

BUROPEAN SYMPOSIUM ON COMPUTER-AIDED PROCESS ENGINEERING

GREEN AND SUSTAINABLE PROCESS SYSTEMS ENGINEERING IN THE DIGITAL AGE

ATHENS - GREECE Royal Olympic Hotel

18-21 JUNE 2023

Final Program

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thematic areas

GREEN AND SUSTAINABLE PROCESS SYSTEMS ENGINEERING IN THE DIGITAL AGE

1 Modelling and optimization for multi-scale integration

- Synthesis, design and optimization methods and algorithms
- Digital twins and data-enabled modelling
- Data engineering in multi-scale integration and decision support

2 Control, scheduling, and operability at the process and enterprise-level

- Advances in scheduling, planning, and supply chain optimization
- Integration of process control with data and network structures
- Decision making for security and resiliency
- Smart operations and knowledge extraction using machine learning and AI

3 Safe and sustainable products by design

- Molecular and materials systems engineering
- Process intensification and additive manufacturing
- Smart and agile manufacturing for the future

4 Green and sustainable processes for the circular economy

- Technology and process integration for circular economy ecosystems
- Integrated biorefineries using thermal and biochemical processes
- Use of waste as a feedstock: modelling and process development applications

5 Systems methods in industrial biotechnology and biomedical applications

- Tools and methods to expand the industrial exploitation of microbial biodiversity
- Simultaneous integration of strain and process design
- Digital twins and embedded models for autonomous bioprocesses
- Novel PAT instruments and biosensors for in-process monitoring

6 Multi-scale energy systems engineering (organized by the EFCE energy section)

- Energy efficiency and renewable energy integration
- Energy management and process system engineering in energy applications
- CO2 capture, usage and sequestration
- Mitigating Global Warming impact of industrial processes
- Water–Energy-Waste nexus, energy storage, power to renewable fuels and hydrogen

7 Sustainable supply chains and ecosystems

- Systems paradigms for eco-efficiency and intelligence in supply chains
- Social engagement and incentivization: methods and tools
- Urban systems engineering and social network models
- Life Cycle Analysis in the Digital Age

8 Education and knowledge transfer

- Interactive environments, pen science and education
- Best practices in design education
- Promoting systems thinking in engineering curricula

introduction

Dear Colleagues and Friends,

Welcome to the 33rd European Symposium on Computer-Aided Process Engineering (ESCAPE-33) that takes place in Athens from Sunday, June 18th to Wednesday, June 21st, 2023. The ESCAPE-33 event is organized under the auspices of the European Federation of Chemical Engineering (EFCE Event No. 776), the CAPE Working Party (CAPE-WP), the Technical Chamber of Greece, the Pan Hellenic Association of Chemical Engineers, and the National Technical University of Athens.

ESCAPE-33 addresses emerging and significant challenges in **Process Systems Engineering as our field is a driver to rebuild industry with a systemic and holistic approach**. Contributions relate to the sustainable development of chemical processes, the development and the systematic evaluation of processing technologies and process innovations, and research promoting **circular economy** paradigms including social aspects and social engagement networks to incentivize and involve citizens. The conference recognizes the exceptional importance of **industrial biotechnology** as a driver and enabler for new chemistries, alongside **Artificial Intelligence** and data engineering as a technological challenge with an apparent impact on many systems technologies. Overall, ESCAPE 33 covers up-to-date topics in Process Systems Engineering and has attracted a significant and diversified number of people from academia, research institutions, and industrial organizations worldwide. Conference themes include modelling and optimization for multi-scale integration; control, scheduling, and operability at the process and enterprise-level; safe and sustainable products by design; green and sustainable processes for the **circular economy**; systems methods in **industrial biotechnology** and biomedical applications; multi-scale energy systems engineering (organized by the EFCE energy section); sustainable supply chains and ecosystems; and education and knowledge transfer.

The conference has attracted over 800 abstracts. The review process involved reviews of abstracts, reviews of manuscripts and, thanks to generous and persistent assistance from as many as 185 reviewers, converged to a final selection of 620 oral and poster presentations from 57 countries (possibly the largest cohort of presenters at an ESCAPE series conference). The scientific program is rounded up by 6 plenary speakers, 19 invited speakers, as well as 4 hands-on workshops that are freely available to all conference attendants. These workshops address process simulation, AI methods and applications, advanced optimization tools and machine learning, as well as the development of new courses and curricular. The conference further hosts a professional career event (jointly with IChemE) and a networking event with a purpose to connect PSE with the SusChem community in Europe (jointly organized with the Sustainable and Safe by Design community coordinated by IRISS).

The conference honors the late Professor Chris Floudas with a special session that attributes credit to his legacy, contributions, and the unremitting impact of his work on the community. ESCAPE holds a separate session in the memory of late Prof Jiri Klemes, a former CAPE WP Chair and a commanding figure in process and energy integration. Further to that, the conference recollects and honors our early pioneers in process simulation with a special event (Chess on CHESS) to credit the contribution of late Prof Rudy Motard and the CHESS simulator in process flowsheeting. As a highlight of the conference, ESCAPE '33 is proud to announce the George Stephanopoulos Award in Process Systems Engineering, a new and generous award that is co-sponsored by the National Technical University of Athens, the EFCE-CAPE Working Party, and the AIChE-CAST Division. The award, expected to start from next year, will select winners between European and North American nominees in alternate years. The award will be announced by the President of EFCE at the Welcome Reception on Sunday 18th June.

ESCAPE '33 is coordinated with guided visits to major archeological sites and museums, cultural events in Athens, including options to attend theatrical performances, and guided tours of the monuments that marked the contemporary face of Old Athens.

We're looking forward to welcoming you in Athens and we wish you an exciting and enjoyable time at this historical and beautiful city.

Antonis Kokossis Professor, National Technical University of Athens School of Chemical Engineering, Greece Michael C. Georgiadis, Professor, Aristotle University of Thessaloniki School of Engineering, Greece Stratos Pistikopoulos Professor, Texas A&M Energy Institute School of Chemical Engineering Director, USA

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LOCAL ORGANIZING COMMITTEE

CHAIR BOARD

Antonis Kokossis (Chair) National Technical University of Athens

Michael Georgiadis (Co-chair) Aristotle University of Thessaloniki

Ioannis Kookos (Co-chair) University of Patras

Konstantina Kosmidou (Treasurer) National Technical University of Athens

Polyxeni Lazaropoulou (Secretary) National Technical University of Athens

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Kostas Pyrgakis National Technical University of Athens

Melina Psycha National Technical University of Athens

Theodoros Damartzis Aristotle University of Thessaloniki

Nikolaos A. Diangelakis Technical University of Crete

Athanasios Papadopoulos Centre for Research & Technology Hellas (CERTH)

Effie Marcoulaki National Centre for Scientific Research 'Demokritos'

Chrysoula Kappatou Imperial College London

INTERNATIONAL SCIENTIFIC COMMITTEE

Representatives of the CAPE / PSE and related scientific and technical communities from all around the world have been invited to join the International Scientific Committee. The list of ISC members includes core members, topic coordinators and reviewers: Antonis Kokossis

Professor, National Technical University of Athens School of Chemical Engineering, Greece

Michael C. Georgiadis Professor, Aristotle University of Thessaloniki School of Engineering, Greece

Stratos Pistikopoulos Professor, Texas A&M Energy Institute School of Chemical Engineering Director, USA



INTERNATIONAL SCIENTIFIC COMMITTEE MEMBERS EUROPE

- Cristhian P. Almeida-Rivera
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- Victor M. Zavala
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• Dominic C. Y. Foo

• Iftekhar A Karimi

- Ali Elkamel
- Paul Stuart

INTERNATIONAL SCIENTIFIC COMMITTEE MEMBERS ASIA

INTERNATIONAL SCIENTIFIC COMMITTEE MEMBERS AFRICA

plenary speakers





PLENARY SESSION 1

Gregory Stephanopoulos, MIT

How can PSE concepts and methods help accelerate progress in biotechnology

Sunday June 18th, 2023
 17:30-18:30
 Olympia Hall



PLENARY SESSION 3

Larry Biegler, Carnegie Mellon University

Strategies and Tools for Optimization-Driven Modeling: A New Era for CAPE Tuesday June 20th, 2023 Op:00-10:00 Olympia Hall



PLENARY SESSION 2

Fengqi You, Cornell University

Tying Deep Learning to Process Systems Engineering for Sustainable Materials, Energy Systems, and Climate Change Mitigation

i Monday, June 19th, 2023
 ③ 09:00-10:00
 ② Olympia Hall



PLENARY SESSION 4

Venkat Venkatasubramian, Columbia University

Quo Vadis ChatGPT? Challenges and Opportunities in Process Systems Engineering

Wednesday, June 21st, 2023
 09:00-10:00
 Olympia Hall



PLENARY SESSION 5

Tony Kiss, Delft University

Turning ideas into innovations in CAPE
Wednesday, June 21st, 2023
13:30-14:00
Olympia Hall



PLENARY SESSION 6

David Bogle, University College London

Stretching Process Systems Engineering
Wednesday, June 21st, 2023
14:00-14:30
Olympia Hall

invited speakers



Claire Adjiman Imperial College London UK



Antonio Del Rio Chanona Imperial College London, UK



Marianthi lerapetritou Bob and Jane Gore Centennial Chair, University of Delaware, USA



Christos Maravelias Anderson Family Professor in Energy and the Environment, Princeton University, USA



Maria M. Papathanasiou Imperial College London UK



Bhavik Bakshi William G Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, USA



Sebastian Engell Head of Process Dynamics and Operations GroupTU Dortmund, Germany



Georgios Kontogeorgis Professor, Technical University of Denmark



Francois Marechal EPFL, Switzerland



Constantinos Theodoropoulos Professor, University of Manchester, UK



Fabrizio Bezzo Professor, University of Padova, Italy



Chrysanthos Gounaris Carnegie Mellon University, USA



Carl Laird Professor, Department of Chemical Engineering, Carnegie Mellon University, USA



Ruth Misener Imperial College UK



Petar Varbanov Head of SPIL – Sustainable Process Integration Laboratory, NETME Centre



Marc-Olivier Coppens Ramsay Memorial Professor in Chemical Engineering, University College London, UK



Vassily Hatzimanikatis EPFL, Switzerland



Costas Maranas Pennsylvania State University USA



Michael O'Donohue Senior Research ManagerInrae



general information

Conference Venue

ROYAL OLYMPIC HOTEL, 28-34 Athanasiou Diakou Str., 117 43, Athens, Greece Website: www.royalolympic.com

Registration Secretariat Operating Hours

The Registration Secretariat will be situated at the Conference Venue and will be operating according to the following schedule:

Sunday 18/6/2023	→	14:00 - 19:30
Monday 19/6/2023	→	08:00 - 18:30
Tuesday 20/6/2023	→	08:00 - 18:30
Wednesday 21/6/2023	→	08:00 - 15:30

Coffee Breaks & Light Lunches

Coffee Breaks & Light Lunches will be offered to all registered participants, according to the time schedule announced in the Scientific Program.

Conference Badges

It is essential that all participants wear their personal badge at all times in the Conference area, as it is the official entrance pass to scientific sessions. The badge is mandatory also for the Welcome Cocktail to be held on Sunday June 19th following the Welcome Speeches and the Opening Plenary Session of the Conference.

Certificates of Attendance

A Certificate of Attendance will be sent to all registered participants after the Conference via email.

Scientific presentations and PC reception

The Symposium Hall offer full audio-visual equipment. A PC Reception desk will be available at the Symposium area. All presentations should be clearly labeled with the author's name and session's title. All speakers are kindly requested to deliver their presentations at least 2 hours prior to the session they participate.

Posters

Posters will be presented on poster panels according to the information that has been sent to the presented authors. A list of the poster board numbers will be also displayed at the entrance of each POSTER hall.

Internet Access

Wifi will be available in all Conference areas. Network: escape33

Overflow

The ESCAPE 33 will hold its plenary meetings in **Olymplia Hall** and will use the **Halls Attica** & **Templar** as overflow rooms to accommodate all participants who cannot be accommodated in the plenary room.

Social Activities

Welcome Reception:

- June 19th, at 18.30 20.30 hrs.
- The Welcome Reception will be held at the Roof Garden of the Royal Olympic Hotel.

Gala Dinner:

- June 20th, at 19.30 23.30 hrs.
- The Gala Dinner will be held at Zappeion Mansion.
- Cost per person: € 80 (limited seats available)

ATH.ENACARD

The Organizers offer to all Registered Participants a free 5-day ticket which is valid for all Athens Urban Transport Organizations means: buses, trolley-buses, trams & metro lines.

This ticket type is not valid for Airport EXPRESS bus line, and metro line for the route part Koropi-Airport.

Insurance & Liability

The Organizers accept no liability for any personal injury, loss or damage of property or additional expenses incurred to conference participants either during the conference or as result of delays, strikes or any other circumstances. Participants are requested to make their own arrangements with respect to health and travel insurance.

Congress Secretariat and Travel Agency



TITITI

17, Asklipiou Str., 106 80 Athens – Greece Tel.: +30 210 3634 944 E-mail: info@era.gr Website: www.era.gr

venue floor plan

Exhibititors



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program at-a-glance

SUNDAY, JUNE 18, 2023

09:30-16:30	Attica Hall CAPE WORKING PARTY				
10:00-16:00	Conf. Room I PROCESS SIMULATION WORKSHOP	Conf. Room II MACHINE LEARNING WORKSHOP	Conf. Room III HANDS-ON WITH OMLT: THE OPTIMIZATION AND MACHINE LEARNING TOOLKIT WORKSHOP		
16:00-17:00					
12:30-17:15	Templar Hall CHESS ON CHESS ESCAPE 33 pays tribute to our pioneers in process simulation. CHESS: Chemical Engineering Simulation Systems				
14:00-17:30	REGISTRATIONS				
17:15-17:30	Olympia Hall WELCOME ADDRESSES				
17:30-18:30	Olympia Hall PLENARY SESSION 1				
18:30-20:30	Roof Garden WELCOME COCKTAIL				

MONDAY, JUNE 19, 2023

	Track 1	Track 2	Track 3	Track 4	Track 5	Track 6	
08:00-09:00			REGISTR	ATIONS			
08:45-09:00			Olympia Hall OPEN		ſ		
09:00-10:00			• Olympia Hall PLEN	NARY SESSION 2			
10:00-10:20		♀ Olyn	npia Foyer & Kallirhoe	Room COFFEE B	REAK		
10:20-12:30	• Olympia Hall \$1-01: Operations and Supply Chains (I)	Templar Hall S1-02: Operations and Control (I)	♥ Attica Hall \$1-03: Sustainable and Circular Systems (I)	♥ Conf. Room I S1-04: Biobased Systems (I)	Conf. Room II S1-05: Industrial Biotechnology (I)	Conf. Room III S1-06: Advances in Optimization (I)	
12:30-13:30	• Olympia Foyer LUNCH	& Kallirhoe Room BREAK	♥ Attica Hall IChemE presents: Carrer opportunities in computer aided process engineering – your questions answered		Conf. Room IV EURECHA MEETING		
13:30-14:30	P	♥ Kallirhoe Hall OSTER SESSION Posters of Theme	1-A 1	PC	• Olympia Foyer OSTER SESSION 1 Posters of Theme 2	- B	
14:30-16:30	Olympia Hall THE UNREMITTING LEGACY OF PROFESSOR FLOUDAS - SEVEN YEARS LATER						
16:30-16:50	Olympia Foyer & Kallirhoe Room COFFEE BREAK						
16:50-18:20	Olympia Hall S2-01: Data Driven Applications (I)	Templar Hall S2-02: Operations and Control (II)	Attica Hall S2-03: Advances in Optimization (II)	Conf. Room I S2-04: Data Driven Applications (II)	Conf. Room II S2-05: Education and Knowledge Transfer	Conf. Room III S2-06: Modeling And Optimization (I)	



