ESCAPE-21

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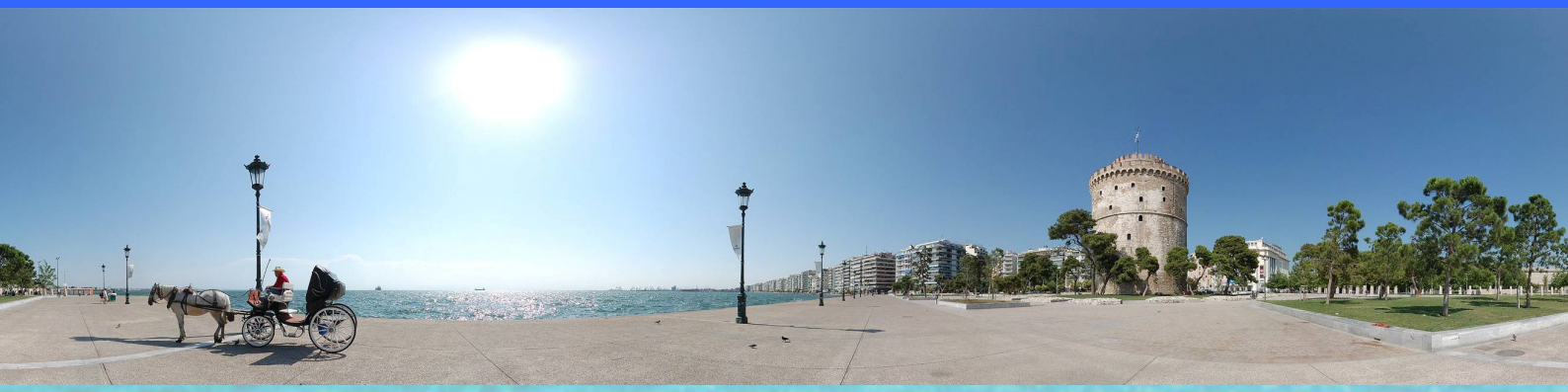

PROGRAMME BOOK




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

Programme Index

Welcome of the NOC Chairman

Welcome to ESCAPE-21. Welcome to Thessaloniki, Greece

On behalf of the National Organizing Committee (NOC) it gives me great pleasure to welcome you to Thessaloniki, Greece, on the occasion of the 21st European Symposium on Computer-Aided Process Engineering.

The Symposium programme includes 8 plenary lectures, 6 keynote lectures, 175 oral presentations and 227 poster presentations. Delegates from more than 45 Countries have travelled to Thessaloniki to participate in ESCAPE-21 to be held in Porto Carras Grand Resort in Chalkidiki.

The world is undergoing a global technology revolution that is integrating developments in **nanotechnology**, **materials technology**, **biotechnology**, and **information technology** at an accelerating pace. Future technological developments will continue to integrate innovations from multiple scientific disciplines in a **"convergence"** that will have profound effects on society.

The manufacturing and process industries are very diverse and cover a wide range of specific production systems ranging from extracting minerals to assembly of very complex products, with all intermediate processing steps in a long chain of industrial suppliers and customers. Extracting from this wide variety of businesses and processes, some general research priorities is far from easy. Despite the diversity of industrial production systems, the following research trends appear to be common to the majority of manufacturing and process industries.

- **New Business Models**
- **Adaptive Production Systems**
- **Networking in Manufacturing and Production Systems**
- **Knowledge-based Engineering**
- **Sustainable Production Systems**

The symposium programme reflects these challenges and I trust that you will be inspired by the presentations and discussions with friends and experts participating in ESCAPE-21.

The cultural programme is centred around the theme of spouce appreciation and offers a unique chance to meet with some very distinct elements of the cultural heritage of Greece as well as the natural beauty of Chalkidiki peninsula through the planned events for accompanying persons: (i) A City Tour of Thessaloniki and its Museums and (ii) A Boat Trip to the "Holy Mount of Athos".

On Tuesday evening, during the Symposium's Gala Dinner, you will have the opportunity to enjoy Greek traditional cuisine, "live" Greek music and a lot of Greek dancing.

Many thanks to all the plenary and keynote speakers, contributors, participants and sponsors of ESCAPE-21. Especially, I would like to thank the personnel of the Laboratory of Polymer Reaction Engineering at CERTH/AUTh for all their efforts and overtime work in relation to the organization of ESCAPE-21.

Let me take this opportunity to wish you all an exciting technical meeting and an unforgettable stay in Greece.

Thessaloniki, May 29, 2011

Professor Costas Kiparissides
Aristotle University of Thessaloniki

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The ESCAPE-21 organizers wish to express their sincere thanks to all the sponsors and supporting partner organizations.

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Badges

Please wear your badge at all time. Badges have been colour coded as follows:

Plenary and Keynote Speakers	Green
Oral and Poster Presenters	Blue
Symposium Organizers	Red

All participants are required to wear their identification badges when attending sessions and social events. If you lose your badge, please go to the Registration Desk where a new badge will be made for you.

Bank and Currency

An ATM/Cash machine can be found in the hotel's main lobby. For exchanging foreign currency and traveller cheques please contact the hotel's registration desk. However, it is possible to change money in Thessaloniki's Airport. There is usually a handling fee and commission.

Car Parking

Delegate car parking is available free of charge at the designated hotel partking areas.

Chairpersons and Speakers

Please ensure that you are available in your presentation room at least ten minutes before the start of the session. Speakers, please ensure that you have visited the Speaker Preview Room to confirm your audiovisual requirements at least two hours prior to the start of your session. The Speaker Preview Room is located near the ESCAPE-21 Registration Desk (opposite to the ERATO Room, on the Ground Floor of Meliton Hotel, see map of venue).

Credit Cards

Commonly accepted credit cards in hotels, restaurants and stores are Americal Express, Visa, Mastercard and Diners.

First Aid

A fully staffed first aid post will be open at all times during the Symposium. Please contact the hotel's reception desk for additional information.

Free Internet Services

The Symposium Organizers offer free internet connection to all participants and accompanying persons in the Speaker Preview Room (opposite to the ERATO Room, on the Ground Floor of Meliton Hotel, see map of venue). You can also find an internet connection in your room. Please contact the hotel's reception desk for more information.

Language

English is the official language of the Symposium. No translation will be provided.

Lost Property

Enquiries regarding items lost or found can be made at the ESCAPE-21 Registration Desk, which is located near the hotel's receprion desk on the Ground Froor of Meliton Hotel. To minimise losses, please ensure that your Symposium Bag is labelled.

Lunches and Refreshments

Coffee and tea will be served during the official refreshment breaks in the Lounge located near the Conference Rooms (TERPSIHORI, ERATO, THALIA, CHLOE). Lunches will be served in the Athos Restaurant.

Mobile Phones

As a countesy to speakers and other participants, all mobile phones and pages must be turned off before entering technical sessions.

Oral Presentations

The time of an oral presentation is strictly limited to 20 minutes (i.e., 17 min for presentation followed by a 3 minutes questions period). Strict timekeeping is essential to facilitate smooth running of the parallel sessions and of the Symposium in general. All presentations will be given in English.

Please provide a copy of you Power Point-Presentation to the personnel of ESCAPE-21 in the Speaker Preview Room (opposite to the ERATO Room, on the Ground Floor of Meliton Hotel, see map of venue) the day before your scheduled presentation. Speakers, please ensure that you are available in the session room at least ten minutes before the start of your session.

Please send to the Symposium Secretariat a brief CV (3-5 lines) to be handed to your Session Chairman for your paper introduction.

