolo 9, 35131 Padova, Italy*
^b *DICCISM – Dipartimento di Ingegneria Chimica, Università di Pisa, via Diotisalvi 2, 56122 Pisa, Italy*

Process Operations II – TERPSIHORI HALL

Chair: Christos Maravelias (University of Wisconsin, USA)

- 10:50 – 11:10 A new coordination heuristic for plant-wide planning and scheduling
Chaojun Xu^{a,c}, Christian Staud^b, Guido Sand^a, Sebastian Engell^c
^a *Process and Production Optimization, ABB AG Corporate Research Center Ladenburg, Germany*
^b *The Faculty of Mathematics and Computer Sciences, Heidelberg University, Germany*
^c *Process Dynamics and Operations Group, Department of Biochemical and Chemical Engineering Technische Universität Dortmund, Germany*

- 11:10 – 11:30 Batch sizing in multi-stage, multi-product batch production systems
Norbert Trautmann, Philipp Baumann, Nadine Saner, Tobias Schäfer
University of Bern, Department of Business Administration, CH-3012 Bern, Switzerland
- 11:30 – 11:50 Optimization of closed-loop supply chains under uncertain quality of returns
M Isabel Gomes^a, Luis J Zeballos^{b,c}, Ana P Barbosa-Povoa^d, Augusto Q Novais^b
^a *CMA, FCT, Universidade Nova de Lisboa, Monte de Caparica, 2825-114 Caparica, Portugal*
^b *Unidade Modelação e Optimização de Sistemas Energéticos, Laboratório Nacional de Energia e Geologia, Lisboa*
^c *Universidad Nacional del Litoral – Fac. de Ingeniería Química, Santa Fe, Argentina*
^d *Centre for Management Studies, Instituto Superior Técnico, UTL, Lisboa Portugal*
- 11:50 – 12:10 Complex network optimization in FMCG
Ali Mehdizadeh^a, Nilay Shah^a, Peter M.M. Bongers^b, Cristhian Almeida-Rivera^b
^a *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London Technology and Medicine, United Kingdom*
^b *Unilever Research Vlaardingen, Oliver van Noortlaan 120, POBox 114, 3130 AC Vlaardingen, The Netherlands*
- 12:10 – 12:30 Integrated refinery planning under product demand uncertainty
Edith Ejikeme-Ugwu^a, Songsong Liu^b and Meihong Wang^a
^a *Process Systems Engineering Group, School of Engineering, Cranfield University, MK43 0AL, UK*
^b *Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, London WC1E 7JE, UK*

Energy Systems Engineering II – MARINA II

Chair: Iftekhar Karimi (NUS, Singapore)

- 10:50 – 11:10 Computational support as efficient sophisticated approach in waste-to-energy systems
Keynote **Petr Stehlik**
Presentation *Institute of Process and Environmental Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, 61669 Brno, Czech Republic*
- 11:10 – 11:30 Sustainable LCA-based MIP synthesis of biogas processes
Lidija Čuček^a, Rozalija Drobež^b, Bojan Pahor^c, Zdravko Kravanja^a
^a *University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova ulica 17, Maribor 2000, Slovenia*
^b *Scientific Research Centre Bistra Ptuj, Slovenski trg 6, 2250 Ptuj, Slovenia*
^c *Perutnina Ptuj, Potrčeva 10, 2250 Ptuj, Slovenia*
- 11:30 – 11:50 Ontology-driven design of an energy management system
Karel Macek, Karel Mařík, Petr Stluka
Honeywell Prague Laboratory, V Parku 23/26, Prague 148 00, Czech Republic
- 11:50 – 12:10 Synthesis of flexible palm oil-based regional energy supply chain
Dominic C. Y. Foo^a, Raymond R. Tan^b, Hon Loong Lam^c, Mustafa Kamal^d, Jiri J. Klemeš^c
^a *Department of Chemical and Environmental Engineering, University of Nottingham Malaysia, Broga Road, 43500 Semenyih, Selangor, Malaysia*
^b *Chemical Engineering Department, De La Salle University, 2401 Taft Avenue, Manila, Philippines*
^c *Centre for Process Integration and Intensification, CPI2, Faculty of Information Technology, University of Pannonia, Egyetem u. 10, 8200, Veszprém, Hungary*
^d *Center of Lipids Engineering Applied Research (CLEAR), Faculty of Chemical Engineering, Universiti Teknologi Malaysia, Semarak Road, 54100 Kuala Lumpur, Malaysia*
- 12:10 – 12:30 Methodology for maximising the use of renewables with variable availability
Andreja Nemet, Jiri J. Klemeš, Petar S. Varbanov
Centre for Process Integration and Intensification - CPI2, Research Institute of Chemical and Process Engineering, Faculty of Information Technology, University of Pannonia, Egyetem utca 10, 8200 Veszprém, Hungary

12:50 – 14:10 Lunch

12:50 – 14:10 Computers & Chemical Engineering Board Mtg (by invitation only)

14:10 – 15:50 Oral Presentations – 5 Parallel Sessions

Environmental Systems Engineering I – TERPSIHORI HALL

Chair: Il Moon (Yonsei University, Korea)

