

ISCRE 27 – POSTER SESSION 1

MONDAY, JUNE 12, 2023

5:00 pm to 7:00 pm

Poster Presenters are in **bold**

AUTOMATED LIQUID-PHASE KINETIC MODEL CONSTRUCTION: A NOVEL MODELING APPROACH APPLIED TO CYCLOHEXANE OXIDATION

Kevin De Ras, Connor Huntwork, Gust Popelier, Unni Kurumbail, Lander Nelis, Joris W. Thybaut, Ive Hermans and Kevin M. Van Geem

(Poster #3)

ULTRASOUND-ASSISTED ESTERIFICATION OF LIGNIN TO BIOLUBRICANTS

Dalma Schieppati, Gregory S. Patience and Daria C. Boffito

(Poster #47)

THERMO-PHOTO DRM OVER NANOROD SHAPED CERIUM DIOXIDE DECORATED WITH NICKEL

Kristijan Lorber, Janez Zavašnik, Jordi Sancho-Parramon, Matej Bubaš, Matjaž Mazaj and Petar Djinović

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EFFECT OF CALCINATION ATMOSPHERE ON CERIA-ZIRCONIA SUPPORTED NI CATALYSTS FOR CARBON DIOXIDE REFORMING OF METHANE

Hyun-Seog Roh and Beom-Jun Kim

(Poster #53)

MICROWAVE POLYMERIZATION OF D,L-LACTIDE TO POLYLACTIC ACID

Nicolas Patience, Daria Camilla Boffito and Xavier Banquy

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AUTOTHERMAL SABATIER REACTOR FOR CO₂ HYDROGENATION TO RENEWABLE NATURAL GAS: EXPERIMENTAL PROOF-OF-CONCEPT AND PARAMETER SENSITIVITY ANALYSIS

Yichen Zhuang and **David Simakov**

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DESIGN OF A MINIATURISED CSTR FOR KINETIC STUDIES USING INLINE RAMAN SPECTROSCOPY

Eleni Grammenou, Chen Tang, Georgios Gkogkos and Asterios Gavriilidis

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DYNAMIC OPERATION OF REACTORS: CLASSIFYING KINETICS FOR QUASI STEADY STATE ENHANCEMENT

Austin Morales, Praveen Bollini and Michael Harold

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EFFECTS OF OPERATIONAL CONDITIONS ON SONOCHEMICAL DEGRADATION OF PHENOL

Daisuke Kobayashi, Hinako Hasegawa, Mari Shiina and Miyu Moriyama

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MULTIPHYSICS-MULTISCALE NON-CATALYTIC GAS-SOLID REACTION MODEL FOR INDUSTRIAL HYDROGEN DIRECT REDUCTION PROCESS

Patrícia Metolina, Alexander Ariyoshi Zerwas, Anthony G. Dixon and Roberto Guardani

(Poster #110)

STUDY ON THE HYDRODYNAMICS OF STRUCTURED PACKING: LIQUID HOLDUP AND PRESSURE DROP OF A NOVEL 3D-PRINTED PACKING

Biao Sun

(Poster #116)

A NEW PHOSGENATION REACTION MECHANISM FOR PREPARING DIISOCYANATE BASED ON FLASHING ATOMIZATION

Zitong Hou, Jianyong Mao, Haifeng Chen, Jijun Ge and **Rongshan Bi**

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INVESTIGATION OF KINETIC PROCESS DYNAMICS FOR HYDROGENATION OF CARBON OXIDES UNDER REALISTIC CONDITIONS

Robert Güttel, Max Gäßler, Simon Hermann, Dominik Meyer and Jens Friedland

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THE EFFECT OF PROMOTERS, TEMPLATE, AND HYDROTHERMAL PROCESSING TIME ON KFI-TYPE ZEOLITE ACTIVITY FOR METHANOL TO DME CONVERSION

Alireza Lotfollahzade Moghaddam, Mohammad Ghavipour, Jan Kopyscinski and Melanie Hazlett

(Poster #156)

FLUIDISED BEDS FOR STRONGLY EXOTHERMIC REACTIONS – RESULTS OF PILOT SCALE INVESTIGATIONS

Philipp Riechmann and Tilman Schildhauer (**Emanuele Moiola**)

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CU-BASED CATALYSTS FOR THE CONVERSION OF CO₂ INTO JET FUEL

Christopher Panaritis, Ergys Pahija, Brian Rutherford, Charles-David Guerette, Martin Couillard, Bussaraporn Patarachao, Jalil Shadbahr, Farid Bensebaa, Gregory S. Patience and Daria C. Boffito

