

escape _
Graz | AUSTRIA **28**
June 10th to 13th | 2018



— **28th European Symposium** on Computer Aided Process Engineering

Technical Program

June 10th to 13th, 2018

Congress Graz



Event No. 745



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The technical program on ConfOrganizer is available via:

<https://escape28.conforganizer.net/program/sessions>



The technical program is available as a PDF via:

https://www.tugraz.at/fileadmin/user_upload/Events/Escape28/ScientificProgram/1_TechnicalProgramm.pdf



The book of abstracts is available as a PDF via (password required):

https://www.tugraz.at/fileadmin/user_upload/Events/Escape28/ScientificProgram/2_BookOfAbstracts.zip



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Welcome!

The 28th European Symposium on Computer-Aided Process Engineering (ESCAPE) takes place in Graz, Austria from Sunday, June 10th to Wednesday, June 13th, 2018.

ESCAPE28 is jointly organized by TU Graz and TU Wien (Austria), and the Scientific Coordination Team also spans Brno University of Technology (Czech Republic). The vision was to collaborate in organizing the event, which - besides traditional themes - also offers a platform for topics that were not explicitly mentioned in the two previous editions of ESCAPE: food, (bio-)pharma, bioresources, and the open science movement.

The themes of ESCAPE28 have been selected after a comprehensive discussion with the CAPE Working Party members and the scientific community. These include: Model Development and Simulation; Methods, Software and Tools; Open Science Movement and Education; Process Synthesis, Process Design and Life Cycle Modelling; Process Operation and Control; Bioresources, Bioprocesses and Biomedical Systems; Environment and Energy; Food, (Bio-)Pharma, and Fine Chemicals.

ESCAPE28 attracted 321 contributions from five continents (Europe, Americas, Africa, Asia and Australia), and the International Scientific Committee (ISC) selected 163 oral presentations out of these contributions. 4 plenaries given by renowned experts from academia and industry, as well as 16 keynote lectures, given by leaders in their field, round up the scientific program.

We would like to cordially thank the nine topic coordinators, as well as the 96 members of the ISC. None of this would have been possible without them.

We hope you enjoy ESCAPE28, as well as one of the most beautiful cities in the heart of Europe: Graz, the cultural capital of Europe in 2003!



Stefan Radl
On behalf of the Local Organization Committee

Scientific Committee

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Jiří J. Klemeš (Brno University of Technology, CZ)
Petar S. Varbanov (Brno University of Technology, CZ)
Thomas Wallek (Graz University of Technology, AUT)

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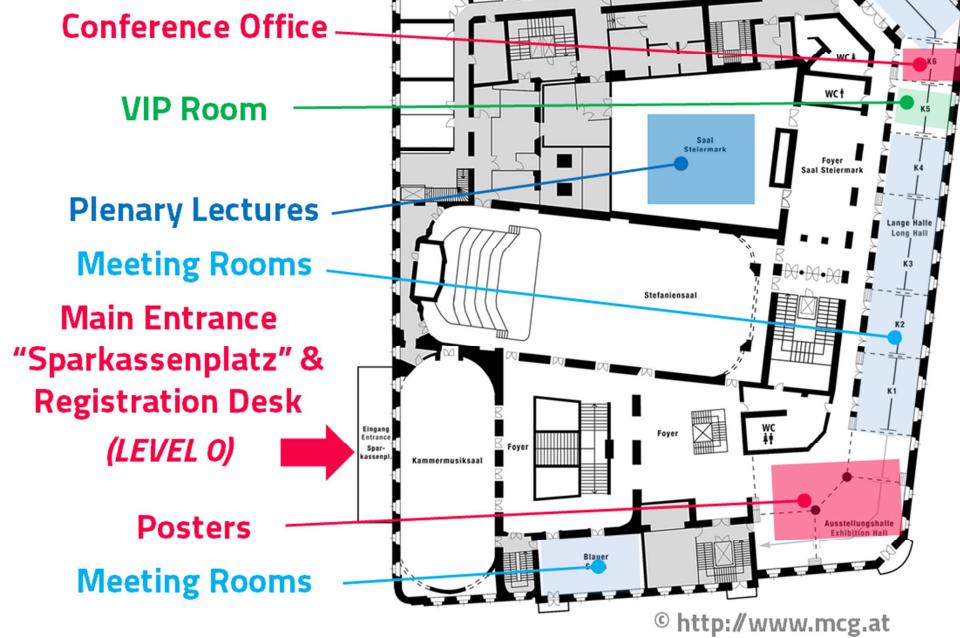
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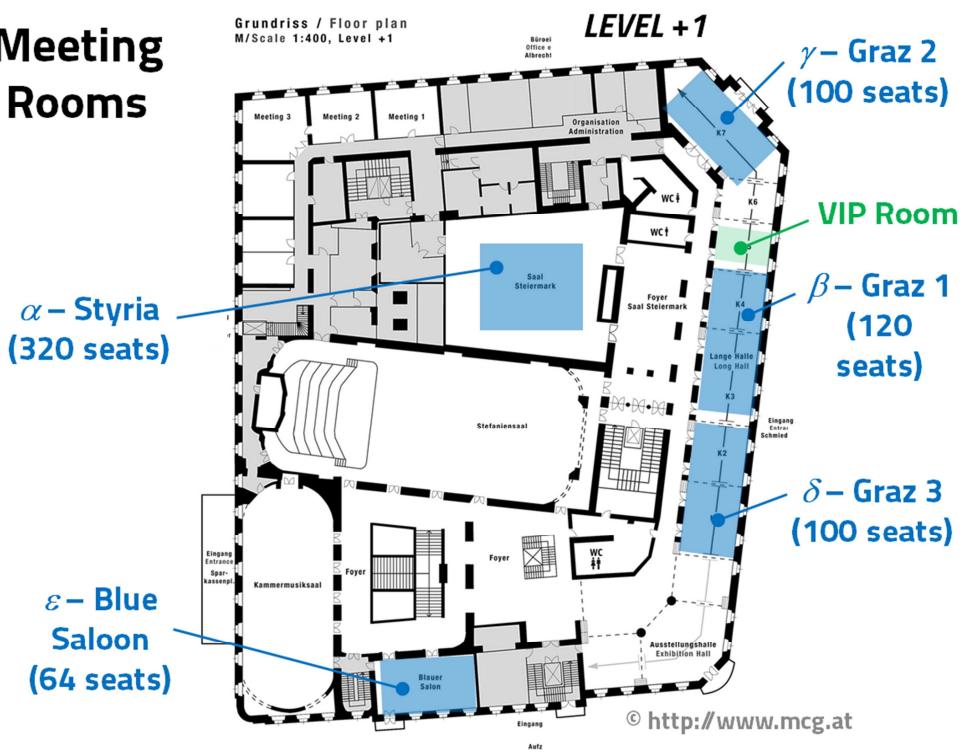
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Conference Venue

Building Overview



Meeting Rooms



About Graz

Locations

The conference venue is **Congress Graz**, which is near the main square (tram stop "Hauptplatz/Congress"). At the main square, walk towards the "**Casino|Congress**" sign, then pass the sign on the right and walk into Albrechtgasse. Take the next left, and walk towards the Vapiano restaurant. The main entrance of Congress Graz is on the left hand side on **Sparkassenplatz 1**, just opposite the Vapiano restaurant. Visit escape28.tugraz.at for further details.

Note: the **CAPE Business Meeting on Sunday, Jun 10**, will take place at TU Graz main building located at **Rechbauerstraße 12**. Visit escape28.tugraz.at for further details.

Transport & Tram

You can walk most distances in Graz. For longer distances you may want to take the tram. Note, **the tram is FREE in the inner city** (main to Jakomini square + 1 Stop, see the "**AltstadtBIM**" sticker and our "[About Graz](#)" page).

Technicalities

Currency: 1 Euro is the official currency. **1 USD is approx. 0.84 EUR. 1 EUR is approx. 1.20 USD**. Credit and debit cards are widely accepted, also in taxis.

Electricity is supplied at the European standard (**220 volts A/C, 50 Hz**, two round pin type outlets).

Shops are typically open from 07:30 to 19:00 hrs, Monday through Friday, and 07:30 to 18:00 on Saturdays. Only at main station and the airport you will find shops that are open on Sundays (typically 6:00 to 22:00 hrs).

Emergency: **dial 112**, this number works even on cell phones without a SIM card. Calls are answered in German and also in English. Direct numbers are:

122 - fire brigade

133 - police

144 - rescue/ambulance

Themes and Topics

THEME 1: Model Development and Simulation

- Topic 1.1 Models and closure development
- Topic 1.2 Meta models and multi-scale models
- Topic 1.3 Property prediction
- Topic 1.4 Environmental, social and risk models

THEME 2: Methods, Software and Tools

- Topic 2.1 Numerical methods
- Topic 2.2 Optimization
- Topic 2.3 Big data management

THEME 3: Open Science Movement and Education

- Topic 3.1 Open source, open data, open educational resources
- Topic 3.2 Computer aided education
- Topic 3.3 Educational aspects in CAPE and PSE

THEME 4: Process Synthesis, Process Design and Life Cycle Modelling

- Topic 4.1 Process and supply chain synthesis
- Topic 4.2 Integrated process and product design
- Topic 4.3 Intensification and micro/nano applications

THEME 5: Process Operation and Control

- Topic 5.1 Process monitoring and control
- Topic 5.2 Safety, fault detection and diagnosis
- Topic 5.3 Planning and scheduling
- Topic 5.4 Decision support applications
- Topic 5.5 Process operation

THEME 6: Bioresources, Bioprocesses and Biomedical Systems

- Topic 6.1 Bioreactor applications
- Topic 6.2 Biorefineries
- Topic 6.3 Pulp & paper applications
- Topic 6.4 Biomolecular and genetic engineering

THEME 7: Environment and Energy

- Topic 7.1 Waste treatment and waste-to-energy applications
- Topic 7.2 Separation and purification processes
- Topic 7.3 Heat and power integration
- Topic 7.4 Carbon mitigation

THEME 8: Food, (Bio-)Pharma, and Fine Chemicals

- Topic 8.1 Process simulation and advanced control
- Topic 8.2 Particulate processes & pharma applications
- Topic 8.3 (Bio-)reactive flow models

Session Overview¹

Sunday, June 10th

Business Meeting (by invitation only) from 10:30 to 16:00 hrs

CAPE WP Business Meeting chaired by Prof Jiří Klemeš, and Dr Petar Varbanov

In **TU Graz Main building, Rechbauerstraße 12, room HS II**

Registration from 15:00 to 18:00 hrs

In **Congress Graz, Registration Area, Entrance/Level 0**

Welcome Reception from 18:00 to 19:30 hrs

In **Congress Graz, Foyer, Level +1**

Monday, June 11th

	α Track	β Track	γ Track	δ Track	ε Track
07:30 - 08:40	<i>Registration</i>				
08:40 - 09:00	Opening Ceremony				
09:00 - 09:45	Plenary Lecture 1: Pistikopoulos (Texas A&M)				
09:45 - 10:15	<i>Coffee Break 1.1</i>				
10:15 - 11:55	OralPres K1 THEME 1	OralPres THEME 5	OralPres THEME 4	OralPres K2 THEME 6	OralPres THEME 7
11:55 - 13:25	<i>Lunch Break 1</i>				
13:25 - 14:45	OralPres K1 THEME 2	OralPres THEME 5	OralPres K2 THEME 4	OralPres THEME 1	OralPres THEME 7
14:45 - 15:15	<i>Coffee Break 1.2</i>				
15:15 - 16:35	OralPres K1 THEME 4	OralPres THEME 5	OralPres THEME 2	OralPres K2 THEME 1	OralPres THEME 7
16:35 - 18:00	Poster Session 1 - THEME 3, THEME 4, THEME 6, THEME 7, THEME 8				

¹ OralPres ... Oral Presentations, K1...keynote in first slot of session, K2...keynote in second slot of session.