Posters

For each poster, there will be a 3 minutes oral presentation. For your oral presentation you are allowed to use strictly two slides. Strict timekeeping is essential to maintain smooth running of the session. Please provide a copy of you Power Point-Presentation to the personnel of ESCAPE-21 in the Speaker Preview Room (opposite to the ERATO Room, on the Ground Floor of Meliton Hotel, see map of venue) the day before your scheduled presentation.

Following the oral presentations, there will be an open poster/exhibition/discussion session running from 19:40 to 21:30 in the OLYMPIC HALL 3. All posters should be put up by early morning on May 30, 2011, on the designated poster stands (according to the paper ID number and its thematic area). All posters should be removed at 18:00 on May 31, 2011. Please note that the ESCAPE-21 Organization Committee will not be responsible for posters that are not removed at that time.

Registration

The ESCAPE-21 Registration Desk will be open at the following times:

Sunday 29 May	13:00 – 18:30
Monday 30 May	08:30 – 18:00
Tuesday 31 May	08:30 – 18:00
Wednesday 1 June	08:30 – 15:00

Security

Any security problems or concerns should be reported to a uniformed member of hotel staff.

Smoking Policy

Please note that smoking is not allowed in session halls and poster area.

Speaker Preview Room

The Speaker Preview Room is located in the lobby of Meliton hotel (opposite to the ERATO Room, on the Ground Floor of Meliton Hotel). The Speaker Preview Room will be open during the following hours:

Sunday 29 May	13:00 – 18:30
Monday 30 May	08:30 – 18:00
Tuesday 31 May	08:30 – 18:00
Wednesday 1 June	08:30 – 15:00

Special Diets

Please contact the ESCAPE-21 Symposium Secretariat for any special dietary requirement. If you have not notified the Secretariat in advance, please do so during your registration.

Tour Bookings

If you wish to participate in the planned tours and have not pre-booked, please contact the ESCAPE-21 personel at the Registration Desk. Bookings will be accepted on a first come, first served basis.

Taxis

Taxis can be hired by contacting the hotel's personnel or the ESCAPE-21 Secretariat.

Transport

The Symposium Organizers offer a bus transportation service free of charge to all participants and accompanying persons. Shuttle buses will depart from Makedonia Airport in Thessaloniki to Porto Carras Grand Resort and return. The trip takes approximately 90 min. For additional information, please look at the ESCAPE-21 website www.escape-21.gr

Symposium Theme

The **European Symposium on Computer Aided Process Engineering (ESCAPE)** series presents the latest innovations and achievements of leading professionals from the industrial and academic communities. The **ESCAPE** series serves as a forum for engineers, scientists, researchers, managers and students to present and discuss progress being made in the area of Computer Aided Process Engineering (**CAPE**).

European industries large and small are bringing innovations into our lives, whether in the form of new technologies to address environmental problems, new products to make our homes more comfortable and energy efficient or new therapies to improve the health and well-being of European citizens. Moreover, the European Industry needs to undertake research and technological initiatives in response to humanity's **"Grand Challenges"**, described in the declaration of Lund, namely, Global Warming, Tightening Supplies of Energy, Water and Food, Ageing Societies, Public Health, Pandemics and Security.

Thus, the Technical Theme of **ESCAPE 21** will be **"Process Systems Approaches for Addressing Grand Challenges in Energy, Environment, Health, Bioprocessing & Nanotechnologies"**.

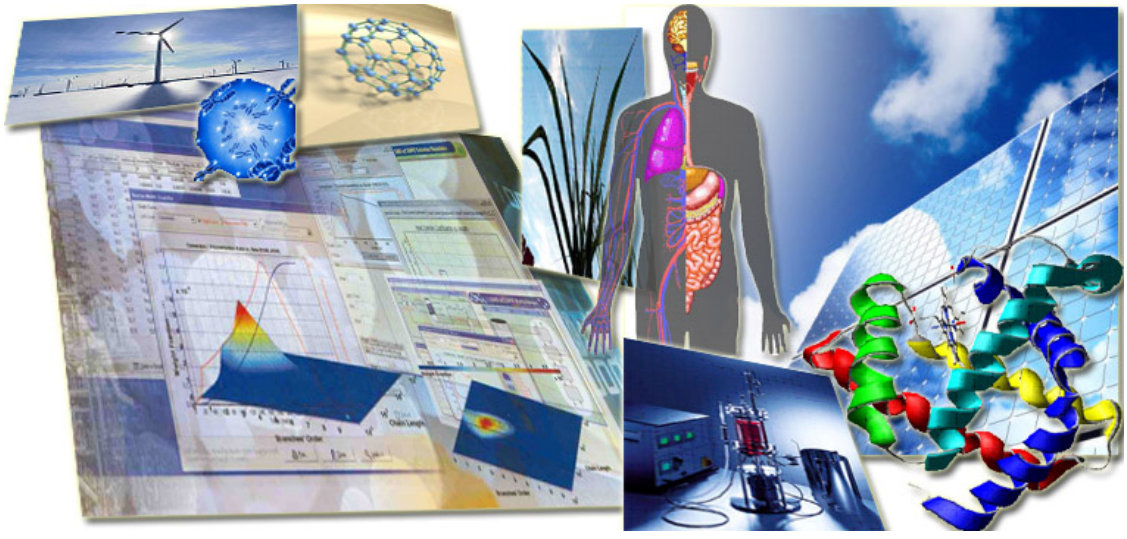
In particular, the Technical Programme of **ESCAPE 21** will cover the following process systems engineering topics and grand challenges:

Process Systems Engineering

- Multi-scale Modeling
- Synthesis and Design
- Optimization and Control
- Production Operations
- Training and Education

Grand Challenges

- Environmental Systems Engineering
- Bioprocess Systems Engineering
- Biomedical Systems Engineering
- Materials and Molecular Systems Engineering
- Energy Systems Engineering



Plenary Speakers

Professor Mike Doherty

University of California Santa Barbara, USA

"Multi-scale models for the design of crystalline solids"

Michael F. Doherty is Professor of Chemical Engineering and Department Chair at the University of California Santa Barbara. He received his B.Sc. in Chemical Engineering from Imperial College, University of London in 1973, and his Ph.D. in Chemical Engineering from Trinity College, University of Cambridge in 1977. His research interests include process systems engineering with particular emphasis on crystal engineering, and separation with chemical reaction. He is the holder of four patents, has published over 200 technical papers and given over 200 invited lectures. He has received numerous honors and awards for his teaching and research, including the Alpha Chi Sigma Award for Chemical Engineering Research (2004), and three divisional research awards from the AIChE. In 2008 he was named one of the "One Hundred Chemical Engineers of the Modern Era (post 1945) by the AIChE.

Dr. Conchita Jiménez-González

GlaxoSmithKline, USA

"Addressing key green engineering challenges - The role of process systems engineering"

Concepción Jiménez-González is Director and Team Leader of Operational Sustainability at the Sustainability and Environment department of GlaxoSmithKline, where she is responsible for the development and deployment of global strategy and programs to integrate Sustainability into the GSK operations and product development. She currently serves in the Governing Board of the American Chemical Society's Green Chemistry Institute (ACS GCI) and co-chairs the ACS GCI Pharmaceutical Roundtable. Conchita was also member of the US EPA's Board of Scientific Counselors, Technology for Sustainability Sub-Committee. In addition, she serves in the National Board of Directors of the Society of Hispanic Professional Engineers as National Vice-President. She holds a Ph.D. in Chemical Engineering from North Carolina State University; Raleigh NC; an M.S. in Environmental Engineering from ITESM; Monterrey, México and a B.S. in Chemical and Industrial Engineering at the Chihuahua Institute of Technology, México. Following the Spanish tradition, she is also known as Conchita.