TUESDAY, JUNE 20, 2023

	Track 1	Trac	k 2	Track 3	Track 4	Trac	:k 5	Track 6
08:00-09:00		REGISTRATIONS						
09:00-10:00				♥ Olympia Hall PLE	NARY SESSION 3			
10:00-10:20			Q Olyn	npia Foyer & Kallirhoe	Room COFFEE B	REAK		
10:20-12:30	 Olympia Hall S3-01: Properties and Materials (I) 	♥ Temp S3-(Ene Syster	ar Hall)2: rgy ns (I)	♥ Attica Hall S3-03: Operations and Supply Chains (II)	Conf. Room I S3-04: Sustainable and Circular Systems (II)	Conf. S3- Process In & Intens (In Men Prof Jiri	Room II 05: Itegration ification noriam: Klemes)	Conf. Room III S3-06: Industrial Biotechnology (II)
12:30-13:30	Olympia Foyer & Kallirhoe Room LUNCH BREAK		Conf. Room IV COMPUTERS & CHEMICAL ENGINEERING - EDITORIAL BOARD MEETING		Conf. Room II IRISS - SUSCHEM INTERNAL MEETING		Room II USCHEM . MEETING	
13:30-14:30	Vallirhoe HallVPOSTER SESSION 2-APOSTPosters of Theme 5-8Poster		Olympia Foyer ER SESSION 2-B ers of Theme 3-4	Conf. Room II IRISS THEMATIC SESSION ON SSbD in the a I		♥ (TITA cemen in the j a ne	Conf. Room III N: Digitalizing t manufacturing journey towards et-zero world	
14:30-16:30	Olympia Hall S4-01: Properties and Materials (II)	♥ Temp S4-(Opera and Su Chain	ar Hall)2: tions ıpply s (III)	♥ Attica Hall S4-03: Industrial Biotechnology (III)	♥ Conf. Room I S4-04: Biobased Systems (II)	♥ Conf. S4- Sustaina Circular (II	Room II 05: Ible and Systems I)	Conf. Room III S4-06: Hydrogen and Carbon Capture (I)
16:30-16:50	Olympia Foyer & Kallirhoe Room COFFEE BREAK							
16:50-18:35	 Olympia Hall S5-01: Operations and Control (III) 	♥ Temp S5-(Sustaina Circular Sy	ar Hall)2: ble and stems (IV)	♥ Attica Hall \$5-03: Industrial Biotechnology (IV)	Conf. Room I 55-04: Biobased Systems (III)	♥ Conf. S5- Modelli Optimiz	Room II 05: ng and ation (II)	Conf. Room III S5-06: Hydrogen and Carbon Capture (II)
19:30-23:30	Zappeion Mansion ESCAPE33 Gala Dinner							

WEDNESDAY, JUNE 21, 2023

	Track 1	Track 2	Track 3	Track 4	Track 5	Track 6
08:00-09:00	REGISTRATIONS					
08:30-09:00		9 C	Olympia Hall Present	ation of ESCAPE	34	
09:00-10:00			Olympia Hall PLE	NARY SESSION 4		
10:00-10:20		Olym	npia Foyer & Kallirhoe	Room COFFEE B	REAK	
10:20-12:30	Olympia Hall S6-01: Energy Systems (II)	♥ Templar Hall S6-02: Modelling and Optimization (III)	 Attica Hall S6-03: Data Driven Applications (III) 	Conf. Room I 56-04: Energy Systems (III)	♥ Conf. Room II S6-05: Process Integration and Intensification (II)	Conf. Room III WORKSHOP on Course Development
12:30-13:30	Olympia Foyer & Kallirhoe Room LUNCH BREAK					
13:30-14:00	Olympia Hall PLENARY SESSION 5					
14:00-14:30	Olympia Hall PLENARY SESSION 6					
14:30-14:55	Olympia Hall EURECHA Student Contest Problem					
14:55-15:30	Olympia Hall Awards & Closing Ceremony					



ESCAPE 33 EUROPEAN SYMPOSIUM Octailed program







SUNDAY, JUNE 18, 2023

Ø 09:30 − 16:30	♥ Attica Hall
CAPE WORKING PARTY	
10:00 – 16:00	♥ Conf. Room I
PROCESS SIMULATION WORKSHOP	
Workshop Coordinator: Prof. Dominic Foo	Participants need to register in advance
10:00 – 16:00	♥ Conf. Room III
HANDS-ON WITH OMLT: THE OPTIMIZATION AND MACHINE LEARN	NING TOOLKIT WORKSHOP
Presented by: Carl D. Laird, Chemical Engineering Department, CMU	Participants need to register in advance
10:00 – 17:00	♥ Conf. Room II
MACHINE LEARNING WORKSHOP	
Workshop Coordinator: Prof. Antonio Rio	Participants need to register in advance
12:30 – 17:15	♥ Templar Hall
CHESS ON CHESS ESCAPE 33 pays tribute to our pioneers in process simulation. CHESS: Che	mical Engineering Simulation Systems Participants need to register in advance
✓ 14:00 – 17:30	
REGISTRATIONS	
17:15 – 17:30	♥ Olympia Hall
WELCOME ADDRESSES	
17:30 – 18:30	🖓 Olympia Hall
PLENARY SESSION 1 Chairs: Prof. Antonios Kokossis, Prof. Vassily Hatzimanikatis	
How can PSE concepts and methods help accelerate progress in bioto Prof. Gregory Stephanopoulos, Willard Henry Dow Professor in Chemical Engine	e chnology ering, MIT
18:30 – 20:30	? Roof Garden
WELCOME COCKTAIL	For Registered participants only

ESCAPE 33 EUROPEAN SYMPOSIUM ON COMPUTER-AIDED PROCESS ENGINEERING 18-21 JUNE 2023 ATHENS-GREECE **MONDAY, JUNE 19, 2023** Ø 08:00 – 09:00 REGISTRATIONS 08:45 - 09:00 **O**lympia Hall **OPENING CEREMONY** ♥ Olympia Hall Ø 09:00 – 10:00 **PLENARY SESSION 2** Chairs: Prof. Ignacio Grossman, Prof. Flavio Manenti Tying Deep Learning to Process Systems Engineering for Sustainable Materials, Energy Systems, and Climate Change Mitigation Prof. Fenggi You, Chair Professor, Cornell University 10:00 - 10:20 Olympia Foyer & Kallirhoe Room COFFEE BREAK 10:20 – 12:30 Olympia Hall SESSION S1-01: Operations and Supply Chains (I) Track 1 Machine learning-based decomposition for complex supply chains 306 Niki Triantafyllou^a, Stavros Papaiakovou^b, Andrea Bernardi^a, Matthew Lakelin^c, Nilay Shah^a, Antonis Kokossis^b, Maria M. Papathanasiou^a ^a The Sargent Centre for Process Systems Engineering, Imperial College London, London, UK, SW72AZ ^b School of Chemical Engineering, National Technical University of Athens, 9, Iroon Polytechniou St, Athens, Greece, 15780 ^c TrakCel Limited, 10/11 Raleigh Walk, Cardiff, CF10 4LN UK Multistage Economic NMPC for Gas Pipeline Networks with Uncertainty 801 Sakshi Naik, Robert Parker, Lorenz T. Biegler Carnegie Mellon University, Pittsburgh, PA 15289, USA Data-Driven Robust Model Predictive Control on Building Climate Control with Renewable Energy 180 Wei-Han Chen, Fengqi You Cornell University, Ithaca, New York, 14853, USA Real-time optimization of a chemical plant with continuous flow reactors via reinforcement learning 243 Min Wu^a, Furkan Elmaz^b, <u>Ulderico Di Caprio</u>^a, Dries De Clercq^c, Siegfried Mercelis^b, Peter Hellinckx^b, Leen Braeken^a, Florence Vermeire^d and M. Enis Leblebici^a ^a Center for Industrial Process Technology, KU Leuven, Agoralaan Building B, 3590 Diepenbeek, Belgium ^b Faculty of Applied Engineering, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium ^c Ajinomoto Bio Pharma Services, Cooppallaan 91, 9230 Wetteren, Belgium ^d Chemical Reactor Engineering and Safety, KU Leuven, Celestijnenlaan 200f, 3001 Leuven, Belgium Lumped-Parameter Heat Exchanger Models for the Robust Dynamic Modelling of Power 807 **Generation Cycles** <u>Oliver Ward</u>^a, Federico Galvanin^a, Nelia Jurado^b, Chris Clements^c, Mohamad Abdallah^d, Daniel Blackburn^c, Eric Fraga^a ^a Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, UK

- ^b Department of Mechanical Engineering, University College London, Torrington Place, London, WC1E 7JE, UK
- ^c United Kingdom Atomic Energy Authority, Culham Science Centre, Abingdon, OX14 3DB, UK
- ^d Formerly at United Kingdom Atomic Energy Authority, Culham Science Centre, Abingdon, OX14 3DB, UK





MONDAY, JUNE 19, 2023



10:20 - 12:30

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SESSION S1-03: Sustainable and Circular Systems (I)

Evaluating the potential of current and emerging alternatives to enable a Sustainable Circular 786 Economy

Vyom Thakker¹, Amrita Sen¹, George Stephanopoulos^{2,3}, <u>Bhavik R. Bakshi¹</u>

¹ William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, Ohio

² The Global KAITEKI Center, Arizona State University, Tempe, Arizona 85287, USA

³ Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA



Attica Hall

Track 3

MONDAY, JUNE 19, 2023

23	Modeling strategies in multi-scale food-energy-water nexus system optimization <u>Marcello Di Martino</u> ^{a,b} , Patrick Linke ^{a,c} , Efstratios N. Pistikopoulos ^{a,b} ^a Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, USA ^b Texas A&M Energy Institute, Texas A&M University, College Station, TX, USA ^c Department of Chemical Engineering, Texas A&M University at Qatar, Education City, Doha, Qatar			
232	 Waste integration for sustainable operation of WWTP's Elena C. Blanco^a Mariano Martín^a Pastora Vega^b ^a Department of Chemical Engineering, University of Salamanca, 37008 Salamanca, Spain ^b Department of Computer Science, University of Salamanca, 37008 Salamanca, Spain 			
418	The Infinity Reactor: A new conceptual design for a more cost-efficient CO2 to methanol route <u>Hilbert Keestra</u> , Edwin Zondervan, Wim Brilman University of Twente, Drienerlolaan 5, 7522 NB Enschede, The Netherlands			
712	Generalized First-Principles Suite for Dynamic Modeling of Circular Solid Waste Thermal Treatments: a Sewage Sludge Oxy-Gasification Case Study <u>Francesco Negri</u> ^{a,c} , Anna Nova ^{a,b} , Andrea Galeazzi ^{a,b} , Francesco Gallo ^c , Flavio Manenti ^{a,b} ^a Politecnico di Milano, CMIC Dept. "Giulio Natta", Piazza Leonardo da Vinci 32, Milan 20133, Italy ^b Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali, Via Giusti 9, Firenze 50121, Italy ^c Itelyum Regeneration spa, Via Tavernelle 19, Pieve Fissiraga 26854, Lodi, Italy			
33	Optimal design of refineries for low-density polyethylene (LDPE) waste upcycling Borja Hernández, Dionisios G. Vlachos, Marianthi G. Ierapetritou Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware, USA			
0 10	0:20 – 12:30	🖓 Conf. Room		
SESSI	ON S1-04: Biobased Systems (I)	Track 4		
879	Algorithmic generation of bioinspired 3D scaffolds for T cell-based cancer immunotherapy Matthew Chin, Barry Reid, <u>Marc-Olivier Coppens</u> Centre for Nature Inspired Engineering & Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE, United Kingdom			
212	Hybrid dynamic model of monoclonal antibody production using CHO cells <u>Mariana Monteiro</u> , Cleo Kontoravdi Sargent Centre for Process Systems Engineering, Department of Chemical Engineeering, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom			
529	9 Hybrid modelling and data-driven parameterization of monoclonal antibody cultivation processes: Shifts in cell metabolic behavior Sara Badr ^a , Kota Oishi ^a , Kozue Okamura ^a , Sei Murakami ^b , Hirokazu Sugiyama ^a ^a Department of Chemical System Engineering, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, 113-8656, Tokyo, Japan ^b Manufacturing Technology Association of Biologics, 2-6-16, Shinkawa, Chuo-ku, 104-0033, Tokyo, Japan			
330	Development of a holistic Python package for optimal selection of in kinetic model discrimination Maerthe Theresa Tillmann ^{a,b} Federico Galvanin ^a	f experimental design criteria		

<u>Maerthe Theresa Tillmann</u>^{a,o}, Federico Galvanin^a

^a Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE, UK

^b Faculty of Mechanical Engineering, RWTH Aachen University, Eilfschornsteinstraße 18, 52062 Aachen, Germany





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249	Mechanistic modeling of product formation in recombinant Escherichia coli cultivations <u>Don Fabian Müller</u> ^a , Philipp Pably ^a , Daniel Wibbing ^c , Julian Kager ^d , Christoph Herwig ^{a,b} ^a Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Gumpendorfer Straße 1a, 1060 Vienna, Austria ^b Competence Center CHASE GmbH, 4040 Linz, Austria ^c Festo SE & Co. KG, 73770 Denkendorf, Germany ^d Department of Chemical and Biochemical Engineering, Technical University of Denmark, Lyngby, Denmark				
153	Innovative process for manufacturing pharmaceutical mini-tablets using 3D printing Varun Sundarkumar, Wanning Wang, Zoltan K. Nagy, Gintaras Reklaitis Davidson School of Chemical Engineering, Purdue University, West Lafayette Indiana 47906 USA				
2 1	0:20 – 12:30 Conf. Room II				
SESS	ON S1-05: Industrial Biotechnology (I) Track 5				
874	Computer-Aided Cellular Process Engineering Vassily Hatzimanikatis EPFL				
583	Analysis of Salmonella Typhimurium growth in the murine intestine using metabolic network reconstruction <u>E. Vayena</u> ^a , L. Fuchs ^b , H. Mohammadi Peyhania ^c , B. Nguyen ^b , W. D. Hardt ^b , V. Hatzimanikatis ^a ^a Laboratory of Computational Systems Biotechnology, EPFL, 1015, Lausanne, CH ^b Institute of Microbiology, D-BIOL, ETH Zurich, 8093 Zurich, CH ^c Present address: pRED, Roche Glycart AG, 8952 Schlieren, CH				
864	On the systematic development of large-scale kinetics using stability criteria and high-throughput analysis of curated dynamics from genome-scale models Konstantinos Mexis, <u>Stefanos Xenios</u> , Antonis Kokosis Department of Process Engineering, NTUA, Iroon Politechniou 6 Zografou, Athens, Greece				
764	Data-driven prediction of peptide-MHC binding using oscillations of physicochemical properties <u>Hyeju Song</u> , Chris A. Kieslich Auburn University, Auburn, AL 36849, USA				
622	Towards a unified multi-scale strategy for bio-manufacturing process development Thomas Bisgaard ^a , Nima Nazemzadah ^b , Eduardo Krebs Kleingesinds ^a , Negin Yousefi ^a , Christian Beenfeldt ^b , <u>Seyed Soheil Mansouri</u> ^a ^a PROSYS, Department of Chemical and Biochemial Engineering, Technical University of Denmark, Søltofts Plads, Buidling 228A, 2800 Kongens Lyngby, Denmark ^b Knowledge Hub Zealand, Holbækvej 141 B, DK-4400, Kalundborg				
165	 Machine learning-supported cybergenetic modeling, optimization and control for synthetic microbial communities Sebastián Espinel-Ríos^a, Katja Bettenbrock^a, Steffen Klamt^a, José L. Avalos^b, Rolf Findeisen^c ^a Analysis and Redesign of Biological Networks, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, 39106 Magdeburg, Germany ^b Department of Chemical and Biological Engineering, Princeton University, 08544 Princeton, United States ^c Control and Cyber-Physical Systems Laboratory, Technical University of Darmstadt, Landgraf-Georg-Straße 4, 64283 Darmstadt, Germany 				

