

IACCHE - XXX INTERAMERICAN CONGRESS OF CHEMICAL ENGINEERING CAIQ2023 - XI ARGENTINIAN CONGRESS OF CHEMICAL ENGINEERING CIBIQ2023 - II IBEROAMERICAN CONGRESS OF CHEMICAL ENGINEERING

Buenos Aires - Argentina - June 4-8, 2023

"The global chemical engineering working for a better future world"

Special Event: Process Systems Engineering Preliminary Technical Program

Monday, June 5, 2023 - 9:00 to 10:30 (Contributed Oral)

UCA Aula Magna

Advances in modelling and model-based systems

1272	9:00-9:15	Predicting activity coefficients at infinite dilution of polymer solutions using Graph Neural Networks	Sanchez Medina, E.I., Kunchapu, S., Sundmacher, K.
1625	9:15-9:30	Hydrogen from wastewater: a phenomenological model for a multi-domain bioreactor	Boese-Cortés, I., Díaz-Alvarado, F. A., Prieto, A. L.
1715	9:30-9:45	Using the aggregation population balance for the surrogate modeling of step-growth polymerization kinetic Monte-Carlo simulations	Bordas, B., Eulig, S., Kurt, S. K., Bamberg, A., Engell, S.
1781	9:45-10:00	Milk spray dryer simulator development	Razmi, R., Woo, M.W., Young, B.R., Yu, W.
1951	10:00-10:15	Accounting for Economics in Attainable-Region-Based Reactor–Separation Network Synthesis: Models, Tradeoffs, and Insights	Pastore de Lima, A.E., Ryu, J., Maravelias, C.T.
1957	10:15-10:30	Stochastic Programming Models for Long-Term Energy Transition Planning	McDonald, M.A., Maravelias, C.T.

UCA Room 7

Advances in Numerical Methods and computational techniques

1929	9:00-9:15	On a revised bound contraction method for the globally optimal synthesis of heat exchanger networks	Eduardo Pacola, Esdras Carvalho, Carolina Carvalho, Miguel Bagajewicz
1950	9:15-9:30	Process design strategies and digital evaluation of extruders for the continuous production of Li-Ion battery slurry	Meza Gonzalez, J.F., Nirschl, H.
2013	9:30-9:45	Global Optimization of a Refinery-Petrochemical Complex using Lagrangean Decomposition	Uribe-Rodríguez, A., <u>Castro, P.M.</u> , Guillén-Gosálbez, G., Chachuat, B.
2131	9:45-10:00	Generalization of a bound contraction methodology for the solution of optimization problems in process systems chemical engineering	Esdras Carvalho, Miguel Bagajewicz
2150	10:00-10:15	A Smart Global Optimization Algorithm for Quadratically Constrained Problems (QCPs)	Pedro Castro
2300	10:15-10:30	Automatic differentiable thermodynamic package	Santos, L.F., Costa, C.B.B., Ravagnani, M.A.S.S., Caballero, J.A.

Monday, June 5, 2023 - 11:00 to 12:30 (Plenary and Keynote)

UCA Aula Magna

11:00-11:30 Marianthi Ierapetritou: Process Systems Engineering Approaches Towards Sustainable Solutions: Path to Circular Economy (Keynote)

11:30 - 12:30 Plenary Lecture



Arturo Jimenez Gutierrez:

Including inherent safety and process intensification as part of the design of chemical processes

Monday, June 5, 2023- 14:00 to 15:30 (Keynote)

UCA Aula Magna

14:00-14:30 Maria Soledad Diaz: PSE challenges to address water management in integrated aquatic and agricultural livestock systems to achieve sustainability goals within a circular economy framework.

14:30-15:00 Miguel Bagajewicz: Set Trimming, Smart and Supersmart Enumeration for the Globally Optimal Design of Chemical Process Equipment.

15:00-15:30 Venkat Venkatasubramanian: Exploiting Physicochemical Knowledge in Machine Learning: Combining Symbolic-AI with Numeric-AI.

