

BOOK OF ABSTRACTS

MaCKiE

**International Conference on Mathematics in
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2025**

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MaCKiE PLENARY

MaCKiE PLENARY

STOCHASTICITY IN BIOREACTION ENGINEERING: OPPORTUNITIES AND CHALLENGES FOR BIOPROCESS INDUSTRIES

Duygu Dikicioglu
Department of Biochemical Engineering, University College London, United Kingdom

Corresponding Author: Duygu Dikicioglu (d.dikicioglu@ucl.ac.uk)

Abstract

Stochasticity in bioreaction and bioprocess engineering refers to the inherent randomness and variability that arise in biological systems due to factors like molecular fluctuations, gene expression noise, variability in enzymatic activity, and environmental conditions. Biological stochasticity can be advantageous not only for the living system, but also for novel bioproduct and bioprocess design and development. Stochastic behaviour allows individual cells or organisms to respond differently to the same stimuli allowing a broader range of phenotypes to be explored. Random mutations introduce variability that can help populations explore better adaptation, thus increasing evolutionary potential. Stochasticity allows flexibility and robustness in uncertain environments preventing the system from committing to a single solution but instead allowing it to explore a range of strategies in parallel. Arguably the most process-relevant characteristic of biological stochasticity is its inherent affinity for exploration allowing living systems exploit beyond known successful strategies, thus ensuring potentially better options, too, to be evaluated.

However, such stochastic behaviour can directly influence the growth performance of cell populations in bioreactors as well as the efficiency of metabolic pathways, leading to varying product yields and quality, in addition to probable process instability. Understanding and modelling these random cellular fluctuations are crucial for optimising bioprocesses, as they can impact everything from cell growth to substrate consumption and product formation. Stochasticity can pose serious challenges rendering process control difficult, decreasing reproducibility, and necessitating sophisticated monitoring and modelling techniques to be implemented to ensure consistent bioprocess performance. Successful control strategies often require incorporating stochastic elements themselves to improve robustness and predictability in large-scale bioproduction systems.

This talk will focus on select examples of molecular, cellular, and process level stochasticity in mammalian and microbial systems for bioprocessing applications, with a particular focus on how this emergent behaviour can be handled employing model-driven approaches.

MaCKiE KEYNOTE

MaCKiE KEYNOTE 1**NANOCONFINEMENT EFFECTS ON DIFFUSION AND REACTION IN POROUS MATERIALS, HETEROGENEITY, AND WHAT WE COULD LEARN FROM NATURE FOR APPLICATIONS.**

Marc-Olivier Coppens

Centre for Nature-Inspired Engineering and Department of Chemical Engineering, University College London,
London WC1E 7JE (United Kingdom)

Corresponding Author: Marc-Olivier Coppens (m.coppens@ucl.ac.uk)

Abstract

Diffusion in nanoporous materials is a fascinating topic of great practical relevance, e.g., for catalytic and molecular separation processes. Despite decades of intensive experimental and theoretical work, there are still gaps in our understanding of diffusion fundamentals. Recent insights into which processes limit the overall transport in porous materials could influence the design criteria and the operation of important processes that apply nanoporous materials, including those for environmental processes relevant to sustainable development – from increasing product selectivity in catalysis and membrane separations, to materials for electrochemical devices and biomedical engineering. Such insights result from more sophisticated experimental characterization tools and molecular simulations but also progress in materials synthesis.

Diffusion in ordered, uniform microporous materials with strong nanoconfinement effects has been extensively studied, e.g., in zeolites, metal organic frameworks and carbon nanotubes. Most materials, however, are heterogeneous, and this introduces surprises that matter in applications. I will discuss the impact of heterogeneity and nanoconfinement on molecular transport and reactions, focusing on Knudsen diffusion in amorphous alumina with its fractal rough surface, and surface barriers in zeolite crystals. I will show how heterogeneity can be embraced, how thinking holistically across length scales is essential, and how nature can teach us lessons to design better catalysts.

PHYSICS-INFORMED TRANSFER LEARNING AND MACHINE LEARNING BASED OPTIMIZATION IN CHEMICAL ENGINEERING

Erdal Aydin
Department of Chemical and Biological Engineering
Koç University, Turkiye

Corresponding Author: Erdal Aydin (eydin@ku.edu.tr)

Abstract

Dynamic processes in chemical engineering, such as wastewater treatment and visbreaking, present significant modeling challenges due to their nonlinearities, complexities, and uncertainties. Developing traditional mechanistic models, while grounded in first principles, often is time-consuming and these models are difficult to apply to complex industrial systems. Conversely, purely data-driven methods, especially recurrent neural networks (RNNs), offer powerful tools for capturing nonlinear dynamic behavior but frequently require large, high-quality datasets and are vulnerable to overfitting and noisy data.