- 14:10 – 14:30 Modelling and process integration of carbon dioxide capture using membrane contactors
J. Albo, J. Cristóbal, A. Irabien
Departamento Ingeniería Química y Química Inorgánica. Universidad de Cantabria, Av de los Castros s/n. 39005 Santander. Spain
- 14:30 – 14:50 Determination of bioremediation strategies in eutrophic water bodies through the formulation of an optimal control problem based on a 3D ecological model
Vanina Estrada^{a,b}, Sabrina Belén Rodríguez Reartes^{a,c}, M. Soledad Diaz^{a,c}
^a *Planta Piloto de Ingeniería Química PLAPIQUI (UNS-CONICET)*
^b *Department of Biology, Biochemistry and Pharmacy, Universidad Nacional del Sur*
^c *Department of Chemical Engineering, Universidad Nacional del Sur Camino La Carrindanga Km 7, 8000 Bahía Blanca, Argentina*
- 14:50 – 15:10 Integration of carbon footprint minimization into the process design of SWRO desalination pretreatment
Matan Beery^a, Günter Wozny^a, Jens-Uwe Repke^b
^a *Institute of Process and Plant Technology, TU Berlin, Sekr. KWT 9, Strasse des 17. Juni 135, 10623 Berlin, Germany*
^b *Institute of Thermal, Environmental and Natural Products Process Engineering, TU Bergakademie Freiberg, Leipziger Strasse 28, 09599 Freiberg, Germany*
- 15:10 – 15:30 Multiscale whole-systems design and analysis of CO₂ capture and transport networks
Niall Mac Dowell, Ahmed Alhajaj, Murthy Konda and Nilay Shah
Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College, London SW7 2AZ, UK
- 15:30 – 15:50 CO₂ sustainable recovery network cluster for carbon capture and sequestration
J. Duque^a, A.P.F.D. Barbosa-Póvoa^b, A.Q. Novais^a
^a *Unidade de Modelação e Optimização de Sistemas Energéticos, UMOSE- LNEG, Estrada do Paço do Lumiar, 22, 1649-038 Lisboa, Portugal*
^b *Centro de Estudos de Gestão, CEG-IST, Instituto Superior Técnico, Universidade Técnica de Lisboa, Av. Rovisco Pais, 1049-001, Lisboa, Portugal*

Bioprocess Systems Engineering I – MARINA I

Chair: Gurkan Sin (DTU, Denmark)

- 14:10 – 14:30 Model-driven design based on sensitivity analysis for a synthetic biology application
Nikolaos Anesiadis^a, William R. Cluett^a, Radhakrishnan Mahadevan^{a,b}
^a *Department of Chemical Engineering and Applied Chemistry, University of Toronto, 200 College Street, Toronto, M5S 3E5, Canada*
^b *Institute of Biomaterials & Biomedical Engineering, University of Toronto, 164 College Street, Toronto, M5S 3G9, Canada*
- 14:30 – 14:50 Microbial strain design for biochemical production using mixed-integer programming techniques
Joonhoon Kim, Jennifer L. Reed, and Christos T. Maravelias
Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA
DOE Great Lakes Bioenergy Research Center, University of Wisconsin-Madison, Madison, WI 53706, USA
- 14:50 – 15:10 A Comprehensive multi-scale modeling of heterogeneities in Mammalian cell culture processes
Srinivas Karra, Brian Sager, M. Nazmul Karim
Department of Chemical Engineering, Texas Tech University, Lubbock, TX-79409, USA
- 15:10 – 15:30 Population balance modelling of homogeneous and heterogeneous cellulose hydrolysis
Philip Engel^a, Benjamin Bonhage^a, Douglas Pernik^a, Roberto Rinaldi^b, Patrick Schmidt^{a,c}, Helene Wulfhorst^a, Antje C. Spiess^a

^a RWTH Aachen University, AVT-Enzyme Process Technology, 52056 Aachen, Germany

^b MPI for Coal Research, 45470 Mülheim an der Ruhr, Germany

^c now: TU Dortmund, Laboratory of Fluid Separations, 44227 Dortmund, Germany

- 15:30 – 15:50 A combined growth kinetics, metabolism and gene expression model for 3D ESC bioprocesses
David Yeo, Alexandros Kiparissides, Efstratios Pistikopoulos, Athanasios Mantalaris
Biological Systems Engineering Laboratory, Department of Chemical Engineering, Imperial College, London SW7 2AZ

Control II – ERATO HALL

Chair: Sten Bay Jorgensen (DTU, Denmark)

- 14:10 – 14:30 Plantwide control of a cumene manufacture process
Vivek Gera^a, Nitin Kaistha^a, Mehdi Panahi^b, Sigurd Skogestad^b
^a Chemical Engineering, Indian Institute of Technology Kanpur, 208016, Kanpur, India
^b Chemical Engineering Department, NTNU, 7491, Trondheim, Norway
- 14:30 – 14:50 Comparison of gradient estimation methods for real-time optimization
Bala Srinivasan, Grégory François and Dominique Bonvin^a
Ecole Polytechnique Montreal, Montreal, H3C 3A7 Canada
^a Laboratoire d'Automatique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
- 14:50 – 15:10 Plantwide control design of a postcombustion CO₂ capture process
Marc-Oliver Schach^a, Rüdiger Schneider^b, Henning Schramm^b, Jens-Uwe Repke^a
^a Institute of Thermal, Environmental and Natural Products Process Engineering, TU Bergakademie Freiberg, Leipziger Straße 28, 09596 Freiberg, Germany
^b Siemens AG Energy Sector, Fossil Power Generation, Industriepark Höchst, 65926 Frankfurt am Main
- 15:10 – 15:30 Receding Nonlinear Kalman (RNK) filter for nonlinear constrained state estimation
Raghunathan Rengaswamy^a, Shankar Narasimhan^b, Vidyashankar Kuppuraj^a
^a Department of Chemical Engineering, Texas Tech University, 6th street and canton, Lubbock, TX 79409, USA
^b Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai 600036, India
- 15:30 – 15:50 An improved formulation for the process control structure selection based on economics problem
Andreas Psaltis, Ioannis K. Kookos, Costas Kravaris
Department of Chemical Engineering, University of Patras, 26504 Rio, Patras, Greece

Molecular/Material Systems Engineering II – CHLOE HALL

Chair: Krist Gernaey (DTU, Denmark)

- 14:10 – 14:30 Simultaneous prediction of phase behaviour and second derivative properties with a group contribution approach (SAFT- γ Mie)
Vasileios Papaioannou, Thomas Lafitte, Claire S. Adjiman, Amparo Galindo and George Jackson
Department of Chemical Engineering, Centre for Process Systems Engineering, South Kensington Campus, Imperial College London, SW7 2AZ, UK
- 14:30 – 14:50 A lattice Boltzmann method for non ideal gases based on the gradient theory of interfaces
E.S. Kikkinides^a, M.E. Kainourgiakis^b, A.G. Yiotis^b and A.K. Stubos^b
^a Department of Mechanical Engineering, University of Western Macedonia, Bakola & Sialvera Str., 50100 Kozani, Greece
^b Environmental Research Laboratory, National Center for Scientific Research "Demokritos", 15310 Ag. Paraskevi, Athens, Greece
- 14:50 – 15:10 Simultaneous design of ionic liquids and azeotropic separation processes
Brock C. Roughton^a, John White^a, Kyle V. Camarda^a, and Rafiqul Gani^b
^a Department of Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS 66049 USA
^b CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark
- 15:10 – 15:30 Chemicals-based formulation design: Virtual experimentations