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\oslash	10:20 – 12:30	
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Conf. Room III

SESSI	ON S1-06: Advances in Optimization (I)	Track 6		
752	Optimization of Process Families for Deployment of Carbon Cap Learning Surrogates Georgia Stinchfield ^a , Bashar L. Ammari ^a , Joshua C. Morgan ^{c,d} , John Carl D. Laird ^a ^a Carnegie Mellon University, 5000 Forbes Ave., Pittsburgh, PA, 15232 ^b Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM, 87185 ^c National Energy Technology Laboratory (NETL), 626 Cochran Mill Road, Pittsburgh METL Support Contractor, 626 Cochran Mill Road, Pittsburgh, PA, 15236	oture Processes using Machine n D. Siirola ^b , Miguel Zamarripa ^{c,d} , argh, PA, 15236		
782	Modeling hierarchical systems via nested generalized disjunctive Hector D. Perez, Ignacio E. Grossmann Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh 15207, USA	e programming		
129	Approaches to Reduce Optimization Time for Stochastic Optimi Chemical Processes Fanyi Duanmu, Dian Ning Chia, Eva Sorensen Department of Chemical Engineering, University College London (UCL), Torringt	zation of Complex		
17	Automated Kinetic Model Discovery – A Methodological Frame Miguel Ángel de Carvalho Servia ^a , Ilya Orson Sandoval ^a , Dongda Z King Kuok (Mimi) Hii ^c , Ehecatl Antonio del Rio Chanona ^a ^a Department of Chemical Engineering, Imperial College London, South Kensin ^b Department of Chemical Engineering, The University of Manchester, M13 9PL, ^c Department of Chemistry, Imperial College London, 82, Wood Lane, London V	work Thang ^ь , Klaus Hellgardtª, gton, London SW7 2AZ, UK UK V12 0BZ, UK		
286	A hybrid forecasting framework for the energy sector <u>Stefanos G. Baratsas</u> ^{a,b} , Funda Iseri ^{a,b} , Efstration N. Pistikopoulos ^{a,b} ^a Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, USA ^b Texas A&M Energy Institute, Texas A&M University, College Station, TX 77843, USA			
150	Modeling Commercial Fleet Charging & Regulation Strategies via James Owens ^{a,b} , Emre Gençer ^a ^a MIT Energy Initiative, Massachusetts Institute of Technology, 400 Main Str., Can ^b Department of Chemical Engineering, Massachusetts Institute of Technology, 2	Data-driven Optimization abridge, MA 02142, USA 25 Ames Str., Cambridge, MA 02142, USA		
2 12	:30 – 13:30 LUNCH BREAK	♥ Olympia Foyer & Kallirhoe Room		
2 12	:30 – 13:30			
ICHEN	IE PRESENTS: Carrer opportunities in computer aided as engineering – your questions answered	Participants need to register in advance		
2 12	:30 – 13:30	♥ Conf. Room IV		
EUREC	CHA MEETING			



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 13:30 – 14:30 POSTER SESSION 	for detailed poster program scan the QR Codes
Kallirhoe Hall POSTER SESSION 1-A Posters of Theme 1	Olympia FoyerPOSTER SESSION 1-BPosters of Theme 2
2 14:30 – 16:30	♥ Olympia Hall
THE UNREMITTING LEGACY OF PROFESSOR FLO	UDAS - SEVEN YEARS LATER
 Opening Remarks Efstratios Pistikopoulos University Distinguished Professor, Texas A&M University Prof Rafiqul Gani CEO, PSE for SPEED Company Limited, Denmark-Thailand PSE-inspired discovery tools in metabolic networks and protein design Costas Maranas Pennsylvania State University Optimisation algorithms for molecular design Claire Adjiman Imperial College London Professor Floudas' continuing legacy: Automatically designing microreactor experiments Ruth Misener Imperial College UK	 Adventuring on the PSE Outskirts: Robust Optimal Vehicle Routing Chrysanthos Gounaris Carnegie Mellon University Cutting plane decomposition algorithms for global optimization driven by machine learning and advanced data analytics Antonios Kokossis Chair of the Local Organizing Committee, School of Chemical Engineering NTUA, Department of Process Analysis and Plant Design Remarks George Floudas University of Ioannina Closing Remarks Stefanos Baratsas Texas A&M Energy Institute Thanks Ismini Flouda
16:30 – 16:50	♥ Olympia Foyer & Kallirhoe Room
COFFE	EBREAK



SESSION S2-01: Data Driven Applications (I)

Data-driven predictive model for irrigation management in greenhouses under CO₂ enrichment and high solar radiation <u>Ikhlas Ghiat</u>, Rajesh Govindan, Tareq Al-Ansari College of Science and Engineering, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar

Development of a Deep Learning-based Schedule-Aware Controller: Toward the Integration of Scheduling and Control

<u>M. Abou El Oassime</u>^{a,b}, A. Shokry^a, A. Espuña^c, E. Moulinesa^b

^a École polytechnique, Paris, France

- ^b Emines School of Industrial Management, BenGuerir, Morocco
- ° Universitat Politècnica de Catalunya, Barcelona, Spain

♥ Olympia Hall

Track 1

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748	A novel neural network bounds-tightening procedure for multiple Dustin Kenefake ^{a,b} , Rahul Kakaodkar ^{a,b} , Moustafa Ali ^{a,b} , Efstratios N. ^a Texas A&M Energy Institute, Texas A&M University, College Station, USA ^b Artie McFerrin Department of Chemical Engineering, Texas A&M University, Co	arametric programming & control Pistikopoulos ^{a,b} Ilege Station, USA
826	Development of a Centralized Classifier for Decentralized Decisi <u>Marco S. Reis</u> , Eugeniu Strelet, Joel Sansana, Margarida J. Quina, L Tiago J. Rato Univ Coimbra, CIEPQPF, Department of Chemical Engineering, Rua Sílvio Lima, F 3030-790 Coimbra, Portugal	on Making .icínio M. Gando-Ferreira, Pólo II – Pinhal de Marrocos,
357	Fault Detection and Diagnosis for Chemical Processes based on Continuous Wavelet Transform <u>Chinatsu Ukawa</u> ^a , Yoshiyuki Yamashita ^b ^a Department of Food and Energy Systems Science, Graduate School of Bio-App Tokyo University of Agriculture and Technology, 2-24-16 Naka-cho, Koganei, Tok ^b Department of Chemical Engineering, Tokyo University of Agriculture and Techn Tokyo 184-8588, Japan	Deep Neural Networks with lications Systems Engineering, ryo 184-8588, Japan nology, 2-24-16 Naka-cho, Koganei,
515	Online real-time multi-parameter optimization solution based on Xuerong Gu ^a , <u>Siyu Yang</u> ^{a,b} ^a School of Chemistry and Chemical Engineering, South China University of Techr ^b Guangdong Key Laboratory of Green Chemical Products Technology, South China 510640, PR China	parallel EGO algorithm nology, Guangzhou, 510640, PR China ina University of Technology, Guangzhou,
2 10	6:50 – 18:20	♥ Templar Hall
SESS	ION S2-02: Operations and Control (II)	Track 2
522	Dynamic Modeling and Control of CO2 Capture Systems with a <u>Panagiotis Kazepidis</u> ^{a,b} , Athanasios I. Papadopoulos ^a , Panos Seferlis ^a Chemical Process & Energy Resources Institute (C.P.E.R.I.), Center for Research a <u>PO</u> Box 60361, 57001, Thermi-Thessaloniki, Greece	Biphasic Solvent ^{,a,b} and Technology Hellas (CE.R.T.H.),
	^b Department of Mechanical Engineering, Aristotle University of Thessaloniki, P.O. I	Box 484, 54124 Thessaloniki
485	 ^b Department of Mechanical Engineering, Aristotle University of Thessaloniki, P.O. I Real-time control and scheduling decision making in fermentation Isuru A. Udugama^a, Keegan K. Hall^a, Christoph Bayer^b, Brent R. Young ^a Ahuora – Centre for Smart Energy Systems, School of Engineering, University of ^b Department of Process Engineering, TH Nürnberg, Nürnberg, 90489, Germany ^c Industrial Information and Control Centre, Department of Chemical & Materials Auckland, 1010, New Zealand 	Box 484, 54124 Thessaloniki on-based food process operations g ^c , Timothy G. Walmsley ^a Waikato, Hamilton, 3240, New Zealand Engineering, The University of Auckland,
485	 ^b Department of Mechanical Engineering, Aristotle University of Thessaloniki, P.O. I Real-time control and scheduling decision making in fermentation Isuru A. Udugama^a, Keegan K. Hall^a, Christoph Bayer^b, Brent R. Young ^a Ahuora – Centre for Smart Energy Systems, School of Engineering, University of bepartment of Process Engineering, TH Nürnberg, Nürnberg, 90489, Germany ^c Industrial Information and Control Centre, Department of Chemical & Materials Auckland, 1010, New Zealand Machine learning-based product concentration estimation, real-temultivariable control of an experimental electrochemical reactor Berkay Çıtmacı^a, Junwei Luo^a, Joon Baek Jang^a, Carlos Morales-Gui ^a Dept. of Chemical and Biomolecular Engineering, University of California, Los Age 	Box 484, 54124 Thessaloniki on-based food process operations g ^c , Timothy G. Walmsley ^a Waikato, Hamilton, 3240, New Zealand Engineering, The University of Auckland, time optimization, and io^a , <u>Panagiotis D. Christofides^{a,b} ingeles 90095, USA</u>
485	 ^b Department of Mechanical Engineering, Aristotle University of Thessaloniki, P.O. I Real-time control and scheduling decision making in fermentation <u>Isuru A. Udugama</u>^a, Keegan K. Hall^a, Christoph Bayer^b, Brent R. Young ^a Ahuora – Centre for Smart Energy Systems, School of Engineering, University of ^b Department of Process Engineering, TH Nürnberg, Nürnberg, 90489, Germany ^c Industrial Information and Control Centre, Department of Chemical & Materials Auckland, 1010, New Zealand Machine learning-based product concentration estimation, real-t multivariable control of an experimental electrochemical reactor Berkay Çıtmacı^a, Junwei Luo^a, Joon Baek Jang^a, Carlos Morales-Gui ^a Dept. of Chemical and Biomolecular Engineering, University of California, Los Ange A machine learning dynamic modelling scheme for wastewater t particle swarm optimization and neural networks Teo Protoulis^a Ioannis Kalogeropoulos^{b,c}, Ioannis Kordatos^a, Haralan ^a Department of Electrical and Electronic Engineering, University of Athens, Heroog ^c Systemica - G.Vangelatos & Co L.P., Ethnikis Antistaseos 70, Athens, Greece 	Box 484, 54124 Thessaloniki In-based food process operations g ^c , Timothy G. Walmsley ^a Waikato, Hamilton, 3240, New Zealand Engineering, The University of Auckland, Eime optimization, and fo ^a , <u>Panagiotis D. Christofides</u> ^{a,b} ingeles 90095, USA eles 90095, USA reatment plants using cooperative nbos Sarimveis^b, Alex Alexandridis ^a Ancient Olive Grove Campus, Thivon 250 & on Polytechneiou 9, Zografou, Greece



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325	Optimal energy management in greenhouses using distributed hybrid DRL-MPC framework Benjamin Decardi-Nelson, Fengqi You Cornell University, Ithaca, New York, 14853, USA	
614	Process as a battery: Robust dynamic optimal operation of zeolite respect to the carbon footprint of electric power Robin Semrau, Sebastian Engell TU Dortmund University, August-Schmidt-Straße 1, 44227 Dortmund, Germany	e crystallization in a COBR with
2 10	6:50 – 18:20	♥ Attica Hall
SESSI	ON S2-03: Advances in Optimization (II)	Track 3
681	Global optimization of symbolic surrogate process models based o <u>Tim Forster</u> , Daniel Vázquez, Gonzalo Guillén-Gosálbez Department of Chemistry and Applied Biosciences, Institute for Chemical and Bioer Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland	on Bayesian learning ngineering, ETH Zurich,
345	A graph classification approach to determine when to decompose of Ilias Mitrai, <u>Prodromos Daoutidis</u> Department of Chemical Engineering & Materials Science, University of Minnesota,	optimization problems Minneapolis, 55455 MN, USA
731	Hybrid Modeling and Multi-Fidelity Approaches for Data-Driven Br Suryateja Ravutla ^a , Jianyuan Zhai ^b , Fani Boukouvala ^a ^a Department of Chemical & Biomolecular Engineering, Georgia Institute of Technol ^b Engineering & Data Sciences, Cargill Inc, Shanghai, 200031, China	ranch-and-Bound Optimization
765	An inverse optimization approach to decision-focused learning <u>Rishabh Gupta</u> , Qi Zhang Department of Chemical Engineering &Materials Science, University of Minnesota, I	Minneapolis, MN 55455, USA
428	Stable two-stage scenario generation via game-theoretic optimisat <u>Georgios L. Bounitsis</u> , Lazaros G. Papageorgiou, Vassilis M. Charitopo The Sargent Centre for Process Systems Engineering, Department of Chemical Engineering Torrington Place, London WC1E 7JE, UK	tion pulos ineering, University College London,
410	An Event-Based Continuous-Time MILP for Short-Term Crude Oil S <u>İrem Marttin</u> ^{a,b} , Sena Kurban ^a , Gizem Kuşoğlu Kaya ^a , Özgür Kabak ^b , Y. ^a Turkish Petroleum Refinery, 41780, Körfez, Kocaeli, Turkey ^b Industrial Engineering Department, Faculty of Management, Istanbul Technical Un	cheduling İlker Topcu ^ь iversity, 34367, Sarıyer, Istanbul, Turkey
() 1/	4·50 18·20	9 Conf Poom I
SESSI	ON \$2-04: Data Driven Applications (II)	Track 4
105	Machine-Learning-Powered process design for the recycling of w. Luca Bosetti, Benedikt Alexander Winter, Johanna Lindfeld and And Energy and Process System Engineering, ETH Zurich, 8092 Zurich, Switzerland	aste polyurethane Iré Bardow
717	Data-driven modeling to predict the rate of Boil-off Gas (BOG) g storage tank Suraj Prakash Singh ^a , Rajagopalan Srinivasan ^{a,b} , I. A. Karimi ^c ^a Department of Chemical Engineering, Indian Institute of Technology Madras, Ch ^b American Express Lab for Data Analytics, Risk & Technology, Indian Institute of Te ^c Department of Chemical and Biomolecular Engineering, National University of Su	eneration in an industrial LNG nennai 600036, India echnologuy Madras, Chennai 600036, India ingapore, Singapore