Monday, June 5th, 2023 - 16:30 to 17:30 (Contributed Oral)

UCA Aula Magna

Advances in numerical methods and computational techniques

1285	16:30-16:45	Stability region of parameters in MINLP problems: Designing a water network in Santiago, Chile	Arenas-Araya, F., <u>Díaz-Alvarado.</u> <u>F.A.</u>
1512	16:45-17:00	A Study on Different Mathematical Formulations for Multiperiod Blending with Applications of Rare-earth Element and Critical Mineral Recovery From Produced Water	Ovalle, D., Pulsipher, J.L., Drouven, M.G., Laird, C.D., <u>Grossmann, I. E.</u>
1579	17:00-17:15	Identifying simple process designs of methanol production from renewables by multi-objective optimization using the FluxMax approach	Svitnič, T., Sundmacher, K.
2984	17:00-17:15	Sustainable Process Design Opportunities	Jakkraphat Kongcharoenkitkul, Teng Zhou, <u>Rafiqul Gani</u>

UCA Room 7

Advances in Process Control, Operation and Intelligent Systems

2899	16:30-16:45	Data-driven modeling for Process Monitoring and Fault Diagnosis of Biomanufacturing Processes	Sivaram, A., Bisgaard, T., Khorasani, M. R., <u>Mansouri, S. S.</u>
3053	16:45-17:00	Unsupervised Fault Detection of Pharmaceutical Processes using Long Short-Term Memory Autoencoders	Mohammad Aghaee, Stephane Krau, Melih Tamer, <u>Hector</u> <u>Budman</u>
2185	17:00-17:15	Learning models from data: Evaluation on the performance of Kaizen Programming for symbolic regression	Ferreira, J., Pedemonte, M., Torres, A.I.
2302	17:15-17:30	AI-ML Based Digital Twin for Operational Excellence in Process Systems – A Case Study of Large-Scale Water Distribution Networks	Parth Brahmbhatt, Abhilasha Maheshwari, <u>Ravindra D. Gudi</u>

Monday, June 5, 2023 - 18:30 to 19:30 (Contributed Oral)

UCA Aula Magna

Advances in modelling and model-based systems

1816	18:30-18:45	Resolved simulation of solid bowl centrifuges as an aspect of advancing digitalization in solid/liquid separation	Baust, H.K., Gleiß, M., Nirschl, H.
1824	18:45-19:00	Evaluation of mathematical models in the estimation of physicochemical properties of binary gasoline and oxygenant mixtures	N.D. Patiño, P.A. Ruiz, M.A. Noriega, J.E. Pachón

UCA Room 7

Advances in Methods and Tools for Biotechnology

1298	18:30-18:45	Integrated design of biorefineries from wine production residues	Taifouris, M., <u>Martin, M.,</u> El- Halwagi, M.
2308	18:45-19:00	Green hydrogen production in a sugarcane biorefinery: an optimization approach	Wheeler, J., Machin Ferrero, L.M., Ploper, A., Sánchez Collado, F.E., Mele, F. D
2897	19:00-19:15	An Integrated Methodology for Product Design Including Sustainability Criteria and Palm Oil Value Chain Requirements	Montañez, M., Serna, J., Narváez- Rincón, P. C.
3106	19:15-19:30	SAF production process from bio-syngas through Fischer- Tropsch synthesis coupled to olefins upgrading in a zeolite bed: simulation and techno-economic feasibility assessment	Pedro L. Cruz, Daniel Martínez del Monte, Javier Dufour



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Tuesday, June 6, 2023 - 9:00 to 10:30 (Contributed Oral)

UCA Aula Magna

Advances in modelling and model-based systems

2315	9:00-9:15	Process modeling and simulation of Solketal production from glycerol: Optimization of the reactive system	Nishiyama, F.E., Cordeiro, P.H.Y., Machado, G. D., Bonfim-Rocha, L., Costa, C.B.B.
2845	9:15-9:30	Internal mass balance verification improves machine learning-based models	Hoyos, J.D., Noriega, M.A., Riascos, C.A.M.
2933	9:30-9:45	Work and heat integration considering rigorous thermodynamic properties	Rossato, I.G., Costa, C.B.B., Ravagnani, M.A.S.S., <u>Pavão, L.V.</u>
3082	9:45-10:00	A Study of the effect of the fluidization regime on the Oxidative Dehydrogenation of Ethane	Durán-Pérez, J.F., <u>Castillo-Araiza</u> , <u>C.O.</u>
2179	10:00-10:15	Measurements in Optimization models	Schamber, N.A., Andersen, F.E., Bindlish, R.
1321	10:15-10:30	Sustainability Optimization and Simultaneous Design of an Integrated Cyanobacteria-Based Biorefinery and its HEN	Ramos, M., Ramos, F.D., Lasry Testa, R., Estrada, V.G., Diaz, M.S.