Elisa Conte, Rafiqul Gani

CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

15:30 – 15:50 Controlling particle size in a novel spinning disc continuous stir tank and settler reactor for the continuous synthesis of titania

M.K. Akindeju, P.H. Ong

Department of Chemical Engineering, Curtin University of Technology Box U1987, Perth, WA 6845, Australia

Energy Systems Engineering III – MARINA II

Chair: Rajagopalan Srinivasan (NUS, Singapore)

14:10 – 14:30 Low temperature process design: Challenges and approaches for using exergy efficiencies

Danahe Marmolejo-Correa, Truls Gundersen

Department of Energy and Process Engineering, Norwegian University of Science and Technology, NTNU. Kolbjoern Hejes v 1B, NO-7491, Trondheim, Norway

14:30 – 14:50 Reduce costs and energy consumption of deethanizing and depropanizing fractionation steps in NGL recovery process

Nguyen Van Duc Long, Moonyong Lee

School of Chemical Engineering and Technology, Yeungnam University, Gyeongsan 712-749, South Korea

14:50 – 15:10 Long-term planning of wind farm siting in the electricity grid

Jingjie Xiao^a, Bri-Mathias S. Hodge^b, Andrew L. Liu^a, Joseph F. Pekny^b, Gintaras V. Reklaitis^b

^a School of Industrial Engineering, Purdue University, West Lafayette, IN 47907

^b School of Chemical Engineering, Purdue University, West Lafayette, IN 47907

15:10 – 15:30 Modeling fluid flow of Vipertex enhanced heat transfer tubes

David J. Kukulka^a and Rick Smith^b

^a State University of New York College at Buffalo, 1300 Elmwood Avenue, Buffalo, New York, 14222, USA

^b Vipertex™, 658 Ohio Street, Buffalo, New York 14203

15:30 – 15:50 Analysis of Integrated Gasification Combined Cycle (IGCC) power plant based on climate change scenarios with respect to CO₂ capture ratio

Kyungtae Park^a, Kyusang Han^a and En Sup Yoon^{a,b}

^a School of Chemical and Biological Engineering, Seoul National University, Seoul, 151-742, Korea

^b ASRI, Automation and Systems Research Institute, Seoul, 151-742, Korea

15:50 – 16:20 Coffee Break

16:20 – 18:00 Oral Presentations – 5 Parallel Sessions

Environmental Systems Engineering II – TERPSIHORI HALL

Chair: Mario Eden (Auburn University, USA)

16:20 – 16:40 A systematic methodology for the synthesis of unit process chains using Life Cycle Assessment and Industrial Ecology Principles

Léda Gerber, Jérôme Mayer, François Maréchal

Industrial Energy Systems Laboratory (LENI), Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

16:40 – 17:00 Minimization of the life cycle impact of chemical supply chain networks under demand uncertainty

Rubén Ruiz-Femenia^b, José A. Caballero^b and Laureano Jiménez^a

^a Universitat Rovira i Virgili, Av. Països Catalans 26, Tarragona 43007, Spain

^b Universidad de Alicante, Apartado de Correos 99, Alicante 03080, Spain

17:00 – 17:20 Evaluation of CO₂ absorption-desorption cycle by dynamic modeling and simulation

Ana-Maria Cormos, Jozsef Gaspar, Paul-Serban Agachi

Babes – Bolyai University, Faculty of Chemistry and Chemical Engineering, 11 Arany Janos Street, RO-400028, Cluj – Napoca, Romania

- 17:20 – 17:40 Integrating economic, environmental and social indicators for sustainable supply chains
 Peng Cheng Wang^a, Iskandar Halim^b, Arief Adhitya^b, Rajagopalan Srinivasan^{a,b}
^a Department of Chemical and Biomolecular Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 117576, Singapore
^b Institute of Chemical and Engineering Sciences, A*STAR (Agency for Science, Technology and Research), 1 Pesek Road, Jurong Island, Singapore 627833, Singapore
- 17:40 – 18:00 Increasing the understanding of the BP Texas city refinery accident
 Davide Manca, Sara Brambilla, Alessandro Villa
 CMIC Department, Politecnico di Milano, 20133 MILANO, ITALY
- 18:00 – 18:20 Towards a generic simulation environment for multiscale modelling based on tool integration
 Yang Zhao, Cheng Jiang, Aidong Yang
 Chemical and Process Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford GU2 7XH, UK

Biomedical Systems Engineering II – MARINA I

Chair: Gurkan Sin (DTU, Denmark)

- 16:20 – 16:40 Towards in silico models of decomplexification in human endotoxemia
 Jeremy D. Scheff^a, Pantelis Mavroudis^b, Steve E. Calvano^c, Stephen F. Lowry^c, Ioannis P. Androulakis^{a,b,c}
^a Department of Biomedical Engineering, Rutgers University, 599 Taylor Road, Piscataway, NJ, USA 08854
^b Department of Chemical and Biochemical Engineering, Rutgers University, 98 Brett Road, Piscataway, NJ, USA 08854
^c Department of Surgery, UMDNJ-Robert Wood Johnson Medical School, Clinical Academic Building, 125 Patterson Street, New Brunswick, NJ, USA 08901
- 16:40 – 17:00 Multi-scale modeling of PLGA microparticle drug delivery systems
 Ashlee N. Ford^a, Daniel W. Pack^a, Richard D. Braatz^{a,b}
^a Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, 600 South Mathews Avenue, Urbana, IL 61801, USA
^b Department of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Room 66-372, Cambridge, MA 02139, USA
- 17:00 – 17:20 Disease classification through integer optimisation
 Chrysanthi Ainali^{a,b}, Frank Nestle^b, Lazaros G. Papageorgiou^c, Sophia Tsoka^a
^a Centre for Bioinformatics, Department of Informatics, School of Natural and Mathematical Sciences, King's College London, Strand, London, WC2R 2LS, UK
^b St John's Institute of Dermatology, King's College London School of Medicine, Tower Wing, Guy's Hospital, Great Maze Pond, London SE1 9RT, UK
^c Centre for Process Systems Engineering, Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, UK
- 17:20 – 17:40 From chemical process diagnosis to cancer prognosis: An integrated approach for diagnosis and sensor/marker selection
 Lyamine Hedjazi^{a,b}, Marie-Véronique Le Lann^{a,b}, Tatiana Kempowsky-Hamon^{a,b}, Joseph Aguilar-Martin^{a,b}, Florence Dalenc^c, Gilles Favre^c, Laurène Despenes^{d,b}, Sébastien Elgue^{d,b}
^a CNRS, LAAS 7, avenue du Colonel Roche, F-31077 Toulouse, France
^b Université de Toulouse, UPS, INSA, INP, ISAE, LAAS, F-31077 Toulouse, France
^c INSERM U563 and Institut Claudius Regaud, F-31300 Toulouse, France
^d CNRS, LGC, INP-ENSIACET, 4 allée Emile Monso, F-31030 Toulouse, France
- 17:40 – 18:00 A variational Bayesian approach for dosage regimen individualization
 J. M. Laínez, L. Mockus, G. Blau, S. Orçun, and G.V. Reklaitis
 Purdue University, School of Chemical Engineering, West Lafayette, IN 47907 USA
- 18:00 – 18:20 Physiologically based pharmacokinetic modeling and predictive control: an integrated approach for optimal drug administration