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MODELLING OF CYCLIC CO₂ ADSORPTION AND IN SITU METHANATION OVER DUAL FUNCTION MATERIALS: A PARAMETRIC STUDY

Alessio Tauro, **Fabio Salomone**, Emanuele Giglio, Samir Bensaid and Raffaele Pirone

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THE SYNERGISTIC EFFECT OF IRON-BASED CATALYSTS AND TETRALIN ON THE PARTIAL UPGRADING OF OIL SAND BITUMEN

Moataz Abdrabou, Xue Han, Yimin Zeng and **Ying Zheng**

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ZrO₂ AS A PROMOTER ON BIMETALLIC PD-PT/AL₂O₃ DIESEL OXIDATION CATALYSTS

Azam Movasati and Melanie Hazlett

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BLACK LIQUOR VALORIZATION VIA REACTIVE DISTILLATION AND HETEROGENEOUS CATALYSIS: MASS TRANSPORT AND REACTIVITY

Laura Reyes, Clemence Nikitine, Lea Vilcocq and **Pascal Fongarland**

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IMPROVING EFFICIENCY AND DE-RISKING OF FIXED-BED REACTOR SCALE-UP VIA ADVANCED PROCESS MODELING

Stepan Spatenka and Vasco Manacas

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UNVEILING PRODUCTION OF ALKALINE EARTH METALS FROM DOLOMITE BY METHANOTHERMIC REDUCTION

Javad Vahabzadeh Pasikhani, Mohammad Khajouei, Mohammad Latifi and Jamal Chaouki

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MIXING AND FLOW CHARACTERIZATION IN AN SMX STATIC MIXER

Athanasios Kritikos, Ravendra Singh, Fernando Muzzio and George Tsilomelekis

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SELECTIVE REDUCTION OF O₂ FOR THE SYNTHESIS OF H₂O₂ VIA H₂ AND HYDROXYQUINONE MEDIATORS

Mayank Tanwar, Jason Adams, David Flaherty and Matthew Neurock

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IMPACT OF CATALYST MICROSTRUCTURE AND SOOT DEPOSITS ON HYDROCARBON AND CO PROFILES IN CATALYTIC FILTER MEASURED BY SPACI-MS

Miroslav Blazek, Aldo Lanza, Emily Price, Lucy Phillipson, Djamela Bounechada, Petr Koci, Andrew York and **Martin Sourek**

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COUPLING CHEMICAL LOOPING AIR SEPARATION WITH THE ALLAM CYCLE

Syed Saqline, Lizhong Yang, Alessandro Romagnoli and **Wen Liu**

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CATALYST SYNTHESIS FOR METHANE CRACKING REACTION WITH CONTROLLED CARBON GROWTH

Xinlong Chen, Xin Pang and **Clémence Fauteux-Lefebvre**

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RTD GUIDES MITIGATION STRATEGIES TO MINIMIZE FORMING EXPLOSIVE MIXTURES

Mahdi Sharifian, Christian Patience and Gregory Patience

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CFD-DEM MODELING OF LABORATORY-SCALE BINARY FLUIDIZED BED: VALIDATION WITH RADIOACTIVE PARTICLE TRACKING (RPT) EXPERIMENTS

Subi Nath and **Shantanu Roy**

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NUMERICAL ANALYSIS AND OPTIMIZATION OF GAS INLET CONFIGURATION OF A STATIC MIXER BASED HIPOXTM REACTOR

Lvliang Wang, **Yanxia Xu**, Yuanyuan Qian and Xuejing Yang

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MODELING THE EFFECT OF TEMPERATURE, CO, AND H₂O ON THE NO_x UPTAKE AND RELEASE BEHAVIOR IN PD/CHA PASSIVE NO_x ADSORBERS

Marvi Kaushik, Rajeshwari C. Kamble, M. Ali Haider and Divesh Bhatia

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PREPARATION AND CHARACTERIZATION OF PITCH-DERIVED CARBON MOLECULAR SIEVES (CMS) FOR BIOGAS SEPARATION

Byeong-Hoon Lee, **Hye-Min Lee** and Byung-Joo Kim

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EFFECT OF FLUID PROPERTIES ON FLOW UNIFORMITY IN PARALLEL MICROCHANNELS

Bhalaji Moorthy, **V M Rajesh** and Karan Gupta

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Sn-BETA ZEOLITE CONVERTS LACTOSE FROM CHEESE WHEY TO LACTIC ACID IN A FLUIDIZED BED REACTOR