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156	Polymer Grade Transition Control via Reinforcement Learning Trained with a Physically Consistent Memory Sequence-to-Sequence Digital Twin Zhen-Feng Jiang ^a , David Shan-Hill Wong ^a , Jia-Lin Kang ^b , Yuan Yao ^a , Yao-Chen Chuang ^c , ^a Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30043, Taiwan ^b Department of Chemical & Materials Engineering, National Yunlin University of Science & Technology, Yunlin 64002, Taiwan ^c Center for Energy and Environmental Research, National Tsing Hua University, Hsinchu 30043, Taiwan
295	Machine learning enabled modelling and sensitivity analysis for the power generation from a 660 MW supercritical coal power plant <u>Waqar Muhammad Ashraf</u> , Vivek Dua Sargent centre for Process Systems Engineering, Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE, UK
797	Fusion and integrated correction of chemometrics and machine learning models based on data reconciliation Pál P. Hanzelik ^{a,b} , Alex Kummer ^b , Ádám Ipkovich ^b , János Abonyi ^b ^a Dombóvári út 28, Budapest, Hungary
151	Achieving Operational Excellence by Combining Material Tracking and On-line Polymer Analysis and Classification data in an all-in-one Integrated Decision Support System Symeon Kassianides, Symon Doe, Sanja Micunovica, Artemis Theodoropoulou, Charis Komodromos, Sofia Louloudi Hyperion Systems Engineering Ltd., 36 Athalassis Street, Geri-Nicosia, 2201, Cyprus
2 1	6:50 – 18:20 ♀ Conf. Room II
SESS	ION S2-05: Education and Knowledge Transfer Track 5
300	Designing an interactive environment to share educational materials and resources. Application to the Geomatics Hub at UniLaSalle Beauvais <u>Réjanne Le Bivic</u> , Sébastien Ottavi, Pierre Saulet, Pauline Louis, Arnaud Coutu Institut Polytechnique UniLaSalle, 19 rue Pierre Waguet, 60000 BEAUVAIS, France
369	Immersive learning through simulation: implementing twin screw extrusion in Unity <u>Pedro Santos Bartolomé</u> ^a , Daniel Just ^b , Ariana Bampouli ^a , Simon Kemmerling ^b , Aleksandra Buczko ^b , Tom Van Gerven ^a ^a Process Engineering for Sustainable Systems (ProcESS), KU Leuven. Celestijnenlaan 200F, 3001, Leuven, Belgium ^b Fraunhofer-Institut für Chemische Technologie ICT, Polymer Engineering. Joseph-von-Fraunhofer-Str. 7, Pfinztal, Germany
141	Integrating Python in the (bio)chemical engineering curriculum: challenges and opportunities <u>Fiammetta Caccavale</u> , Carina L. Gargalo, Krist V. Gernaey, Ulrich Krühne PROSYS, Dept. of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads, Building 228 A, 2800 Kgs. Lyngby, Denmark
406	An Educational Workshop for Effective PSE Course Development Daniel R. Lewin ^a , Edwin Zondervan ^b , Meik Franke ^b , Anton A. Kiss ^c , Stefan Krämer ^d , Mar Pérez-Fortes ^e , Artur M. Schweidtmann ^c , Petronella M. (Ellen) Slegers ^f , Ana Somoza-Tornos ^c , Pieter L.J. Swinkels ^c , Bart Wentink ^g ^a Department of Chemical Engineering, Technion. I. I. T., Haifa 32000, Israel ^b Department of Chemical Engineering, University of Twente, the Netherlands ^c Department of Chemical Engineering, TU Delft, the Netherlands ^d Bayer AG, Engineering & Technology, Leverkusen, Germany ^e Engineering, Systems and Services, TU Delft, the Netherlands ^f Operations Research and Logistics, Wageningen University & Research, the Netherlands ^g BASE SE, Carporate Technology, Ludwigshafen, Germany



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858	A Cloud-based Collaborative Interactive Platform for Education an Process Modelling <u>Vinay Gautam</u> , Alberto Rodríguez-Fernández, Heinz A. Preisig Department of Chemical Engineering, Norwegian University of Science & Technolog	nd Research in Dynamic y, Trondheim, 7491, Norway
197	An Online Course for Teaching Process Simulation <u>Daniel R. Lewin</u> ^a , Assaf Simon ^a , Sapir Lifshiz Simon ^a , Asia Matatyaho ^a ^a Department of Chemical Engineering, Technion. I. I. T., Haifa 32000, Israel ^b Centre for the Promotion of Learning and Teaching, Technion, Haifa 32000, Israel	Ya'akobiª, Abigail Barzilai ^ь
2 1	6:50 – 18:20	♥ Conf. Room III
SESS	ON S2-06: Modeling and Optimization (I)	Track 6
80	Efficient physical model building algorithm using equations extrac Shota Kato, Manabu Kano Department of Systems Science, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyo	eted from documents
320	Architecture and Design of a Modern Commercial Process Simulat Ian Boys ^a , <u>Jochen Steimel^b</u> ^a AVEVA, 26561 Rancho Parkway South, Lake Forest, CA 92630, USA ^b AVEVA, Mainzer Landstraße 178-190, 60327 Frankfurt, Germany	or
343	Data augmentation for machine learning of chemical process flow Lukas Schulze Balhorn, Edwin Hirtreiter, Lynn Luderer, Artur M. Schw Process Intelligence Research, Department of Chemical Engineering, Delft Universi- Delft 2629 HZ, The Netherlands	sheets eidtmann ity of Technology, Van der Maasweg 9,
290	Sustainable Development Goals assessment of carbon capture on Valentina Negri, Margarita A. Charalambous, Juan D. Medrano-Garci Institute for Chemical and Bioengineering, Department of Chemistry and Applied I Vladimir-Prelog-Weg 1, Zürich 8093, Switzerland	- board ía , Gonzalo Guillén-Gosálbez Biosciences, ETH Zürich,
828	Extended Multiple-Curve Resolution framework for the calibration <u>Daniel Casas-Orozco</u> , Jaron Mackey, Ilke Akturk, Gintaras V. Reklaitis Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, 4	n of first-principles models , Zoltan K. Nagy 7907,USA
	Symbolic regression-based method for developing a physics-infor a manufacturing process <u>Utsav Awasthi</u> , George M. Bollas Department of Chemical and Biomolecular Engineering, Pratt and Whitney Institut University of Connecticut, 159 Discovery Dr, Storrs, CT, 06269, USA	med surrogate model for e of Advanced Systems Engineering,



TUESDAY, JUNE 20, 2023

08:00 - 09:00

REGISTRATIONS Ø 09:00 – 10:00 **Q** Olympia Hall **PLENARY SESSION 3** Chairs: Prof. Stratos Pistikopoulos, Prof. Robin Smith Strategies and Tools for Optimization-Driven Modeling: A New Era for CAPE Prof. Lorenz Biegler, Covestro University Professor, Carnegie Mellon University (⁄) 10:00 - 10:20 Olympia Foyer & Kallirhoe Room COFFEE BREAK 10:20 - 12:30 **O**lympia Hall SESSION S3-01: Properties and Materials (I) Track 1 774 Academic and Industrial Views on the Future of Applied Thermodynamics Georgios M. Kontogeorgis¹, Jean-Charles de Hemptinne², Ralf Dohrn³, Ioannis G. Economou⁴, Antoon ten Kate⁵, Susanna Kuitunen⁶, Miranda Mooijer⁷, Ljudmila Fele Žilnik⁸, Maria Grazia De Angelis⁹, Velisa Vesovic¹⁰ ¹ Center for Energy Resources Engineering (CERE), Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800, Lyngby, Denmark ² IFP Energies nouvelles, 1 et 4, avenue de Bois-Préau,92852 Rueil-Malmaison Cedex, France ³ Bayer AG, Process Technologies, Building E41, 51368 Leverkusen, Germany ⁴ Texas A&M University at Qatar, Chemical Engineering Program, PO Box 23874, Doha, Qatar ⁵ Nouryon, Zutphenseweg 10, 7418 AJ Deventer, The Netherlands ⁶ Neste Engineering Solutions Oy, PO Box 310, FI-06101 Porvoo, Finland ⁷ Shell Global Solutions, Shell Technology Centre Amsterdam, Grasweg 3, 1031 HW Amsterdam, The Netherlands ⁸ Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Ljubljana, Slovenia ^o Institute for Materials and Processes, School of Engineering, University of Edinburgh, Edinburgh, UK ¹⁰ Department of Earth Science and Engineering, Imperial College London, UK Intelligent Process Flowsheet Synthesis and Design using Extended SFILES Representation 119 Vipul Mann^a, Rafiqul Gani^{b,c}, Venkat Venkatasubramanian^a ^a Columbia University, New York, NY 10027, USA ^b PSE for SPEED Company, Charlottenlund, DK-2920, Denmark ^c Sustainable Energy and Environment Thrust, The Hong Kong University of Science and Technology (Guangzhou), Guangzhou, China Connectivity Matrix-based Descriptors with Deep Learning for Estimation of Pure Component 217 **Properties** Qiong Pan^a, Xiaolei Fan^b, Jie Li^a ^a Centre for Process Integration, Department of Chemical Engineering, School of Engineering, The University of Manchester, Manchester M13 9PL, UK ^b Department of Chemical Engineering, School of Engineering, The University of Manchester, Manchester M13 9PL, UK 302 S-GNN: State-Dependent Graph Neural Networks for Functional Molecular Properties Adem R.N. Aouichaoui, Alessandro Cogliati, Jens Abildskov, Gürkan Sin Process and Systems Engineering Centre (PROSYS), Department of Chemical and Biochemical Engineering, Technical

University of Denmark, Søltofts Plads, Building 228A, 2800 Kgs. Lyngby, Denmark





Kostas Blekos, Effie Marcoulaki

Agia Paraskevi 15310, Greece

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GREEN AND SUSTAINABLE PROCESS SYSTEMS ENGINEERING IN THE DIGITAL AGE

A Bayesian-based screening framework for optimal development of safe-by-design nanomaterials

System Reliability and Industrial Safety Laboratory, National Centre for Scientific Research "Demokritos", P.O. Box 60037,

An approach for modelling simultaneous fluid-phase and chemical-reaction equilibria



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	in multicomponent systems via Lagrangian duality: The Reactive <u>Felipe A. Perdomo</u> ^a , George Jackson ^a , Amparo Galindo ^a , Claire S. A ^a Department of Chemical Engineering, Sargent Centre for Process Systems Engir and Engineering, Imperial College London, South Kensington Campus, London	HELD algorithm djiman ^a neering, Institute for Molecular Science SW7 2AZ, UK
2 10):20 – 12:30	🕈 Templar Hall
SESS	ON S3-02: Energy Systems (I)	Track 2
94	Mechanistic model for inkjet printing and applications in perovsk Naveen Bhati ^a , Mohammad Khaja Nazeeruddin ^b , <u>François Maréchala</u> ^a Industrial Process and Energy Systems Engineering, Ecole Polytechnique Fedéra ^b Group for Molecular Engineering of Functional Materials, Institute of Chemical S Polytechnique Fedérale de Lausanne, Sion, 1951, Switzerland	tite solar cells engineering a ble de Lausanne, Sion, 1951, Switzerland Sciences and Engineering, Ecole
702	Dynamic Simulation to Verify Operability of LNG Plants with Post Jaleel Valappil Bechtel Energy, 3000 Post Oak Boulevard, Houston, TX - 77407, USA	t Combustion Carbon Capture
654	Multiscale design & analysis of templated zeolite for Li-O2 battery Khizar Hayat ^{a,b} , Daniel Bahamon ^{a,b} , Lourdes F. Vega ^{a,b} , Ahmed Al Ha ^a Research and Innovation Center on CO2 & Hydrogen (RICH Center), Khalifa Univ ^b Department of Chemical Engineering, Khalifa University, P.O. Box 127788, Abu E	with improved discharge capacity jaj ^{a,b} versity, P.O. Box 127788, UAE Dhabi, UAE
433	Combining Operational and Design Optimization Decisions with Capture Retrofit Analysis Zachary Kilwein, Pengfei Cheng, Joseph Scott, Matthew Realff, Fan School of Chemical and Biomolecular Engineering, Georgia Institute of Technology	Hybrid Models for Direct Air i Boukouvala gy, Atlanta, USA
561	Molecule design beyond group counts – Integrated design of pro superstructures <u>P. Rehner</u> , J. Schilling, A. Bardow Energy and Process Systems Engineering, ETH Zurich, Switzerland	ocesses and molecule
108	In Silico solvent selection for optimum lignin depolymerisation provide the selection for optimum lignin depolymerisation provide the selection of the selectio	rocess acher ^a , erland

^c Bloom Biorenewables SA, 1723 Marly, Switzerland

Track 4

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2 10	0:20 – 12:30	♥ Attica Hall
SESSI	ON S3-03: Operations and Supply Chains (II)	Track 3
123	 Process Design and Bayesian Optimization of 5-Hydroxymethylfe Yuqing Luo^a, Zhaoxing Wang^{a,b}, Prahalad Srinivasan^a, Dionisios G. V ^a Department of Chemical and Biomolecular Engineering, University of Delaware, 19716, USA ^b Catalysis Center for Energy Innovation, RAPID Manufacturing Institute, and Dela Delaware, Newark, Delaware 19716, USA 	urfural Hydrodeoxygenation 'lachos ^{a,b} , <u>Marianthi lerapetritou</u> ^{a,b} , 150 Academy Street, Newark, Delaware, aware Energy Institute (DEI), University of
804	A new time-bucket MILP formulation for optimal lot-sizing and s make-and-fill process Roderich Wallrath ^{a,b} , Florian Seanner ^c , Matthias Lampe ^a , <u>Meik Frank</u> ^a Bayer AG, Kaiser-Wilhelm Allee 1, 51368 Leverkusen, Germany ^b University of Twente, Faculty of Science and Technology, Sustainable Process Te Optimization, Drienerlolaan 5, 7522 NB Enschede, The Netherlands ^c SimPlan Systems GmbH, Sophie-Scholl-Platz 6, 63452 Hanau, Germany	cheduling of an industrial ce ^b echnology, Process Design and
798	The Integration of Drug Substance and Drug Product Manufactur for Model-based End-to-End Process Development Charalampos Christodoulou ^a , <u>Samir Diab</u> ^b , Gabriele Bano ^c , Magdal Simeone Zomer ^b ^a GlaxoSmithKline, Gunnels Wood Road, Stevenage SG1 2NY, UK ^b GlaxoSmithKline, Park Road, Ware SG12 0DP, UK ^c GlaxoSmithKline, 1250 S Collegeville Rd, Collegeville (PA) 19426, USA	i <mark>ring Models: The Missing Link</mark> ini Aroniada ^ь , Neil Hodnettª,
787	A Computational Pipeline to Optimize 3D Scaffolds for Cancer In Lucy Todd ^a , Matthew Chin ^a , Marc-Olivier Coppens ^a ^a Centre for Nature Inspired Engineering & Department of Chemical Engineering Place, London WC1E 7JE, UK	mmunotherapy 1, University College London, Torrington
222	Multi-period optimisation of oligopolies with contracts: A coopera Asimina Marousi ^a , Jose M. Pinto ^b , Lazaros G. Papageorgiou ^a , Vassili ^a Department of Chemical Engineering, Sargent Centre for Process Systems Engi Torrington Place, London WC1E 7JE, UK ^b Linde Digital Americas, 10 Riverview Drive, Danbury CT 06810, USA	tive approach to customer fairness is M. Charitopoulos ^a ineering, University College London,
237	On discrete time chemical production scheduling MILP models of Amin Samadi ^a , Nathan Adelgren ^b , Christos T. Maravelias ^{a,b} ^a Department of Chemical and Biological Engineering, Princeton University, Prince ^b Andlinger Center for Energy and the Environment, Princeton University, Princeton	ontaining record keeping variables eton, NJ 08540, USA on, NJ 08540, USA
() 1()·20 – 12·30	Conf. Room I

10:20 – 12:30

SESSION S3-04: Sustainable and Circular Systems (II)

Ъ Investigation of economic and environmental tradeoffs of spatially explicit biomass supply chains 124 towards the production of net-negative biofuels Eric G. O'Neill^{a,b}, Caleb H. Geissler^{a,b}, Christos T. Maravelias^{a,b,c}

^a Deprartment of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544, USA

- ^b DOE Great Lakes Bioenergy Research Center, USA
- ^c Andlinger Center for Energy and the Environment, Princeton University, Princeton, NJ, 08544, USA