Tuesday, June 12th

	α Track	β Track	γ Track	δ Track	ε Track
08:30 - 09:15		Plenary Lecture 2: Klamt (COSMOlogic)			
09:15 - 09:45		<i>Coffee Break 2.1</i>			
09:45 - 11:45	OralPres K1 THEME 5	OralPres K2 THEME 2	OralPres THEME 1	OralPres THEME 4	OralPres THEME 8
11:45 - 13:00		<i>Lunch Break 2</i>			
13:00 - 13:45		Plenary Lecture 3: You (Cornell)			
13:50 - 15:10	OralPres K1 THEME 1	OralPres THEME 5	OralPres K2 THEME 7	OralPres THEME 4	OralPres THEME 7&4
15:10 - 15:40		<i>Coffee Break 2.2</i>			
15:40 - 16:40	OralPres K1 THEME 5	OralPres THEME 5	OralPres K2 THEME 7	OralPres THEME 1	OralPres THEME 3
16:40 - 18:00		Poster Session 2 - THEME 1, THEME 2, THEME 5			
20:00 - 23:00		<i>Conference Banquet (Schlossberg Restaurant, ticket required)</i>			

Business Meeting (by invitation only) from 11:45 to 13:00 hrs

CACE Advisory Board Meeting chaired by Prof Efstratios Pistikopoulos
In room **zeta - VIP Room (20)**

Wednesday, June 13th

	α Track	β Track	γ Track	δ Track	ε Track
09:00 - 10:20	OralPres K1 THEME 7	OralPres THEME 5	OralPres K2 THEME 4	OralPres THEME 1	OralPres THEME 2
10:20 - 10:50	<i>Coffee Break 3</i>				
10:50 - 12:10	OralPres K1 THEME 5	OralPres K2 THEME 8	OralPres THEME 7	Workshop THEME 2	OralPres THEME 2
12:10 - 13:40	<i>Lunch Break 3</i>				
13:40 - 14:25	Plenary Lecture 4: Jimenez-Gonzales (GSK)				
14:25 – 15:00	Award Ceremony				
15:00 - 15:15	Preview to ESCAPE29 & Farewell				
15:30 - 20:30	<i>Excursion to Zotter Chocolate Factory (ticket required)</i>				

PSE Workshop

The “**PSE Workshop on Advanced process modelling**” will take place on **Wednesday, Jun 13, 10:50 to 12:10** hrs in room “**delta - Graz 3 (100)**”. Please register via [THIS LINK](#), which is also provided in the ConfOrganizer program.

Excursion

The meeting point for the **Excursion to Zotter Chocolate Factory** on **Wednesday, Jun 13, 15:30 to 20:30** hrs is the **Poster Hall**.

Detailed Technical Program²

Sunday, June 10th

Business Meeting (by invitation only) from 10:30 to 16:00 hrs

CAPE WP Business Meeting chaired by Prof Jiří Klemeš, and Dr Petar Varbanov

In **TU Graz Main building, Rechbauerstraße 12, room HS II**

Registration from 15:00 to 18:00 hrs

In **Congress Graz, Registration Area, Entrance/Level 0**

Welcome Reception from 18:00 to 19:30 hrs

In **Congress Graz, Foyer, Level +1**

Monday, June 11th

Registration

on **Monday, Jun 11, from 07:30 to 08:40 hrs**

In **Congress Graz, Registration Area, Entrance/Level 0**

Opening Ceremony

on **Monday, Jun 11, 08:40 to 09:00 hrs**

In room **alpha - Styria (320)**

Prof Harald Kainz, Rector of TU Graz

Prof Jiří Klemeš, CAPE Chair

Dr Petar Varbanov, CAPE Secretary

Ass.Prof Stefan Radl, Local Organization Team

² OralPres ... Oral Presentations, K1...keynote in first slot of session, K2...keynote in second slot of session. The number in brackets after the title of the contribution is the ConfOrganizer abstract id.

Changes after May 23rd 2018 are not reflected in the printed program. Please see

<https://escape28.conforganizer.net> for the final program.

Plenary Lecture 1: Pistikopoulos (Texas A&M)

on **Monday, Jun 11, 09:00 to 09:45** hrs

Chaired by Prof Jiří Klemeš, and Dr Petar Varbanov

In room **alpha - Styria (320)**

- | | |
|-------|---|
| 09:00 | Multi-Parametric Optimization in Smart Manufacturing & Process Intensification (584) |
| | Efstratios Pistikopoulos |

Coffee Break 1.1

on **Tuesday, Jun 12, 09:45 to 10:15** hrs

OralPresK1 - THEME 1 - 1.1.alpha

on **Monday, Jun 11, 10:15 to 11:55** hrs

Chaired by Asc. Prof Davide Manca, and Prof Fengqi You

In room **alpha - Styria (320)**

- | | |
|-------|---|
| 10:15 | Keynote Lecture:

The Ordinary Kriging Metamodel in Multivariate Dynamic Modeling and Multistep Ahead Prediction (544)

Ahmed Shokry, Antonio Espuña |
| 10:35 | Exploiting meta-modeling approach to investigate the effect of oil characteristics on the optimal operating conditions and biodiesel properties (377)

Pulkit Chhabra, Li Zhou, Iftekhar A. Karimi, Markus Kraft |
| 10:55 | Surrogate-based modeling in flotation processes (507)

Achref Rabhi, Moulay Abdellah Chkifa, Saad Benjelloun, Abderrazak Latifi |
| 11:15 | Simulation and Analysis of Indian Residential Electricity Consumption Using Agent-Based Models (470)

Sohini Dhar, Babji Srinivasan, Rajagopalan Srinivasan |
| 11:35 | Influence of cylinder-to-particle diameter ratio and filling speed on bed porosity of random packed beds of spheres (234)

Johanna Fernengel, Jennie von Seckendorff, Olaf Hinrichsen |

OralPres - THEME 5 - 1.1.beta

on **Monday, Jun 11, 10:15 to 11:55** hrs

Chaired by Dr Stefania Tronci, and Dr Radoslav Paulen

In room **beta - Graz 1 (120)**

- | | |
|-------|---|
| 10:15 | A discrete-time scheduling model for continuous power-intensive processes considering fatigue of equipment (120)

Andreas Obermeier, Christoph Windmeier, Erik Esche, Jens-Uwe Repke |
| 10:35 | New Continuous-time Scheduling Formulation for Multilevel Tree-like Pipeline Systems (144)

Pedro Castro, Hossein Mostafaei |
| 10:55 | New approaches for scheduling of multitasking multipurpose batch processes in scientific services facilities (211)

Nikolaos Rakovitis, Jie Li, Nan Zhang |

- 11:15 **Network formulations for the design and scheduling of multiproduct batch plants with parallel lines (447)**
Floor Verbiest, Tânia Pinto-Varela, Trijntje Cornelissens, Ana Barbosa-Povoa
- 11:35 **Logistics optimization for dispositions and depooling of distillates in oil-refineries: closing the production scheduling and distribution gap (390)**
Brenno Menezes, Jeffrey Kelly, Ignacio Grossmann

OralPres - THEME 4 - 1.1.gamma

on **Monday, Jun 11, 10:15 to 11:55 hrs**

Chaired by Asc. Prof Selen Cremaschi, and Prof Zorka Novak Pintarič

In room **gamma - Graz 2 (100)**

- 10:15 **Processing Systems Synthesis with Embedded Reliability Consideration (567)**
Ákos Orosz, Zoltán Kovács, Ferenc Friedler
- 10:35 **Balancing costs, safety and CO₂ emissions in the design of hydrogen supply chains (119)**
Anton Ochoa Bique, Leonardo K. K. Maia, Fabio La Mantia, Davide Manca, Edwin Zondervan
- 10:55 **Evaluating the effect of separation and reaction systems in industrial symbiosis (374)**
Ana Somoza-Tornos, Moisès Graells, Antonio Espuña
- 11:15 **Preliminary economic assessment of reactive distillation using a navigation method (479)**
Rahma Muthia, Anton Kiss
- 11:35 **Optimal on-grid hybrid power system for eco-industrial parks planning and influence of the geographical position (444)**
Florent Mousqué, Marianne Boix, Stéphane Negny, Ludovic Montastruc, Louis Genty, Serge Domenech

OralPresK2 - THEME 6 - 1.1.delta

on **Monday, Jun 11, 10:15 to 11:55 hrs**

Chaired by Prof Heinz A. Preisig, and Prof Antonis Kokossis

In room **delta - Graz 3 (100)**

- 10:15 **Combined basic and fine chemical biorefinery concepts with integration of processes at different technology readiness levels (420)**
Sara Badr, Jane Yee Yap, Mathias Janssen, Elin Svensson, Stavros Papadokonstantakis
- 10:35 **Keynote Lecture:**
Model-based fed-batch algal cultivation strategy for enhanced starch production (566)
Gonzalo Figueroa Torres, Constantinos Theodoropoulos
- 10:55 **Adaptation of a Monte Carlo method to the hydrotreating of bio-oil model compounds (368)**
Ana Costa da Cruz, Jan Verstraete, Nadège Charon, Jean-François Joly
- 11:15 **Enzymatic keratin hydrolysis: Dynamic modelling, parameter estimation and validation (323)**
Alistair Rodman, Francesco C. Falco, Dimitrios Gerogiorgis, Krist V. Gernaey
- 11:35 **Dynamic Modeling of Butanol Production from Lignocellulosic Sugars (296)**
Cansu Birgen, Heinz A. Preisig

OralPres - THEME 7 - 1.1.epsilonon **Monday, Jun 11, 10:15 to 11:55 hrs**

Chaired by Prof Ana Carvalho, and Prof Stéphane Negny

In room **epsilon - Blue Saloon (64)**

10:15	Including Agricultural and Organic Waste in Food-Water-Energy-Waste Nexus Modelling and Decision-Making (467) <u>Daniel Garcia</u> , Fengqi You
10:35	An Energy, Water and Food Nexus Approach to Enhancing Food Production Systems through CO2 Fertilization (495) <u>Tareq Al-Ansari</u> , Rajesh Govindan, Anna Korre, Zhenggang Nie, Nilay Shah
10:55	Energy and water integration for the design of sustainable total textile waste refinery (502) <u>Athanassios Nikolakopoulos</u> , Antonis Kokossis
11:15	Optimal integrated facility for waste processing (23) <u>Edgar Martín</u> , Apoorva Sampat, Victor Zavala, <u>Mariano Martin</u>