Professor Ignacio Grossmann

Carnegie Mellon University, USA

"State-of-the-art and progress in discrete and continuous optimization for process systems engineering"

Professor Ignacio E. Grossmann is the R. R. Dean University Professor of Chemical Engineering at Carnegie Mellon University. He obtained his B.S. degree at the Universidad Iberoamericana, Mexico City, in 1974, and his M.S. and Ph.D. at Imperial College in 1975 and 1977, respectively. He is currently director of the "Center for Advanced Process Decision-making," an industrial consortium that involves 20 petroleum, chemical, engineering and software companies. He is a member of the National Academy of Engineering and his major awards include the 1994 Computing in Chemical Engineering Award of AIChE, the 1997 William H. Walker Award of AIChE, 2009 Warren Lewis Award of AIChE, Fellow of INFORMS and AIChE, Top 15 Most Cited Author in Computer Science by ISI, 2003 Computing Society Prize of INFORMS. He was also named "One of the Hundred Chemical Engineers of the Modern Era" by AIChE in 2008. His research interests are in the areas of process synthesis, energy integration, planning and scheduling of batch and continuous processes, supply chain optimization, stochastic programming, and mixed-integer and logic-based optimization. He has authored more than 300 papers, several monographs on design cases studies, and the textbook "Systematic Methods of Chemical Process Design."

Professor Zheng Li

Tsinghua University, China

"Perspectives on the energy system of China"

Zheng Li got his bachelor and master degrees from Department of Thermal Engineering, Tsinghua University in 1986 and 1988. He then worked for three years in the industry, before he returned to Tsinghua University and got his PhD in 1994. He became a faculty member of Department of Thermal Engineering at the end of 1994, a full professor in 2000, and Changjiang Scholar Professor in 2008. He is now the Dean of Department of Thermal Engineering. He founded Tsinghua BP Clean Energy Research and Education Center in 2003 and has been the director of the center ever since. Prof. Li was awarded the National Award of Science and Technology of China in 2006 for his contribution to the development of simulation technologies for circulating fluidized bed power plants. Besides technical studies, Prof. Li also works on energy strategy and policy study for China and leads several national and international research projects.

Professor Manfred Morari

ETH Zurich, Switzerland

"The role of theory in control practice"

Manfred Morari was appointed head of the Department of Information Technology and Electrical Engineering at ETH Zurich in 2009. He was head of the Automatic Control Laboratory from 1994 to 2008. Before that he was the McCollum-Corcoran Professor of Chemical Engineering and Executive Officer for Control and Dynamical Systems at the California Institute of Technology. He obtained the diploma from ETH Zurich and the Ph.D. from the University of Minnesota, both in chemical engineering. His interests are in hybrid systems and the control of biomedical systems. In recognition of his research contributions he received numerous awards, among them the Donald P. Eckman Award, the John R. Ragazzini Award and the Richard E. Bellman Control Heritage Award of the Automatic Control Council, the Allan P. Colburn Award and the Professional Progress Award of the AIChE, the Curtis W. McGraw Research Award of the ASEE, Doctor Honoris Causa from Babes-Bolyai University, Fellow of IEEE and IFAC, the IEEE Control Systems Field Award, and was elected to the National Academy of Engineering (U.S.). Manfred Morari has held appointments with Exxon and ICI plc and serves on the technical advisory boards of several major corporations.

Professor Achim Noack

Bayer CropScience, Germany

"Innovation at Bayer CropScience"

Achim Noack – Member of the Board of Management and designated Head of Industrial Operations & QHSE*. Achim Noack (50) was appointed to the company's Board of Management effective June 1, 2010. As of October 1, 2010, Noack has assumed responsibility for Industrial Operations & QHSE (Quality, Health, Safety and Environment) in succession to Dr. Wolfgang Welter, who retired in September 2010.Achim Noack was born in Hamburg on July 17, 1959. After studying chemical engineering at the University of Dortmund, he joined Bayer AG in 1986 as a process engineer with the former Crop Protection Business Group. After five years he transferred to Engineering in the Central Technology Division, moving after two years to Kansas City, Missouri, U.S.A., to serve as Project Manager for the Crop Protection Business Group. Noack returned to Germany in 1997 as Plant Manager for the Organic Chemicals Business Group in Krefeld-Uerdingen. Two years later he was placed in charge of engineering support for agrochemical active ingredients in Germany. In 2000 he was named Head of the Corporate Engineering Department and, shortly thereafter, Chief Technology Officer of Bayer Corporation, U.S.A., in Pittsburgh, Pennsylvania. After the establishment of Bayer Technology Services (BTS) in 2002, he headed the Bayer Technology Services Americas office. Noack was appointed the company's Managing Director in mid-2005. In this function Noack pursued a systematic growth strategy, continuing the development of the former Central Technology Division into a flexible, customer-focused service provider.

**QHSE = Quality, Health, Safety and Environment*

Professor George Stephanopoulos

Massachusetts Institute of Technology (MIT), USA

"Nanoscale process systems engineering: Design, fabrication, monitoring and control"

George was born in Kalamata, Greece, in 1947. He received his Diploma in Chemical Engineering from National Technical University of Athens in 1970, and his M.E. from McMaster University in 1971. During the period 1971-1974 he worked with Art Westerberg at the University of Florida on his PhD degree. He started his academic career in the University of Minnesota as Assistant Professor and soon he was promoted to Professor. In September of 1980 he took on a chaired professorship at his Greek alma matta and taught there until January 1984, when he joined the faculty at MIT; first as the J. R. Mares and then as the A. D. Little Professor of Chemical Engineering. After a two-year leave of absence (2000-02) from MIT as Chief Technology Officer and Managing Executive Officer of Mitsubishi Chemical Corporation (MCC), he returned to MIT and continued as Managing Director, Member of the Board of MCC until 2005. George's research interests and scientific developments have covered many aspects of Process Systems Engineering applied at various systems, such as: networks of chemical or biochemical reactions; integrated manufacturing systems within the scope of a national economy or corporate business; city traffic networks and intercity transportation networks and nanoscale processes (his current focus and love). With his scientific work he has been distinguished in the scientific community, he has been selected as one of the 100 Chemical Engineers of the Modern Era, he has been awarded by several Chemical Engineering Societies and Councils, he has been invited for honorary lectureships at several well known Universities and Congresses, while he has been a member of several editorial boards. George has authored/co-authored 7 books and co-edited 8. He has co-authored more than 210 papers. Over the years he has mentored more than 40 PhD students, with 16 of them in academic positions around the world.

Professor Venkat Venkatasubramanian

Purdue University, USA

"Process Systems Engineering in the Era of Watson: Challenges and Opportunities in Cyberinfrastructure and Informatics"

Professor Venkat Venkatasubramanian is Reilly Professor of Chemical Engineering at Purdue University. He earned his PhD in Chemical Engineering (with a Minor in Theoretical Physics) from Cornell University, M.S. in Physics from Vanderbilt University, and B. Tech. in Chemical Engineering from the University of Madras, India. Venkat worked as a Research Associate in Artificial Intelligence at Carnegie-Mellon University and taught at Columbia University before joining Purdue in 1988. His research contributions have been in the areas of process fault diagnosis and risk management complex engineered systems, pharmaceutical informatics, molecular products design, and complex adaptive systems. Prof. Venkatasubramanian has over 190 refereed publications, and delivered 130+ invited lectures and seminars, including 21 keynote/plenary lectures, at various international conferences and institutions all over the world. He has authored/co-authored a three-volume CACHE case study and two books, while he co-edited two more books. Thirty two doctoral and ten master students have graduated under Venkat's supervision or co-supervision, while he has offered his consultancy service to several major global corporations and institutions. Venkat has gained great recognition for his outstanding teaching record and research contribution both from the academia and the industry and has been honored with a number of awards for excellence in teaching and research (e.g., Norris Shreve Award for Outstanding Teaching in Chemical Engineering, special honor Purdue bestows for excellence in teaching, Team Research Excellence Award from the College of Engineering, Purdue University, nominated as “one of the fifty R&D stars in the United States whose achievements are shaping the future of our industrial culture and America's technology policy” etc.). Venkat’s other interests include comparative theology, classical music, and cricket.