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648	Evaluation of centralized/decentralized configuration schemes of CO2 electrochemical reduction-based supply chains <u>Thijmen Wiltink</u> , Stijn Yska, Andrea Ramirez, Mar Pérez-Fortes Department of Engineering, Systems, and Services, Faculty of Technology, Policy, and Management, Delft University
	of Technology, Jaffalaan 5, 2628 BX Delft
311	Resilience-aware multi-scale integration of distributed energy systems <u>Natasha J. Chrisandina</u> ^a , Shivam Vedant ^{b,c} , Eleftherios lakovou ^{b,d} , Efstratios N. Pistikopoulos ^{a,b} , Mahmoud M. El-Halwagi ^{a,b,g} ^a Artie McFerrin Department of Chemical Engineering, Texas A&M University, 3122 TAMU, 100 Spence St., College Station, USA
	 ^b Texas A&M Energy Institute, Texas A&M University, College Station, TX, 77843, USA ^c Department of Multidisciplinary Engineering, Texas A&M University, College Station, USA ^d Department of Engineering Technology and Industrial Distribution, Texas A&M University, College Station, USA
	^g Gas and Fuels Research Center, Texas A&M Engineering Experiment Station, College Station, USA
117	Developing a Comprehensive Decision Support Optimization Model for Biofuel Supply Chain Brook Tesfamichael ^a , <u>Ludovic Montastruc</u> ^{b,c} , Stéphane Negny ^{b,c} ^a Addis Ababa University, Addis Ababa Institute of Technology, School of Chemical & Bio Engineering, Addis Ababa, Ethiopia ^b Université de Toulouse, INP-ENSIACET, LGC (Laboratoire de Génie Chimique), 4, allée Emile Monso, Toulouse Cedex 04, France ^c CNRS, LGC (Laboratoire de Génie Chimique), oulouse Cedex 04, France
396	Gray and hybrid green ammonia price sensitivity to market fluctuations: the Russia-Ukraine war case Andrea Isella ^a , Alberto Lista ^a , Gabriele Colombo ^b , Raffaele Ostuni ^b , <u>Davide Manca^a</u> ^a PSE-Lab, Process Systems Engineering Laboratory, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy ^b Casale SA, Via Giulio Pocobelli 6, 6900 Lugano, Switzerland
45	Strategic participation of a gas-fired power plant in interdependent electricity and natural gas markets under carbon emission trading schemes <u>Christos N. Dimitriadis</u> , Evangelos G. Tsimopoulos, Michael C. Georgiadis Department of Chemical Engineering, Aristotle University of Thessaloniki, University Campus, Thessaloniki, 54124, Greece
() 10	0:20 – 12:30 ♀ Conf. Room II
SESSI	ON \$3-05: Process Integration and Intensification (In Memoriam: Prof. Jiri Klemes)
873	Resource Efficiency and Sustainability - Energy and Process Integration Championed by Professor Jiří Jaromír Klemeš <u>Petar Varbanov</u> Head of SPIL – Sustainable Process Integration Laboratory, NETME Centre, FME, Brno University of Technology – VUT Brno, Czech Republic
372	Systematic Development of Strategies for the Decarbonization of Process Utility Systems Julia Jiménez-Romero, Adisa Azapagic, Robin Smith Department of Chemical Engineering, The University of Manchester, Oxford Road, Manchester M13 9PL, UK
685	Optimization of large-scale energy systems to achieve carbon emissions neutrality <u>Sanja Potrč</u> ^a , Andreja Nemet ^a , Lidija Čuček ^a , Petar Varbanov ^b , Zdravko Kravanja ^a ^a Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia ^b Sustainable Process Integration Laboratory – SPIL, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology – VUT Brno, Technicka 2896/2, 616 69 Brno, Czech Republic
582	Design and optimization of a shared heat exchanger network for an integrated rSOC system Xinyi Wei ^{a,b} , Shivom Sharma ^a , Francois Marechal ^a , Jan Van Herle ^b ^a IPESE, EPFL Valais Wallis, 1950 Sion, Switzerland, ^b GEM, EPFL Valais Wallis, 1950 Sion, Switzerland

A novel industrial biotechnology approach to valorize fatty acids to bioplastics: scope for scale-up

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and process efficiency using an integrated approach

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	Pantelis Vasilakis ^a , Kostas Pyrgakis ^a , Melina Psycha ^a , Antonino Biunc ^a Chemical Engineering National Technical University of Athens, Athens, Greece ^b REWOW srl, Via Ciasca 9, 70124, Bari, Italy	lo ^ь , Antonis Kokossisª
835	Fully Electrified Conversion of Low-Quality Plastic Waste to Poly <u>Kristiano Prifti</u> ^{a,b} , Andrea Galeazzi ^{a,b} , Adrián Pacheco-López ^{a,c} , Antor ^a Politecnico di Milano, CMIC Department "Giulio Natta", Piazza Leonardo da Vir ^b Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali, ^c Department of Chemical Engineering, Universitat Politècnica de Catalunya, Esco Eduard Maristany 16, Barcelona 08019, Spain	mer Precursors nio Espuña ^c , Flavio Manenti ^{a,b} nci, 32, Milan 20133, Italy Via Giusti 9, 50121 Firenze, Italy ola d'Enginyeria de Barcelona Est, C /
146	Design of CO2 Capture and Mineralization Systems: Integrated R Controllability Assessment in Parallel Infrastructures <u>Thomas Prousalis</u> ^a , George Gkizas ^b , Athanasios I. Papadopoulos ^b , P ^a Y Squared P.C., 57019, Perea, Greece ^b Chemical Process & Energy Resources Institute, Centre for Research & Technolo c Department of Mechanical Engineering, Aristotle University of Thessaloniki, 541	Process Optimization and anos Seferlis ^c 19y Hellas, Thermi, Thessaloniki, Greece 24, Thessaloniki, Greece
2 10	0:20 – 12:30	♥ Conf. Room III
SESS	ON S3-06: Industrial Biotechnology (II)	Track 6
872	IBISBA - A Systems-oriented Research Infrastructure in Industrial Michael O'Donohue IBISBA	Biotechnology
775	Dynamic studies of metabolism empowered by Al Ljubisa Miskovic, Subham Choudhury, Vassily Hatzimanikatis Institute of Chemical Sciences and Engineering, School of Basic Sciences, Ecole F (EPFL), Switzerland	Polytechnique Fédérale de Lausanne
626	Upgrading an Industry 3.0 fermentation plant: A small step forward towards the future Mads Orla Kaiser-Albaek Fermentation Pilot Plant, Novozymes A/S, Bagsvaerd, Denmark	
698	Combined metabolic modeling and experimental data for enhan <u>Anita L. Ziegler</u> ^{a,*} , Melanie Filbig ^{b,*} , Johannes Parschau ^{a,b} , Till Tiso ^b , ^a Process Systems Engineering (AVT.SVT), RWTH Aachen University, Aachen, Gern ^b Institute of Applied Microbiology (iAMB), Aachen Biology & Biotechnology (ABBt), * Equally contributing authors	ced biotechnological production Lars M. Blank ^b , Alexander Mitsos ^a nany RWTH Aachen University, Aachen, Germany
313	Switching Multi-Objective Dynamic Optimization (MODO) for the P Juan C. Acosta-Pavas ^a , Carlos. E Robles-Rodríguez ^a , Jérôme Morch Claire Dumas ^a , Arnaud Cockx ^a , <u>César A. Aceves-Lara</u> ^a ^a TBI, Université de Toulouse, CNRS, INRAE, INSA, Toulouse, France ^b ToulouseWhite Biotechnology (TWB), INRAE, 135 Avenue de Rangueil, 31077 To	Production of Value-Added Products ain ^a , David Camilo Corrales ^b , pulouse, France
	Combined Devestor contrations and all help constants to the	an also a materia atom of

Combined Bayesian optimization and global sensitivity analysis for the optimization of 216 simulation-based pharmaceutical processes Niki Triantafyllou, Nilay Shah, Maria M. Papathanasiou, Cleo Kontoravdi The Sargent Centre for Process Systems Engineering, Imperial College London, London, United Kingdom, SW72AZ





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Track 1

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2 12:30 – 13:30	Olympia Foyer & Kallirhoe Room
LUNCH BRE	E A K
2 12:30 – 13:30	♥ Conf. Room IV
COMPUTERS & CHEMICAL ENGINEERING - EDITORIAL BC	ARD MEETING
2 12:30 – 13:30	♥ Conf. Room II
IRISS -SUSCHEM INTERNAL MEETING (Participation at the in	nternal meeting is by invitation only)
13:30 – 14:30	♥ Conf. Room II
IRISS THEMATIC SESSION ON SSbD	Participants need to register in advance
2 13:30 – 14:30	♥ Conf. Room III
TITAN: DIGITALIZING CEMENT MANUFACTURING IN THE	JOURNEY TOWARDS A NET-ZERO WORLD
Digitalizing cement manufacturing in the journey towards Othon Manis, Manufacturing Digitization & Data Management Directo Mr Panagiotis Papadeas, Environmental and Quality Director, Titan (a net-zero world r, Titan Cement Company SA Cement Company SA
13:30 – 14:30	for detailed poster program scan the QR Codes
POSTER SESSION	
Vallirhoe Hall POSTER SESSION 2-A Posters of Themes 5-8	Olympia FoyerPOSTER SESSION 2-BPosters of Themes 3-4
2 14:30 – 16:30	የ Olympia Hall

SESSION S4-01: Properties and Materials (II)

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Monte Carlo Simulation of Photo Induced Atom-Transfer Radical Polymerization for Microscopic Properties

<u>Rui Liu</u>^a, Xiaowen Lin^a, Antonios Armaou^{b,c,d}, Xi Chen^{a,e}

- ^a State Key Laboratory of Industrial Control Technology, College of Control Science and Engineering, Zhejiang University 310027, Hangzhou China
- ^b Chemical Engineering Department, University of Patras, Patras 26504, Greece
- ^c Chemical Engineering & Mechanical Engineering Departments, Pennsylvania State University, College Park, PA 16802 USA
- ^d College of Mechanical Engineering, Wenzhou University, 325035 Wenzhou China
- ^e National Center for International Research on Quality-targeted Process Optimization and Control, Zhejiang University 310027, Hangzhou China

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833	 Feature Embedding of Molecular Dynamics-Based Descriptors for Modeling Electrochemical Separation Processes H. K. Gallage Dona^{a,1}, T. Olayiwola^{b,1}, L. A. Briceno-Mena^b, C. G. Arges^c, R. Kumar^a, J. A. Romagnoli^b ^a Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803, USA ^b Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803, USA ^c Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 160802, USA
504	 ¹ Equal contribution Solvent pre-selection for extractive distillation using Gibbs-Helmholtz Graph Neural Networks Edgar Ivan Sanchez Medina^a, Kai Sundmacher^{a,b} ^a Chair for Process Systems Engineering, Otto-von-Guericke University, Universitätsplatz. 2, Magdeburg, 39106, Germany ^b Process Systems Engineering, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, Magdeburg, 39106, Germany
568	Improving Model Robustness with Transfer Learning for Product Property Models <u>Per Julian Becker</u> , Loic Iapteff, Benoit Celse IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France
750	The influence of biomass characteristics and their uncertainties on the production of sustainable aviation fuel <u>Moaaz Shehab</u> ^{a.b.c} , Diego Freire Ordóñez ^c , Mai Bui ^c , Kai Moshammer ^a , Edwin Zondervan ^b ^a Physikalisch Technische Bundesanstalt (PTB), Bundesallee 100, Braunschweig 38116, Germany ^b Twente University, Drienerlolaan 5, Enschede 7522 NB, the Netherlands ^c Imperial College London, Exhibition Rd, South Kensington, London SW7 2BX, UK
120	Substitution of hexane in vegetable oil extraction using Computer Aided Molecular Design <u>Mohamad Nehmeh</u> ^{a,b} , Ivonne Rodriguez-Donis ^a , Vincent Gerbaud ^b , Sophie Thiebaud-Roux ^a ^a Laboratoire de Chimie Agro-Industrielle, Université de Toulouse, INRAE, INP, Toulouse (Fr) ^b Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INP, UPS, Toulouse (Fr)
436	Molecular Modelling and Optimization of Diesel Hydrotreating Processes Xiaolin Bi ^a , Nan Zhang ^a , Robin Smith ^a ^a Centre for Process Integration, Department of Chemical Engineering, University of Manchester, Oxford Road, Manchester, M13 9PL,UK
422	Modeling aqueous multi-electrolyte systems for the simulation and optimization of concentrated brine processes Wajeha Tauqir, Adaeze C. Maduako, Xi Yang, <u>George M. Bollas</u> Department of Chemical and Biomolecular Engineering, UTC Institute for Advanced Systems Engineering, University of Connecticut, 159 Discovery Dr, Storr, CT, 06269, USA
2 14	I:30 – 16:30 ♀ Templar Hall
SESSI	ON S4-02: Operations and Supply Chains (III) Track 2
214	Supply Chain Optimization Considering Disruption Demand Uncertainty Oluwadare Badejo ^a , Marianthi Ierapetritou ^a ^a Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, 19711, USA
446	Reinforcement Learning for inventory management in multi-echelon supply chains Guoquan Wu ^c , Miguel Ángel de Carvalho Servia ^b , <u>Max Mowbray</u> ^a ^a Department of Chemical Engineering, University of Manchester, Oxford Road, Manchester, M1 3AL, UK ^b Sargent Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, SW7 2AZ, UK ^c Department of Chemical and Biomolecular Engineering, National University of Singapore, 117585, Singapore





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98	Supply chain optimal planning for revalorization of empty plastic pesticide and fertilizer containers Sergio Iván Martínez-Guido ^a , Rubén Bernabé-Martínez ^b , Claudia Gutiérrez-Antonio ^a , Salvador Hernandéz ^c ^a Universidad Autónoma de Querétaro, El Marqués, Querétaro, 76265, Mexico ^b PRANA Proyectos de Reciclaje y Acciones por la Naturaleza, Tuxtla Gutiérrez-Chiapas, 29000, Mexico ^c Universidad de Guanajuato, Guanajuato, 36050, Mexico
438	Life-cycle assessment of marine biofuels from thermochemical liquefaction of different olive residues in Spain Sivaramakrishnan Chandrasekaran, <u>Puck Wammes</u> , John A. Posada Delft University of Technology, Mekelweg 5, Delft and 2628 CD, the Netherlands
616	Analyzing the Large-Scale Supply of Low-Carbon Hydrogen in Germany Paul Sizaire, Emre Gençer MIT Energy Initiative, Massachusetts Institute of Technology, 400 Main Street, Cambridge, MA 02142, USA
413	Hydrogen infrastructure planning for heat decarbonisation in Great Britain <u>Margarita E. Efthymiadou</u> , Vassilis M. Charitopoulos, Lazaros G. Papageorgiou The Sargent Centre for Process Systems Engineering, Department of Chemical Engineering, University College London (UCL), Torrington Place, London WC1E 7JE, UK
407	Life Cycle Assessment of Two Liquid Organic Hydrogen Carriers Camille Bontron ^a , <u>Diogo Rodrigues^b</u> , Catarina G. Braz ^b , Henrique A. Matos ^b ^a INP-ENSIACET, 4 All. Emile Monso, CS 44362, 31030 Toulouse Cedex 4, France ^b Centro de Recursos Naturais e Ambiente, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal
65	 MINLP modelling and optimization of the supply chain for the renewable production of methanol in Mexico Nereyda Vanessa Hernández-Camacho^a, Fernando Israel Gómez-Castro^a, José María Ponce-Ortega^b, Mariano Martín^c ^a Universidad de Guanajuato, Campus Guanajuato, División de Ciencias Naturales y Exactas, Departamento de Ingeniería Química, Noria Alta S/N, Guanajuato, Guanajuato 36050, Mexico ^b Universidad Michoacana de San Nicolás de Hidalgo, Departamento de Ingeniería Química, Francisco J. Múgica S/N, Morelia, Michoacán 58060, Mexico ^c Universidad de Salamanca, Departamento de Ingeniería Química, Pza. Caídos 1-5, Salamanca 37008, Spain
	I:30 – 16:30 ♀ Attica Hall
SESSI	ON S4-03: Industrial Biotechnology (III) Track 3
397	Optimal dosing of thyroid hormones in hypothyroid patients with an individualized compartmental model Davide Manca, Federico Appiani, Giovanni Colombo PSE-Lab, Process Systems Engineering Laboratory, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy
641	A systematic mixed-integer linear programming approach for the solution of large-scale metabolism and protein expression (ME-models) O. Oftadeh, P. Salvy, M. Masid, M. Curvat, L. Miskovic, V. Hatzimanikatis