*Lunch Break 1*on **Monday, Jun 11, 11:55 to 13:25 hrs****OralPresK1 - THEME 2 - 1.2.alpha**on **Monday, Jun 11, 13:25 to 14:45 hrs**

Chaired by Prof Truls Gundersen, and Dr Mirko Skiborowski

In room **alpha - Styria (320)**

13:25	Keynote Lecture: Approximation Algorithms for Process Systems Engineering (579) <u>Dimitrios Letsios</u> , Georgia Kouyialis, <u>Ruth Misener</u>
13:45	Ordinary Kriging: a Machine Learning tool applied to Mixed-integer Multiparametric approach (496) <u>Gicela Luperá Calahorrano</u> , Mohammad Hamed Ardakani, Antonio Espuña
14:05	A Relaxed Knapsack-Problem Based Decomposition Heuristic For Large-Scale Multistage Stochastic Programs (484) <u>Zuo Zeng</u> , <u>Selen Cremaschi</u>
14:25	A Bilevel Decomposition Method for the Simultaneous Synthesis of Utility Systems, Rankine Cycles and Heat Exchanger Networks (219) <u>Cristina Elsido</u> , Emanuele Martelli, Ignacio Grossmann

OralPres - THEME 5 - 1.2.betaon **Monday, Jun 11, 13:25 to 14:45 hrs**

Chaired by Prof Ana Barbosa-Povoa, and Prof Sebastian Engell

In room **beta - Graz 1 (120)**

13:25	Smarter process engineering across the plant life-cycle: CAPE 4.0 in industrial practice (445) <u>Rolf-Dieter Becher</u> , Michael Imle, <u>David Elixmann</u>
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- 13:45 **Optimisation of water supply systems in the water – energy nexus: Model development and implementation to support decision making in investment planning (501)**
 Emilia Kondili, Christiana Papapostolou
- 14:05 **Optimal operation of a subsea compression system subject to degradation (196)**
 Adriaen Verheylewegen, Julie Marie Gjøby, Johannes Jäschke
- 14:25 **Planning the Drilling Rig Activities – Routing and Allocation (503)**
 Mohammad Sadegh Tavallali, Marzieh Zare

OralPresK2 - THEME 4 - 1.2.gamma

on **Monday, Jun 11, 13:25 to 14:45 hrs**

Chaired by Prof Stéphane Negny, and Prof Ana Carvalho

In room **gamma - Graz 2 (100)**

- 13:25 **Heat pump assisted azeotropic DWC for enhanced biobutanol separation (441)**
 Iulian Patrascu, Costin Sorin Bildea, Anton Kiss
- 13:45 **Keynote Lecture:**
 Thermodynamic Network Flow Approach for Chemical Process Synthesis (574)
 Kai Sundmacher, Georg Liesche, Dominik Schack, Karsten Hans Georg Rätze
- 14:05 **Selection of fractionation pathways and intermediates for mixed consumer products (195)**
 Alberto Castiglioni, Jochem Jonkman, Renzo Akkerman, Albert van der Padt
- 14:25 **Understanding the dynamic behavior of Semicontinuous Distillation (510)**
 Pranav Bhaswanth Madabhushi, Edgar Iván Sánchez Medina, Thomas A. Adams II

OralPres - THEME 1 - 1.2.delta

on **Monday, Jun 11, 13:25 to 14:45 hrs**

Chaired by Prof Constantinos Theodoropoulos, and Ass. Prof Zhihong Yuan

In room **delta - Graz 3 (100)**

- 13:25 **Kinetic Modeling of Methanol Synthesis - Impact of Catalyst Deactivation (199)**
 Carsten Seidel, Andreas Jörke, Bert Vollbrecht, Andreas Seidel-Morgenstern, Achim Kienle
- 13:45 **Closure Development for Multi-Scale Fluidized Bed Reactor Models: A CLR Case Study (524)**
 Stefan Radl, Federico Municchi, Schalk Cloete, Jan Hendrik Cloete, Stefan Andersson, Joana Francisco Morgado, Thomas Gurker, Rosa Quinta-Ferreira, Christoph Kloss, Christoph Goniva, Shahriar Amini
- 14:05 **Modelling of biomass residence time distribution and xylan depolymerization kinetics analysis in a Pilot-Scale Pretreatment Continuous Tubular Reactor (468)**
 Felicia Rodríguez, Arturo Sanchez
- 14:25 **Modeling the Effect of Temperature on Microalgal Growth under Outdoor Conditions (105)**
 Pooya Darvehei, Parisa A. Bahri, Navid Reza Moheimani

OralPres - THEME 7 - 1.2.epsilon

on **Monday, Jun 11, 13:25 to 14:45 hrs**

Chaired by Prof Rene Hofmann, and Prof Edwin Zondervan

In room **epsilon - Blue Saloon (64)**

- 13:25 **Optimum Utilization of Biomass for the Production of Power and Fuels using Gasification** (475)
Ahmed AlNouss, Gordon McKay, Tareq Al-Ansari
- 13:45 **Use of artificial intelligence to detect failures in the process of delignification of sugarcane bagasse from supercritical carbon dioxide** (464)
Isabelle Cunha Valim, Artur S.C. Rego, Alex Queiroz, Vinnicius Brant, Antônio Fidalgo Neto, Cecília Vilani, Bruno Santos
- 14:05 **Sequential Flowsheet Optimization: Maximizing the Exergy Efficiency of a High-Pressure Water Scrubbing Process for Biogas Upgrade** (106)
Alberto Penteado, Jan Christian Schöneberger, Erik Esche, Hamid Reza Godini, Günter Wozny, Jens-Uwe Repke

Coffee Break 1.2

on **Monday, Jun 11, 14:45 to 15:15 hrs****OralPresK1 - THEME 4 - 1.3.alpha**

on **Monday, Jun 11, 15:15 to 16:35 hrs**

Chaired by Prof Zorka Novak Pintarič, and Asc. Prof Selen Cremaschi

In room **alpha - Styria (320)**

- 15:15 **Keynote Lecture:**
Synthesis, design and analysis of energy efficient sustainable process alternatives (586)
Rafiqul Gani, Ramsagar Vooradi, Sarah Babu Anne
- 15:35 **Systematic tool for sustainable synthesis and design of flexible processes and supply chains under uncertainty** (562)
Klavdija Žirngast, Žan Zore, Lidija Čuček, Zorka Novak Pintarič, Zdravko Kravanja
- 15:55 **Extended Value Chain Synthesis towards the Design of Multi-feedstock Algae Biorefineries** (188)
Melina Psycha, Antonis Kokossis
- 16:15 **A System Dynamics Framework for Supply Chain Sustainability Assessment: A Case Study in Process Industries** (222)
Naoum Tsolakis, Eleftheria Ntonou, Nikolaos Trokanas

OralPres - THEME 5 - 1.3.beta

on **Monday, Jun 11, 15:15 to 16:35 hrs**

Chaired by Dr Radoslav Paulen, and Prof Moisès Graells

In room **beta - Graz 1 (120)**

- 15:15 **Toward the cooperative-based control of chemical plants** (314)
Bogdan Dorneanu, Evgenia Mechleri, Harvey Arellano-Garcia

- 15:35 **Dynamics and MPC of an Evaporative Continuous Crystallization Process** (175)
Marcellus Moraes, Mauricio B de Souza Jr, Argimiro Resende Secchi
- 15:55 **System identification for a system subjected to persistent disturbances** (455)
Roberto Mei, Massimiliano Grosso, Federico Desotgiu, Michela Mulas, Stefania Tronci
- 16:15 **Leveraging the Power of Big Data Analytics for Process Scheduling under Uncertainty using a Stochastic Robust Optimization Approach** (59)
Chao Ning, Fengqi You

OralPres - THEME 2 - 1.3.gamma

on **Monday, Jun 11, 15:15 to 16:35** hrs

Chaired by Prof Zdravko Kravanja, and Dr Miloš Bogataj

In room **gamma - Graz 2 (100)**

- 15:15 **Simulation-Based Optimization of Chemical Processes using the Extended Cutting Plane Algorithm** (376)
Juan Javaloyes-Antón, Jan Kronqvist, José A. Caballero
- 15:35 **A hierarchical approach for solvent selection based on successive model refinement** (88)
Kai Fabian Kruber, Jan Scheffczyk, Kai Leonhard, André Bardow, Mirko Skiborowski
- 15:55 **Comparison of reformulations of the Duran-Grossmann model on Work and Heat Exchange Network Synthesis (WHENS)** (415)
Haoshui Yu, Matias Vikse, Truls Gundersen
- 16:15 **Ensuring (n-1)-reliability in the optimal design of distributed energy supply systems** (33)
Dinah Elena Hollermann, Dörthe Hoffrogge, Maike Hennen, André Bardow

OralPresK2 - THEME 1 - 1.3.delta

on **Monday, Jun 11, 15:15 to 16:35** hrs

Chaired by Ass. Prof Zhihong Yuan, and Prof Constantinos Theodoropoulos

In room **delta - Graz 3 (100)**

- 15:15 **Comparative Life Cycle Assessment of Ethylene from Wet Shale Gas and Biomass** (64)
Minbo Yang, Xueyu Tian, Fengqi You
- 15:35 **Keynote Lecture:**
Process network modelling for the assessment of environmental impacts (341)
Raul Calvo-Serrano, Gonzalo Guillen Gosálbez
- 15:55 **Mixed-integer multiparametric Meta-Modeling: a Machine Learning tool applied to Reactive Scheduling** (387)
Gicela Lupera Calahorrano, Ahmed Shokry, Georgios Kopanos, Antonio Espuña

OralPres - THEME 7 - 1.3.epsilon

on **Monday, Jun 11, 15:15 to 16:35** hrs

Chaired by Prof Edwin Zondervan, and Prof Rene Hofmann

In room **epsilon - Blue Saloon (64)**

- 15:15 **Reduced model describing efficient extraction of hydrogen transported as co-stream in the natural gas grid** (249)
Werner Liemberger, Martin Miltner, Michael Harasek

15:35	Flow diagram of waste double base propellant treatment including fluidized bed reactor (408) <u>Raymoon Hwang, Jiheon Lee, Inkyu Lee, Hyunsoo Kim, Jungsoo Park, Oh Min, Il Moon</u>
15:55	Energy Efficient Hybrid Gas Separation with Ionic Liquid (571) <u>Xinyan Liu, Xiaodong Liang, Xiangping Zhang, Suojiang Zhang, Georgios M. Kontogeorgis, Rafiqul Gani</u>
16:15	Parameter estimation for modelling of organophilic pervaporation (63) <u>Andras Jozsef Toth, Eniko Haaz, Szabolcs Solti, Nora Valentini, Anita Andre, Daniel Fozer, Tibor Nagy, Peter Mizsey</u>