UCA Room 7

Advances in Process and Product synthesis, design and optimization

1505	9:00-9:15	The Impact of Small Modular Reactors and Nuclear Technologies in the Energy Transition	Tovar-Facio, J., Martín, M., Ponce-Ortega, J. M., Grossmann, I. E.
1705	9:15-9:30	Water influence on total annual cost for CO ₂ separation through a two-stage membrane system	Arias, A.M., Kraft, R.A., Scenna, N.J., Mores, P.L.
1673	9:30-9:45	Comparative Study of Hydrogen and Natural Gas Networks: Simulation and Network Design Optimization	D.H. Jamali, C. Ganzer, <u>K.</u> <u>Sundmacher</u>
1908	10:00-10:15	Use of Proxy Set Trimming for the Optimal Basic Design of Process Equipment	Andre Nahes, SungYoung Kim, André L. H. Costa, <u>Miguel J.</u> <u>Bagajewicz</u>
1928	9:45-10:00	Set Trimming procedure and Smart Enumeration for the globally optimal design of cooling towers	Eduardo Pacola, Andre Nahes, Ana Levy, Esdras Carvalho, Andre Costa, Miguel Bagajewicz
1884	10:15-10:30	Advanced Systems Configurations for Targeting Zero Liquid Discharge in Industrial Wastewater Management	Rishabh Jain, Abhilasha Maheshwari

Tuesday, June 6, 2023 - 11:00 to 12:30 (Plenary and Keynote)

UCA Aula Magna

11:00-11:30 Christos Maravelias: Process Synthesis Redefined: How Studying Renewable Energy Systems Led to New Classes of Problems (Keynote)

11:30 - 12:30 Plenary Lecture



Andre Bardow

Betting on Molecules: PSE Tools to Capture the Jackpot at the Climate Casino

Tuesday June 6, 2023 - 14:00 to 15:30 (Keynote)

UCA Aula Magna

14:00-14:30 Hirokazu Sugiyama: Bridging PSE and pharma: Challenges and opportunities for modeling, simulation, and optimization

14:30-15:00 Ana Carvalho: Environmental and social Life Cycle Assessment: A powerful tool for Process Systems Engineering

15:00-15:30 Benham Khadim and Sander Dubbelman: The use of Hansen Solubility Parameters in Cosmetic Formulations: first experience in Henkel and the way forward



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Wednesday, June 7, 2023 - 9:00 to 10:30 (Contributed Oral)

UCA Aula Magna

Advances in Process and Product Synthesis, Design and Optimization

2071	9:00-9:15	Globally Optimal Design of Distillation Columns using Enumeration Techniques	Lucas Santos de Jesus, Alice Peccini, Eduardo Mach, Argimiro Secchi, Andre Costa, Miguel Bagajewicz
2143	9:15-9:30	An optimization model for the development of a sustainable empty pesticide containers management system in Buenos Aires Province, Argentina	Sorichetti, A.E., González Prieto, M., Bandoni, J.A., Savoretti, A.A.
2233	9:30-9:45	Multi-objective optimization applied in CAMD design for extraction solvents selection: Lactic acid/water and acetic acid/water cases study	Roa-Gómez, V.A., Serrato, J.C.
2245	9:45-10:00	Study of flow rate manipulation effects on crude oil heat exchangers considering fouling phenomena on shell and tube side	de Cesaro, J.P.V., Maruyama, V., Mele, F.D., Ravagnani, M.A.S.S., Costa, C.B.B.
2474	10:00-10:15	Optimisation-based investigation of uncertainty towards the decarbonisation of the domestic heat sector: a Great Britain case study	Vassilis M. Charitopoulos
2538	10:15-10:30	Synthesis of cost-optimal Organic Rankine Cycles coupled to heat exchanger networks	Correa, V.H., Ravagnani, M.A.S.S., Costa, C.B.B, <u>Pavão</u> , <u>L.V.</u>