The social programme planned for ESCAPE-21 is centered around the theme of spouse appreciation and aims to motivate the participation of all spouses and accompanying persons. Swimming, sunbathing, short excursions and other social activities will be available.

Welcome Reception

Sunday 29 May, 2011, 20:30 – 22:30

All registered participants and registered accompanying persons are invited to join the hosts of ESCAPE-21 Symposium in the Welcome Reception, taking place by the central swimming pool of Meliton Hotel. Wine, beer, soft drinks and canapés will be served under the tunes of a "live" instrumental band to complement the evening. Entry is by ticket only.

Poster Cocktail

Monday 30 May, 2011, 19:40 – 21:40

You are invited to enjoy our cocktail party during the evening poster exhibition session to take place in the Olympic Hall. Greek wines, beer, "ouzo", "tsipouro" and a variety of Greek cheeces will be served, kindly provided by our Symposium sponsors.

Symposium Gala Dinner

Tuesday 31 May, 2011, 20:15 – 24:00

All registered participants and registered accompanying persons are invited to join the hosts of ESCAPE-21 Symposium in the Symposium Gana Dinner, taking place by the central swimming pool of Meliton Hotel. The Symposium Gala will be held in true Greek style. The evening will begin with an "ouzo" drink reception. The dinner menu includes traditional Greek dishes and a barbecue. Different local wines will be served throughout the evening. A "live" music band and a "traditional Greek folk dancing group" will play and dance during the evening. It is hoped that everyone will join in the spirit of evening – listening, watching and taking part in both the music and dance. Entry is by ticket only.

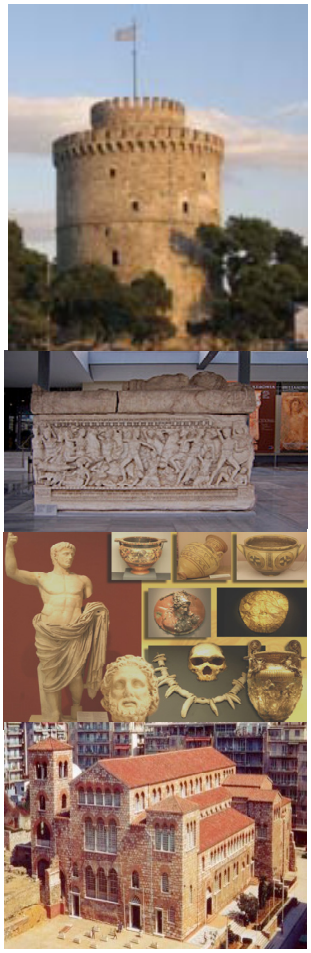
General Information

Accompanying persons will have a unique chance to meet with some very distinct elements of the cultural and religious heritage of Greece as well as the natural beauty of Thessaloniki and Chalkidiki peninsula through the following single-day excursions.

The excursions will be realised upon sufficient participation. Although advance booking for the excursions is highly recommended, accompanying persons who wish to participate, at the last minute, in any of the excursions, can check for availability at the ***ESCAPE-21 Registration Desk***.

The tour assembly point is the lobby of Meliton Hotel, Porto Carras Grand Resort. Please note that all tours will depart from the car park area, in front of Meliton Hotel, promptly according to the programme of each excursion.

➢ Tour 1: *Thessaloniki-City tour and Monuments* (Monday 30th of May)



A full-day coach tour to Thessaloniki, the city of Alexander the Great with a history of over 2300 years. En route the tour will pass through the uptown where you can see the Venetian castles and walls "securing" the city and traditional neighbourhoods still alive just few hundred meters away from the commercial city centre. Moving down town you can have a panoramic view of the city and Thermaikos bay, you will stop at the church of Saint Dimitrios, the patron of the City, and the church's undercroft, you will pass by the Galerius Arc, the church of Saint Sophia and you will enter the commercial area of the city. The next stop is at the Archaeological Museum of Thessaloniki, where the sculptures and all the museum collection allow a recursion over the history of Thessaloniki and Macedonia from prehistoric times to Late Antiquity. The tour ends at the area of the White Tower, the "landmark" of the city, where you can have free time for sightseeing and lunch at the roof garden of the Royal Theatre before departing back to Porto Carras Resort.

Tour time-schedule

09:15 - 11:15	Departure from Meliton hotel - Arrival at Thessaloniki
11:15 - 12:45	Sightseeing over the city monuments (uptown, Saint Dimitrios church, Galerius Arc, Saint Sophia church
12:45 - 14:10	Visit the Archaeological Museum of Thessaloniki
14:15 - 16:00	Tour in the area of White Tower, walking by the sea, lunch at the roof garden of the Royal Theatre of Thessaloniki.
16:00 - 17:45	Departure from Thessaloniki - Arrival at Porto Carras Meliton hotel

Price: 30€/person depending on participation, includes coach transfer will luxury bus and ticket for the Archaeological Museum and English guide during the tour.

➢ Tour 2: *The Holy Mount of Athos-the Cradle of Orthodoxy & Monasticism* (Tuesday 31st of May)

A full-day tour that combines a charming cruise in the deep blue sea of Chalkidiki and acquaintance with the "treasure" of the Christian Orthodox Monasticism. Mount Athos, being one of the most gorgeous districts of Greece, with a very varied magnificence of scenery, ranges along the third peninsula of Chalkidiki and it is home to over 20 Eastern Orthodox monasteries. During this tour you will have the chance to visit the coastal monasteries and to admire the mountainous landscape on the one hand and the sea on the other. The location of Mount Athos

ideally shapes the indispensable frame for the creation of a remote habitat within which its ascetic population chose to build their state and live. Being on board you will learn the history of this self-governed monastic state that has existed for over 1000 years according to the spirit and religion of the Byzantines. Upon your arrival at the port of Ouranoupolis you will pass from the spirit of monasticism back to the mundane life. The picturesque village of Ouranoupolis with its small fishing harbour, the golden beaches, the clear blue sea, the unspoiled natural beauty is the place where heritage and nature are in harmony. In Ouranoupolis you will have some free time to do independent sightseeing, to buy local hand-made products and have a lunch by the sea before heading back to Porto Carras Resort

Tour time-schedule

09:30-10:00	Departure from Meliton hotel - Arrival at Panagia bay and boarding on "Ioanna" boat.
10:00-14:00	Tour over the coastal monasteries (English guide on the boat)
14:00	Arrival at the port of Ouranoupolis village
14:00-16:00	Tour in the village - Lunch at a local tavern by the sea
16:00-17:30	Departure from the port of Ouranoupolis - Arrival at Panagia bay
18:00	Arrival at Porto Carras Meliton hotel by bus

Price: 60-70€/person depending on participation, includes coach transfer will luxury bus, cruise to Mount Athos and lunch by the sea in Ouranoupolis.