Paula Andrea Rivera Quintero, Daria C Boffito and Gregory S Patience

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MODELLING OF HEAT AND MASS TRANSPORT IN SINGLE PELLET STRING REACTORS WITH DIFFERENT LEVELS OF DETAIL

Christian Bauer, Tabea Gros, Hanh My Bui and Olaf Hinrichsen

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CATALYTIC CONVERSION OF METHANOL AND ETHANOL TO BIOFUELS OVER COPPER/HYDROXYAPATITE

Daniel Alejandro Valdivieso-Vera, **M. Olga Guerrero-Perez**, Ivan Alonso Santos-López, Isabel Barroso-Martín, Enrique Rodríguez-Castellón, Gerardo Antonio Flores-Escamilla and Edward Handy Brent

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INTENSIFIED ANTIVIRAL PERFORMANCE OF MICRO-STRUCTURED METAL FOAM IN WATER

Jinghan Zhao and Emily Yi Wai Chiang (**Stephen Vanderburgt**)

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PREDICTION OF MARINE FUEL TYPE BASED ON SPECTRAL DATA AND SULPHUR CONTENT USING SUPPORT VECTOR MACHINES

Njideka Chima-Amaeshi, Chris O'Malley, Mark Willis and Paul Winstone

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SUSTAINABLE AVIATION GASOLINE: PROCESS DESIGN BASED ON SIMULATION AND EXPERIMENT

Dorela Dhamo, Jannis Kühn, Simon Lüttin, Michael Rubin and Roland Dittmeyer

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ON THE HEAT AND MASS TRANSPORT DURING THE CO₂ METHANATION REACTION IN A SINGLE PELLET STRING REACTOR

Tabea Gros, Christian Bauer, Hanh My Bui and Olaf Hinrichsen

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ENHANCED CARBON CAPTURE BY EXFOLIATED LAYERED DOUBLE HYDROXIDES: STRUCTURE EVOLUTION & PERFORMANCE

Rija Ansari, **Deepak Kirpalani**, Jeff Fraser, Douglas Vick and Simona Moisa

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OPTIMIZATION OF OLEFINS YIELD AND A NEW KINETIC MODEL FOR FISCHER-TROPSCH SYNTHESIS ON A PROMOTED IRON CATALYST

Arash Yahyazadeh, Ajay K Dalai and Lifeng Zhang

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FIXED BED CHROMATOGRAPHIC REACTOR FOR THE PRODUCTION OF 2, 2-DIMETHOXYPROPANE

Akash Shinde and Sanjay Mahajani

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SCALE-OUT STRATEGY FOR FLOW UNIFORMITY USING SPIRAL AND NON-SPIRAL PARALLEL MICRO/MILLI CHANNELS

Devang Patel, V M Rajesh and **Karan Gupta**

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AQUEOUS-PHASE OXIDATION OF METHANE ON Fe-SILICALITE-1: ROLE OF FRAMEWORK Fe

Balashanmugam Venu Gopal, Niket S. Kaisare and Parasuraman Selvam

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KEY PROCESS PARAMETERS TO INFLUENCE SPACE-TIME YIELD AND PRODUCT RATIO OF SYNGAS FERMENTATION

Lukas Perret, Nikolaos Boukis and Joerg Sauer

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PROCESS MODELLING OF THE SYNTHESIS OF POLYPROPYLENE: FROM LAB TO INDUSTRY

Anna Konopka, Johanna Fernengel, Richard Walter Fischer and Olaf Hinrichsen

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AN INTEGRATED MODELING PLATFORM FOR SCREENING CO₂ CAPTURE MATERIALS

Ashish Mhadeshwar, Jayashree Kalyanaraman, Anantha Sundaram, Joseph Falkowski, Jonathan Szlachta, Rodrigo Neumann Barros Ferreira, Binquan Luan, Ricardo Ohta, Felipe Oliveira, Mathias Steiner and Yogesh Joshi

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EFFECT OF CATALYTIC STRUCTURES ON FLUID FLOW AND HEAT TRANSFER CHARACTERISTICS USING STRUCTURE-RESOLVED CFD SIMULATIONS

Kuldeep Singh, **Ankita Kumari**, Olaf Hinrichsen and Vivek V. Buwa

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AUTOTHERMAL DRY REFORMING OF METHANE AT HIGH TEMPERATURE AND ELEVATED PRESSURE UNDER A NICKEL SPINELIZED CATALYST PREPARED FROM A METALLURGICAL RESIDUE