UCA Room 7

Advances in Numerical Methods and Computational techniques

2451	9:00-9:15	Multi-objective simultaneous optimization of a heat exchanger network integrated with organic Rankine cycle	Ribeiro, R.B., Ravagnani, M.A.S.S, Costa, C.B.B.
3062	9:15-9:30	Molecular superstructures to increase the resolution of molecular design beyond counting groups	Philipp Rehner, Johannes Schilling, <u>André Bardow</u>
3077	9:30-9:45	Passive mixing enhancement in microchannel flows using flexible structures	Gaurav Singh
1821	9:45-10:00	Optimization framework based on a sensitivity analysis for the identification of the critical design variables	Maria de los A. Villarreal-de- Aquino, Jaime D. Ponce-Rocha, Eduardo S. Perez-Cisneros, Verónica Rodríguez-López, Edgar I. Murillo-Andrade, Divanery Rodriguez-Gomez, Ricardo Morales-Rodríguez
1921	10:00-10:15	Optimization of an alternative structure for producing ethyl lactate by reactive distillation	Valvassore, M.S., Costa, C.B.B.

Wednesday, June 7, 2023 - 11:00 to 12:30 (Plenary and Keynote)

UCA Aula Magna

11:00-11:30 Argimiro Secchi: Optimization and Control of Variants of Simulated Moving Bed (Keynote)

11:30 - 12:30 Plenary Lecture



E. N. (Stratos) Pistikopoulos

Multi-Scale Energy Systems Engineering - Methodologies & Tools (Plenary)

Wednesday, June 7, 2023 - 14:00 to 15:30 (Keynote)

UCA Aula Magna

14:00-14:30 Amornchai Arpornwichanop: Process Systems Engineering in Developing Sustainable Biorefinery

14:30-15:00 Jose Pinto: Enterprise-wide optimization of industrial gas value chains in the face of disruptions.

15:00-15:30 Seyed Soheil Mansouri: A unified multi-scale strategy for bio-manufacturing process development.

Wednesday, June 7, 2023 - 16:30 to 17:30 (Contributed Oral)

UCA Aula Magna

Advances in process control, operation, and intelligent systems

2343	16:30-16:45	Economic model predictive control for mitigating the COVID-19 impact based on social distancing policies and vaccination	Silva, D.M., Secchi, A.R.
2522	16:45-17:00	Feature Engineering and Machine Learning for High- Throughput Screening of Single and Binary Metal Catalysts with Simple Adsorbates	Alexander J. Summers, <u>Q. Peter</u> <u>He</u>
2894	17:00-17:15	Coupling neural networks and evolutionary algorithms as a strategy to find cost-efficient operational conditions for the degradation of pharmaceutical pollutants using Advanced Oxidation Processes	Acosta-Angulo, B., Lara-Ramos, J., Diaz-Angulo, J., Niño-Vargas, A, Machuca, Martínez, F.
3063	17:15-17:30	Exploiting machine-learning thermodynamics for process design of the polyurethane waste recycling	Bosetti, L., Winter, B.A., Lindfeld, J., Schilling, J., <u>Bardow</u> , <u>A.</u>

UCA Room 7

Advances in process and/or product synthesis, design, and optimization

2993	16:30-16:45	Modeling and Simulation of the Fischer-Tropsch Synthesis for Diesel Production	Santos, M.F., Bresciani, A.E., Bassani, G.S., Alves, R.M.B.
2995	16:45-17:00	Mixed-Integer Optimization using Quantum Computing in Process Systems Engineering	Ashfaq Iftakher, Monzure-Khoda Kazi, M. M. Faruque Hasan
3064	17:00-17:15	Environmental Benefits of Solvent-Based Separation for Multilayer Plastic Films Recycling	Munguia-Lopez, A.C., Goreke, D., Sanchez-Rivera, K.L., Aguirre-Villegas, H.A., Avraamidou, S., Huber, G.W., Zavala, V.M.
3085	17:15-17:30	Synthesis of a Continuous Multi-Stage Fluidized Bed System for CO2 Capture Utilizing Temperature Swing Adsorption	Yuri Souza Beleli, José Luis de Paiva, Marcelo Martins Seckler, Galo Antonio Carrillo Le Roux