- **Tour 3:** ***Acquaintance with the Mountainous Chalkidiki*** **(Tuesday 31st of May)**

A full-day coach tour to Petralona Cave created 5 million years ago and bejewelled with stalagmites and stalactites, and to the adjacent Anthropological Museum, where thousands of fossils and other findings are deposited. The tour continues with a magnificent wooded route crossing the Holomontas Mount towards the Arnaia village, one of the most picturesque and historic mountainy villages of Chalkidiki, where you can meet the local culture and buy handmade products. There would be free time for shopping, further sightseeing and lunch before departing back to Porto Carras Resort.

Tour time-schedule

09:30 - 10:45	Departure from Meliton hotel - Arrival at Petralona Cave
10:45 - 12:15	Visit the Petralona Cave (English guide included) and museum
12:15 - 13:30	Departure from Petralona Cave - Arrival at Arnaia village
13:30 - 16:15	Tour in the village, visit churches, buy traditional handmade products (woven materials, honey, olive oil, etc.), lunch at local taverns
16:15 - 17:45	Departure from Arnaia village -Arrival at Porto Carras Meliton hotel

Price: 30€/person depending on participation, includes coach transfer will luxury bus and ticket for the Petralona Cave and museum.

SUNDAY, 29 May 2011

	OLYMPIC HALL	TERPSIHORI HALL	ERATO HALL	THALIA HALL	CHLOE HALL	MARINA I	MARINA II
12:30 – 16:30	*Lunch*			CAPE WP Mtg			
14:00 – 18:30	*Registration*						
20:30 – 22:30	*Welcome Reception*						

MONDAY, 30 May 2011

	OLYMPIC HALL	TERPSIHORI HALL	ERATO HALL	THALIA HALL	CHLOE HALL	MARINA I	MARINA II
08:30 – 09:00	Welcome & Opening Remarks						
09:00 – 09:40	Plenary *Achim Noack*						
09:40 – 10:30	Plenary *George Stephanopoulos*						
10:30 – 10:50	*Coffee Break*						
10:50 – 12:40				***Oral Presentations***			
		Synthesis/Design I	Optimization I		Molecular/Materials Systems Engineering I	Biomedical Systems Engineering I	Energy Systems Engineering I
12:40 – 14:20	*Lunch*						
				IEA Annex I Luncheon Mtg			
14:20 – 15:00	Plenary *Ignacio Grossmann*						
15:00 – 15:40	Plenary *Zheng Li*						
15:40 – 16:00	*Coffee Break*						
16:00 – 17:40		Process Operations I	Optimization II		Synthesis/Design II	Training and EURECHA	Multi-scale Modeling I
17:40 – 19:40				***Poster Presentations***			
		Poster Session 3 • *Process Operations* • *Multi-scale Modeling*	Poster Session 2 • *Optimization and Control*		Poster Session 1 • *Synthesis/Design* • *Molecular / Material System Engineering* • *Biomedical System Engineering*	Poster Session 4 • *Training and Education* • *Environmental Systems Engineering* • *Bioprocess Systems Engineering*	Poster Session 5 • *Energy Systems Engineering*
19:40 – 21:40	*Poster Session – with beer, wine, "ouzo" & snacks*						

TUESDAY, 31 May 2011

	OLYMPIC HALL	TERPSIHORI HALL	ERATO HALL	THALIA HALL	CHLOE HALL	MARINA I	MARINA II
08:30 – 09:10	Plenary *Conchita J. González*						
09:10 – 09:50	Plenary *Mike Doherty*						
09:50 – 10:20	ESCAPE22 & PSE2012 presentations						
10:20 – 10:50	*Coffee Break*						
10:50 – 12:30				***Oral Presentations***			
		Process Operations II	Control I		Synthesis/Design III	Multi-scale Modeling II	Energy Systems Engineering II
12:30 – 14:10	*Lunch*						
				Computers & Chem. Eng. Board Mtg & Luncheon			
14:10 – 15:50		Environmental System Engineering I	Control II		Molecular/Materials Systems Engineering II	Bioprocess Systems Engineering I	Energy Systems Engineering III
15:50 – 16:20	*Coffee Break*						
16:20 – 18:20		Environmental System Engineering II	Optimization III		Bioprocess Systems Engineering II	Biomedical Systems Engineering II	Energy Systems Engineering IV
20:15 – 24:00	*Symposium Gala Dinner*						

WEDNESDAY, 1 June 2011

	OLYMPIC HALL	TERPSIHORI HALL	ERATO HALL	THALIA HALL	CHLOE HALL	MARINA I	MARINA II
08:30 – 09:10	Plenary *Venkat Venkatasubramanian*						
09:10 – 09:50	Plenary *Manfred Morari*						
10:00 – 11:40				***Oral Presentations***			
		Process Operations III	Control III		Multi-scale Modeling III	Bioprocess Systems Engineering III	Energy Systems Engineering V
11:40 – 12:00	*Coffee Break*						
12:00 – 13:40		Process Operations IV	Optimization IV		Control IV	Synthesis/Design IV	Energy Systems Engineering VI
13:40 – 15:00	*Lunch*						
15:00	*End of the Conference*						