Pantelis Sopasakis, Panagiotis Patrinos, Stefania Giannikou, Haralambos Sarimveis
 National Technical University of Athens, School of Chemical Engineering, 9 Heroon Polytechniou Str., GR- 157 80, Athens, Greece

Bioprocess Systems Engineering II – CHLOE HALL

Chair: Athanasios Mantalaris (Imperial, UK)

16:20 – 16:40 A framework for model-based optimization of bioprocesses under uncertainty: Identifying critical parameters and operating variables

Ricardo Morales-Rodriguez^a, Anne S. Meyer^b, Krist V. Gernaey^c, Gürkan Sin^a

^a CAPEC, ^b BIOENG, ^c PROCESS, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

16:40 – 17:00 Population balance modelling of influenza virus replication during vaccine production – Influence of apoptosis

Thomas Müller^a, Robert Dürr^b, Britta Isken^b, Josef Schulze-Horse^b, Udo Reich^{a,b}, Achim Kienle^{a,b}

^a Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

^b Max-Planck-Institut für Dynamik komplexer technischer Systeme, Sandtorstrasse 1, D- 39106 Magdeburg, Germany

17:00 – 17:20 Systematic data and knowledge utilization to speed up bioprocess design

Jun Zhang^a, Anthony Hunter^b, Yuhong Zhou^a

^a Department of Biochemical Engineering, University College London, Torrington Place, London, WC1E 7JE, U.K.

^b Department of Computer Science, University College London, Gower Street, London, WC1E 6BT, U.K.

17:20 – 17:40 Prediction of activation of metabolic pathways via dynamic optimization

Gundian M. De Hijas-Liste, Eva Balsa-Canto, Julio R. Banga

(Bio)Process Engineering Group, IIM-CSIC, Eduardo Cabello 6, Vigo 36208, Spain

17:40 – 18:00 Standards for continual scheduling of batch operations

Charles Siletti^a, Demetri Petrides^b, Dimitri Vardalis^c

^a Intelligen, Inc. 700 Walton Ave., Mt. Laurel, NJ 08054 USA

^b Intelligen, Inc. 2326 Morse Ave, Scotch Plains, NJ 07076 USA

^c Intelligen Europe, Thessaloniki, Greece

18:00 – 18:20 Optimization of a sequencing batch reactor process for waste water treatment using a two step nitrification model

M.N. Cruz Bournazou^a, K. Hooshiar^a, H. Arellano-Garcia^a, G. Lyberatos^{b,c}, C. Kravaris^b, G. Wozny^a

^a Chair of Process Dynamics and Operation, Berlin Institute of Technology, Sekr. KWT-9 Str. des 17. Juni 135, D-10623 Berlin, Germany

^b Department of Chemical Engineering, University of Patras, 26504 Patras, Greece

^c Institute of Chemical Engineering and High Temperature Chemical Processes, FORTH, Patras, Greece

Optimization III – ERATO HALL

Chair: Vivek Dua (UCL, UK)

16:20 – 16:40 Plant-wide optimisation and control of a multi-scale pharmaceutical process

Mayank P. Patel^a, Nilay Shah^a, Robert Ashe^b

^a CPSE, Dept. Chemical Engineering, Imperial College, London, SW7 2AZ, UK

^b AM Technology, The Heath Bus. & Tech. Park, Runcorn, Cheshire, WA7 4QX, UK

16:40 – 17:00 The Coulomb glass – Modeling and computational experience with a large scale 0-1 QP Problem

Ray Pörn^a, Otto Nissfolk^b, Fredrik Jansson^c, Tapio Westerlund^b

^a Novia University of Applied Sciences, Wolffskavägen 33, 65200 Vaasa, Finland

^b Process Design and Systems Engineering Laboratory, Åbo Akademi University, Biskopsgatan 8, 20500 Turku, Finland

^c Department of Physics and Center for Functional Materials, Åbo Akademi University, Porthansgatan 3, 20500 Turku, Finland

17:00 – 17:20 Multiobjective optimization of the pulp/water storage towers in design of paper production systems

Aino Ropponen, Miika Rajala, Risto Ritala

Tampere University of Technology, Department of Automation Science and Engineering, P.O. BOX 692, FI-33101 Tampere, Finland

- 17:20 – 17:40 Deterministic global optimization of kinetic models of metabolic networks: outer approximation vs. spatial branch and bound
Carlos Pozo^a, Gonzalo Guillen-Gosalbez^a, Albert Sorribas^b, Laureano Jimenez^a
^a *Departament d'Enginyeria Quimica, Universitat Rovira i Virgili, Tarragona, Spain*
^b *Departament de Ciències Mèdiques Bàsiques, Universitat de Lleida, Lleida, Spain*
- 17:40 – 18:00 Model based optimisation of a cyclic reactor for the production of hydrogen
Filip Logist, Joost Lauwers, Benoît Trigaux, Jan F. Van Impe
BioTeC & OPTeC - Chemical Engineering Dept., Katholieke Universiteit Leuven, W. de Croylaan 46, B-3001 Leuven, Belgium
- 18:00 – 18:20 Integration of ontology and knowledge-based optimization in process synthesis applications
F. Ceceļja^a, A. Kokossis^b, Du Du^a
^a *Process & Information Systems Engineering, FEPS, University of Surrey, Guildford, U.K*
^b *School of Chemical Engineering, National Technical University of Athens, Zografou Campus, Athens, Greece*