Wednesday, June 7, 2023 - 18:30 to 19:30 (Contributed Oral)

UCA Aula Magna

Advances in Process Control, Operation, and Intelligent Systems

2785	18:30-18:45	Simulation Optimization based Irrigation Control via Dynamic Crop Growth Simulation Models	Jisung, Jang, Q. Peter He
1670	18:45-19:00	Fault Forewarning for Chemical Processes through Adaptive Transformer Network	Ruoshi Qin, <u>Jinsong Zhao</u>
1815	19:00-19:15	Smart centrifuges: Digitalisation and process control tools challenged with a recycling process chain	Sinn, T., Nirschl, H., Gleiss, M.
3079	19:15-19:30	Smartphone-based voice controllable microfluidic device for automatic bacterial DNA extraction	Hoang Khang Bui, Woo-Sik Kim, <u>Tae Seok Se</u>

UCA Room 7

Advances in Planning, Scheduling, and supply chain management

1620	18:30-18:45	Detailed transportation planning for daily supply of forest biomass at an electricity generation plant	Melchiori, L., Nasini, G., <u>Corsano,</u> <u>G</u> .
2944	18:45-19:00	Ontologies in Chemical Engineering: Are we following the right track	Henning, G.P.
2079	19:00-19:15	Optimization model for expansion planning of reliable and resilient power systems under extreme scenarios	Seolhee Cho, Javier Tovar-Facio, John D. Siirola, Benjamin P. Omell, Jaffer H. Ghouse, <u>Ignacio</u> <u>E. Grossmann</u>
3015	19:15-19:30	Optimizing crude oil operations scheduling using Similarity Index decomposition	García García-Verdier, T., Montes, D., Gutiérrez, G., Méndez, C., de Prada, C.



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UCA Room 7 - Extra session PSE *Thursday June 8*

Color codes for session topics

Color codes for session topics		
Advances in Methods and Tools for Biotechnology		
Advances in Process Control, Operation, and Intelligent Systems		
Advances in Planning, Scheduling and Supply Chain Management		
Advances in process and/or product synthesis, design, and optimization		

1428	9:00-9:15	Simultaneous Globally Optimal Heat Exchanger Network and Heat Exchanger Synthesis	<u>Diego Oliva</u> , Julia Lemosb, André L. H. Costab, Miguel J. Bagajewicz
3160	9:15-9:30	A Trust Region Filter Method for Expensive Black-Box Optimization with High Sampling Efficiency	Runzhe Liang, <u>Zhihong Yuan</u> , <u>Lorenz T. Biegler</u>
2601	9:30-9:45	An MILP-based framework to the logistical problem of an industrial gas supply chain	Sergio G. Bonino, Luis J. Zeballos, Akash Moolya, Jose Lainez, Jose M. Pinto, Ignacio E. Grossmann, Carlos A. Méndez
2921	9:45-10:00	Redefining PRoduct ONTOlogy to improve intra and cross-domain interoperability	Vegetti, M.,Leone, H.P., Henning, G.P.
2680	10:00-10:15	Model Predictive Control applied to a gas compression system of an offshore platform	Giraldo, S.A.C., Lima, D.M., Guedes, T.A.L, Campos, M.M., Lima, M.L., Ribeiro, L.D., Secchi, A.R.
2236	10:15-10:30	Genome-scale metabolic model for the toxic bloom- forming cyanobacteria Microcystis aeruginosa	Lasry Testa, R. D., Privitera Signoretta, I. E., Diaz, M. S., Estrada, V.
	10:30-11:00	BREAK	