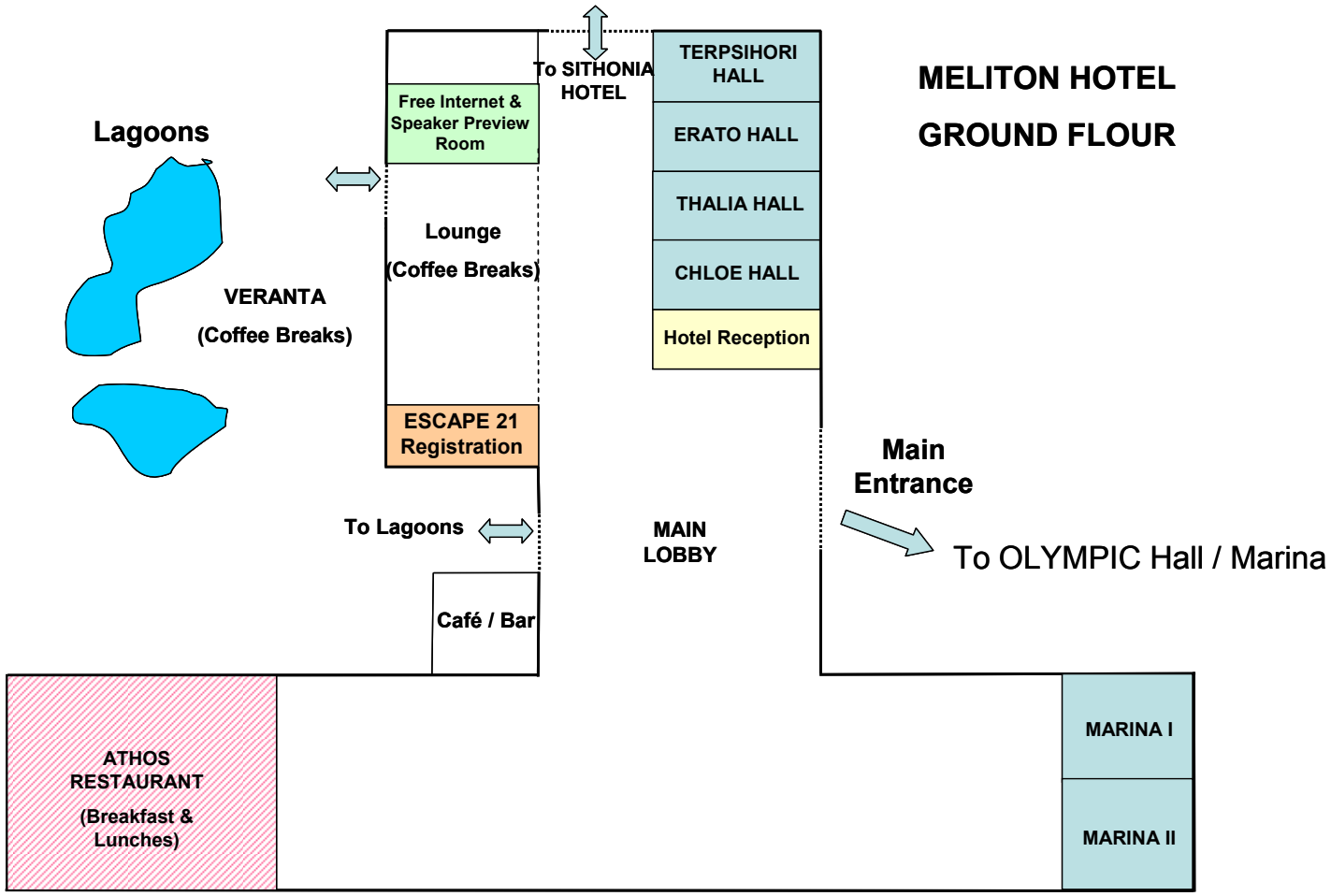
Map of Venue


Thessaloniki
Airport
Ancient Stagira
Olympiada
Stratoni
Arnea
Petralona (Cave)
Poligiros
Ierissos
Ouranoupoli
Olynthos
Ag. Nikolaos
Nikiti
Mount Athos
N. Kalikratia
Mount Olympus
N. Moudania
Sithonia
N. Potidea
N. Marmaras
Sarti
Porto Carras
Sykia
Kassandria
Hanioti
Kassandra


Olympic Hall
Meliton Hotel
Marina
Sithonia Hotel
Lagoons

Map of Venue

5	Golf and Country club
7	Tennis, Football, Volleyball
9	Casino
10	Perjali Restaurant
11	Children playground
13	Pefko Restaurant
15	Beach with umbrella
14	Athos Restaurant
16	Marina
17	Olympic Hall
18	Zefuros Restaurant
19	Port Captain Yacht Club
20	Boutique
21	Mini Market
22	Hotel Village Inn
23	Gina Bachauer Hall
24	Administrations Offers
25	Meltemi Bar
26	Apollo Theatre
27	Sailing Centre
28	Diving Centre



SUNDAY, 29 MAY 2011

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

14:00 – 18:30 Registration

20:30 – 22:30 Welcome 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 *Keynote Presentation*
Development of a synthesis tool for Gas-To-Liquid complexes
***Jan van Schijndel*[a], *Nort Thijssen*[a], *Govert Baak*[a], *Abhijeet Avhale*[a], *Jerome Ellepola*[a], *Johan Grievink*[b]**
[a] *Shell Global Solutions International BV, P.O.Box 38000, Amsterdam, 1030 BN, The Netherlands*
[b] *Delft 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 Siougkrou, 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 *Keynote Presentation* High-throughput methods for in silico discovery of peptides, proteins, and post-translational modifications in proteomics
*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 *Keynote Presentation* PSE in pharmaceutical process development
***Krist V. Gernaey**, Albert E. Cervera and John M. Woodley*
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 Nooraii[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 Perl[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 Presentation
Andreas A. 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

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 Presentation
Virginie Chambost, Behrang Mansoornejad, ***Paul Stuart***
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) – THALIA HALL

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

Chairs: Luis Puigjaner (UPC, Spain)
Michael Georgiadis (AUTh, 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 *(Tsinguha 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 Górak[a]
[a] *Laboratory of Fluid Separations, Department of Biochemical and Chemical Engineering, TU Dortmund University, Emil Figge Strasse70, 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 Long Distance Operator Training
Yiannis Bessiris[a], Dionyssia Kyriakopoulou[a], Fadi Ghajar[b], Curtis Steuckrath[b]
[a] *Hyperion Systems Engineering, 38 Strovolou Avenue, CY-2018 Nicosia, Cyprus*
[b] *Saudi Aramco, Saudi Arabia*

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 Austarlia, 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

1. 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*

2. Retrofit design of a pharmaceutical batch process considering green chemistry and engineering principles
A. Banimostafa, S. Papadokonstantakis, K. Hungerbühler
Swiss federal institute of technology (ETH), Zurich 8093, Switzerland

3. 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*

4. 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*

5. Spatiotemporal pattern formation in an electrochemical membrane reactor during deep CO removal from reformate 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*

6. 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

7. 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*

8. A novel process design for the hydroformylation of higher alkenes
M. Müller[a,c], V.A. Merchan[a,c], H. Arellano-Garcia[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*

9. 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. Kiil[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 Techonology 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 (F^3)" 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 Quimica, Universitat Rovira i Virgili, Av. Paisos Catalans, 26, 43007, Tarragona, Spain*
[c] *Departament d'Enginyeria Mecanica, 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, Hibarigaoka 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. Ghadrdan[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 CO_2
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 CO_2 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. Jardini[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. Pantelelis[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 Panoskaltsis[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 Panoskaltsi[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 Panoskaltsis[b], Athanasios Mantalaris[a], Michael C. Georgiadis[a], EfstratiosN. 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
Deparment 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 Mošať 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
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. Coccola[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. Garea, 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, aafety 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
[a] IBB – Instituto Superior Técnico/UTL, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal

[b] IDMEC – Instituto Superior Técnico/UTL, Av. Rovisco Pais, 1, 1049-001 Lisboa, Portugal
[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. Baltsas[b], C. Kiparissides[a,b]
[a] Department of Chemical Engineering, AUTH, Thessaloniki, 541 24, Greece
[b] Centre for Research and Technology Hellas,Therssaloniki, 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]
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[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]
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[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-Figueredo[a], O.R. Ayala[b], S. Aguilar[b], O. Aroche[b], A. Loukianov[b], A. Sánchez[b]
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[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]
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[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 C_4 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 Sílvio Lima, 3030-790, Coimbra, Portugal

42. Free radicals copolymerization optimization, system: acrylonitrile-vinyl acetate in CSTR
S.V. Vallecillo-Gómez, J.C. Tapia-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
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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*
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[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 Politecnica 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 Elzakker[a], E. Zondervan[a], C. Almeida-Rivera[b], I.E. Grossmann[c], P.M.M. Bongers[b,d]
[a] *Dep. Chem. And Chem. Eng., Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, the Netherlands*
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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*
[c] *Unilever R&D Vlaardingen, the Netherlands*

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. 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

13. 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*

14. 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]
[a] *Technological Ecudational Institute of Larissa, Department of Project Management, 41110 Larissa, Greece*
[b] *Center for Research & Technology Hellas (CERTH), Chemical Process Industry Research Institute (CPERI), Laboratory of Environmental Fuels and Hydrocarbons (LEFH), 6th klm Harilaou-Thermi Rd, Thermi, Thessaloniki 57001,Greece*
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[e] *Texas A&M University, Department of Chemical Engineering, College Station, TX 77843-3122, USA*

15. 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*

16. 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

17. Simulation-based reactive scheduling in tomato processing plant with raw material uncertainty
A. Koulouris, I. Kotelida
Alexandrion Technological Educational Institute of Thessaloniki, 57400 Sindos, Greece

18. 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

19. 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

20. 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

21. 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

22. 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. Hangos[d], I.T. Cameron[a]
[a] School of Chemical Engineering, The University of Queensland, Brisbane, Australia 4072
[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