Poster Session 1

on **Monday, Jun 11, 16:35 to 18:00** hrs

in the **Poster Hall**

Tuesday, June 12th

Plenary Lecture 2: Klamt (COSMOlogic)

on **Tuesday, Jun 12, 08:30 to 09:15** hrs

Chaired by Prof Anton Friedl, and Ass. Prof Thomas Wallek

In room **alpha - Styria (320)**

08:30	COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics (583) <u>Andreas Klamt</u>
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Coffee Break 2.1

on **Tuesday, Jun 12, 09:15 to 09:45** hrs

OralPresK1 - THEME 5 - 2.1.alpha

on **Tuesday, Jun 12, 09:45 to 11:45** hrs

Chaired by Prof Tânia Pinto-Varela, and Dr Pedro Castro

In room **alpha - Styria (320)**

09:45	Keynote Lecture: Global Optimization Algorithm for Multi-period Design and Planning of Centralized and Distributed Manufacturing Networks (389) <u>Cristiana Lara, Ignacio Grossmann</u>
10:05	Oil product distribution planning via robust optimization (114) <u>Camilo Lima, Susana Relvas, Ana Barbosa-Povoa, Juan M. Morales</u>
10:25	A heuristic neighborhood search-based approach for the solution of resource-task network scheduling problems (35) <u>Giancarlo Dalle Ave, Xing Wang, Iiro Harjunkoski, Sebastian Engell</u>
10:45	Robust Process Scheduling under Uncertainty with Regret (60) <u>Chao Ning, Fengqi You</u>

- 11:05 **Tackling the complexity of designing multiproduct multistage batch plants with parallel lines: the application of a cooperative optimization approach** (152)
 Floor Verbiest, Trijntje Cornelissens, Johan Springael
- 11:25 **Production Scheduling of Multi-Stage, Multi-Product Food Process Industries** (306)
Georgios P. Georgiadis, Chrysovalantou Ziogou, Georgios Kopanos, Manuel Garcia, Daniel Cabo, Miguel Antonio López, Michail Georgiadis

OralPresK2 - THEME 2 - 2.1.beta

on **Tuesday, Jun 12, 09:45 to 11:45** hrs

Chaired by Prof Ruth Misener, and Dr Gonzalo Guillen Gosálbez

In room **beta - Graz 1 (120)**

- 09:45 **Towards a quantitative Food-Energy-Water Nexus metric to facilitate decision making in process systems: A case study on a dairy production plant** (247)
Styliani Avraamidou, Aaron Milhorn, Owais Sarwar, Efstratios Pistikopoulos
- 10:05 **Keynote Lecture:**
Optimization of centralized and/or distributed utility production in Total Site (171)
Andreja Nemet, Zdravko Kravanja
- 10:25 **Integrating Real-time Operational Constraints in Planning of Water and Energy Supply** (54)
Negar Vakilifard, Parisa A. Bahri, Martin Anda, Goen Ho
- 10:45 **Robust design of multi-energy systems with long-term energy storage** (488)
Paolo Gabrielli, Florian Fürer, Portia Murray, Kristina Orehoungi, Jan Carmeliet, Matteo Gazzani, Marco Mazzotti
- 11:05 **Economic and environmental benefits of waste-based energy closed-loop integration in process industries under uncertainty** (428)
Shabnam Morakabatchiankar, Kefah Hjaila, Fernando D. Mele, Moisès Graells, Antonio Espuña
- 11:25 **Operational Optimization for Integrated Cooling Water Systems with Chemical Processes** (394)
Fei Song, Nan Zhang, Robin Smith, Yujiao Zeng, Jie Li, Xin Xiao

OralPres - THEME 1 - 2.1.gamma

on **Tuesday, Jun 12, 09:45 to 11:45** hrs

Chaired by Prof Bernhard Peters, and Dr Norbert Asprion

In room **gamma - Graz 2 (100)**

- 09:45 **A CFD investigation of the effect of particle sphericity on wellbore cleaning efficiency during oil and gas drilling** (324)
Emmanuel Epelle, Dimitrios Gerogiorgis
- 10:05 **Resolved Numerical Analysis of Drying on a Vibrating Grate** (402)
Bernhard Peters, Mohammad Mohammad Mohseni, Marc Demouling, Thorsten Kläs
- 10:25 **Direct Reduction of Iron Ore in Fluidized Beds** (493)
Mustafa Efe Kinaci, Thomas Lichtenegger, Simon Schneiderbauer
- 10:45 **Thermal and hydraulic performance of pillow-plate heat exchangers** (416)
Olga Arsenyeva, Julian M. Tran, Eugeny Y. Kenig

- 11:05 **Prediction of stability and thermal conductivity of nanofluids for thermal energy storage applications** (110)
Bashar Mahmoud, Michael Fairweather, Lee Mortimer, Jeffrey Peakall, Hugh Rice, David Harbottle
- 11:25 **A multi-fluid approach to simulate separation of liquid-liquid systems in a gravity settler** (46)
Anurag Misra, Cyrille Bonamy, Luís M. de Souza, Lena Hohl, Markus Illner, Jens-Uwe Repke, Matthias Kraume, Dominique Thévenin

OralPres - THEME 4 - 2.1.delta

on **Tuesday, Jun 12, 09:45 to 11:45** hrs

Chaired by Prof François Maréchal, and Prof Antonio Espuña

In room **delta - Graz 3 (100)**

- 09:45 **Surrogate-based optimization approach to the development of membrane networks in gas separation** (93)
Jose Graciano, Rita Alves, Benoit Chachuat
- 10:05 **Retrofit of Mass Exchange Networks Using a Reduced Superstructure Synthesis Approach** (283)
Adeniyi Isafiade
- 10:25 **Sustainable supply chain: monetization of environmental and social impacts** (424)
Cátia da Silva, Ana Barbosa-Povoa, Ana Carvalho
- 10:45 **Endpoint-oriented Life Cycle Optimization Models for Sustainable Design and Operations of Shale Gas Supply Chains with Modular Manufacturing** (50)
Jiayao Gao, Fengqi You
- 11:05 **Optimal Strategic Planning for Shale Water Management** (225)
Alba Carrero, Juan A. Reyes, José A. Caballero, Ignacio Grossmann
- 11:25 **Techno-economic assessment of a lignocellulosic biorefinery coproducing ethanol and xylitol or furfural** (44)
Aristide Giuliano, Diego Barletta, Isabella Da Bari, Massimo Poletto

OralPres - THEME 8 - 2.1.epsilon

on **Tuesday, Jun 12, 09:45 to 11:45** hrs

Chaired by Prof Sandro Macchietto, and Ass. Prof Stefan Radl

In room **epsilon - Blue Saloon (64)**

- 09:45 **A Process System Approach to Nose-to-Brain Delivery of Biopharmaceutics** (358)
Costas Kiparissides, Aleck Alexopoulos, Filippos Karageorgos, Athina Vasileiadou, Vasileios Bourganis
- 10:05 **Model predictive control of anesthesia** (316)
Adriana Savoca, Jessica Barazzetta, Giuseppe Pesenti, Davide Manca
- 10:25 **Models for designing hydrogen peroxide decontamination processes in sterile drug product manufacturing** (169)
Keisho Yabuta, Haruka Futamura, Koji Kawasaki, Masahiko Hirao, Hirokazu Sugiyama

- 10:45 **Automatic controller failure detection with application in model based control of an *E. coli* fed-batch** (463)
 Sophia Ulonska, Julian Kager, Christoph Herwig
- 11:05 **Dynamic modelling and simulation of reactive transport phenomena in an amperometric blood glucose biosensor** (326)
 Fergus McIlwaine, Dimitrios Gerogiorgis
- 11:25 **A novel dynamic model of plate heat exchangers subject to fouling** (512)
 Sandro Macchietto, Shunfeng Guan

*Lunch Break 2*on **Monday, Jun 11, 11:45 to 13:00** hrs**Business Meeting (by invitation only) from 11:45 to 13:00 hrs****CACE Advisory Board Meeting** chaired by Prof Efstratios PistikopoulosIn room **zeta - VIP Room (20)****Plenary Lecture 3: You (Cornell)**on **Tuesday, Jun 12, 13:00 to 13:45** hrs

Chaired by Prof Rafiqul Gani, and Ass. Prof Stefan Radl

In room **alpha - Styria (320)**

- 13:00 **Resilient Design and Operations of Chemical Process Systems** (56)
 Jian Gong, Fengqi You

OralPresK1 - THEME 1-2.2.alphaon **Tuesday, Jun 12, 13:50 to 15:10** hrs

Chaired by Asc. Prof Stavros Papadokonstantakis, and Asc. Prof Davide Manca

In room **alpha - Styria (320)**

- 13:50 **Keynote Lecture:**
 Good modelling practice for process engineering: pitfalls and requirements to develop fit for purpose models (585)
 Ingmar Nopens
- 14:10 **Model-based Design of Experiments Using a Flowsheet-Simulator** (85)
 Norbert Asprion, Juliane Ritter, Roger Böttcher, Michael Bortz
- 14:30 **Kinetic Modeling of Precipitation Terpolymerization for Functional Microgels** (256)
 Franca Janssen, Agnieszka Ksiazkiewicz, Michael Kather, Leif Kröger, Adel Mhamdi, Kai Leonhard, Andrij Pich, Alexander Mitsos
- 14:50 **From Process Graph to Process Simulation with Proper Model Documentation** (515)
 Arne Tobias Elve, Heinz A. Preisig, Tore Haug-Warberg

OralPres - THEME 5 - 2.2.betaon **Tuesday, Jun 12, 13:50 to 15:10** hrs

Chaired by Asc. Prof Yuan Yao, and Prof Marco Reis

In room **beta - Graz 1 (120)**

- 13:50 **Learning operation strategies from alarm management systems by temporal pattern mining and deep learning (182)**
Gyula Dörgő, Péter Pigler, Máté Haragovics, János Abonyi
- 14:10 **Application of CFD modelling to external reactor vessel cooling (210)**
Marco Colombo, Michael Fairweather
- 14:30 **Towards Obviating Human Errors in Real-time through Eye Tracking (465)**
Umair Mohd I, Babji Srinivasan, Rajagopalan Srinivasan
- 14:50 **Fault detection of fermentation processes (448)**
Ernie Che Mid, Vivek Dua