Energy Systems Engineering IV – MARINA II

Chair: *Paul Stuart (Ecole Polytechnique Montreal, Canada)*

- 16:20 – 16:40 Energy systems analysis for a renewable transportation sector
*Dharik S. Mallapragada, Navneet R. Singh, Rakesh Agrawal**
School of Chemical Engineering, Purdue University, 480 Stadium Mall Drive, West Lafayette, Indiana, 47907, USA.
**Corresponding Author email: agrawalr@purdue.edu*
- 16:40 – 17:00 BOG handling method for energy savings in LNG receiving terminal
Chansaem Park, Youngsub Lim, Sangho Lee, Chonghun Han
School of Chemical and Biological Engineering, Seoul National University, San 56-1, Shillim-doong, Kwanak-ggu, Seoul, 1511-742, Korea
- 17:00 – 17:20 Co-production of ethanol, hydrogen and biogas using agro-wastes. Conceptual plant design and NPV analysis for mid-size agricultural sectors
Arturo Sanchez^a, Victor Sevilla-Guitron, Gabriela Magaña, Paulina Melgoza, Hector Hernandez^b
^a *Cinvestav Unidad Guadalajara, Av. Científica 1145, Zapopan 45015, México*
^b *Dept. de Ingeniería Química, Universidad de Guanajuato, Gto, México*
- 17:20 – 17:40 Optimization of LNG plants – challenges and Strategies
Magnus G. Jacobsen, Sigurd Skogestad
Norwegian University of Science and Technology, 7491 Trondheim, Norway
- 17:40 – 18:00 Process synthesis with heat and power integration of thermochemical coal, biomass, and natural gas hybrid energy processes
Richard C. Baliban, Josephine A. Elia, Christodoulos A. Floudas
Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, 08540, USA
- 18:00 – 18:20 Reynolds number effects on particle dispersion and deposition in turbulent square duct flows
J.F.W. Adams, J. Yao and M. Fairweather
Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT, UK

20:30 Conference Dinner

08:30 – 09:50 Plenary Session 4 - OLYMPIC HALL

Chairs: Ferenc Friedler (University of Pannonia, Hungary)
Stratos Pistikopoulos (Imperial, UK)

08:30 – 09:10 Process systems engineering in the era of Watson: Challenges and opportunities in cyberinfrastructure and informatics

Venkat Venkatasubramanian (*Purdue University, USA*)

09:10 – 09:50 The role of theory in control practice

Manfred Morari (*ETH Zurich, Switzerland*)

10:00 – 11:40 Oral Presentations

Multi-scale Modelling III – CHLOE HALL

Chair: Fabrizio Bezzo (University of Padoa, Italy)

10:00 – 10:20 Multiscale modeling of chemical vapor deposition of silicon

N. Cheimarios^a, S. Garnelis^a, G. Kokkoris^b, A.G. Boudouvis^a

^a *School of Chemical Engineering, National Technical University of Athens, Athens 15780, Greece*

^b *Institute of Microelectronics, National Center for Scientific Research "Demokritos", Athens 15310, Greece*

10:20 – 10:40 Modelling of micro- and nano-patterned electrodes for the study and control of spillover processes in catalysis

I. Bonis, S. Valiño-Pazos, I.S. Fragkopoulou, C. Theodoropoulos

School of Chemical Engineering and Analytical Science, University of Manchester, Sackville Street, Manchester M13 9PL, UK

10:40 – 11:00 Multiscale modeling of a silicon solar wafer manufacturing process

Ruo Chen Liu, German Oliveros, Seetharaman Sridhar^a, B. Erik Ydstie

Dept. of Chemical (and) Material Science Engineering, Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh PA 15213, USA

11:00 – 11:20 Modeling of a batch emulsion copolymerization reactor in the presence of a chain transfer agent: estimability analysis parameters identification and experimental validation

B. Benyahia^{a,b}, M. A. Latifi^a, C. Fonteix^a, F. Pla^a

^a *Laboratoire Réactions et Génie des Procédés, CNRS-ENSIC 1 rue Grandville, BP 20451, 54001 Nancy Cedex, France*

^b *Process Systems Engineering Laboratory, Department of Chemical Engineering, MIT, 77 Massachusetts Avenue, Cambridge MA 02139, USA*

11:20 – 11:40 Integration of generic multi-dimensional model and operational policies for batch cooling crystallization

Noor Asma Fazli Abdul Samad, Ravendra Singh, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani

Department of Chemical and Biochemical Engineering, Søtofts Plads, Building 229, Technical University of Denmark, DK-2800, Lyngby, Denmark

Process Operations III – TERPSIHORI HALL

Chair: Lazaros Papageorgiou (UCL, UK)

10:00 – 10:20 Optimal scheduling of multi-level tree-structure pipeline networks

Diego C. Cafaro, Jaime Cerdá

INTEC (UNL-CONICET), Güemes 3450, (3000) Santa Fe, Argentina

10:20 – 10:40 Recipe-based batch process engineering tool for process development workflow

Jae Hyun Cho, Junghwan Kim, Il Moon

Department of Chemical and Biomolecular Engineering, Yonsei University 262 Seongsanno, Seodaemun-gu, Seoul 120-749, Republic of Korea

- 10:40 – 11:00 Integrated supply chain planning for multinational pharmaceutical enterprises
Naresh Susarla, I A Karimi
Department of Chemical & Biomolecular Engineering, National University of Singapore, Singapore
- 11:00 – 11:20 A continuous-time MILP to compute schedules with minimum changeover times for a make-and-pack production
Philipp Baumann, Norbert Trautmann
Department of Business Administration, University of Bern, Switzerland
- 11:20 – 11:40 Scenario-based strategic SC design and analysis for the Forest Biorefinery
Behrang Mansoornejad^a, Efstratios N. Pistikopoulos^b, Paul Stuart^a
^a NSERC Environmental Design Engineering Chair Department of Chemical Engineering, École Polytechnique, 2920 Chemin de la Tour, Pavillon Aisenstadt, Montreal H3C 3A7, Canada
^b Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College, London SW7 2AZ, UK