Muhammad Irfan Malik, Nicolas Abatzoglou and Inés Esma Achouri

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STEADY STATE MULTIPLICITY FEATURES AND SPATIAL INHOMOGENEITIES DURING METHANE OXIDATION ON Pt-Pd/Al₂O₃ MONOLITH CATALYST

Jonathan Ratcliff and **Michael Harold**

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CATALYTIC CONVERSION OF WOOD RESIDUES INTO ETHYL LEVULINATE AND LEVULINIC ACID
Naima El Mehdi, Sanaz Safa, **Mathieu Sarrazin**, Raymond Le Van Mao and Yacine Boumghar
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CARBON DIOXIDE ADSORPTION: ISOTHERM AND TEMPERATURE EFFECT ON BREAKTHROUGH CURVE
Jose Antonio Colin Luna, Margarita M Gonzalez Brambila, Jesús Miguel, Jacinto Nava and **Julio César García Martínez**
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EFFECT OF PRESSURE ON DIRECT REDUCTION OF MINERAL IRON CARBONATE WITH HYDROGEN
Sascha Kleiber, Astrid Loder, Matthäus Siebenhofer and Susanne Lux
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DEEP LEARNING METHODS FOR ACCELERATING THE SCREENING OF M-CERIA CATALYST FOR REVERSE WATER GAS SHIFT REACTION
Yue Yu, Kishore Kandasamy, Kira Selby, David Simakov, Aiping Yu, Pascal Poupart, Ricardo Fukasawa and Luis Ricardez-Sandoval
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HEAT TRANSFER STUDY IN A LIQUID CONTAINING GAS-SOLID FLUIDIZED BED TO CONVERT FRUCTOSE TO VALUE-ADDED CHEMICALS
Zahra Khani, Joshua Brinkerhoff and Gregory Patience
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NEAR AND SUPERCRITICAL WATER AS A TUNABLE SOLVENT FOR RECYCLING MULTILAYER PLASTIC FILMS
Madison Reed and Michael Timko
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EVALUATING THE EFFECT OF SEVERAL PARAMETERS ON THE LIMITS OF KINETIC AND MASS TRANSFER CONTROLLED REGIONS BY USING A 1+1D MODEL FOR THE SCR WITH DUAL-LAYER CATALYSTS
Paôlla Chrystine Pinheiro Patrício, Melanie Jane Hazlett and Alex De Visscher
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EXPANDED-RANGE PHOTOTHERMAL CONTINUOUS GAS-PHASE CO₂ REDUCTION OVER METAL-DOPED MOLYBDENUM SULFIDE / TITANIUM OXIDE HETEROJUNCTIONS
Arturo Sanz Marco, Jose L. Hueso, Victor Sebastian, Francisco Balas and **Jesus Santamaria**
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INTEGRATED SUPERCRITICAL HYDROTHERMAL MINERALIZATION FOR WASTE TO CARBON CAPTURE

David Kenney, Michael Timko and Andrew Teixeira

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PARAMETERS ESTIMATION FOR TOTH AND LANGMUIR MODELS ON ZEOLITE 13X IN THE CO₂ ADSORPTION PROCESS

E. Oliverio Ruiz-González, J. César García-Martínez, E. Ramírez-Castelan, S. Núñez-Correa, M. Mercedes González-Brambila, J. Guadalupe Pacheco-Sosa, A. Karina Medina-Mendoza and J. Antonio Colin-Luna (**Emigdio Gregorio Zamora Rodea**)

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MODELING OF TRANSPORT-KINETIC INTERACTIONS IN VARIOUS CONFIGURATIONS OF EGG-SHELL CATALYST PARTICLES

Anuradha Nagaraj and **Patrick Mills**

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CATALYTIC METHANE PYROLYSIS OVER IRON-ALUMINA FOR THE PRODUCTION OF CARBON-NEUTRAL HYDROGEN

Enrico Sartoretti, Piercosimo Vedele, Fabio Salomone, Chiara Novara, Fabrizio Giorgis, Massimiliano Antonini and **Samir Bensaid**

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CYCLOADDITION REACTION OF CO₂ WITH EPOXIDE USING GUANIDINIUM FUNCTIONALIZED Zr-MOF CATALYSTS UNDER ATMOSPHERIC PRESSURE, SOLVENT AND CO-CATALYST-FREE CONDITIONS

Syedeh Molood Masoom Nataj, Frédéric-Georges Fontaine and Serge Kaliaguine

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LARGE-SCALE EPOXIDATION OF TERPENES IN THE AQUEOUS PHASE

Yacoub Mahamat Ahmat, Hilaire Mossak Kamkui and Serge Kaliaguine

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