This lecture explores recent advances in integrating physical knowledge into machine learning models to overcome these limitations, with a focus on two main areas: We first examine innovative physics-informed training methodologies designed to embed governing differential equations directly into neural network loss functions, and hybrid recurrent architectures that integrate physics-based and data-driven components. These approaches improve model generalization, reduce overfitting, and yield more compact, robust neural networks through hyper-parameter optimization. In parallel, transfer learning is leveraged to address the challenges of noisy, sparse, or incomplete data commonly encountered in industrial applications. By transferring knowledge from physics-based simulation models and related industrial plants, prediction performance in an industrial wastewater treatment plant is significantly improved, with validation accuracy gains exceeding 50%. This synergy between physics-informed modeling and transfer learning underscores a promising pathway for robust, data-efficient process modeling.

The second part of the lecture delves into embedding physics-informed neural network models within optimization frameworks to facilitate faster and more reliable decision-making for complex chemical processes. By utilizing piecewise linear approximations and physics-informed training, neural network surrogates are developed that enable near-global optimal solutions with substantially reduced computational effort. Case studies demonstrate that physics-informed surrogates not only improve solution quality but also accelerate computation times compared to conventional approaches.

MaCKiE KEYNOTE 3

TOP-DOWN AND BOTTOM-UP MULTISCALE METHODOLOGY FOR MODELING AN INDUSTRIAL-SCALE CATALYTIC REACTOR

Carlos O. Castillo-Araiza

Laboratory of Catalytic Reactor Engineering Applied to Chemical and Biological Systems, Department of Process and Hydraulic Engineering, Universidad Autónoma Metropolitana, Mexico City 09340, Mexico

Corresponding Author: Carlos O. Castillo-Araiza (coca@xanum.uam.mx)

Abstract

This key-note lecture aims to elucidate the application of a combined top-down and bottom-up multiscale methodology for the modeling of an industrial catalytic reactor. While this methodology has been applied in our laboratory to both chemical and biological reaction systems for over 15 years, this presentation exemplifies its application to the selective catalytic oxidation of ethane to produce ethylene. Due to the thermodynamic and kinetic constraints inherent to selective oxidation reactions, the wall-cooled packed-bed reactor is selected as the reference technology, a configuration that remains highly relevant in current industrial practice. The selection of this reactor technology also reinforces the relevance of the fundamental research developed in our laboratory, as it addresses a longstanding modeling gap in which, despite its extensive industrial use for over a century, there is still no widely accepted paradigm-based mathematical model capable of reliably simulating its performance under industrial operating scenarios.

The modeling begins with a top-down multiscale approach, developing a pseudo-continuous model of the heterogeneous reactor using conventional experimental data and theoretical frameworks. Regime analysis and sensitivity studies are used to identify dominant transport limitations. A bottom-up approach then complements this, using Particle-Resolved Simulations (PRS) to characterize transport phenomena under realistic conditions and determine accurate transport descriptors. In parallel, Density Functional Theory (DFT) is used to derive a microkinetic model. These microscale insights are integrated into the reactor-scale model, yielding a robust multiscale framework that offers key advantages over conventional approaches:

- (i) Transport phenomena that typically limit industrial-scale reactor modeling are no longer approximated using macroscopic approaches. Instead, PRS data informs the models, enhancing accuracy and relevance in the characterization of transport phenomena;
- (ii) Parameters involved in the microkinetic model are constrained within uncertainty ranges determined by DFT calculations, improving its reliability; and
- (iii) To ensure consistency across scales, the Volume Average Method is applied to enhance the soundness of pseudo-continuous models developed using reactor engineering principles.

This top-down and bottom-up multiscale methodology reduces uncertainties in modeling transport and reaction mechanisms and supports the rational design of intensified catalytic reactors. Its versatility also enables application to a wide range of chemical and biological systems, reinforcing its value as a modern tool for industrial reactor design.