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POSTER SESSION

Advances in modelling and model-based systems

1468	Determination and Model Evaluation of Pure Dissolution Kinetics of Potassium Sulfate Using In-Situ Dynamic Image Analysis	Moraes, Marcellus G. F., Lima, Fernando A. R. D., Barreto Jr., Amaro G., Lage, Paulo L.C., Souza Jr., Maurício B., Secchi, Argimiro R.
1809	Resolved simulation of the filtration process in a chamber filter press	Baust, H.K., Fränkle, B., Gleiß, M. 1, Nirschl, H.
1926	Workflow and Planning Data-Driven Model to Optimize Efficiency in Fracture Spacing for Multi Well-Pad Operations on Vaca Muerta Formation	Benvenutti, L., Borio, D.O., Bandoni J.A.
2433	Integrated Water Quality Models for Optimal Design and Control of Restoration Strategies	Fritz, L.J., Siniscalchi, A.G., Ramos, F. 1,2, Díaz, M.S, Estrada, V.G.
2727	Simulation of a NGCC power plant with CO2 capture: Exhaust gas conditioning strategies	Belzunce, P.S., García Lagos, M.V., Rodríguez, M.L.
3194	Application of Dynamic Modifier Estimation to an Industrial Propane- propylene Splitter	Erika Oliveira-Silva, Cesar de Prada, Daniel Navia

Advances in numerical methods and computational techniques

1454	Towards Automating Simultaneous Process Synthesis and Design Using Bayesian Optimization	Fischer C.D., Martínez E.C.
2101	Optimal design of chemical absorption-based carbon capture using an equation-oriented approach	Pedrozo, H. A., Valderrama- Rios C. M., Zamarripa, M., Morgan, J., Osorio-Suárez, J.P., <u>Uribe-Rodríguez, A.</u> , Diaz, M. S., Biegler L. T.
2132	Minimization of installation and operation costs in water distribution networks using a bound contraction methodology	Maria Izabela Silva, Eduardo Pacola, Carolina Carvalho, Esdras Carvalho
2340	User friendly EOMMM for rational mixed micelles design	Schulz, E., Durand, G.A.
2486	Dynamic optimization for sustainable management for a Salt Lake basin with a water-food-energy-carbon nexus approach	Siniscalchi, A., Schulz, E., Lara, R.J., <u>Diaz M. S</u>

Advances in process control, operation and intelligent systems

Advances in process and/or product synthesis, design and optimization

1563	Design of greener cycloaddition reactions. Selection of ionic liquids (ILs) from their actual microstructural composition	Adam, C. G., Fernández, J. L., Della Rosa C. D., Bravo, Ma V., Martini, Ma B.
2533	Water Source Diagram (WSD) Method: Application in Batch Processes	de Oliveira, P.P., Francisco, F.S., Pessoa, F.L.P., <u>Queiroz, E.M</u>
2662	Technical and economic assessment of anion exchange membrane electrolysis for green hydrogen production	De la Ossa, D., Ramírez, G. E., Uribe - Rodríguez, A.
2763	Food emulsion system formulation using computer aided design tools	Hernández-Ochoa R., Navarrete R., López-Malo, A., Palou E. Ramírez-Corona, N.

2984	Sustainable Process Design Opportunities	Jakkraphat Kongcharoenkitkul, Teng Zhou, <u>Rafiqul Gani</u>
2986	Chemical analysis and substitution in products and their manufacturing processes	Nichakorn Kuprasertwong, Jakkraphat Kongcharoenkitkul, Rafiqul Gani
3161	Sustainable design and capacity expansion planning for the integrated chemical process under endogenous uncertainty	Yuxuan Xu1, Lifeng Zhang, Zhihong Yuan

Advances in Planning, Scheduling and Supply Chain Management

	1647	Optimal design of the supply chain for the ready mix-concrete production in the Metropolitan Region of Buenos Aires.	Paulo, C.I., Cordoba, G.P., Irassar, E.F.
		The Use of the Roadmap to verify trends related to the minimization of calcium carbonate scale in oil and gas production and exploration systems	Daás, A. A, Figueiredo, M.A.G, Corrêa, H. L.
	1886	Different perspectives to assess the supply chain performance considering sustainability criteria	Vanzetti, N., <u>Corsano, G.</u> , Montagna, J.M.
	3164	Multistage stochastic programming for the facility location of a modular mobile closed-loop supply chain	Ge, Congqin ¹ , Zhang, Lifeng, Yang, Wenhui ¹ , <u>Yuan, Zhihong</u>