

ISCRE 27 – POSTER SESSION 2

TUESDAY, JUNE 13, 2023

4:30 pm to 6:30 pm

Poster Presenters are in **bold**

KINETICS AND REACTION MECHANISM OF LIMONENE EPOXIDATION WITH HYDROGEN PEROXIDE PROMOTED BY Al_2O_3

Vincenzo Russo, Giuseppe Rossi, Wander Perez Sena, Rosa Turco, Martino Di Serio, Kari Eranen, Dmitry Murzin and Tapio Salmi (**Tommaso Cogliano**)

(Poster #16)

ENERGY STORAGE IN IRON: KINETIC ANALYSIS OF IRON OXIDE REDUCTION WITH HYDROGEN

Carola Kuhn, Steffen Tischer and Olaf Deutschmann

(Poster #59)

ON THE DYNAMICS OF ELECTRIFICATION OF HETEROGENEOUS CATALYTIC REACTORS

Rucha Railkar and Dionisios Vlachos

(Poster #62)

AB INITIO MODELLING OF THE SIZE EFFECT IN RUTHENIUM NANOPARTICLES FOR AMMONIA PRODUCTION

Matej Huš, Luka Skubic, Sašo Gyergyek and Blaž Likozar

(Poster #74)

HYDROGEN PRODUCTION AND CARBON CAPTURE BY METHANE PYROLYSIS IN A FIXED BED REACTOR

Manas Mokashi, Patrick Lott, Akash Shirsath, Ahmet Celik, Heinz Müller, Steffen Tischer, Lubow Maier, Johannes Bode, David Schlereth, Frederik Scheiff, Dieter Flick, Michael Bender, Kai Ehrhardt and Olaf Deutschmann

(Poster #79)

MODELING AND ANALYSIS OF THE BIOETHANOL-TO-JET FUEL PROCESS

Hyeon Park, **Yubeen Jung**, Ho-Jeong Chae, Young-Woong Suh, Young-Min Chung and Myung-June Park

(Poster #105)

CATALYST DESIGN ASPECTS FROM FIRST PRINCIPLES FOR SELECTIVE GLYCEROL HYDRODEOXYGENATION TO 1,3-PROPANEDIOL

Ajin Rajan and Jithin John Varghese

(Poster #108)

KINETIC MODEL OF THE THERMAL AND CATALYTIC AGEING OF THE AXLEBOX GREASE

Léa Camousseigt, Aurélie Galfre, Françoise Couenne, Camella Oumahi, Sandrine Muller and Melaz Tayakaout

(Poster #118)

CONVERSION OF THE DEBRIS-TREATED ASH INTO CESIUM-ADSORBENT USING ALKALI REACTION

Takaaki Wajima

(Poster #128)

INVESTIGATION OF SIMULTANEOUS AMMONIA SYNTHESIS AND ABSORPTION EQUILIBRIUM BY GIBBS FREE ENERGY MINIMIZATION

Theresa Kunz and Robert Güttel

(Poster #129)

INTENSIFYING BIOMASS AND SOLID WASTE PYROLYSIS BY CHEMICAL LOOPING

Lukas C. Buelens, Varun J. Singh, Guillaume Lambert, Hilde Poelman, Kevin M. Van Geem and Vladimir V. Galvita (**Michiel Van Cauwelaert**)

(Poster #136)

REVISITING MICROKINETICS OF OXIDATIVE COUPLING OF METHANE IN THE AGE OF UNCONVENTIONAL SUPPORTS

Gontzal Lezcano, Shekhar Kulkarni, Vijay Velisoju, Natalia Realpe and Pedro Castaño

(Poster #137)

BRIDGING LAB-SCALE STUDIES TO PROCESS DESIGN FOR THE CHEMICAL CONVERSION OF BIOMASS TO LEVULINATE ESTERS

Joanne Woloszyn, R. Tom Baker and **Clémence Fauteux-Lefebvre**

(Poster #148)