Bioprocess Systems Engineering III – MARINA I

Chair: Athanasios Mantalaris (Imperial, UK)

- 10:00 – 10:20 Global sensitivity analysis in bioreactor networks
Maria Paz Ochoa, Patricia M. Hoch
Planta Piloto de Ingeniería Química – CONICET – 8000 Bahia Blanca, Argentina Universidad Nacional del Sur – Departamento de Ingeniería Química – 8000 Bahia Blanca, Argentina
- 10:20 – 10:40 Graph theory augmented recursive MILP approach for identifying multiple minimal reaction sets in metabolic networks
Sudhakar Jonnalagadda^a, Rajagopalan Srinivasan^{a,b}
^a Institute of Chemical and Engineering Sciences, Agency for Science, Technology and Research, 1, Pesek Road, Jurong Island, Singapore, 627833
^b Dept of Chemical and Biomolecular Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore
- 10:40 – 11:00 Robust optimal control of a biochemical reactor with multiple objectives
Filip Logist^a, Boris Houska^b, Moritz Dieh^b, Jan F. Van Impe^a
^a BioTeC & OPTEC - Chemical Engineering Dept., Katholieke Universiteit Leuven, W. de Croylaan 46, B-3001 Leuven, Belgium
^b SCD & OPTEC, Electrical Engineering Dept., Katholieke Universiteit Leuven, Kasteelpark Arenberg 10, 3001 Leuven, Belgium
- 11:00 – 11:20 Toward online control of glycosylation in MAbs
Melissa M. St. Amand, Anne S. Robinson, Babatunde A. Ogunnaike
University of Delaware, 150 Academy Street, Newark, DE USA
- 11:20 – 11:40 Methodological approach for modeling of multi-enzyme in-pot processes
Paloma A. Santacoloma^a, Alicia Roman-Martinez^b, Gürkan Sin^b, Krist V. Gernaey^a, John M. Woodley^a
^a PROCESS, ^b CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søtofts Plads, B. 229, 2800-Kgs. Lyngby, Denmark

Control III – ERATO HALL

Chair: Ioannis Kookos (University of Patras, Greece)

- 10:00 – 10:20 Integrated process and control design by the normal vector approach: Application to the Tennessee-Eastman process
Diego A. Muñoz^{a,b}, Johannes Gerhard^a, Ralf Hannemann^a, Wolfgang Marquardt^a
^a Aachener Verfahrenstechnik, RWTH Aachen University, 52064 Aachen, Germany.
^b Research Group on Mathematics, Universidad Pontificia Bolivariana, Med.-Colombia
- 10:20 – 10:40 Reliable optimal control of a fed-batch fermentation process using ant colony optimisation and bootstrap aggregated neural network models
Jie Zhang, Yiting Feng, Mahmood Hilal Al-Mahrouqi

School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU, UK

- 10:40 – 11:00 Nonlinear state estimation with delayed measurements. Application to polymer processes
Ruben Galdeano, Mariano Asteasuain, Mabel C. Sanchez
PLAPIQUI (CONICET – UNS), Camino la Carrindanga km 7, Bahia Blanca 8000, Argentina
- 11:00 – 11:20 System identification using wavelet analysis
Zdenek Vána^a, Samuel Privara^a, Jiri Cigler^a, Heinz A. Preisig^b
^a *Department of Control Engineering, CTU in Prague, Prague, Czech Republic*
^b *Department of Chemical Engineering, NTNU, Trondheim, Norway*
- 11:20 – 11:40 Optimal controlled variable selection using a nonlinear simulation-optimization framework
Mahdi Sharifzadeh, Nina F. Thornhill
Centre for Process System Engineering (CPSE), Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

Energy Systems Engineering V – MARINA II

Chair: *Andreas Linninger (University of Illinois, USA)*

- 10:00 – 10:20 Optimal location of gasification plants for electricity production in rural areas
Mar Pérez-Fortes^{a,b}, Pol Arranz-Piera^b, José Miguel Laínez^c, Enric Velo^b, Luis Puigjaner^a
^a *Dept. of Chemical Engineering-CEPIMA, UPC, ETSEIB, Av. Diagonal 647, Barcelona, E08028, Spain*
^b *Institute of Sustainability, Science & Technologies, IS, UPC, Pl. Eugeni Güell 6, Barcelona, E08034, Spain*
^c *School of Chemical Engineering, Purdue University, West Lafayette, IN, USA*
- 10:20 – 10:40 An integrated approach to optimal pipeline routing, design, operation and maintenance
Eftychia C. Marcoulaki^a, Ioannis A. Papazoglou^a, Nathalie Pixopoulou^b
^a *Laboratory of System Reliability and Industrial Safety, National Centre for Scientific Research “Demokritos”, PO Box 60228, Athens 15310, Greece*
^b *Penspen Limited, 405 Messogeion Avenue, Athens 15343, Greece*
- 10:40 – 11:00 Ethanol from corn: screening options and power supply improvement to ethanol plant in Italy
Marco Soldà, Franjo Cecelja, Aidong Yang, Piyalap Manakit
PRISE Centre for Process and Information System Engineering University of Surrey, Guildford, UK
- 11:00 – 11:20 General methodology for exergy balance in a process simulator
Ali Ghannadzadeh^{a,b,c}, Raphaële Thery-Hetreux^{a,b}, Olivier Baudouin^c, Philippe Baudet^c, Pascal Floquet^{a,b}, Xavier Joulia^{a,b}
^a *Université de Toulouse; INPT, UPS; Laboratoire de Génie Chimique; 4, Allée Emile Monso, F-31030 Toulouse, France*
^b *CNRS; Laboratoire de Génie Chimique; F-31030 Toulouse, France*
^c *ProSim SA, Stratège Bâtiment A, BP 27210, F-31672 Labège Cedex, France*
- 11:20 – 11:40 Strategic planning of petroleum supply chains
Leão José Fernandes^{a,b}, Susana Relvas^a, Ana Paula Barbosa-Póvo^a
^a *CLC, EN 366, Km 18, 2050 Aveiras de Cima, Portugal*
^b *CEG-IST, UTL, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*