OralPresK2 - THEME 7 - 2.2.gamma

on **Tuesday, Jun 12, 13:50 to 15:10 hrs**

Chaired by Ass. Prof Andras Jozsef Toth, and Mr Daniel Garcia

In room **gamma - Graz 2 (100)**

- 13:50 **Total Site Utility Systems Structural Design Considering Environmental Impacts (73)**
Timothy Walmsley, Xuexiu Jia, Petar Varbanov, Jiří Klemeš, Yutao Wang
- 14:10 **Keynote Lecture:**
Extensions for Multi-Period MINLP Superstructure Formulation for Integration of Thermal Energy Storages in Industrial Processes (117)
Anton Beck, Rene Hofmann
- 14:30 **Innovative Temperature Swing Adsorption Simulation Model for Biogas Upgrading (246)**
Hannes Vogtenhuber, Elisabeth Sonnleitner, Franz Helminger, Rene Hofmann, Gerhard Schöny, Veronika Wilk, Andreas Werner, Hermann Hofbauer
- 14:50 **Packed bed sorption enhanced methane reforming on CaO/CuO/Al2O3(NiO) catalyst (262)**
Giuseppe Diglio, Piero Bareschino, Erasmo Mancusi, Francesco Pepe, Dawid Hanak, Vasilije Manovic

OralPres - THEME 4 - 2.2.delta

on **Tuesday, Jun 12, 13:50 to 15:10 hrs**

Chaired by Prof François Maréchal, and Asc. Prof Ricardo Morales-Rodriguez

In room **delta - Graz 3 (100)**

- 13:50 **Towards the Synthesis of Modular Process Intensification Systems with Safety and Operability Considerations – Application to Heat Exchanger Network (337)**
Yuhe Tian, M. Sam Mannan, Zdravko Kravanja, Efstratios Pistikopoulos
- 14:10 **Comparative Performance Analysis of Industrial Scale Catalytic Steam Reformer with Membrane Steam Reformer (328)**
Arun Senthil Sundaramoorthy, Arun Prem Anand Natarajan, Sundaramoorthy Sithanandam
- 14:30 **An Integrated Reactive Separation Process for Co-Hydrotreating of Vegetable Oils and Gasoil to Produce Jet Diesel (491)**
Miriam García-Sánchez, Mauricio Sales-Cruz, Teresa Lopez-Arenas, Tomás Viveros-García, Alberto Ochoa-Tapia, Eduardo Perez-Cisneros

- 14:50 **A Multi-stage and Multi-level Computer Aided Framework for Sustainable Process Intensification (570)**
Nipun Garg, Georgios M. Kontogeorgis, John M. Woodley, Rafiqul Gani

OralPres - THEME 7 & THEME 4 - 2.2.epsilon

on **Tuesday, Jun 12, 13:50 to 15:10** hrs

Chaired by Prof Mariano Martin, and Prof João M. Silva

In room **epsilon - Blue Saloon (64)**

- 13:50 **Dynamic simulation of a post-combustion CO₂ capture pilot with assessment of solvent degradation (151)**
Hana Benkoussas, Grégoire Leonard, Madalina Ioana Burca, Ana-Maria Cormos
- 14:10 **Integration of Renewable Energy Sources into Petroleum Refining for Sustainable Production of Transportation Fuels (436)**
Mohamed Al Jamri, Robin Smith, Jie Li
- 14:30 **Design and Analysis of Edible Oil Processes Containing Lipids (365)**
Olivia A. Perederic, Sten Appel, Bent Sarup, John M. Woodley, Georgios M. Kontogeorgis, Rafiqul Gani

Coffee Break 2.2

on **Tuesday, Jun 12, 15:10 to 15:40** hrs

OralPresK1 - THEME 5 - 2.3.alpha

on **Tuesday, Jun 12, 15:40 to 16:40** hrs

Chaired by Dr Pedro Castro, and Prof Tânia Pinto-Varela

In room **alpha - Styria (320)**

- 15:40 **Keynote Lecture:**
Risk assessment for the design and scheduling optimization of periodic multipurpose batch plants under demand uncertainty (170)
Miguel Vieira, Helena Paulo, Corentin Vilard, Tânia Pinto-Varela, Ana Barbosa-Povoa
- 16:00 **Process Scheduling under Ambiguity Uncertainty Probability Distribution (61)**
Chao Shang, Cen Guo, Fengqi You
- 16:20 **Scheduling of a Multiproduct and Multiple Destinations Pipeline System with Repumping Operations (78)**
William Hitoshi Tsunoda Meira, Leandro Magatão, Susana Relvas, Lúcia V. R. Arruda, Flávio Neves-Jr, Ana Barbosa-Povoa

OralPres - THEME 5 - 2.3.beta

on **Tuesday, Jun 12, 15:40 to 16:40** hrs

Chaired by Dr Babji Srinivasan, and Prof Costas Kiparissides

In room **beta - Graz 1 (120)**

- 15:40 **An Integrated Medium-Term Energy Planning Model For Interconnected Systems (238)**
Apostolos Elekidis, Nikolaos Koltsaklis, Michail Georgiadis

- 16:00 **Mixed Integer Linear Programming Formulation for Sensible Thermal Energy Storages (77)**
Martin Koller, Rene Hofmann
- 16:20 **A two-stage stochastic programming approach to integrated day-ahead electricity commitment and production scheduling (187)**
Egidio Leo, Sebastian Engell

OralPresK2 - THEME 7 - 2.3.gamma

on **Tuesday, Jun 12, 15:40 to 16:40 hrs**

Chaired by Prof Emanuele Martelli, and Prof Michael Fairweather

In room **gamma - Graz 2 (100)**

- 15:40 **Optimisation of Integrated Bioenergy and Concentrated Solar Power Supply Chains in South Africa (459)**
Massimo Liu, Koen H. Van Dam, Antonio Marco Pantaleo, Miao Guo
- 16:00 **Keynote Lecture:**
Integration of carbon dioxide and hydrogen supply chains (290)
Anton Ochoa Bique, Bui Huu Tuan Nguyen, Grazia Leonzio, Christos Galanopoulos, Edwin Zondervan
- 16:20 **Combining biomass, natural gas and carbonless heat to produce liquid fuels and electricity (274)**
Leila Hoseinzade, Thomas A. Adams II

OralPres - THEME 1 - 2.3.delta

on **Tuesday, Jun 12, 15:40 to 16:40 hrs**

Chaired by Prof Sandro Macchietto, and Prof Bernhard Peters

In room **delta - Graz 3 (100)**

- 15:40 **Data-driven predictive degradation modeling for batch processes: a case study on heat exchanger fouling (362)**
Ouyang Wu, Ala Eldin Farag Bouaswaig, Stefan Marco Schneider, Fernando Moreno Leira, Lars Struen Imsland, Matthias Roth
- 16:00 **Dull or bright you still get electric delight: A new approach to the design of all-weather panels (478)**
Sahar Hajizeinalibioki, Daniel Sebastia-Saez, Oleksiy Klymenko, Harvey Arellano-Garcia

OralPres - THEME 3 - 2.3.epsilon

on **Tuesday, Jun 12, 15:40 to 16:40 hrs**

Chaired by Ass. Prof Michael Harasek, and Ass. Prof Stefan Radl

In room **epsilon - Blue Saloon (64)**

- 15:40 **Combining Open Source and Easy Access in the field of DEM and coupled CFD-DEM: LIGGGHTS®, CFDEM®coupling and CFDEM®workbench (548)**
Alice Hager, Christoph Kloss, Christoph Goniva
- 16:00 **A study on computational improvements for the Eddy Dissipation Concept by operator splitting and tabulation (194)**
Eva-Maria Wartha, Markus Bösenhofer, Michael Harasek

- 16:20 **Active learning of process control** (293)
 Manuel Rodriguez, Alberto Prada Palos, Ismael Diaz, Emilio González Gómez

Poster Session 2

on **Tuesday, Jun 12, 16:40 to 18:00** hrs
in the **Poster Hall**

Conference Banquet (Ticket Required)

on **Tuesday, Jun 12, 20:00 to 23:00** hrs
in **Schlossberg Restaurant**

Wednesday, June 13th

OralPresK1 - THEME 7 - 3.1.alpha

on **Wednesday, Jun 13, 09:00 to 10:20** hrs
Chaired by Mr Daniel Garcia, and Ass. Prof Andras Jozsef Toth
In room **alpha - Styria (320)**

- 09:00 **Keynote Lecture:**
Numerical Representation for Heat Exchanger Networks Binding Topology and Thermodynamics (454)
 Petar Varbanov, Timothy Walmsley, Michael Walmsley, Jiří Klemeš, Zdravko Kravanja
- 09:20 **Simultaneous Optimization of Multistream Heat Exchangers** (69)
 Yingzong Liang, Keat Ping Yeoh, Pui Ying Lee, Ergys Pahija, Chi Wai Hui
- 09:40 **Use of excess heat from ethylene recycling in a low-density polyethylene production plant** (38)
 Rodolfo Matos, Isabel M. João, João M. Silva
- 10:00 **A Heat Load Distribution Method for Retrofitting Heat Exchanger Networks** (266)
 Hür Büütün, Ivan Kantor, Alberto Mian, François Maréchal

OralPres - THEME 5 - 3.1.beta

on **Wednesday, Jun 13, 09:00 to 10:20** hrs
Chaired by Prof Sigurd Skogestad, and Prof Jose Romagnoli
In room **beta - Graz 1 (120)**

- 09:00 **Incorporating Systems Structure in Data-Driven High-Dimensional Predictive Modeling** (212)
 Marco Reis
- 09:20 **Real-Time Nonlinear State Estimation for Smart Manufacturing in Polymerization Reactors** (500)
 Santiago Salas, Jorge Chebeir, Stefania Tronci, Roberto Baratti, Jose Romagnoli

- 09:40 **Dynamic Real-time Optimization of Batch Membrane Processes using Pontryagin's Minimum Principle (213)**
Radoslav Paulen, Ayush Sharma, Miroslav Fikar
- 10:00 **Control of the Steady-State Gradient of an Ammonia Reactor using Transient Measurements (347)**
Harro Bonnowitz, Julian Straus, Dinesh Krishnamoorthy, Esmaeil Jahanshahi, Sigurd Skogestad

OralPresK2 - THEME 4 - 3.1.gamma

on Wednesday, Jun 13, 09:00 to 10:20 hrs

Chaired by Prof Rafiqul Gani, and Prof Antonio Espuña

In room **gamma - Graz 2 (100)**

- 09:00 **An engineering tool to screen and integrate biomass valorization paths in multiple-feedstock biorefineries (37)**
Konstantinos Pyrgakis, Antonis Kokossis
- 09:20 **Keynote Lecture:**
Optimization-based process synthesis for integrated crystallizer-wet mill system for improved crystal shape control (300)
Botond Szilagyi, Zoltan Nagy
- 09:40 **Thermo-economic evaluation of solid-oxide electrolysis integrated biomass-to-liquid systems (193)**
Ligang Wang, Mar Perez Fortes, Stefan Diethelm, Jan Van Herle, François Maréchal

OralPres - THEME 1 - 3.1.delta

on Wednesday, Jun 13, 09:00 to 10:20 hrs

Chaired by Prof Fengqi You, and Ass. Prof Thomas Wallek

In room **delta - Graz 3 (100)**

- 09:00 **Property Prediction of Pharmaceuticals for Designing of Downstream Separation Processes (425)**
Getachew S. Molla, Lukasz Ruszcynski, Jens Abildskov, Gürkan Sin
- 09:20 **Analyzing the link between GE-model parameter regression and optimal process design (236)**
Mirko Skiborowski, Philipp Temmann, Christoph Brandenbusch
- 09:40 **Development of predictive models for organic solvent nanofiltration based on a data-driven approach (275)**
Rebecca Goebel, Tobias Glaser, Ilka Niederkleine, Mirko Skiborowski