23. 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

24. 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

25. 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

26. Simulation-based dynamic optimization under uncertainty of a industrial biological process
Guillermo A. Durand[a], Aníbal 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) Bahia Blanca, Argentina
[b]Depto. Ingeniería de Procesos, Universidad Nacional de Tucumán, Av. Independencia 1800, (4002) San Miguel de Tucumán, Argentina

27. 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

28. Detailed mathematical modelling of Liquid-Liquid extraction columns
M. Jaradat[a,c], M. Attarakih[b,c], H.J. Bart[a,c]
[a] Chair of Separation Science and Technology, TU Kaiserslautern, POB 3049, 67653 Kaiserslautern, Germany
[b] Faculty of Eng. Tech., Chem. Eng. Dept., Al-Balqa Applied University, POB 15008, 11134 Amman, Jordan
[c] Centre of Mathematical and Computational Modelling, TU Kaiserslautern, Germany

29. 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

30. Application of computer-aided multi-scale modelling framework – Aerosol case study
M. Heitzig[a], C. Gregson[b], G. Sin[a], R. Gani[a]
[a] CAPEC, Department of Chemical & Biochemical Engineering, Technical University of Denmark, Søltofts Plads, Bld. 227, 2800 Kgs. Lyngby, Denmark
[b] Firmenich Inc., 250 Plainsboro Road, Plainsboro, NJ, 08536, USA

31. 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*

32. 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*

33. 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

34. 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*

35. 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*

36. 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*

37. 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

38. 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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39. 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*
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[c] *Department of Chemical Engineering, University College London, London,UK*
[d] *Department of Chemical Engineering, College of Engineering and Petroleum, Kuwait University, Kuwait*

40. 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

41. 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*

42. 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

43. 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*

44. General-purpose graphics processing units application for diffusion simulation using cellular automata
A.Kolnoochenko, P. Gurikov, N. Menshutina
CAPE Department, MUCTR, Moscow, Russia

45. 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

46. 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

47. 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

48. 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. 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

2. 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

3. 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

4. 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*

5. 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

6. Multilevel strategies for the retrofit of a large industrial water system
H. Tokos[a], Z.N. Pintarič[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

7. 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]
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[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

8. 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

9. 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

10. 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
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11. 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

12. 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]
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13. Sustainability in chemical processes: Application of different environmental methodologies to evaluate process alternatives
A.N. Mendes[a], A. Carvalho[b], H.A. Matos[a]
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14. Design and simulation of eco-efficient biodiesel manufacture
S. Couto[1], T.M. Mata[1,a], A.A. Martins[1,b], B. Moura[1], J. Magalhães[1], N.S. Caetano[2,a]
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15. 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

16. 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]
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17. 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

18. 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

19. Multi-objective optimization of integrated bioethanol-sugar supply chains considering different LCA metrics simultaneously
A. Kostin[a], F.D. Mele[b], G. Guillén-Gozálbez[a]
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20. 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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21. 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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22. 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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Bioprocess Systems Engineering

23. Dynamic modelling of the margarine production process
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24. 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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25. 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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26. 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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[d] *Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK*

27. Optimizing cyanobacteria metabolic network for ethanol production
Cecilia Paulo[a], Jimena Di Maggio[a], Vanina Estrada[a,c], M. Soledad Diaz[a,b]
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28. Techno-economic analysis under uncertainty for early stage design of the forest biorefinery
Eemeli Hytönen, Paul Stuart

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29. BIOCORE– A systems integration paradigm in the real-life development of a lignocellulosic biorefinery
Aikaterini D. Mountraki[α], Athanassios Nikolakopoulos[α], Bouchra Benjelloun Mlayah[b], Antonis C. Kokossis[α]
[α] *School of Chemical Engineering, National Technical University of Athens, Greece*
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30. 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

31. 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 Morais[a], Igor R. S. Victorino[a], Eduardo C. Vasco de Toledo[b], Maria Regina Wolf Maciel[a], Rubens Maciel Filho[a]
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[b] *Petrobras SA, Paulínia Refinery (REPLAN), Paulínia, São Paulo, Brazil*

32. 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]
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[b] *Chemical Process Engineering Research Institute, Centre for Research and Technology Hellas, P.O. Box 60361, 57001, Thermi, Thessaloniki, Greece*

33. 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

34. Bioprocessing of exopolysaccharides (EPS): CFD characterization of bioreactor conditions
Serafim Vlaev[a], Konstantza Tonova[a], Kostantsa Pavlova[b], Mohammed Elqotbi[c]
[a] *Insitute 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*

35. 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

36. Glycerol metabolic conversion to succinic acid uing Actinobacillus succinogenes: A metabolic network-based analysis
Michael Binns[a], Anestis Vlysidis[a], Colin Webb[a], Constantinos Theodoropoulos[a], Pedro de Atauri[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*

37. Desing and operation of a continuos reactor for acid pretreatment of lignocellulosic biomass
Mauricio Sales-Cruz[a], Edgar Ramírez-Jiménez[b], Teresa López-Arenas[a]
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38. 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*
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39. Simulations of hydrodynamical stress in stirred-tank bioreactors using CFD technology
Y. Verkholaz[a], P. Lavrov[a], E. Guseva[a], N. Menshutina[a], J. Boudrant[b]
[a] *Mendeleyev University of Chemical Technology of Russia High Technology Department Building 9, Miusskaya square, 125047, Moscow, Russian Federation*
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40. System inversion of multidimensional population balance systems
Henrique Menarin[a] and Naim Bajcinca[a,b]

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[b] Technische Universit¨ at Berlin, Einsteinufer 17, 10857 Berlin, Germany

41. 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. Kokossis[a]
[a] School of Chemical Engineering, National Technical University of Athens, Greece
[b] Faculty of Engineering and Physical Sciences, University of Surrey, UK

42. 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.

43. Evaluating Bioprocess Technologies under Uncertainty
Charles Siletti[a], Demetri Petrides[b]
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44. Kinetic modelling of cytosolic glucose metabolism
Ning Chen[a,b], Karen Polizzi[c], Cleo Kontoravdi[a,b]
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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
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[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]
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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]
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[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]
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[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]
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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]
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12. Modeling post-combustion CO_2 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*
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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*
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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]
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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]
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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]
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22. Site-wide process integration for low grade heat recovery
Ankur Kapil[a], Igor Bulatov[a], Robin Smith[a], Jin-Kuk Kim[b]
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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]
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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*
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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]
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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]
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[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 Krajnik[b], Petar Sabev Varbanov[a], Jiří Jaromír Klemeš[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]
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34. The role of energy consumption in batch process scheduling and optimization
Mate Hegyhati, Ferenc Friedler
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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
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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 Aníbal 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. 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 – 21:40 Poster Session – with beer, wine, "ouzo" & snacks

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

Chairs: David Bogle (UCL, UK)
Antonis 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] *Frauenhofer 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 electrodialysis 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 Bommareddy[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 Wisconcin, 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 Neherlands*

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 Presentation
Petr Stehlík
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], Jirí 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, Jirí J. Klemeš, Petar S. Varbanov
Centre for Process Integration and Intesification - CPI$_2$, Research Institute of Chemical and Process Engineering, Faculty of Information Technology, University of Pannonia, Egyetem utca 10, 8200 Veszprém, Hungary

12:30 – 14:10 Lunch

12:30 – 14:10 Computers & Chemical Engineering Board Mtg & Luncheon (by invitation only) – THALIA HALL