Laboratory of Computational Systems Biotechnology, EPFL, 1015, Lausanne, CH

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846	Improving accuracy scores of neural network driven QSAR models of mutagenicity Alexander D. Kalian ^a , Emilio Benfenati ^b , Olivia J. Osborne ^c , Jean-Lou C.M. Dorne ^d , David Gott ^c , Claire Potter ^c , Miao Guo ^a , Christer Hogstrand ^a ^a King's College London, Franklin-Wilkins Building, 150 Stamford St., London SE1 9NH, United Kingdom ^b IRCCS - Istituto di Ricerche Farmacologiche Mario Negri, Via Mario Negri 2, 20156 Milano, Italy ^c Food Standards Agency, 70 Petty France, London SW1H 9EX, United Kingdom ^d European Food Safety Authority (EFSA), Via Carlo Magno 1A, 43126 Parma, Italy
248	Workflow for adaptation, analysis and application of mechanistic models for experimental planning of protein refolding processes Jan Niklas Pauk ^{a,b} , Chika Linda Igwe ^{a,b} , Christoph Herwig ^b ^a Competence Center Chase GmbH, Altenberger Straße 69, 4040 Linz, Austria ^b Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Gumpendorfer Straße 1a, 1060 Vienna, Austria
559	 Parameter estimation combined with model reduction techniques for identifiability analysis of biological models <u>Michael Binns</u>^a, Alessandro Usai^b, Constantinos Theodoropoulos^b ^a Department of Chemical and Biochemical Engineering, Dongguk University-Seoul, 30 Pildong-ro 1-gil, Jung-gu, Seoul 04620, Republic of Korea ^b Department of Chemical Engineering, Biochemical and Bioprocess Engineering Group, The University of Manchester, Manchester M13 9PL, United Kingdom
73	Integrating hybrid modelling and transfer learning for new bioprocess predictive modelling Sam Kay ^a , Harry Kay ^a , Alexander W. Rogers ^a , Dongda Zhang ^a ^a Department of Chemical Engineering, University of Manchester, Oxford Road, Manchester, M1 3AL, UK
199	Closed-loop optimization of high-throughput robotic platforms for reproducible bioprocess development Federico M. Mione ^a , Judit Aizpuru ^b , Martin F. Luna ^a , Pablo Rodriguez Bahamon ^b , Jong Woo Kim ^b , Ernesto C. Martinez ^{a,b} , <u>M. Nicolas Cruz Bournazou^b</u> ^a INGAR (CONICET-UTN), Avellaneda 3657, S3002GJC Santa Fe, Argentina ^b KIWI-biolab, Bioprocess Engineering, TU Berlin, Ackerstrasse 76, 13355 Berlin, Germany
365	Digital Twins in Pilot Scale Fermentation: Non-Linear State Estimation for Improving Induction Timing Mads Stevnsborg ^a , Kurt Selle ^b , Ryan Barton ^b , Oscar A. Prado-Rubio ^{a,c} , Carina Gargalo ^a , Krist V. Gernaey ^a , Gary Gilleskie ^b , Jakob K. Huusom ^a ^a PROSYS, Dept. of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads, Building 228A, 2800 Kgs. Lyngby, Denmark ^b Golden LEAF, BTEC, NC State University, 27695 Raleigh, NC, USA ^c Departamento de Ingeniería Química, Universidad Nacional de Colombia – 170003 Manizales, Colombia
2 14	•:30 – 16:30 Conf. Room I
SESS	ON S4-04: Biobased Systems (II) Track 4
520	Profit Allocation in Industrial Symbiosis Networks: Utility Exchanges <u>Fabian Lechtenberg</u> , Antonio Espuña, Moisès Graells Department of Chemical Engineering, Universitat Politècnica de Catalunya, Barcelona 08019, Spain
554	Synthesis and optimization of NGL separation as a complex energy-integrated distillation sequence Qing Li ^{a,b} , Adrian J. Finn ^c , Stephen J. Doyle ^b , Robin Smith ^b , Anton A. Kiss ^a

- Qing Li^{a,b}, Adrian J. Finn^c, Stephen J. Doyle^b, Robin Smith^b, Anton A. Kiss^a
 - ^a Department of Chemical Engineering, Delft University of Technology, Van der Maasweg 9, 2629 HZ, Delft, The Netherlands
 - ^b Centre for Process Integration, Department of Chemical Engineering, The University of Manchester, Sackville Street, Manchester, M13 9PL, United Kingdom
 - ^c Costain, Costain House, 1500 Aviator Way, Manchester Business Park, Manchester, M22 5TG, United Kingdom







287	A Chance-Constrained Programming Approach to Optimal Planning of Low-carbon Transition of a Natural Gas Supply System: A Case Study of China Jiaqi Zhang, Pei Liu, Zheng Li Tsinghua BP Clean Energy Research and Education Centre, Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, China
118	Multi-stage optimization for marketing industrial flexibility <u>Martin Fischer</u> , Karl-Wilhelm Schenzel, René Hofmann Institute of Energy Systems and Thermodynamics, TU Wien, Getreidemarkt 9/302, 1060 Vienna, Austria
18	DynHeat: Heat Exchanger Network Design for Batch Processes via Dynamic Optimization Dörthe Franzisca Hagedorn ^a , Sören Demandt ^a , Florian Joseph Baader ^{b,c} , Christiane Reinert ^a , Niklas von der Aßen ^a ^a Institute of Technical Thermodynamics, RWTH Aachen University, Schinkelstr. 8, 52062 Aachen, Germany ^b Energy & Process Systems Engineering, Department of Mechanical & Process Engineering, ETH Zurich, Zürich, Switzerland ^c Institute of Energy & Climate Research, Energy Systems Engineering (IEK-10), Forschungszentrum Jülich GmbH, Jülich, Germany
62	Optimal Design of Heat Integrated Hybrid Dividing Wall Columns by Vapor Recompression Dian Ning Chia, Fanyi Duanmu, Eva Sorensen Department of Chemical Engineering, University College London (UCL), Torrington Place, London WC1E 7JE, UK
473	Hybrid Dynamic Surrogate Modelling for a Once-Through Steam Generator Sindre Stenen Blakseth ^{a,b} , Leif Erik Andersson ^a , Rubén Mocholí Montañés ^a , Marit Jagtøyen Mazzetti ^a ^a Department of Gas Technology, SINTEF Energy Research, Trondheim, Norway ^b Department of Mathematical Sciences, Norwegian University of Science and Technology, Trondheim, Norway
11	GHG emission reduction via multiple fuel options in carbon-constrained industrial clusters Christelle Bechara ^a , <u>Sabla Y. Alnouri^b</u> ^a Baha and Walid Bassatne Department of Chemical and Petroleum Engineering, American University of Beirut, P.O. Box 11-0236, Riyad El-Solh, Beirut, Lebanon ^b Gas Processing Center, College of Engineering, Qatar University, Doha, Qatar

2 14:30 – 16:30

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Conf. Room II

Track 5

SESSION S4-05: Sustainable and Circular Systems (III)

Decarbonization of energy-intensive industries: sustainable implementation of CO2 recycling within the industrial symbiosis

Marta Rumayor, Javier Fernández-González, Antonio Domínguez-Ramos, Angel Irabien Universidad de Cantabria, Departmento de Ingenierías Química y Biomolecular, Av. Los Castros s/n, Santander, Spain

Enviro-economic assessment of sustainable aviation fuel production from direct CO2 hydrogenation <u>Andrea Bernardi</u>^{a,b}, Daniel Bagan Casan^b, Andrew Symes^c, Benoit Chachuat^{a,b}

^a The Sargent Centre for Process Systems Engineering, Imperial College London,UK

- ^b Department of Chemical Engineering, Imperial College London, UK
- ° OXCCU Tech Ltd, Oxford, UK

- ^a Max Planck Institute for Dynamics of Complex Technical Systems, Process Systems Engineering, Sandstorstr. 1, 39106 Magdeburg, Germany
- ^b Chair for Process Systems Engineering, Otto-von-Guericke University, Universitätsplatz 2, 39106 Magdeburg, Germany

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60	 Waste valorisation within the Energy-Water-Food Nexus: A hybrid techno-geospatial optimisation approach Mohammad Alherbawi, Sarah Namany, Maryam Haji, Gordon McKay, Tareq Al-Ansari College of Science and Engineering, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar 	
803	Model-based Optimisation of Regional Nutrient Flow and Recover Environmental Sustainability Purusothmn Nair S Bhasker Nair ^a , Nan-Hua Nadja Yang ^a , Wei Zhang ^a Department of Engineering Science, University of Oxford, Parks Road, Oxford C ^b Department of Chemical Engineering, College of Engineering, Design and Physic Kingston Lane, Uxbridge UB8 3PH, UK	ery for Resource and J ^a , Kok Siew Ng ^{a,b} , Aidong Yang ^a IX1 3PJ, UK iical Sciences, Brunel University London,
639	Life cycle assessment of Pine needle-based electricity generation Pratham Khaitan, Ankush Halba, <u>Pratham Arora</u> Hydro and Renewable Energy Department, Indian Institute of Technology Roorke	n in India e, Roorkee-247667, India
724	 Prediction of biomedical waste generation in sanitary emergencies for urban regions using multivariate recurrent neural networks Nicolas Galvan-Alvarez, David Rojas-Casadiego, Viatcheslav Kafarov, <u>David Romo-Bucheli</u> Universidad Industrial de Santander, Bucaramanga, Santander, Colombia 	
813	Computer simulation of a plastic waste gasification-solid oxide for system using Aspen Plus Mahmudul Hassan Riyad, Sadman Fakid, <u>Nahid Sanzida</u> Department of Chemical Engineering, Bangladesh University of Engineering and	Jel cell power generation Technology, Dhaka-1000, Bangladesh
2 14	4:30 – 16:30	Conf. Room III
I SESSI	4:30 – 16:30 ION S4-06: Hydrogen and Carbon Capture (I)	Conf. Room III Track 6
14 SESSI 207	4:30 – 16:30 ON S4-06: Hydrogen and Carbon Capture (I) A Power-to-Gas energy system: modeling and operational optim supply and storage <u>Yifan Wang</u> , Luka Bornemann, Christiane Reinert, Niklas von der Aß Institute of Technical Thermodynamics, RWTH Aachen University, Schinkelstr. 8, 5.	Conf. Room III Track 6 ization for seasonal energy Gen 2062 Aachen, Germany
1/ SESSI 207	 4:30 – 16:30 ON S4-06: Hydrogen and Carbon Capture (I) A Power-to-Gas energy system: modeling and operational optim supply and storage Yifan Wang, Luka Bornemann, Christiane Reinert, Niklas von der Affinstitute of Technical Thermodynamics, RWTH Aachen University, Schinkelstr. 8, 5. Multiobjective optimization of distributed energy systems design environmental and exergy) analysis Bogdan Dorneanu^a, Sayeef Miah^b, Evgenia Mechleri^b, Harvey Arella ^a LS Prozess und Anlagentechnik, Brandenburgische Technische Universität Cottbus ^b Department of Chemical and Process Engineering, University of Surrey, Guildford 	♥ Conf. Room III Track 6 ization for seasonal energy ien 2062 Aachen, Germany n through 3E (economic, no-Garcia ^a s-Senftenberg, Cottbus D-03046, Germany d GU27XH, UK
 1/ SESSI 207 332 466 	 4:30 – 16:30 ON S4-06: Hydrogen and Carbon Capture (I) A Power-to-Gas energy system: modeling and operational optim supply and storage Yifan Wang, Luka Bornemann, Christiane Reinert, Niklas von der AB Institute of Technical Thermodynamics, RWTH Aachen University, Schinkelstr. 8, 5. Multiobjective optimization of distributed energy systems design environmental and exergy) analysis Bogdan Dorneanu^a, Sayeef Miah^b, Evgenia Mechleri^b, Harvey Arella ^a LS Prozess und Anlagentechnik, Brandenburgische Technische Universität Cottbus ^b Department of Chemical and Process Engineering, University of Surrey, Guildfor Electrification of ethylene production: exploring the potential of Julia L. Tiggeloven^a, André P.C. Faaij^{a,b}, Gert Jan Kramer^a, Matteo G^a Copernicus Institute of Sustainable Development, Utrecht University, the Netherl^b TNO Energy Transition, the Netherlands 	Conf. Room III Track 6 ization for seasonal energy den 2062 Aachen, Germany a through 3E (economic, no-Garcia ^a s-Senftenberg, Cottbus D-03046, Germany d GU27XH, UK flexible operation iazzani ^a lands

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857	Evaluation of Factors Affecting Novel Technology Developmen Pooja Zen Santhamoorthy, <u>Selen Cremaschi</u> Department of Chemical Engineering, Auburn University, AL 36849, USA	nt using Mathematical Programming
468	An MINLP model for the optimal design of CO2 transportation infrastructure in industrial clusters Jude O. Ejeh ^a , Sergey B. Martynov ^b , <u>Solomon F. Brown</u> ^a ^a Department of Chemical & Biological Engineering, The University of Sheffield, Mappin Street, Sheffield, S1 3JD, UK ^b Department of Chemical Engineering, University College London, London, WC1E 7JE, UK	
15	5 Optimal ship-based CO2 transport chains from Mediterranean emission points to the North Sea <u>Federico d'Amore</u> , Matteo C. Romano Politecnico di Milano, Department of Energy, via Lambruschini 4, IT-20156 Milano, Italy	
642	Evaluation of alternative carbon based ethylene production in Technology screening & value chain impact assessment James Tonny Manalal, Mar Pérez-Fortes, Paola Ibarra Gonzalez, A Department of Engineering, Systems and Services, Faculty of Technology Polic of Technology, Jaffalaan 5, 2628BX, Delft, the Netherlands	a petrochemical cluster: Andrea Ramirez Ramirez and Management, Delft University
2 1	6:30 – 16:50	♥ Olympia Foyer & Kallirhoe Room
	COFFEE BREAK	
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U 1	6:50 – 18:35	🕈 Olympia Hall
SESS	ION S5-01: Operations and Control (III)	Track 1
834	Fault detection using Fourier neural operator <u>Jyoti Rani</u> ^a , Tapas Tripura ^c , Umang Goswami ^a , Hariprasad Kodam ^a Department of Chemical Engineering, Indian Institute of Technology Delhi, N ^b Yardi School of Artificial Intelligence, Indian Institute of Technology Delhi, N ^c Department of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute of Technology Delhi, Neuroperative Statement of Applied Mechanics, Indian Institute Statement State	ana ^{a,b} , Souvik Chakraborty ^{b,c} New Delhi-110016, India ew Delhi-110016, India v Delhi-110016, India
145	 Application of Bayesian Optimization in HME Batch Concentration Process <u>Chong Liu</u>^a, Cheng Ji^a, Chengyu Han^a, Chenxi Gu^b, Jindong Dai^a, Wei Sun^a, Jingde Wang^a ^a College of Chemical Engineering, Beijing University of Chemical Technology, North Third Ring Road 15, Chaoyang Distric Beijing, 100029, China ^b Shijiazhuang Lonzeal Pharmaceutical Co., Ltd., No. 16 West Ring Road, Shenze County Industrial Park, Shijiazhuang, Hebrovice, 052560, China 	
815	 Unsupervised anomaly detection model for diesel off-spec color change triggered by flooding <u>A. Eren Vedin</u>^a, Sadık Odemis^b, Aysegul Sener^b, Gizem Kayar^b, Mammad Aliyev^b ^a SOCAR Turkey, Vadistanbul, Istanbul 34485, Turkey ^b SOCAR STAR Oil Refinery, Aliaga, Izmir 35800, Turkey 	
637	Moisture & Throughput Control in an Integrated Pharmaceutical Purification Platform using Pharma Inyoung Hur, Daniel Casas-Orozco, Gintaras Reklaitis, Zoltan K. Nagy Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN 47907 USA	
579	Residence Time Distribution characterization in a Continuous PCA and PLS-DA modeling Pau Lapiedra Carrasquer ^a , Satyajeet S. Bhonsale ^a , Liang Li ^b , Jan F ^a BioTeC+, KU Leuven, Gebroeders De Smetstraat 1, Gent 9000, Belgium ^b Janssen Pharmaceutica, Turnhoutseweg 30, Beerse Antwerp 2340, Belgium	Manufacturing tableting line using