FAST MODELS FOR CO₂ ADSORPTION IN A FIXED BED WITH POROUS SORBENTS

Govind Tak, Swapna Rabha and **Himanshu Goyal**

(Poster #157)

THREE-SCALE REDUCED ORDER CONTINUUM MODELS FOR REAL TIME SIMULATIONS OF CATALYTIC MONOLITH REACTORS

Ram Ratnakar and Vemuri Balakotaiah

(Poster #176)

RENEWABLE PRODUCTION OF ADIPATES FROM ALDARIC ACIDS BY HETEROGENEOUS CATALYSIS

Miha Grilc, Florian M. Harth, Brigita Hočevar and Blaž Likozar
(Poster #177)

ICE LAYER CRYSTALLIZATION FOR A BINARY SYSTEM: EXPERIMENTAL STUDY AND MODELING BY THE PHASE-FIELD METHOD

Xiaoqian Huang, Aurélie Galfré, Françoise Couenne and Claudia Cogné
(Poster #186)

ELECTRO-MECHANICAL PISTON REACTOR TO DRIVE PROPANE PYROLYSIS

Aya Abousrafa, Mamoun Al-Rawashdeh and Patrick Linke
(Poster #190)

ELECTRICALLY-HEATED CATALYTIC PARTIAL OXIDATION OF METHANE OVER STRUCTURED CATALYSTS

Nooshin Moradi Kazerooni and Gregory Scott Patience
(Poster #202)

A METHODOLOGY FOR SOLID MINERAL CHARACTERIZATION WITHIN ORGANIC WASTE AND THROUGHOUT THEIR TRANSFORMATION: A FOCUS ON PHOSPHORUS

Christian Del Valle Velasco, Fabrice Béline and Céline Vaneeckhaute
(Poster #207)

NON-LINEAR ASYMMETRIC CONVECTION IN CRYOGENIC INSULATION LAYERS OF LNG AND LH2 STORAGE TANKS

Swapnil Sharma and Vemuri Balakotaiah
(Poster #221)

RECYCLING FORMALDEHYDE TO HYDROGEN VIA STEAM REFORMING ON ALKALI PROMOTED Pt/ZrO₂ CATALYSTS

Michela Martinelli, Elijah S. Garcia, Zahra Rajabi, Caleb D. Watson, Donald D. Cronauer, A. Jeremy Kropf and Gary Jacobs
(Poster #226)

RECYCLING TECHNOLOGIES FOR POLYMETHYL METHACRYLATE AND POLYCARBONATE IN AUTOMOTIVE INDUSTRY

Tien Dat Nguyen, Nooshin Saadatkhah, Yanfa Zhuang, Minh-Tan Ton-That, Adrien Faye, Karen Stoeffler and Gregory Patience
(Poster #235)

MICROWAVE-ASSISTED NICKEL AND VANADIUM REMOVAL FROM CRUDE PETROLEUM OIL USING D2EHPA: A KINETIC STUDY

Amin Solouki, Mohammad Monzavi and Jamal Chaouki

(Poster #238)

CARBON BLACK PRODUCED BY PLASMA IN BENZENE SOLUTION APPLIED AS THE CONDUCTIVE AGENT IN SUPERCAPACITOR

Gyeong-Geun Lee, Chan-Seo You and **Sang-Chul Jung**

(Poster #242)

DEVELOP A SUSTAINABLE PROCESS TOWARD THE RECOVERY OF HARD-TO-DISSOLVE MINERALS BASED ON FLASH JOULE HEATING

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

(Poster #255)

ENHANCEMENT OF LIGHT FIELD UNIFORMITY USING INTERNAL COMPONENTS IN A CIRCULAR TUBE REACTOR

Manman Hao, Hao Wang, Xinying Liu, Kuankuan Liu, Runchang Shi and **Yanxia Xu**

(Poster #258)