OralPres - THEME 2 - 3.1.epsilon

on Wednesday, Jun 13, 09:00 to 10:20 hrs

Chaired by Prof Menwer Attarakih, and PhD Marco Voccante

In room **epsilon - Blue Saloon (64)**

- 09:00 **An optimization method to estimate the SOFC market in waste water treatment (282)**
Sonja Sechi, Sara Giarola, Andrea Lanzini, Marta Gandiglio, Gbemi Oluleye, Massimo Santarelli, Adam Hawkes

- 09:20 **Electricity mix assessment of the EU member countries using data envelopment analysis and EffMixF (349)**
Patricia Zurano-Cervelló, Carlos Pozo, Josep María Mateo-Sanz, Laureano Jiménez, Gonzalo Guillen Gosálbez
- 09:40 **Improved modeling of membrane separation in integrated hybrid processes (197)**
Bettina Scharzec, Mirko Skiborowski
- 10:00 **Experimentally Driven Guaranteed Parameter Estimation: a Way to Speed up Model-Based Design of Experiments Techniques (155)**
Arun Pankajakshan, Marco Quaglio, Federico Galvanin

*Coffee Break 3*on **Wednesday, Jun 13, 09:00 to 10:20 hrs****OralPresK1 - THEME 5 - 3.2.alpha**on **Wednesday, Jun 13, 10:50 to 12:10 hrs**

Chaired by Prof Marco Reis, and Asc. Prof Grégoire Leonard

In room **alpha - Styria (320)**

- 10:50 **Keynote Lecture:**
Changing between Active Constraint Regions for Optimal Operation: Classical Advanced Control versus Model Predictive Control (189)
Adriana Reyes-Lúa, Cristina Zotică, Tamal Das, Dinesh Krishnamoorthy, Sigurd Skogestad
- 11:10 **Bayesian estimation of product attributes from on-line measurements in a dropwise additive manufacturing system (554)**
Andrew Radcliffe, Gintaras Reklaitis
- 11:30 **Virtual inflow estimation with simplified tuning using cascaded and Kalman-like least squares observers (430)**
Christoph Josef Backi, Sigurd Skogestad
- 11:50 **A simultaneous parameter and state estimator for polymerization process based on molecular weight distribution (367)**
Jiayuan Kang, Zhijiang Shao, Xi Chen, Lorenz Biegler

OralPresK2 - THEME 8 - 3.2.betaon **Wednesday, Jun 13, 10:50 to 12:10 hrs**

Chaired by Asc. Prof Dimitrios Gerogiorgis, and Prof Zoltan Nagy

In room **beta - Graz 1 (120)**

- 10:50 **Artificial vision system for the online characterization of the particle size distribution of bulk materials on conveyor belts (371)**
Mario Soprana, Andrea C. Santomaso, Pierantonio Facco
- 11:10 **Keynote Lecture:**
Process Simulation of Pharmaceutical Manufacturing Operations – State of the Art (580)
Johannes Khinast

- 11:30 **Process modelling, simulation and technoeconomic optimisation for continuous pharmaceutical manufacturing of (S)-warfarin (322)**
Samir Diab, Dimitrios Gerogiorgis
- 11:50 **A global state feedback linearization and decoupling MPC of a MIMO continuous MSMPR cooling crystallization process (137)**
Ravi Parekh, Brahim Benyahia, Chris Rielly

OralPres - THEME 7 - 3.2.gamma

on **Wednesday, Jun 13, 10:50 to 12:10 hrs**

Chaired by Prof Michael Fairweather, and Prof Emanuele Martelli

In room **gamma - Graz 2 (100)**

- 10:50 **Multi-objective optimization of a carbon dioxide utilization superstructure for the synthesis of formic and acetic acid (366)**
Juan D. Medrano-García, Rubén Ruiz-Femenia, José A. Caballero
- 11:10 **The role of CCS and biomass-based processes in the refinery sector for different carbon scenarios (206)**
Julia Sachs, Sukma Hidayat, Sara Giarola, Adam Hawkes
- 11:30 **Decarbonisation of the Industrial Sector by means of Fuel Switching, Electrification and CCS (74)**
Sandro Luh, Sara Budinis, Thomas Schmidt, Adam Hawkes
- 11:50 **Process design of absorption-membrane hybrid CO₂ capture systems for coal-fired power plant (404)**
Mun-Gi Jang, Sunghoon Lee, Seokwon Yun, Jin-Kuk Kim

PSE Workshop - THEME 2 - 3.2.delta

on **Wednesday, Jun 13, 10:50 to 12:10 hrs**

Chaired by Dr Pieter Schmal, and Dr Christian Triana

In room **delta - Graz 3 (100)**

- 10:50 **PSE Workshop on Advanced process modelling (589)**
Pieter Schmal, Christian Triana

OralPres - THEME 2 - 3.2.epsilon

on **Wednesday, Jun 13, 10:50 to 12:10 hrs**

Chaired by Asc. Prof Ricardo Morales-Rodriguez, and Ass. Prof Michael Harasek

In room **epsilon - Blue Saloon (64)**

- 10:50 **Numerical Evaluation of Different Turbulence Models for Single-Phase Flow in the Outer Pillow-Plate Channel (260)**
Marco Voccante, Mark Piper, Alexander Zibart, Julian M. Tran, Eugeny Y. Kenig
- 11:10 **CFD Modeling of Pulsed Sieve Plate Liquid Extraction Columns using OPOSPM as a Reduced Population Balance Model: Coupled Hydrodynamics and Mass Transfer (357)**
Samer Alzyod, Menwer Attarakih, Hans-Jörg Bart
- 11:30 **Solution of the Population Balance Equation by the Meshless Moving Particle Method (MMPM) (310)**
Menwer Attarakih, Hans-Jörg Bart

- 11:50 **Optimal Chemical Grouping and Sorbent Material Design by Data Analysis, Modeling and Dimensionality Reduction Techniques (302)**

Melis Onel, Burcu Beykal, Meichen Wang, Fabian A. Grimm, Lan Zhou, Fred A. Wright, Timothy D. Phillips, Ivan Rusyn, Efstratios Pistikopoulos

Lunch Break 3

on **Wednesday, Jun 13, 12:10 to 13:40** hrs

Plenary Lecture 4: Jimenez-Gonzales (GSK)

on **Wednesday, Jun 13, 13:40 to 14:25** hrs

Chaired by Prof Jiří Klemeš, and Dr Petar Varbanov

In room **alpha - Styria (320)**

- 13:40 **Developing key PSE skills for the workforce of the future (577)**

Concepción (Conchita) Jiménez-González

Award Ceremony

on **Wednesday, Jun 13, 14:25 to 15:00** hrs

Chaired by Prof Jiří Klemeš, and Dr Petar Varbanov

In room **alpha - Styria (320)**

Preview to ESCAPE29 & Farewell

on **Wednesday, Jun 13, 14:25 to 15:00** hrs

Chaired by Prof Jiří Klemeš, and Dr Petar Varbanov

In room **alpha - Styria (320)**

Excursion (Ticket Required)

The meeting point for the **Excursion to Zotter Chocolate Factory** on **Wednesday, Jun 13, 15:30 to 20:30** hrs is the **Poster Hall**.

Poster Session 1 – THEME 3 / 4 / 6 / 7 / 8

on **Monday, Jun 11, 16:35 to 18:00** hrs

Chaired by Dr Timothy Walmsley, Prof. Zdravko Kravanja, Asc. Prof Grégoire Leonard

In the **Poster Hall**

Slot	Topic	Title (Abstract ID)
1	3.1	Open-use and community-based tools for education in process system engineering: industrial applications from decision automation to data analytics (383) Brenno Menezes , Jeffrey Kelly
2	3.2	An interactive virtual laboratory for process engineering education (489) Diana Ibet Roman-Sanchez , Teresa Lopez-Arenas , Mauricio Sales-Cruz
3	4.1	Multi-objective optimization of sustainability criteria in the design of chemical plants (370) Federico Scotti , Nicola Fabricatore , Davide Manca
4	4.1	Multi-floor process plant layout using mixed-integer optimization (166) Jude Ejeh , Songsong Liu , Lazaros Papageorgiou
5	4.1	Optimal design of biogas supply chains (268) Grégoire Alain Chomette , Theodoros Damartzis , François Maréchal
6	4.1	Eco-design of closed-loop supply chains: application to lead-acid batteries (244) Magno González Rodriguez , Catherine Azzaro-Pantel , Alberto Aguilar-Lasserre
7	4.1	Design, Control and Economic Evaluation of Processes for Isobutyl Acrylate Production (340) Mihai Daniel Moraru , Diana Adela Berinde , Costin Sorin Bildea
8	4.1	Dimethyl Carbonate production process from Urea and Methanol (360) Daniel Vázquez , Juan Javaloyes-Antón , Juan D. Medrano-García
9	4.1	GHG emission analysis of milking of microalgae (393) Sofia Chaudry , Parisa A. Bahri , Navid Reza Moheimani
10	4.1	Superstructure optimization (MINLP) within ProSim Simulator (412) Qiao Zhao , Thibaut Neveux , Mounir Mecheri , Romain Privat , Philippe Guittard , Jean-Noël Jaubert
11	4.1	Process synthesis and optimization of membrane systems with superstructure approach for the mitigation of CO₂ emissions from a coal-fired power plant (391) Sunghoon Lee , Jin-Kuk Kim
12	4.1	Optimization based design of a resilient biomass to energy system (443) Ashish Soren , Yogendra Shastri
13	4.1	Semantically-enabled CAPE platform: Towards a generic and dynamic formulation for the synthesis and optimisation of value chains (449) Eirini Siougkrou , Foteini Barla , Antonis Kokossis
14	4.1	Life cycle assessment of pulp and paper production – A Portuguese case study (457) Andreia Santos , Ana Barbosa-Povoa , Ana Carvalho
15	4.1	Modelling and Analysing Supply Chain Resilience – Flow Complexity (474) João Pires Ribeiro , Ana Barbosa-Povoa