11:40 – 12:00 Coffee Break

12:00 – 13:40 Oral Presentations – 5 Parallel Sessions

Optimization IV – ERATO HALL

Chair: *Christos Maravelias (University of Wisconsin, USA)*

- 12:00 – 12:20 Optimization of simulated moving bed chromatography with fractionation and feedback incorporating an enrichment step
Suzhou Li^a, Yoshiaki Kawajiri^b, Jörg Raisch^{a,c}, Andreas Seidel-Morgenstern^{a,d}

- ^a Max-Planck-Institut für Dynamik of komplexer technischer Systeme, Sandtorstraße 1, D-39106 Magdeburg, Germany
^b School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, 311 Ferst Drive, Atlanta, GA 30332, USA
^c Fachgebiet Regelungssysteme, Technische Universität Berlin, Einsteinufer 17, D-10587 Berlin, Germany
^d Institut für Verfahrenstechnik, Otto-von-Guericke Universität, Universitätsplatz 2, D- 39106 Magdeburg, Germany, Magdeburg, Germany

- 12:20 – 12:40 Calibration of a polyethylene plant model for optimisation of grade changes
Niklas Andersson^a, Per-Ola Larsson^b, Johan Åkesson^b, Staffan Haugwitz^c, Bernt Nilsson^a
^a Dept. of Chemical Engineering, Lund University, Box 124, SE 221 00 Lund, Sweden
^b Dept. of Automatic Control, Lund University, Box 118, SE 221 00 Lund, Sweden
^c Borealis AB, SE-444 86, Stenungsund, Sweden
- 12:40 – 13:00 Superstructure approach to batch process scheduling by S-graph representation
B. Bertok^a, R. Adonyi^a, F. Friedler^a, L.T. Fan^b
^a Department of Computer Science and Systems Technology, University of Pannonia, Egyetem u. 10, H-8200 Veszprém, Hungary
^b Department of Chemical Engineering, Kansas State University, Manhattan, Kansas 66506, USA
- 13:00 – 13:20 A reformulation scheme for parameter estimation of hybrid systems
Ines Mynttinen, Pu Li
Simulation and Optimal Processes Group, Institute of Automation and Systems Engineering, Technische Universität Ilmenau, 98693 Ilmenau, Germany
- 13:20 – 13:40 Dynamic optimization of bioreactors using probabilistic tendency models and bayesian active learning
Ernesto Martínez^a, Mariano Cristaldi^b, Ricardo Grau^b, Joao Lopes^c
^a INGAR (Conicet-UTN), Avellaneda 3657, Santa Fe, S3002 GJC, Argentina
^b INTEC (Conicet-UNL), Güemes 3450, Santa Fe, 3000, Argentina
^c Porto University, Chemistry Dept., R. Anibal Cunha 164, Porto 4099-030, Portugal

Synthesis/Design IV – MARINA I

Chair: Benoit Chachuat (Imperial, UK)

- 12:00 – 12:20 Lipid processing technology: Building a multilevel modeling network
Carlos A. Diaz-Tovar^a, Azizul A. Mustaffa^a, Amol Hukkerikar^a, Alberto Quaglia^a, Gürkan Sin^a, Georgios Kontogeorgis^b, Bent Sarup^c, Rafiqul Gani^a
^a CAPEC, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Soltofts Plads Building 229, Kgs. Lyngby DK-2800, Denmark.
^b CERE, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Soltofts Plads Building 229, Kgs. Lyngby DK-2800, Denmark.
^c Vegetable Oil Technology Business Unit, Alfa Laval Copenhagen A/S, Maskinvej 5, Soborg DK-2860, Denmark
- 12:20 – 12:40 Designing multi-product biopharmaceutical facilities using evolutionary algorithms
Ana S. Simaria^a, Ying Gao^b, Richard Turner^b, Suzanne S. Farid^a
^a The Advanced Centre for Biochemical Engineering, Dept. of Biochemical Engineering, University College London, Torrington Place, London WC1E 7JE, UK.
^b MedImmune Limited, Milstein Building, Granta Park, Cambridge, CB1 6GH, UK
- 12:40 – 13:00 Pareto-navigation in chemical engineering
Norbert Aspöckl^a, Sergej Blagov^a, Oliver Ryll^a, Richard Welke^b, Anton Winterfeld^b, Agnes Dittel^b, Michael Bortz^b, Karl-Heinz Küfer^b, Jakob Burger^c, Andreas Scheithauer^c, Hans Hasse^c
^a BASF SE, Carl-Bosch-Str. 38, 67056 Ludwigshafen, Germany
^b Fraunhofer Institut für Techno- und Wirtschaftsmathematik, Fraunhofer Platz 1, 67663 Kaiserslautern, Germany
^c Lehrstuhl für Thermodynamik, University of Kaiserslautern, Erwin-Schrödinger-Str. 44, 67663 Kaiserslautern, Germany
- 13:00 – 13:20 Design of a sustainable biorefinery
Mehboob Nawaz^a, Edwin Zondervan^b, John Woodley^a, Rafiqul Gani^a
^a Department of Chemical and Biological Engineering, Technical University of Denmark, Lyngby, 2800, Denmark
^b Department of Chemistry and Chemical Engineering, Eindhoven University of Technology, P.O.Box 513, 5600MB, Eindhoven, the Netherlands

- 13:20 – 13:40 Separation circuits analysis and design using sensitivity analysis
Freddy Lucay^{a,b}, Mario E. Mellado^b, Luis A. Cisternas^{a,b}, Edelmira D. Gálvez^{b,c}
^a *Departamento de Ingeniería Química, Universidad de Antofagasta, Chile*
^b *Centro de Investigación Científico tecnológico para la Minería, CICITEM, Chile*
^c *Departamento de Ingeniería Metalúrgica, Universidad Católica del Norte, Chile*

Process Operations IV – TERPSIHORI HALL

Chair: Ana Barbosa (IST, UTL, Portugal)