IMPACT OF ZEOLITE FRAMEWORK ON NOX STORAGE AND RELEASE CYCLE IN PASSIVE NOX ADSORBERS

Marvi Kaushik, Tuhin S. Khan, M. Ali Haider and Divesh Bhatia

(Poster #260)

IMPROVED METHOD FOR CFD MODELLING OF CRYOGENIC FROST FORMATION

Joshua Chang Qai Wong, Biao Sun, Milinkumar Shah and Vishnu Pareek

(Poster #261)

REPRESENTATING HIERARCHICAL CATALYST SUPPORTS BY MEANS OF 3D PORE NETWORK MODELS

Gabriel Ledezma, **Jan J. Verstraete**, Loic Sorbier, Damien Leinekugel-Le Cocq, Elsa Jolimaitrea and Christian Jallut

(Poster #271)

DECIPHERING POLYMERIZATION ROUTES IN HYPERBRANCHED POLYMERS THROUGH KINETIC MODELING

Matthew Coile, Alexander Shaw, Sai Phani Kumar Vangala, Changxia Shi, Eugene Chen and Linda Broadbelt

(Poster #272)

NUMERICAL AND EXPERIMENTAL STUDY OF ULTRASONICALLY-ASSISTED LEACHING OF SPENT CATHODES

Chiara Canciani, Elia Colleoni, Paolo Guida and William Roberts (**Varaha Sarvothaman**)

(Poster #276)

ELECTROSPUN CARBON NANOFIBERS COMPRISING NICKEL MANGANESE SULFIDE AS AN ANODE MATERIAL FOR LITHIUM-ION BATTERIES

Parthasarathi Bandyopadhyay, Erdenebayar Baasanjav, See Hoon Lee and **Sang Mun Jeong**

(Poster #286)

INVESTIGATING THE EFFECT OF IMPURITIES ON THE DRY REFORMING OF BIOGAS FOR HYDROGEN PRODUCTION

Muriel Chaghouri, Carmen Ciotonea, Lucette Haingomalala Tidahy, Fabrice Cazier, Cédric Gennequin and Edmond Abi-Aad

(Poster #293)

A TECHNO-ECONOMIC ASSESSMENT OF THE REUTILISATION OF MUNICIPAL SOLID WASTE INCINERATION ASH FOR CO₂ CAPTURE FROM INCINERATION FLUE GASES BY CALCIUM LOOPING

Lek Hong Lim, Preston Tan, Wei Ping Chan, Andrei Veksha, Gregorz Lisak and **Wen Liu**

(Poster #298)

KINETIC MODELLING OF PLASTIC WASTE THERMOCHEMICAL RECYCLING: POLYETHYLENE TEREPHTHALATE PYROLYSIS

Andrea Locaspi, Marco Mehl, Matteo Pelucchi and Tiziano Faravelli

(Poster #339)

REVEALING THE ROLE OF LITHIUM IONS IN MOLTEN SALT WITH MACHINE LEARNING AIDED META-ANALYSIS, MOLECULAR DYNAMICS AND EXPERIMENT

Ze Sun, Yuxin Luo and Haiou Ni

(Poster #343)

OPTIMIZATION DESIGN OF PHOSGENE DECOMPOSITION TOWER FOR PHOSGENE CONTAINED EXHAUST GAS WITH SODIUM HYDROXIDE SOLUTION

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

(Poster #360)

DOPING AN OXOPHILIC METAL INTO A METAL CARBIDE: UNRAVELLING THE SYNERGY BETWEEN THE MICROSTRUCTURE OF THE CATALYST AND ITS ACTIVITY AND SELECTIVITY FOR HYDRODEOXYGENATION

Sagar Bathla, Chi-Cong Tran, Serge Kaliaguine and Samir Mushrif

(Poster #365)

SOLID COPOLYMER ELECTROLYTES TO ACHIEVE ROOM-TEMPERATURE EFFICIENT ALL-SOLID-STATE LI AND NA METAL BATTERIES

Vincent St-Onge, Jean-Christophe Daigle and Jérôme Claverie (**Florian Marti**)