- 16 4.1 **Multi-scale system modelling under circular bioeconomy** (486)
Miao Guo
- 17 4.2 **Furfural Processes Separation: Design and Optimization Involving Economical, Environmental and Safety Criteria** (41)
Gabriel Contreras-Zarazua, Eduardo Sánchez-Ramírez, José-Antonio Vazquez-Castillo,
Cesar Ramírez-Márquez, Juan-Gabriel Segovia-Hernandez
- 18 4.2 **Alternative processes for obtaining solar grade silicon** (8)
Cesar Ramírez-Márquez, Marta Vidal-Otero, José-Antonio Vazquez-Castillo, Mariano
Martin, Juan-Gabriel Segovia-Hernandez
- 19 4.2 **A framework for optimized sustainable mixture and rigorous separation process design** (378)
Eduardo Sánchez-Ramírez, Jaime David Ponce-Rocha, Juan-Gabriel Segovia-Hernandez,
Fernando Israel Gómez-Castro, Ricardo Morales-Rodríguez
- 20 4.2 **Method of Removing water from Products of Dehydration Reaction of 3-hydroxypropionic acid in Acrylic acid Process** (157)
Jae-Hyeon Yang, Chul-Jin Lee
- 21 4.2 **Process integration as an effective route towards sustainable oil refinery development** (129)
Poland Jelihi, Timo Wassermann, Edwin Zondervan
- 22 4.2 **Experimental Study Of A Biomass Downdraft Gasifier With Multi-Tube Gas Outlets To Improve Synthesis Gases Quality** (133)
Ajaree Suwatthikul, Paisan Kittisupakorn
- 23 4.2 **Design and optimisation of novel cascade refrigeration cycles for LNG production** (136)
Fernando Almeida-Trasvina, Robin Smith
- 24 4.2 **Mathematical modeling and simulation in natural flavors and fragrances bioproduction intensification** (303)
Ivan Červeňanský, Mário Mihal', Jozef Markoš
- 25 4.2 **Analysis and Comparative Study of Stand-Alone Reverse Osmosis Desalination Systems Powered by Pressure Retarded Osmosis** (403)
Jyh-Cheng Jeng, Heng-Yi Chu
- 26 4.2 **Optimal Design and Operation of Hybrid Osmosis Processes for Simultaneous Production of Water and Power under Different Demand Conditions** (401)
Jyh-Cheng Jeng, Heng-Yi Chu
- 27 4.2 **Design of biotechnological production of 2-phenylethanol** (426)
Peter Vargai, Ivan Červeňanský, Mário Mihal', Jozef Markoš
- 28 4.2 **A novel Graphical Gibbs Energy-Driving Force Method for the Optimal Design of Non-reactive and Reactive Distillation Columns.** (485)
Mauricio Sales-Cruz, Rafiqul Gani, Eduardo Perez-Cisneros
- 29 4.2 **Exergy efficiency based design and analysis of utilization pathways of biomasses** (543)
Hongliang Qian, Weiwei Zhu, Chang Liu, Xiaohua Lu, Georgios M. Kontogeorgis, Rafiqul Gani
- 30 4.2 **A General Model-based Methodology for Chemical Substitution** (576)
Spardha Jhamb, Xiaodong Liang, Rafiqul Gani, Georgios M. Kontogeorgis

- 31 4.2 **Integrated Solvent-Membrane and Process Design Method for Hybrid Reaction-Separation Schemes** (539)
Yugu Chen, John M. Woodley, Georgios M. Kontogeorgis, Rafiqul Gani
- 32 4.3 **Feasibility Study of using reactive distillation for the production of renewable aviation fuel** (172)
Claudia Gutiérrez-Antonio, Maritza Soria-Ornelas, Fernando Israel Gómez-Castro, Salvador Hernández
- 33 4.3 **Energy system intensification: compact and multi-stream heat exchanger design** (228)
Somei Hayashi, Kitipat Siemanond
- 34 4.3 **Process innovation through bio-inspired design** (431)
Anne Marie Barthe Delanoe, Stéphane Negny, Jean Marc Le Lann
- 35 4.3 **A model-based approach to design miniaturised structured packings for highly efficient mass transfer in gas/liquid multiphase flow** (476)
Daniel Sebastia-Saez, Zuzana Browne, Harvey Arellano-Garcia
- 36 6.2 **Design of a low-cost process for the production of biodiesel using waste oil as raw material.** (32)
Roberto Gasca-Gonzalez, Fernando Israel Gómez-Castro, Araceli Guadalupe Romero Izquierdo, Eric Zenon-Olvera, Claudia Gutiérrez-Antonio
- 37 6.2 **Feasibility of energy integration for high-pressure biofuels production processes.** (21)
Luis Alberto Villegas-Herrera, Fernando Israel Gómez-Castro, Araceli Guadalupe Romero Izquierdo, Claudia Gutiérrez-Antonio, Salvador Hernández
- 38 6.2 **CFD modelling of organosolv lignin extraction in packed beds** (477)
Michael Harasek, Bahram Haddadi-Sisakht, Christian Jordan, Anton Friedl
- 39 6.2 **Energetic assessment of lignin extraction processes by simulation** (173)
Javier Fernández-Rodriguez, Maria Gonzalez Alriols, Fabio Hernández Ramos, Jalel Labidi
- 40 6.2 **Retro-Techno-Economic-Environmental Analysis (RTEEA) from the cradle: a new approach for process development** (281)
Andrew Milli Elias, Felipe Furlan, Marcelo Perencim de Arruda Ribeiro, Roberto de Campos Giordano
- 41 6.2 **Ontology Modelling for Lignocellulosic Biomass: Composition and Conversion** (381)
Madeleine Bussemaker, Nikolaos Trokanas, Linsey Koo, Franjo Cecelja
- 42 6.2 **Optimization Of Cellulose Hydrolysis In A Non-Ideally Mixed Batch Reactor** (399)
Fenila F, Yogendra Shastri
- 43 6.3 **Managing the diffusion of 'green' pharmaceuticals defined by renewable chemical feedstocks: An illustrative real-world case study** (223)
Naoum Tsolakis, Jagit Singh Srai
- 44 6.4 **Pyrolysis Characteristics and Kinetics of Genetically Engineered Hybrid Poplars for Bio-Oil Production** (522)
Jinsoo Kim, The Ky Vo
- 45 7.1 **Simulation-based Analysis of Sewage Sludge Treatment Considering Regional, Social, and Technological Characteristics.** (179)
Akinori Shimizu, Tatsuya Okubo, Yasunori Kikuchi

- 46 7.1 **Increasing Energy Efficiency in Pulp and Paper Production by Employing a New Type of Latent Heat Storage (198)**
Christoph Zauner, Rene Hofmann, Florian Hengstberger, Bernd Windholz
- 47 7.1 **Optimisation Framework for Wastewater Treatment and Recovery Solutions in an Industrial Park Context (280)**
Edward O'Dwyer, Hongcheng Wang, Ai-jie Wang, Miao Guo, Nilay Shah
- 48 7.2 **Solvent use optimization on polyphenols extraction from grape marc involving economical aspects (79)**
Rodolfo de Mattos, Berta Zecchi, Patricia Gerla, Adrián Ferrari
- 49 7.2 **Population Balance Equation Applied to Microalgae Harvesting (72)**
Chi Wai Hui, Pui Ying Lee, Ergys Pahija, Keat Ping Yeoh, Yingzong Liang
- 50 7.2 **Integrated Process Design and Optimization of a Nitrogen Recovery in Natural Gas Processing with Natural Gas Liquefaction and NGL(Natural Gas Liquid) Recovery (102)**
Yongseok Lee, Youngsub Lim, Chonghun Han
- 51 7.2 **Application of process integration and system analysis for improving energy-efficiency of nitrogen separation process in natural gas processing (411)**
Miae Gim, Jin-Kuk Kim
- 52 7.2 **Optimization of Batch Heteroazeotropic Distillation Operational Strategies with Entrainer Recycle (545)**
Laszlo Hegely, Peter Lang
- 53 7.3 **A computer-aided analysis on regional power and heat energy systems considering socio-economic aspects: A case study on an isolated island in Japan (176)**
Yasunori Kikuchi, Yuko Oshita, Miwa Nakai, Aya Heijo, Yasuhiro Fukushima
- 54 7.3 **A Multi-period Mixed Integer Linear Program for Assessing the Benefits of Power to Heat Storage in a Dwelling Energy System (440)**
Gbemi Oluleye, Nick Kelly, John Allison, Adam Hawkes
- 55 7.3 **Optimal operation of seasonal geothermal energy storage for decarbonizing integrated multi-energy systems (588)**
Paolo Gabrielli, Maria Isabella Yliruka, Marco Mazzotti
- 56 7.4 **Assessing the energy and CO₂ emission reduction potential from ammonia production by chemical looping as innovative carbon capture technology (25)**
Dora Andreea Chisalita, Letitia Petrescu, Ana-Maria Cormos, Calin-Cristian Cormos
- 57 7.4 **Flexible hydrogen and power co-generation based on dry methane reforming with carbon capture (45)**
Szabolcs Szirma, Ana-Maria Cormos, Calin-Cristian Cormos
- 58 7.4 **Techno-Economic Analysis of CO₂ Capture Processes from Coal-fired Power Plants (396)**
Seokwon Yun, Sunghoon Lee, Jin-Kuk Kim
- 59 7.4 **Concentrating High Purity CO₂ from Syngas after Oxy-fuel Combustion by Pressure Swing Adsorption Process (406)**
Cheng-Tung Chou, Bi-Ching Wu, Tien-Lin Wu, Hong-Sung Yang, Chia-Hsuan Shen
- 60 7.4 **Simulation of CO₂ Geological Storage Together with a Water Alternating Gas Process for Oil Production in Fang Oilfield (Thailand) (437)**
Kreangkrai Maneeintr, Hutthapong Yoosook

- 61 7.4 **CO₂ capture and utilization potential within the State of Qatar** (516)
Ali Attiq Al-Yaeeshi, Tareq Al-Ansari, Rajesh Govindan
- 62 8.1 **Model-based process development for a continuous lactic acid bacteria fermentation** (112)
Robert Spann, Anna Eliasson Lantz, Christophe Roca, Krist V. Gernaey, Gürkan Sin
- 63 8.1 **Multi-flowrate optimization of the loading phase of a preparative chromatographic separation** (203)
Anton Sellberg, Niklas Andersson, Mikael Nolin, Anton Löfgren, Bernt Nilsson
- 64 8.1 **Process modelling, design and technoeconomic evaluation for continuous paracetamol crystallisation** (321)
Hikaru G. Jolliffe, Dimitrios Gerogiorgis
- 65 8.2 **Risk based approach for batch release** (123)
Linas Mockus, Gintaras Reklaitis, Kenneth Morris, David LeBlond
- 66 8.2 **Industrial scale experiments towards the development of process evaluation models for continuous pharmaceutical tablet manufacturing** (346)
Kensaku Matsunami, Takuya Nagato, Koji Hasegawa, Masahiko Hirao, Hirokazu Sugiyama
- 67 8.2 **Mathematical modelling of moisture migration in confectionery multicomponent food systems** (286)
Paschalia Mavrou, Rex Thorpe, William Frith, Guoping Lian, Tao Chen