- 12:00 – 12:20 Real-time process management in particulate and pharmaceutical systems
Arun Giridhar, Intan Hamdan, Girish Joglekar, Venkat Venkatasubramanian, Gintaras V. Reklaitis
School of Chemical Engineering, Purdue University, West Lafayette, Indiana USA
- 12:20 – 12:40 Efficient scheduling of batch plants using reachability tree search for timed automata with lower bound computations
Subanatarajan Subbiah, Christian Schoppmeyer, Sebastian Engell
Process Dynamics and Operations Group, Department of Biochemical and Chemical Engineering, Technische Universität Dortmund, Emil-Figge Str. 70, 44227 Dortmund, Germany
- 12:40 – 13:00 A rigorous mathematical formulation to Automated Wet-Etch Station scheduling with multiple wafer-handling robots in Semiconductor Manufacturing Systems
Adrián M. Aguirre^a, Carlos A. Méndez^a, Pedro M. Castro^b
^a *INTEC (UNL-CONICET), Güemes 3450, 3000 Santa Fe, Argentina*
^b *Unidade Modelação e Optimização de Sistemas Energéticos, Laboratório Nacional de Energia e Geologia, Lisboa, Portugal*
- 13:00 – 13:20 Improving supply chain management in a competitive environment
M. Zamarripa^a, A. M. Aguirre^b, C. A. Méndez^b, A. Espuña^a
^a *Universitat Politècnica de Catalunya (UPC), Chem. Engng. Dpt. Barcelona, Spain*
^b *INTEC (UNL-CONICET), Santa Fe, Argentina*
- 13:20 – 13:40 A novel CP approach for scheduling an automated Wet-Etch Station
Juan M. Novas, Gabriela P. Henning
INTEC (UNL-CONICET), Güemes 3450, Santa Fe, CP 3000, Argentina

Energy Systems Engineering VI – MARINA II

Chair: Francois Marechal (EPFL, Switzerland)

- 12:00 – 12:20 Towards second generation bioethanol: Supply chain design and capacity planning
Andrea Zamboni, Sara Giarola, Fabrizio Bezzo
CAPE-Lab, Dipartimento di Principi e Impianti di Ingegneria Chimica, Università di Padova, via Marzolo 9, 35131, Padova, Italy
- 12:20 – 12:40 A mixed-integer programming approach to infrastructure planning for chemical centres: A case study in the UK
Pei Liu^{a,b}, Alan Whitaker^a, Efstratios N. Pistikopoulos^a, Zheng Li^b, Yong Chen^c
^a *Centre for Process Systems Engineering (CPSE), Imperial College London, London SW7 2AZ, U.K.*
^b *State Key Laboratory of Power Systems, Department of Thermal Engineering, Tsinghua University, Beijing 100084, China*
^c *Sinochem Group, Beijing 100031, China*
- 12:40 – 13:00 A multi objective optimization method to integrate heat pumps in industrial processes
Helen Becker, Giulia Spinato, François Maréchal
Industrial Energy Systems Laboratory (LENI), Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
- 13:00 – 13:20 Potential impacts and modelling of the heat value loss due to chelation in natural gas processing and transport

Hunt, D.J., Akindeju, M.K., Obanijesu, E.O., Pareek, V.K, Tade, M.O
Department of Chemical Engineering, Curtin University of Technology, Perth, WA 6845, Australia

- 13:20 – 13:40 An MILP model for the strategic design of the UK bioethanol supply chain
Ozlem Akgul^a, Nilay Shah^b, Lazaros G. Papageorgiou^a
^a *Centre for Process Systems Engineering, University College London (UCL), London WC1E 7JE, UK*
^b *Centre for Process Systems Engineering, Imperial College London, London SW7 2AZ, UK*

Control IV – CHLOE HALL

Chair: Panos Seferlis (AUTh, Greece)

- 12:00 – 12:20 Economic MPC for power management in the smart grid
Tobias Gybel Hovgaard^{a,c}, Kristian Edlund^b, John Bagterp Jørgensen^c
^a *Danfoss Refrigeration and A/C Controls, Nordborgvej 81, 6430 Nordborg, Denmark*
^b *DONG Energy A/S, Kraftværksvej53, 7000 Fredericia, Denmark*
^c *DTU Informatics, Richard Petersens Plads, Building 321, 2800 Lyngby, Denmark*
- 12:20 – 12:40 Role of MPC in building climate control
Samuel Prívar^a, Zdenek Vána^a, Jirí Cigler^a, Frauke Oldewurtel^b, Josef Komárek^c
^a *Department of Control Engineering, CTU in Prague, 121 35 Prague, Czech Republic*
^b *Automatic Control Laboratory, ETH Zurich, 8006, Switzerland*
^c *Technofiber s.r.o, Lazaretn 7, 615 00 Brno, Czech Republic*
- 12:40 – 13:00 Time optimal control of particle size distribution in emulsion polymerization
Ahmad Mansour, Ala Eldin Bouaswaig, Sebastian Engell
Process Dynamics and Operations Group, Technische Universität Dortmund, 44221 Dortmund, Germany
- 13:00 – 13:20 Application of Graphic Processing Unit (GPU) in model predictive control
Arash Sadrieh, Parisa A. Bahri
School of Engineering and Energy, Murdoch University, Western Australia, 6150
- 13:20 – 13:40 Multi-parametric model predictive control of an automated integrated fuel cell testing unit
Chrysovalantou Ziogou^{a,c}, Christos Panos^b, Konstantinos I. Kouramas^b, Simira Papadopoulou^d, Michael C. Georgiadis^c, Spyros Voutetakis^a, Efstratios N. Pistikopoulos^b
^a *Chemical Process Engineering Research Institute (CPERI), Center for Research and Technology Hellas (CERTH) P.O. Box 60361, 57001 Thessaloniki, Greece*
^b *Department of Chemical Engineering, CPSE, Imperial College London, SW7 2AZ London, UK*
^c *University of Western Macedonia, Department of Engineering Informatics and Telecommunications, Kozani 50100, Greece*
^d *Alexander Technological Educational Institute of Thessaloniki, Department of Automation, P.O. Box 141, 57400, Thessaloniki, Greece*

13:40 – 15:00 Lunch

15:00 End of Conference