(Poster #376)

AN AT-LINE MONITORING STRATEGY OF SUGAR ISOMERIZATION VIA ATR-FTIR SPECTROSCOPY FOR RAPID CATALYST DEVELOPMENT

Jakub Konkol and George Tsilomelekis

(Poster #378)

REACTION PARAMETER OPTIMIZATION AND KINETIC STUDY OF FISCHER-TROPSCH SYNTHESIS REACTIONS OVER COMNAG/TITUD-1 CATALYST

Girish Kamath and Ajay K Dalai

(Poster #381)

HOMOGENEOUS AND HETEROGENEOUS CATALYSIS OF GLUCOSE TO LACTIC ACID AND LACTATES: A REVIEW

Thomas Saulnier-Bellemare and Gregory Patience

(Poster #385)

5- HYDROXYMETHYLFURFURAL PRODUCTION FROM PRETREATED LIGNOCELLULOSIC BIOMASS

Hela Hammami

(Poster #390)

LASER-DRIVEN SYNTHESIS OF ADVANCED CARBON-BASED CATALYSTS: SINGLE-ATOM CATALYSTS (SACS) AND CARBON DOTS

Ainhoa Madrid, Gema Martinez, Ekaterina Pakrieva, Reyes Mallada, **Jesus Santamaria** and Jose Hueso

(Poster #409)

CO₂-FREE HYDROGEN PRODUCTION BY PYROLYSIS OF METHANE AND BIOGAS: A COMPARATIVE EXPERIMENTAL STUDY.

Ahmet Celik, Iadh Ben Othman, Heinz Müller, **Patrick Lott** and Olaf Deutschmann

(Poster #423)

PYROLYSIS OF PLASTIC WASTE USING A NICKEL-BASED CATALYST SUPPORTED ON A MINING RESIDUE FOR THE PRODUCTION OF CARBON NANOMATERIALS AND SUSTAINABLE ENERGY CARRIERS

Karen Bechwaty, Salma Belbessai, Ines Esmâ Achouri and Nicolas Abatzoglou

(Poster #424)

CONTINUOUS CATALYTIC CONVERSION OF LACTOSE TO POLYMER GRADE LACTIC ACID IN A SPINNING DISK REACTOR

Maoline Houndedoke, Thomas Saulnier-Bellemare, Daria C. Boffito and Gregory S. Patience
(Poster #434)

A NOVEL HYDROGEN PRODUCTION METHOD BY A CIRCULAR ECONOMY PROCESS

José Jozic García Hernández, Bernardo Jair Esquivel Cortés, Ricardo Montoya González, José Antonio Colín Luna, Oscar Manuel González Brambila, Margarita Mercedes González Brambila and **Julio Cesar Garcia Martinez**
(Poster #436)

ENHANCEMENT OF LIQUID FUEL PRODUCTION USING IRON-ZEOLITE HYBRID CATALYST IN THE FISCHER TROPSCH SYNTHESIS

Min Hye Youn, Deviana Deviana, Geun Bae Rhim, Kwang Young Kim, Kee Young Koo and Dong Hyun Chun
(Poster #443)

INVESTIGATION INTO ELECTROLYTE RECOVERY IN WASTE LITHIUM ION BATTERY RECYCLING

Stephen Vanderburgt, Rafael M. Santos and Emily Yi Wai Chiang
(Poster #449)

PYROLYSIS OF Cu (II) CONTAMINATED PANICUM VIRGATUM BIOMASS: IMPACT OF CONTAMINATION ON YIELDS AND QUALITY OF BY-PRODUCTS.