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^a Indian Institute of Technology Gandhinagar, Gujarat, 382355, India

^b Indian Institute of Technology Madras, Tamil Nadu, 600036, India

^c American Express Lab for Data Analytics, Risk & Technology, Indian Institute of Technology Madras, Tamil Nadu, India

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A comparative study of distributed feedback-optimizing control strategies Vegard Aas, <u>Risvan Dirza</u>, Dinesh Krishnamoorthy, Sigurd Skogestad Department of Chemical Engineering, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

🕗 16:50 – 18:35

♥ Templar Hall

SESSI	ON S5-02: Sustainable and Circular Systems (IV)	Track 2
767	Regional sustainability of food-energy-water nexus considering a modeling and optimization Anupam Satyakam, Rashi Dhanraj, Yogendra Shastri Indian Institute of Technology Bombay, Mumbai 400076, India	water stress using multi-objective
22	Simulation and optimisation of a medium scale industrial reverse Mudhar A. Al-Obaidi ^a , Alanood A. Alsarayreh ^b , <u>Iqbal M. Mujtaba</u> ^c ^a Middle Technical University, Technical Institute of Baquba, Baquba, Dayala – Irac ^b Chemical Engineering Department, Mu'tah University, Al Karak – Jordan ^c Chemical Engineering Department, University of Bradford, Bradford BD7 1DP, U	e osmosis desalination system
268	Predictive Modeling and scale-up of Wet Oxidation for Hydrothe Water treatment Carolin Eva Schuck ^{a,b} , Thomas Schäfer ^b , <u>Konstantinos Anastasakis</u> ^a ^a Department of Biological and Chemical Engineering, Aarhus University, Hangøv ^b Department of Chemical Engineering and Biotechnology, Hochschule Darmstad Stephanstraße 7, Darmstadt 64295, Germany	ermal Liquefaction Process rej 2, Aarhus 8200, Denmark dt – University of applied sciences,
652	Different methods of model-based process optimization present from water industry Dr. Ewa Bozek, Dr. Corinna Busse, Delia Gietmann, Dr. Bernd-Marke Siemens AG, Siemenspromenade 3, Erlangen 91058, Germany	ed on real world examples us Pfeiffer
128	Physics-informed Neural Network based Modeling of an Industri Tuse Asrav ^{a,b} , Ece Serenat Koksal ^{a,b} , Elif Ecem Esenboga ^c , Ahmet Co Duygu Aydin ^c , <u>Erdal Aydin^{a,b}</u> ^a Department of Chemical and Biological Engineering, Koç University, Istanbul 34 ^b Koç University TUPRAS Energy Center (KUTEM), Koç University, Istanbul, 34450, ^c Turkish Petroleum Refineries Corporation, Körfez, Kocaeli 41790, Turkey	al Wastewater Treatment Unit osgun ^c , Gizem Kusoglu ^c , 450, Turkey Turkey
379	Knowledge-based model and simulations to support decision matrix treatment processes Claire Valentin ^a , Frédéric Lagoutière ^b , Jean-Marc Choubert ^c , Franço ^a Univ Lyon, Université Claude Bernard Lyon 1, CNRS, LAGEPP UMR 5007, 43 bou Villeurbanne, France ^b Univ Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Camille Jordan, UM 1918, 69622 Villeurbanne Cedex, France ^c INRAE REVERSAAL, 69625 Villeurbanne, France	aking in wastewater hise Couenneª, Christian Jallutª hlevard du 11 novembre 1918, 69100, IR 5208, 43 boulevard du 11 novembre

decision-making tool

Felipe Buendia^{1,2}, Julie Perrin^{1,2}, Sandra Domenek^{1,2}

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GREEN AND SUSTAINABLE PROCESS SYSTEMS ENGINEERING IN THE DIGITAL AGE

Comparison of different waste management systems in France: Process simulation and

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	¹ Université Paris-Saclay, INRAE, AgroParisTech, UMR SayFood, Campus AgroPar ² Chaire CoPack, 91120 Palaiseau, France	isSaclay, 91120 Palaiseau, France
2 1	6:50 – 18:35	♥ Attica Hall
SESS	ION S5-03: Industrial Biotechnology (IV)	Track 3
753	Global Optimal Explainable Models for Biorefining Jiayang Ren, Kaixun Hua, Heather Trajano, <u>Yankai Cao</u> Department of Chemical & Biological Engineering, University of British Columbia, 2	2360 East Mall, Vancouver V6T 1Z3, Canada
132	Optimal Retrofitting of Conventional Oil Refinery into Sustainable Bio-refinery under Uncertainty Lifeng Zhang ^a , Ana Inés Torres ^b , Bingzhen Chen ^a , Zhihong Yuan ^a , Ignacio E. Grossmann ^b ^a Department of Chemical Engineering, Tsinghua University, Beijing, 100084, China ^b Chemical Engineering Department, Carnegie Mellon UniVersity, Pittsburgh, Pennsylvania 15213, USA	
682	Modeling, simulation & techno-economic analysis of an integrated biorefinery based on halophytes <u>Tutku Taşçı Çilak</u> ^a , Sanketkumar Raval ^a , Sylvia Fasse ^a , Mette H. Thomsen ^b , Axel Gottschalk ^a ^a Institute of Process Engineering, Bremerhaven University of Applied Sciences, An der Karlstadt 8, Bremerhaven, Germany ^b Department for Energy Technology, Aalborg University, Esbjerg Campus, Niels Bohrs Vej 8, 6700 Esbjerg, Denmark	
111	Thermodynamic equilibrium modelling for the optimal performa gasifier for hydrogen production <u>Anamika Kushwah</u> ^a , Tomas Ramirez Reina ^{a,b} , Michael Short ^a ^a University of Surrey, Guildford, GU27XH, UK ^b Institute of Materials Science of Seville, Seville, 41092, Spain	nce of a wood biomass downdraft
327	Superstructure configuration and optimization of the biofuel production perspectives in Austria Safdar Abbas, Ada Josefina Robinson, Stavros Papadokonstantakis Institute of Chemical, Environmental and Bioscience Engineering TU Wien, 1060 Wien, Austria	
86	Troubleshooting high-pressure issues in an industrial biorefinery process by feature-oriented modeling <u>Elia Arnese-Feffin</u> ^a , Pierantonio Facco ^a , Daniele Turati ^b , Fabrizio Bezzo ^a , Massimiliano Barolo ^a ^a CAPE-Lab – Computer-Aided Process Engineering Laboratory, Department of Industrial Engineering, University of Padova, via Marzolo 9, 35131 Padova, Italy ^b Novamont S.p.A., via G. Fauser 8, 28100 Novara, Italy	
841	Process modelling of the hydrothermal liquefaction of oil-palm v and hydrochar production Muhammad Shahbaz ^{a,b} , Mohammad Alherbawi ^a , Prakash Parthasarat Tareq Al-Ansari ^a ^a College of Science and Engineering, Hamad Bin Khalifa University, Qatar Found ^b Centre of Bio-Fuel and Biochemical Research, Department of Chemical Engineer 32610 Bandar Seri Iskandar, Perak, Malaysia	vaste for biocrude hyª, Gordon McKayª, lation, Doha, Qatar ering, Universiti Teknologi PETRONAS,

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(⁄) 16:50 - 18:35 🖓 Conf. Room I SESSION S5-04: Biobased Systems (III) Track 4 Into the Valley of Death Rode the Green Transition 850 Robert Pujan^{a,b}, Heinz A. Preisig^b ^a BNT Chemicals GmbH, PC-Straße 1, 06749 Bitterfeld-Wolfen, Germany ^b NTNU Norwegian University of Science and Technology, Høgskoleringen 5, 7491 Trondheim, Norway 297 Integration of metabolic models in biorefinery designs using superstructure optimisation Lucas Van der Hauwaert^a, Alberte Requeira^{a,b}, Miguel Mauricio-Iglesias^a ^a CRETUS, Department of Chemical Engineering. Universidade de Santiago de Compostela, 15782, Santiago de Compostela, Spain ^b Center for Microbial Ecology and Technology (CMET), Ghent University, B-9000, Ghent, Belgium Closing the balance- the pulp industry as a prosumer in the energy system 697 Julia Granacher^a, Jonas Schnidrig^a, Meire Ellen Gorete Ribeiro Domingos^{a,b}, Rafael Castro-Amoedo^a, François Maréchal^a ^a Ecole Polytechnique Fédérale de Lausanne, Rue de l'industrie 17, 1950 Sion, Switzerland ^b Department of Chemical Engineering, University of Sao Paulo, Brazil Enhanced hot-liquid water pretreatment of biomass with recovery and valorization of side products 805 Tamara Janković^a, Adrie J. J. Straathof^a, Anton A. Kiss^{a,b} ^a Department of Biotechnology, Delft University of Technology, van der Maasweg 9, 2629 HZ Delft, The Netherlands ^b Department of Chemical Engineering, Delft University of Technology, van der Maasweg 9, 2629 HZ Delft, The Netherlands 472 Simulation-based design of regional biomass thermochemical conversion system for improved environmental and socio-economic performance Leonardo L. Corradini^a, Aya Heiho^b, Yuichiro Kanematsu^b, Ryoko Shimono^b, Satoshi Ohara^c, Yasunori Kikuchi^{a,b,c} ^a Department of Chemical Sytem Engineering, the University of Tokyo, 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113-8656, Japan ^b Presidential Endowed Chair "Platinum Society", the University of Tokyo, 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113-8656, Japan ^c Institute for Future Initiatives, the University of Tokyo, 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113-8654, Japan Sustainability assessment of poly(butylene succinate) production and End-of-Life options from 796 wheat straw Sofia-Maria Ioannidou^a, Dimitrios Ladakis^a, Ricardo Rebolledo-Leiva^b, Maria Teressa Moreira^b, Ioannis K. Kookos^c, Apostolis Koutinas^a ^a Department of Food Science and Human Nutrition, Agricultural University of Athens, Iera Odos 75, 118 55 Athens, Greece ^b Department of Chemical Engineering, School of Engineering, Universidade de Santiago de Compostela, D Rúa Lope Gómez de Marzoa, s/n, 15782, Santiago de Compostela, Spain ^c Department of Chemical Engineering, University of Patras, 26504, Rio, Greece Architectural Design of Chemical and Biological Pathways through Parameter Sensitivity Oriented 361 **Mixed Integer Formulations** Emir Topac^a, Emrullah Erturk^a, Ozgun Deliismail^b, Sahin Sarrafi^b, <u>Hasan Sildir</u>^a ^a Department of Chemical Engineering, Gebze Technical University, Kocaeli, 41400, Türkiye ^b SOCAR Turkey R&D and Innovation Co., Izmir, 35800, Türkiye

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2 1	6:50 – 18:35	♥ Conf. Room II
SESS	ION S5-05: Modelling and Optimization (II)	Track 5
97	 Modeling and optimization of cascade reactions of enzymes immode Leandros Paschalidis^{a,b}, Jakob Burger^{a,b} ^a Laboratory of Chemical Process Engineering, Technical University of Munich, Came Sustainability, Uferstraße 53, 94315 ^b SynBioFoundry@TUM, Technical University of Munich, Campus Straubing for Biote Schulgasse 22, 94315, Straubing, Germany 	obilized in porous particles apus Straubing for Biotechnology and echnology and Sustainability,
227	Modeling of a trickle bed reactor: Study of arabinose oxidation of Mouad Hachhach ^a , Vincenzo Russo ^{a,b} , Dmitry Yu. Murzin ^a , Tapio Salr ^a Laboratory of Industrial Chemistry and Reaction Engineering (TKR), Johan Gado Akademi University, Åbo-Turku FI-20500, Finland ^b Università di Napoli Federico II, Chemical Sciences, Complesso Universitario Mo	on gold catalyst extrudates miª olin Process Chemistry Centre (PCC), Åbo onte S. Angelo, Napoli IT-80126, Italy
400	Modelling of iron oxide reduction with hydrogen <u>Emiliano Salucci</u> ^a , Snigdha Ghosh ^b , Vincenzo Russo ^c , Henrik Grénma ^a Åbo Akademi University, Henrikinkatu 2, Turku 20500, Finland ^b IIT (ISM) Dhanbad, Jharkhand, Dhanbad 826001, India ^c University of Naples Federico II, Via Vicinale Cupa Cintia 26, Napoli 80126, Italy	anª, Henrik Saxénª
401	 Parameter estimation approach applied to microalgae-bacteria p <u>Irina Bausa-Ortiz</u>^{a,b}, Raul Muñoz^{a,c}, Smaranda P. Cristea^{a,b}, Cesar de I ^a Institute of Sustainable Processes, Universidad de Valladolid, Dr. Mergelina s/n, ^b Dpt. of Systems Engineering and Automatic Control, School of Industrial Engine Prado de la Magdalena 3-5, Valladolid 47011, Spain ^c Dpt. of Chemical Engineering and Environmental Technology, School of Industria Dr. Mergelina, s/n, Valladolid 47011, Spain 	photobioreactor Prada ^{a,b} Valladolid 47011, Spain eering, Universidad de Valladolid, ial Engineering, Universidad de Valladolid,
839	In-silico investigation of microalgae culture performance in lab a between reactor size and productivity <u>Christos Chatzidoukas</u> , Vasileios Parisis Department of Chemical Engineering, Aristotle University of Thessaloniki (AUTH),	nd pilot scale: The trade-off , P.O. Box: 472, 54124, Thessaloniki, Greece
134	A Combined D-optimal and Estimability Model-Based Design of Crystallization Process Xuming Yuan, Brahim Benyahia Department of Chemical Engineering, Loughborough University, Epinal Way, Lou	Experiments of a Batch Cooling Ighborough, LE11 3TU, United Kingdom
709	 An NN-NMPC for Controlling a Crystallization Process in the Sate Fernando Arrais R. D. Lima^a, Marcellus G. F. de Moraes^b, Amaro G. Maurício B. de Souza Jr.^{a,b} ^a School of Chemistry, EPQB, Universidade Federal do Rio de Janeiro, Av. Horácio Rio de Janeiro, RJ – Brazil ^b PEQ/COPPE – Universidade Federal do Rio de Janeiro, Av. Horácio Macedo, 20 Rio de Janeiro, RJ – Brazil 	urated and Undersaturated Zones Barreto ^a , Argimiro R. Secchi ^{a,b} , o Macedo, 2030, CT, Bloco E, 21941-914, 030, CT, Bloco G, G115, 21941-914,