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 biorestoration 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 Rodriguez Reartes[a,c], M. Soledad Diaz[a,c]
[a] *Planta Piloto de Ingenieria Química PLAPIQUI (UNS-CONICET)*
[b] *Department of Biology, Biochemistry and Pharmacy, Universidad Nacional del Su*
[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 CO_2 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 CO_2 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 Plantewide control design of a postcombustion CO_2 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 Chemial 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 CO_2 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 – 18:20 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 CO_2 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-Horsel[b] , Udo Reichl[a,b], Achim Kienle[a,b]
[a] Otto-von-Guericke-Universitat Magdeburg, Universitatsplatz 2, D-39106 Magdeburg, Germany
[b] Max-Planck-Institut fur Dynamik komplexer technischer Systeme, Sandtorstrase 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 Ciencies Mediques Basiques, 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. Cecelja[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 Engineeering, 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 andd 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

20:15 – 24:00 Symposium Gala 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. Fragkopoulos, C. Theodoropoulos
School of Chemical Engineering and Analytical Science, Univerisity of Manchester, Sackville Street, Manchester M13 9PL, UK

10:40 – 11:00 Multiscale modeling of a silicon solar wafer manufacturing process
Ruochen Liu, German Oliveros, Seetharaman Sridhar[a], B. Erik Ydstie
Dept. of Chemical ([a] Material Science and) 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 Labora tory, 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, Søltofts 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 Ingenieria 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 Diehl[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, Søltofts 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 Prívara[a], Jirí 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[b], Ana Paula Barbosa-Póvoa[b]
[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 Wisconcin, 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. Aníbal 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 Asprion[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 Metalurgica, 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 Engergy 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 Prívara[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 Zrich, 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

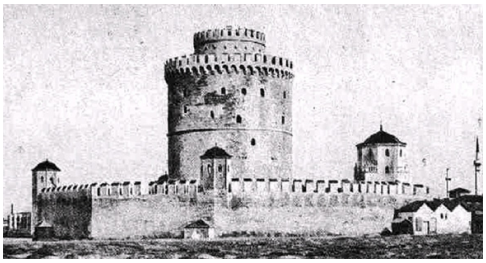
13:00 – 13:20 Application of Graphic Processing Unit (GPU) in model predictive control
Arash Sadrieh, Parisa A. Bahri
School of Engineering and Energy, Murdoch University, Western Australia, 6150

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

The White Tower *(Nikis Avenue, Thessaloniki, Tel: +30 2310 267 832)*



The White Tower once stood with many others, surrounding the medieval city, until the Ottoman Turks destroyed all but two in 1866. Constructed in the 15th century this tower served as a defensive bulwark, an infamous prison, a place of execution, and now is home to a wonderful collection of sculptures, frescoes, and other interesting artefacts from 300 to 1400 AD portraying the amazing history and culture of the city. The White Tower, once known as the Bloody Tower, has become the city's most famous landmark.

Archeological Museum of Thessaloniki *(Hanth Square 6, M. Andronikou Street, Thessaloniki Tel: +30 2310 830 538)*

With a wonderful collection of artifacts from Neolithic times and amazing sculptures from the Archaic to the Late Roman period, this museum is a house of treasures. There are many thematic units that are very significant, and which provide a thorough and unforgettable exhibition of the history of Thessaloniki and the surrounding areas.

Aghia Sofia *(Pavlou Mela Street, Aghia Sofia Square, Thessaloniki Tel: +30 3 1270 253)*

Built in the 8th century, Aghia Sofia is a beautiful Christian church modeled on the magnificent church of Aghia Sofia in Istanbul. The church contains superb mosaics and wall paintings including a wonderful mosaic of The Ascension.

Byzantine Museum *(2 Stratou Avenue, Thessaloniki Tel: +30 2310 868 570)*

Containing the finest collection of Byzantine art in Greece, this museum focuses on preserving, researching, and studying the remains of the Byzantine civilization. The treasures housed in this fine museum include priceless icons, frescoes, sculpted reliefs, mosaics, jewellery, manuscripts, and pottery.

Rotonda *(Dimitriou Gounari Street, Thessaloniki Tel: +30 2310 213 627)*

This monument was built in 306 AD as the mausoleum of the Roman Emperor Galerius. Later the Rotonda became a church dedicated to St. George and wonderful 4th century mosaics were added. After serving as a mosque for the Ottomans, the Rotonda now houses Christian art and occasionally holds art exhibitions and concerts.

Aghios Dimitrios *(Aghiou Dimitriou and Aghiou Nikolaou at Egnatias Street, Thessaloniki Tel: +30 2310 221 3627)*

After the great fire of 1918 the church was restored with the aim of preserving the details of the original. Originally the church was built on the ruins of a Roman bath. Beneath the church is the crypt of the martyr Aghios Demetrios containing sculpture from the 3rd to 5th centuries and Byzantine artifacts.

The City Walls

The City Walls were erected during the time of Theodossios the Great to guard the city from Democracy Square of nowadays across Eptapyrgio up to the site later occupied by the White Tower, a work of the architect Sinan (first half of 16th century).

Modiano Market *Ermou, Thessaloniki*

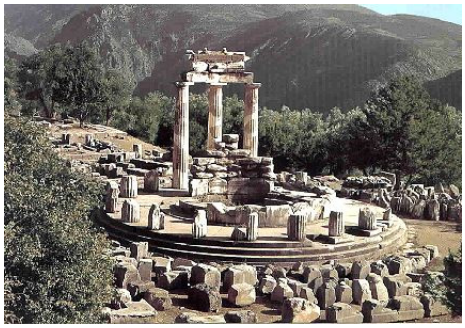
Here, one can not only shop, but eat, drink, listen to the music provided by gypsy musicians and enjoy the culture and diverse crowd visiting the open-air market.

Archaeological Site of Aigai (modern name Vergina): The city of Aigai, the ancient first capital of the Kingdom of Macedonia, was discovered in the 19th century near Vergina, in northern Greece. The most important remains are the monumental palace, lavishly decorated with mosaics and painted stuccoes, and the burial ground with more than 300 tumuli, some of which date from the 11th century B.C. One of the royal tombs in the Great Tumulus is identified as that of Philip II, who conquered all the Greek cities, paving the way for his son Alexander and the expansion of the Hellenistic world.

Dion: Ancient Dion was an important religious center for worshipping the Gods of nearby Mount Olympus. This is where Phillip II came to celebrate his victories and his son Alexander came to make his sacrifices here before going off to conquer the East. While most of the statues which were not only found virtually intact, but with traces of color, are in the nearby museum in the town of Dion, they have been replaced with copies. The Sanctuary of Isis is perhaps the most interesting discovery so far. An earthquake had displaced water and mud and the building was hidden for centuries under 6 feet of water which protected it from vandals. The temple still sits in the water and a copy of the statue of Aphrodite can be seen there.

Meteora: Meteora is from the biggest and most important group of monasteries in Greece after those in Mount Athos. We can locate the first traces of their history from 11th c. when the first hermits settled there. The rock monasteries have been characterized by Unesco as a unique phenomenon of cultural heritage and they form one of the most important stations of cultural map of Greece.

Delphi: At the foot of Mount Parnassos, within the angle formed by the twin rocks of the Phaedriades, lies the Pan-Hellenic sanctuary of Delphi, which had the most famous oracle of ancient Greece. Delphi was regarded as the centre of the world. According to mythology, it is here that the two eagles sent out by Zeus from the ends of the universe to find the navel of the world met. The sanctuary of Delphi, set within a most spectacular landscape, was for many centuries the cultural and religious centre and symbol of unity for the Hellenic world.



And if all this seems like a little too much culture you can always just travel to the Greek Islands…

http://www.gtp.gr

http://www.greekferries.gr/domestic.htm

ESCAPE-21

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