Khadija Olivia Ogoula Igouwe, Dalia Allouss, Ines Esmâ Achouri and Nicolas Abatzoglou
(Poster #452)

ENZYMATIC CO₂ ABSORPTION IN INTENSIFIED PACKED-BED BIOREACTORS: A TECHNO-ECONOMIC ASSESSMENT

Kaven Nguyen, Ion Iliuta, Francis Bougie, Louis-César Pasquier and Maria C. Iliuta
(Poster #455)

MACHINE LEARNING PREDICTIONS OF OIL YIELDS OBTAINED BY PLASTIC PYROLYSIS AND APPLICATION TO THERMODYNAMIC ANALYSIS

Elizabeth Belden, Nikolaos Kazantzis, Randy Paffenroth and Michael Timko
(Poster #469)

INSIGHTS INTO CO-PYROLYSIS OF POLYMER MIXTURES THROUGH EXPERIMENTS, KINETIC MODELING AND MACHINE LEARNING

Barbara Alejandra Perez, J.V. Jayarama Krishna and **Hilal Ezgi Toraman**
(Poster #476)

MODEL-BASED COMPARISON OF NOVEL SINGLE-PASS OPERATED FT REACTOR AND CONVENTIONAL REACTOR TECHNOLOGIES

Zbigniew Urban and **Stepan Spatenka**

(Poster #481)

INVESTIGATION OF PRIMARY DECOMPOSITION OF POLYPROPYLENE USING A PY-GC×GC-FID/TOF-MS SYSTEM

Barbara Perez and Hilal Toraman

(Poster #486)

MECHANISTIC MODELING OF POLYETHYLENE TEREPHTHALATE GLYCOLYSIS USING KINETIC MONTE CARLO FRAMEWORK

SriBala Gorugantu, Nicholas Rorrer, Sabin Adhikari, Ana Morais, Bonnie Buss, Gregg Beckham, Robert Allen, Sanat Kumar and Linda Broadbelt

(Poster #493)

CHAOTROPIC PROMOTION OF DILUTE-ACID LIGNOCELLULOSIC HYDROLYSIS

Timothy Woodard and Michael Timko

(Poster #494)

FISCHER-TRPOSCH SYNTHESIS OVER SPONTANEOUSLY ACTIVATABLE IRON-BASED CATALYSTS IN A SLURRY-PHASE REACTOR

Dong Hyun Chun, Geun Bae Rhim, Kwang Young Kim and Min Hye Youn

(Poster #501)

BIFUNCTIONAL CATALYSTS BEHAVIOUR OF Ni-Pd AND Ni-Pt SUPPORTED ON Zr-PILC IN THE ACTIVITY OF HYDRODEOXYGENATION OF EUGENOL

E. Gregorio Zamora Garcia Rodea, C. Rogelio Tapia-Medina, Deyanira Angeles-Beltran, M. Mercedes Gonzalez-Brambila, J. Guadalupe Pacheco-Sosa, R. Rosas-Cedillo and J. Antonio Colín-Luna

(Poster #505)

DATA RECONCILIATION AND INCREMENTAL IDENTIFICATION FOR NONISOTHERMAL REACTION SYSTEMS

Manokaran Veeramani, Sridharakumar Narasimhan and Nirav Bhatt

(Poster #507)

IMPROVING CHARACTERIZATION OF POLYETHYLENE PYROLYSIS

Run Ze Cao and Cedric Briens

(Poster #520)

MODELING TRANSPORT-KINETIC INTERACTIONS IN COMMERCIAL CATALYST SHAPES FOR SO₂ OXIDATION TO SO₃

Anuradha Nagaraj and **Patrick Mills**

(Poster #526)

A NOVEL REUSABLE NANOCOMPOSITE BASED ON NATURAL CLAY AND Co₃O₄ NANOPARTICLES TO REMOVE Pb(II) AND Cd(II) IONS FROM WATER

Noureddine El Messaoudi, Abdelaziz El Mouden, Valbonë Mehmeti, Abdellah Lacherai and Amane Jada

(Poster #545)

METHACRYLIC ACID FROM POLY(METHYL METHACRYLATE) (PMMA): A NEW APPROACH IN POLYMER REPROCESSING

Olga V. Chub, Jean-Luc Dubois and Gregory Scott Patience

(Poster #570)