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2 16:50 – 18:35 Conf. Room III SESSION S5-06: Hydrogen and Carbon Capture (II) Track 6 Comparing operational strategies for alkaline electrolysis systems considering a probabilistic wind 625 power distribution Lucas Cammann, Johannes Jäschke Department of Chemical Engineering, Norwegian University of Science and Technology, NTNU, N-7491 Trondheim, Norway 273 Optimal production of green hydrogen with grid assistance for enhanced flexibility Christopher Varela^{a,b,c}, Mahmoud Mostafa^a, Edwin Zondervan^d ^a Laboratory of Process Systems Engineering, University of Bremen, Leobener Str. 6, 28359 Bremen, Germany ^b Facultad de Ciencias Naturales y Matemáticas, Escuela Superior Politécnica del Litoral, ESPOL, Campus Gustavo Galindo, Km. 30.5 Vía Perimetral, Guayaquil P.O.Box 09-01-5863, Ecuador ° Centro de Energías Renovables y Alternativas, CERA, Escuela Superior Politécnica del Litoral, ESPOL, Campus Gustavo Galindo, Km. 30.5 Vía Perimetral, Guayaquil P.O. Box 09-01-5863, Ecuador ^d SPT-PSE, University of Twente, 7522NB Enschede, The Netherlands 174 Economic Benefits from Planned Renewable Installations in the US using Hydrogen and Modular **Ammonia Production Units** Apoorv Lal, Fengqi You Cornell University, Ithaca, New York 14853, USA Techno-enviro-economic analysis of H2 economy in China from H2 production to utilization 314 Xiaodong Hong^a, Zuwei Liao^b, Yao Yang^{a,b}, Jingdai Wang^b, Yongrong Yang^b ^a ZJU-Hangzhou Global Scientific and Technological Innovation Center, Hangzhou 311215, China ^b State Key Laboratory of Chemical Engineering, College of Chemical and Biological Engineering, Zhejiang University, Hangzhou 310027, China Planetary Environmental Benefits of CO2-to-Ethylene Direct Bifunctional Catalytic Synthesis 673 Cecilia Salah, Iasonas Ioannou, Stavroula Batsolaki, Gonzalo Guillén-Gosálbez Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences ETH Zürich, Switzerland Techno-economic assessment of a novel reforming process with low energy demand for high-620 purity hydrogen production Athanasios Arampatzis, Theodoros Papalas, Andy N. Antzaras, Angeliki A. Lemonidou Department of Chemical Engineering Aristotle University of Thessaloniki (AUTh), Greece **Process Simulation Approaches to Reduce Commercial Risk of CCS Projects** 38 Ryan Muir^a, Ralph Cos^b, Chloe Smith^b, Stelios Papastratos^c ^a AVEVA, Lake Forest, California, United States of America ^b AVEVA, Munich, Bavaria, Germany ^c AVEVA, Thessaloniki, Greece

I9:30 – 23:30

ESCAPE 33 GALA DINNER

♥ Zappeion Mansion

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30 🛇	3:00 – 09:00	
REGIS	STRATIONS	
30 🛇	3:30 – 09:00	♥ Olympia Hall
Prese	ntation of ESCAPE 34	
09	9:00 – 10:00	오 Olympia Hall
PLEN. Chairs	ARY SESSION 4 s: Prof. Christos Maravelias, Prof. Edwin Zondervan	
Quo \ Prof. \	/adis ChatGPT? Challenges and Opportunities in Process Systems /enkat Venkatasubramanian, Columbia University	Engineering
2 10	0:00 – 10:20	Olympia Foyer & Kallirhoe Room
	COFFEE BREAK	
2 10	0:20 – 12:30	🕈 Olympia Hall
SESSI	ON S6-01: Energy Systems (II)	Track 1
21	Model-Based Design of Experiments for the identification of mic limiting nutrients Alberto Saccardo, Beatriz Felices-Rando, Eleonora Sforza, <u>Fabrizio</u> Department of Industrial Engineering, University of Padova, Via Marzolo 9, Padov	croalgae growth models with <u>Bezzo</u> va 35131, Italy
305	Strategic low-carbon hydrogen supply chain planning under mar <u>Tushar Rathi</u> ^a , Jose M. Pinto ^b , Qi Zhang ^a ^a Department of Chemical Engineering and Materials Science, University of Minn ^b Linde Digital Americas, Linde plc, Danbury, CT 06810, USA	r ket price uncertainty nesota, Minneapolis, MN 55455, USA
658	A Novel Approach for Cost-effective and Sustainable Capacity E Intensification in Chemical Process Industries Chinmoy B. Mukta, Selen Cremaschi, Mario R. Eden Department of Chemical Engineering, Auburn University, Auburn, AL 36849, USA	Expansion Utilizing Process
90	The controlled environment agriculture: a sustainable agrifood p by systems engineering Liang Wang ^{a,d} , Guoping Lian ^{a,b} , Zoe Harris ^a , Mark Horler ^c , Yang War ^a Faculty of Engineering & Physical Sciences, University of Surrey, Guildford, GU2 ^b Unilever R&D Colworth, Sharnbrook, Bedfordshire, MK40 1LQ, UK ^c UK Urban AgriTech, 46 Jamaica Street, Liverpool, L1 0AF, UK ^d National Innovation Center for Digital Fishery, China Agricultural University, Bei	production paradigm empowered ng ^d , <u>Tao Chen</u> ª 27XH, UK jing, 100083, China
187	Modular vs centralized manufacturing supply chain: identifying t <u>Alessandro Di Pretoro</u> , Stéphane Negny, Ludovic Montastruc Laboratoire de Génie Chimique, Université de Toulouse, CNRS/INP, Toulouse, Fr	he best solution under uncertainty
490	Cross-domain Fault Diagnosis for Chemical Processes through Dyna <u>Ruoshi Qin</u> ^a , Jinsong Zhao ^{a,b} ^a State Key Laboratory of Chemical Engineering, Department of Chemical Engine ^b Beijing Key Laboratory of Industrial Big Data System and Application, Tsinghua	mic Adversarial Adaptation Network eering, Tsinghua University, Beijing, China University, Beijing, China

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2 10:20 – 12:30 Templar Hall SESSION S6-02: Modelling and Optimization (III) Track 2 Multi-scale model of solid oxide fuel cell: enabling microscopic solvers to predict physical 557 features over a macroscopic domain Hamid Reza Abbasi^a, Masoud Babaei^a, Arash Rabbani^b, <u>Constantinos Theodoropoulos</u>^a ^a Department of Chemical Engineering, The University of Manchester, Manchester, M13 9PL, UK ^b School of Computing, The University of Leeds, UK From problem specification to converged flowsheet simulations: Integrated workflow in an 244 industrial context Mirko Skiborowski^a, Norbert Asprion^c, Sergej Blagov^c, Michael Bortz^b, Dennis Manuel Heim^b, Kai Fabian Kruber^a, Thulasi Rolland^a, Tobias Seidel^b ^a Hamburg University of Technology, Institute of Process Systems Engineering, Am Schwarzenberg-Campus 4, Hamburg, Germany ^b Fraunhofer Institut für Techno- und Wirtschaftsmathematik, Optimierung, Fraunhofer Platz 1, Kaiserslautern, Germany ^c BASF SE, Process Modeling & Cheminformatics, Carl-Bosch-Str. 38, 67063 Ludwigshafen am Rhein, Germany 37 Multiscale Modeling of Spatial Area-Selective Thermal Atomic Layer Deposition Matthew Tom^a, Sungil Yun^a, Henrik Wang^a, Feiyang Ou^a, Gerassimos Orkoulas^b, Panagiotis D. Christofides^{ac} ^a Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095-1592, USA ^b Department of Chemical Engineering, Widener University, Chester, PA 19013, USA ^c Department of Electrical and Computer Engineering, University of California, Los Angeles, CA 90095-1592, USA Efficient 1D modelling of hot melt extrusion process for pharmaceutical applications 288 Michaela Vasilaki^a, Umair Zafar^b, Ioannis .S. Fragkopoulos^c, <u>Ioannis K. Kookos</u>^a ^a Department of Chemical Engineering, University of Patras, Rio, 26504, Patras Greece ^b Oral Formulation Research, Novo Nordisk A/S, Måløv, Denmark ^c Oral Drug Product Process Development, Novo Nordisk A/S, Måløv, Denmark A novel mathematical formulation for short-term scheduling of multipurpose batch plants in 137 chemical manufacturing Dan Li, Taicheng Zheng, Jie Li Centre for process Integration, Department of Chemical Engineering, University of Manchester, Manchester, M13 9PL, UK A Global Optimization Algorithm for the Solution of Mixed-Integer Quadratic Adjustable Robust 487 **Optimization Problems under Endogenous Uncertainty** Byungjun Lee, Styliani Avraamidou Department of Chemical & Biological Engineering, University of Wisconsin-Madison, 1415 Engineering Dr, Madison, WI 53706, USA 2 10:20 – 12:30 Attica Hall SESSION S6-03: Data Driven Applications (III) Track 3 Multi-fidelity Bayesian Optimisation of Reactor Simulations using Deep Gaussian Processes

- Tom Savage, Nausheen Basha, Omar K. Matar, <u>Antonio del Rio Chanona</u> Imperial College London, London SW7 2BX, United Kingdom.
- **Digital Twin A System for Testing and Training** <u>Michael Schueler</u>, Tanja Mehling Siemens AG, DI PA SW ID MBS OA , Industriepark Hoechst, B598, 65926 Frankfurt

242	A Reinforcement Learning Development for the Exact Jie-Ying Su ^a , Chia-Hsiang Liu ^c , Cian-Shan Syu ^c , Jia-Lir ^a Department of Chemical Engineering, National Tsinghua Univ ^b Department of Chemical & Materials Engineering, National Yu ^c Department of Industrial Engineering & Engineering Manager	Guillotine with Flexibility on Cutting Stock Problem Kang ^b , Shi-Shang Jang ^a ersity, Hsinchu, Taiwan ROC nlin University of Science & Technology, Yunlin, Taiwan ROC nent, National Tsinghua University, Hsinchu, Taiwan ROC
355	Globally Convergent Composite-Step Trust-Region Optimization Duo Zhang ^a , Xiang Li ^b , Kexin Wang ^a , Zhijiang Shao ^a ^a College of Control Science and Engineering, Zhejiang University ^b Department of Chemical Engineering, Queen's University, King	Framework for Model-Based Real-Time ity, Hangzhou, 310027, China gton, ON K7L 3N6, Canada
445	A joint model-based design of experiments approx in geological exploration <u>Philipp Deussen</u> , Federico Galvanin Department of Chemical Engineering, University College Londo	ach for the identification of Kriging models
609	Learning interpretable multi-output models: Kaize for estimating outlet concentrations of a splitter Jimena Ferreira ^{a,b} , Martín Pedemonte ^b , Ana I. Torres ^c ^a Instituto de Ingeniería Química, IIQ, Facultad de Ingeniería, Univ ^b Instituto de Computación, INCO, Facultad de Ingeniería, Univ ^c Department of Chemical Engineering, Carnegie Mellon Universit	n Programming based symbolic regression niversidad de la República, Montevideo, 11600, Uruguay ersidad de la República, Montevideo, 11600, Uruguay ty, 5000 Forbes Ave., Doherty Hall, Pittsburgh, PA, 15213, USA
1 0	0:20 – 12:30	Conf. Room l
SESSI	ON S6-04: Energy Systems (III)	Track 4
188	Computer aided-design of energy efficiency tools Araceli Guadalupe Romero-Izquierdo ^a , Claudia Gutié Salvador Hernández ^b , Juan Fernando García-Trejo ^a ^a Facultad de Ingeniería, Universidad Autónoma de Querétaro, ^b Departamento de Ingeniería Química, Universidad de Guanaj	on a microalgae biorefinery scheme rrez-Antonioª, Fernando Israel Gómez-Castro ^b , Cerro de las Campanas S/N, Querétaro, México Jato, Noria Alta S/N, Guanajuato, México
157	A MILP-based approach to manage logistics in large industrial gas supply chains Sergio G. Bonino ^a , Luis J. Zeballos ^a , Akash Moolya ^c , Jose Lainez ^c , Jose M. Pinto ^c , Ignacio E. Grossmann ^b , <u>Carlos A. Méndez^a</u> ^a Intec (UNL-CONICET), Güemes 3430, Santa Fe 3000, Argentina ^b Carnegie Mellon University, 5000 Forbes, Pittsburgh 15213, USA ^c Praxair, Inc., a Linde company, Connecticut 06810, USA	
701	Dynamic operation for the effective use of green hydrogen in Power-to-X value chains Michael Mock, Hannes Lange, Isabell Viedt, Kumar Rajan Gopa, Jonathan Mädler, Leon Urbas TU Dresden, Chair of Process Control System and Process Systems Engineering Group, Helmholtzstr. 14, Dresden, Germany	
113	A model predictive control approach for recirculating aquaculture systems integrated with sustainable hybrid energy systems <u>Ruosi Zhang</u> ^{a,b} , Tao Chen ^a , Michael Short ^a ^a University of Surrey, Guildford, UK ^b National Innovation Center for Digital Fishery. Beijing. China	
707	Optimal Control for Deriving Policies for Global Su Urmila Diwekar ^{1,2} Apoorva Nisal ² Yogendra Shastri ³	stainability

Conf. Room II

Track 5

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Process Ecology Inc., 401 – 301 14 St. NW, Calgary, AB T2N 2A1, Canada

Methane-to-X: an economic assessment of methane valorisation options to improve carbon circularity Ben Lyons, Andrea Bernardi, Nilay Shah, Benoît Chachuat The Sargent Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, SW7 2AZ, UK

Evaluation of Methane Mitigation Technologies in the Upstream Oil and Gas Sector using the TEAM Digital Platform Marcelo Mathias, Ahad Sarraf Shirazi, Jairo Duran, <u>Alberto Alva-Argaez</u>

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An Automated Approach for Emission Reduction Cost Calculation

Maria Victoria Migo-Sumagang^{a,b}, Raymond R. Tan^a, Kathleen B. Aviso^b, <u>Dominic C. Y. Foo</u>^c

- ^a Department of Chemical Engineering, De La Salle University, 2401 Taft Avenue, 0922 Manila, Philippines
- ^b Department of Chemical Engineering, College of Engineering and Agro-Industrial Technology, University of the Philippines Los Baños, College, Los Baños, Laguna, 4031, Philippines
- ^c Department Chemical and Environmental Engineering/Centre of Excellence for Green Technologies, University of Nottingham Malaysia, Broga Road, 43500 Semenyih, Selangor, Malaysia

🕗 10:20 – 12:30

SESSION S6-05: Process Integration and Intensification (II)

- Heat integration and heat exchanger network design for oxyfuel cement plants Leif E. Andersson^a, Avinash Subramanian^a, Mari Voldsund^a, Rahul Anantharaman^a, Kristina Fleiger^b, Francisco Carrasco^c, Mirko Weber^d ^a SINTEF Energy Research, Sem Sælands vei 11,7043 Trondheim, Norway
 - ^b VDZ Technology gGmbH, Toulouser Allee 71, 41476 Düsseldorf, Germany
 - ° HeidelbergCement AG, Berliner Straße 6, 69120 Heidelberg, Germany
 - ^d Holcim Technology Ltd, Grafenauweg 10, 6300 Zug, Switzerland
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Optimal Design of Anion-pillared Metal-organic Frameworks for Gas Separation Xiang Zhang^a, Kai Sundmacher^{a,b}

- ^a Department for Process Systems Engineering, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, D-39106 Magdeburg, Germany
- ^b Chair of Process Systems Engineering, Otto-von-Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany
- **System identification of scrap metal shredders under minimal process and feedstock information** Manolis Vasileiadis^a, Thomas Papageorgiou^b, Antonis Kokossis^a, <u>Kyriakos Syrmakezis^b</u> ^a National Technical University of Athens, 9 Heroon Polytechniou Str., 15780, Athens, Greece
 - ^b ANAMET S.A., 160 NATO Av., 19300, Aspropyrgos, Greece
- Identifying first-principles models for bubble column aeration using machine learning <u>Peter Jul-Rasmussen</u>^a, Arijit Chakraborty^b, Venkat Venkatasubramanian^b, Xiaodong Liang^a, Jakob Kjøbsted Huusom^a
 - ^a Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads 228A, 2800 Kgs. Lyngby, Denmark
 - ^b Complex Resilient Intelligent Systems Laboratory, Department of Chemical Engineering, Columbia University, New York, NY 10027, USA
- 483 Mathematical Modeling of Anion Exchange Membrane Water Electrolyzer Donggyun Lee, Minsu Kim, Il Moon Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul 03722, Republic of Korea

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