Poster Session 2 – THEME 1 / 2 / 5

on **Tuesday, Jun 12, 16:40 to 18:00** hrs

Chaired by Prof Mauricio Sales-Cruz, Prof Moisès Graells, Prof Luis Puigjaner

In the **Poster Hall**

Slot	Topic	Title (Abstract ID)
1	1.1	Model of a Formaldehyde Absorption System Based on Industrial Data (42) <u>Ana Catarina Braz</u> , Henrique A. Matos, A. Mendes, Jorge F. Rocha, Ricardo P. Alvim
2	1.1	Identification of Mass Flow Dynamics in a Pretreatment Continuous Tubular Reactor (375) <u>Ismael Jaramillo</u> , Arturo Sanchez
3	1.1	Modeling the performance of low-pressure reverse osmosis membrane system for N-nitrosamine rejection (31) <u>Mudhar Al-Obaidi</u> , Chakib Kara-Zaitri, Iqbal Mujtaba
4	1.1	Computer-Aided Simulation of the Volumetric Efficiency of a 2 MW Gas Engine (533) <u>Guillermo Valencia</u> , Franklin Consuegra, Marisol Osorio
5	1.1	Modeling and simulation of the control of the control of the L-acid poly (PLLA) process obtained from renewable sources (471) <u>Juliana L. G. Fidalgo</u> , Ricardo B. Massá, Bruno Santos
6	1.1	Modelling Fenton and photo-Fenton Processes by Combining Design of Experiments and Direct Computer Mapping Based Programmable Structures (494) <u>Francesca Audino</u> , Mónika Varga, Montserrat Pérez-Moya, Moisès Graells, Antonio Espuña, Béla Csukás
7	1.1	Microbubble coalescence during transport in vertical channel flows (149) <u>Kenneth Asiagbe</u> , Michael Fairweather, Derrick Njobuenwu, Marco Colombo
8	1.1	Dynamic Modeling And Simulation Of An Industrial Steam Reforming Furnace (462) <u>Poliana Pastorele da Silva Quirino</u> , Karen Pontes, Flavio Manenti
9	1.1	Incorporating fouling model in plate heat exchanger modelling and design (531) <u>Olexiy Demirskyy</u> , Petro Kapustenko, <u>Olga Arsenyeva</u> , Olexandr Matsegora, Pavlo Arsenyev, Vladimir Tovazhnianskyi, Alisher Khusanov
10	1.1	Graph- Based Modelling with Distributed Systems (517) <u>Heinz A. Preisig</u> , Arne Tobias Elve
11	1.1	Coke Formation Model in Crude Oil Furnace for Maintenance Scheduling (132) <u>Amata Anantpinijwatna</u>
12	1.2	Assessing the performance of industrial ethanol fermentation unit using neural networks (405) <u>Rauber Pereira</u> , Alberto C. Badino, Antonio J. G. Cruz
13	1.2	Model transformations and integration for process plant simulation, optimization and visualization (295) <u>Manuel Rodriguez</u> , Ismael Diaz

- 14 1.2 **Modeling of non-isothermal adsorption process in a silica gel desiccant packed bed** (104)
Siripan Murathathunyaluk, Koranut Srichanvichit, Amata Anantpinijwatna, Prakob Kitchaiya
- 15 1.2 **Surrogate Model for Carbon Dioxide Equilibrium Absorption Using Aqueous Monoethanolamine (MEA)** (504)
Valentin Plesu, Jordi Bonet Ruiz, Alexandra Elena Bonet Ruiz, Alan Chavarria, Petrica Iancu, Joan Llorens
- 16 1.2 **Multi-scale modelling and simulation of Ca-looping cycle process for CO₂ post-combustion capture** (546)
Carla I.C. Pinheiro, Rui Filipe, Miguel Abreu Torres, João M. Silva, Henrique A. Matos
- 17 1.3 **Recursive Model Estimation for the Plasma Parameters Quality Control** (587)
Junmo Koo, Damdae Park, Sangwon Ryu, Gon-Ho Kim, Youn-Woo Lee
- 18 1.3 **COSMO-derived descriptors applied in ionic liquids physical property modelling using machine learning algorithms** (279)
Ismael Diaz, Manuel Rodriguez
- 19 1.3 **Predicting Research and Motor Octane Numbers based on Near Infrared Spectroscopy: Models based on Partial Least Squares Regression and Artificial Neural Networks** (417)
Fernando Martins
- 20 1.4 **Assessing the GHG emissions footprints of newly ultra-sour gas developments in the Middle East region for electricity production** (200)
Alberto Betancourt-Torcat, Mohammed Alkatheri, Ali Almansoori
- 21 1.4 **Multiobjective optimization of eco-industrial parks: evaluation of environmental impacts at the watershed scale** (131)
Laura Garcia de Dios, Marianne Boix, Sabine Sauvage, Iréa Touche, Roxelane Cakir, Ludovic Montastruc, Jose Miguel Sanchez Perez
- 22 1.4 **LCSoft as a tool for Life Cycle Assessment of Environmental Impacts: New LCIA methodologies and interpretation** (20)
Tanathip Rattanatum, Rebecca Frauzeug, Pomthong Malakul, Rafiqul Gani
- 23 1.4 **Life Cycle Assessment of calcium carbonate loop CO₂ capture technology for brown coal power plant unit of the Czech Republic** (529)
Kristina Zakuciova, Vladimir Koci, Karel Ciahotny, Ana Carvalho, Jiri Stefanica, Jana Smutna
- 24 1.4 **Applying new sustainability metric in different natural gas liquid (NGL) recovery configurations to extend investment decision and incorporate sustainability analysis in decision-making process.** (369)
Saad Al-Sobhi, Ahmed AlNouss
- 25 1.4 **Modeling of an air quality monitoring network with high space-time resolution** (442)
Daniele Sofia, Aristide Giuliano, Filomena Gioiella, Diego Barletta, Massimo Poletto
- 26 1.4 **Modeling and advanced dynamic optimization strategies for hydrological and water quality management in continental water bodies** (568)
Amira Siniscalchi, Vanina Estrada, Monica Hoffmeyer, Ruben Lara, Soledad Diaz
- 27 1.4 **Immission assessment inside an industrial ventilated room using CFD** (513)
Valentin Plesu, Alexandra Elena Bonet Ruiz, Petrica Iancu, Jordi Bonet Ruiz, Joan Llorens, Laura Isabel Becerra

- 28 2.1 **Efficient simulation of ion exchange chromatography with application to bioseparations** (19)
Marcus Fechtner, Malte Kaspereit, Achim Kienle
- 29 2.1 **Improving Convergence Behavior of Nonlinear Equation Systems in Intensified Process Models by Decomposition Methods** (261)
Saskia Bublitz, Erik Esche, Jens-Uwe Repke
- 30 2.1 **LES of particle collision and agglomeration in vertical channel flows** (578)
Tosanbami Ogholaja, Derrick Njobuenwu, Michael Fairweather
- 31 2.2 **Simulation/optimization of bio-hydrogenated diesel process with techno-economic analysis** (207)
Phooreerat Tawai, Kitipat Siemanond
- 32 2.2 **Optimizing Decolorization Efficiency of Methylene Blue by Photo-Fenton Process over Fe-Diatomite using Central Composite Design** (264)
Pongsert Sriprom, Varocha Champa, Prakob Kitchaiya, Pornsawan Assawasaengrat
- 33 2.2 **Virtual splitting of shared resource networks for price-based coordination with portfolio tariffs** (22)
Simon Wenzel, Lukas Samuel Maxeiner, Sebastian Engell
- 34 2.2 **Kinetic modeling of plastic waste pyrolysis in a laboratory scale two stage reactor** (145)
Zoltán Till, Tamás Varga, János Sója, Norbert Miskolczi, Tibor Chován
- 35 2.2 **Energy and Exergy analysis for Cryogenic process design/retrofit** (230)
Nattawat Threerachannarong, Kitipat Siemanond
- 36 2.2 **A methodology of a hybrid hydrogen supply network under alternative energy resources of hydrogen footprint constraint for sustainable energy production** (138)
Soonho Hwangbo, ChangKyoo Yoo
- 37 2.2 **Multi-objective Optimization for Plant Design via Tabu Search** (505)
Faiz Mandani, Kyle Camarda
- 38 2.2 **Systematic generation of insulation materials via DEA and Building modelling** (361)
Alba Torres Rivas, Anna Ewertowska, Carlos Pozo, Dieter Boer, Laureano Jiménez
- 39 2.2 **Optimization of cryogenic carbon capture and LNG processes by mathematical programming** (108)
Orakotch Padungwatanaroj, Kitipat Siemanond
- 40 2.2 **Optimization algorithm study for MILP applications of petrochemical supply chain** (540)
Tittawat Fongchantuk, Kitipat Siemanond
- 41 2.2 **Assessment of technology portfolios with enhanced economic and environmental performance for the energy, water and food nexus** (499)
Rajesh Govindan, Tareq Al-Ansari, Anna Korre, Nilay Shah
- 42 2.2 **Parameter Estimation of Biosurfactant Production from Agro-industrial Waste Using Genetic Algorithm** (395)
Ana Campos, Júlia Nogueira, Filipe Coelho, Brunno Santos
- 43 2.2 **Multi-objective optimization of a CO₂-EOR process from the sustainability criteria** (318)
Juan Pablo Gutierrez, Eleonora Erdmann, Davide Manca

44	2.2	Exergy analysis of an extractive distillation column for reducing energy consumption in a bioethanol production process (460) <u>Cristóbal García-García</u> , Danahe Marmolejo-Correa, J. Carlos Cárdenas-Guerra, Ricardo Morales-Rodriguez
45	2.2	Ammonia/Urea Production Process Simulation/Optimization with Techno-Economic Analysis. (235) <u>Jiranart Jeenchat</u> , Kitipat Siemanond
46	2.2	Alternative mixed-integer reformulations of Generalized Disjunctive Programs (560) <u>Miloš Bogataj</u> , Zdravko Kravanja
47	2.2	Optimal synthesis of mass exchange networks through a state-task-representation superstructure. (99) <u>Miguel Angel Velazquez-Guevara</u> , Agustin Ramon Uribe-Ramirez, Fernando Israel Gómez-Castro, Juan-Gabriel Segovia-Hernandez, Salvador Hernández, Jose Maria Ponce-Ortega
48	2.2	Optimal Design Of A Dividing Wall Column For The Separation Of Aromatic Mixture Using Response Surface Methodology (165) <u>Pedro Oliveira</u> , Karen Pontes
49	2.2	Minimum Entropy Based PFR Analysis (433) <u>David Rosa</u> , Paulo Góes, João Manzi
50	2.2	A software tool for optimizing intra-logistic activities (338) <u>Dimitrios Poulimenos</u> , Dimitrios Bechtis, Dimitrios Vlachos, Eleftherios Iakovou
51	2.3	Semantic Networking Facility for the Biorefining Community (421) <u>Edlira Kalemi</u> , Linsey Koo, Franjo Cecelja
52	2.3	Ontology engineering approach to support process of model integration (419) <u>Linsey Koo</u> , Edlira Kalemi, Nikolaos Trokanas, Franjo Cecelja
53	2.3	Towards a Methodology for Reusable Ontology Development: A Case Study in the Process Engineering Domain (386) <u>Nikolaos Trokanas</u> , Linsey Koo, Franjo Cecelja
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