MaCKiE KEYNOTE 4

MULTISCALE MODELING OF ZEOLITE CATALYTIC PROCESS: FROM CRYSTAL TO REACTOR

Xinggui Zhou
State-Key Laboratory of Chemical Engineering and Low-Carbon Technology
East China University of Science and Technology
130 Meilong Road, Shanghai 200237, China

Corresponding Author: Xinggui Zhou (xgzhou@ecust.edu.cn)

Abstract

Industrial zeolite catalysts feature multi-level transport networks governing multiscale flows and diffusion, with reactor-scale (macro) mass transfer dominated by convection in interparticle voids, catalyst pellet-scale (meso) transfer driven by diffusion, and microscale (crystal/active site) processes involving adsorption, surface reactions, and desorption. While surface reactions convert reactants to products, multiscale transport efficiency significantly impacts overall catalytic performance and product distribution. Current research predominantly focuses on single-scale transfer and reaction processes, with limited integration across scales.

This report reports a multiscale coupling methodology integrating continuum models to characterize transfer and diffusion behaviors across crystal, pellet, and reactor scales. Case studies on n-hexane isomerization and benzene alkylation validate the model. For n-hexane isomerization over hierarchically structured ZSM-5 zeolites (HSZs), diffusion limitations from micropores (crystals) and macro/mesopores (pellets) are regulated by adjusting crystal size, porosity, and macro/mesopore dimensions. Introducing intraparticle porosity reduces micropore diffusion barriers, significantly enhancing the conversion compared to conventional zeolites. For benzene alkylation, diffusion limitations in binder (macro/mesopores) and crystals (micropores) are addressed by optimizing crystal size, intracrystalline pores, and binder properties (volume fraction, porosity, pore diameter). Higher binder porosity proves more critical than pore diameter in balancing mass transfer and catalytic activity, with recrystallization altering binder-catalyst interactions. These multiscale models should serve to guide the optimal design of industrial zeolite catalysts.

MaCKiE KEYNOTE 5

ON THE INTERPLAY OF SPATIO-TEMPORAL GRADIENTS IN CATALYTIC KINETICS

Evgeniy A. Redekop

Department of Chemistry, Centre for Materials Science and Nanotechnology (SMN), University of Oslo, Norway

Corresponding Author: Evgeniy A. Redekop (evgeniy.redekop@kjemi.uio.no)

Abstract

Rigorous analysis of the spatio-temporal gradients in the composition, temperature, and, therefore, reaction rates inside chemical reactors have played an essential role in developing quantitatively-sound mathematical models of these devices, with wide-reaching implications for reactor design and, fundamentally, for accurate kinetic measurements. Well-known criteria exist for the assessment of whether such gradients are significant in each particular case or can be ignored to simplify the analysis. In recent decades, both the experimental techniques used to monitor chemical reactions (e.g. effluent analytics and operando spectroscopy) and the computational models used to simulate them (e.g. Computational Transport Phenomena) become increasingly resolved in space and time. These advances provide unprecedented opportunities to quantify the spatio-temporal variations within chemical processes but also challenge us to develop more nuanced frameworks within which such information can be better understood and utilized for deriving new chemical knowledge.

In this talk, I will first discuss a theoretical framework for analyzing spatio-temporal gradients of chemical composition, e.g. gas, pore, and surface species, within a catalytic material at different scales, particularly for evaluating the impact of gradients on chemical kinetics. The framework is motivated by the concepts of “state-defining” and “state-altering” experiments in a Temporal Analysis of Products (TAP) reactor, in which gaseous species traverse the catalyst bed by means of Knudsen diffusion. The framework distinguishes the spatial and temporal components (i.e. marginal variances) of the total composition and/or temperature variance/gradients in the reactor. These distinct components are shown to be interdependent, with their interplay ultimately determining the lower bound of uncertainty in the measured kinetics. After presenting several illustrative examples relevant for TAP experiments, the framework will be extended to operando catalyst characterization data. In particular, it will be applied to meso-scopic mapping of coke deposition inside a catalytic extrudate using 3D Computed Tomography X-Ray Diffraction (CT-XRD). I will conclude by outlining the scope of potential applications of this analysis framework to various sources of space-/time-resolved experimental and simulated data relevant to heterogeneous catalysis and beyond.

MaCKiE KEYNOTE 6

SYNERGISTIC MODELING OF MULTIPHASE REACTORS: BLENDING CFD, MACHINE LEARNING AND DATA

Shantanu Roy
Indian Institute of Technology Delhi – Abu Dhabi, UAE

Corresponding Author: Shantanu Roy (roys@iitdabudhabi.ac.ae)

Abstract

The grand challenges of the global energy transition and the urgent demand for sustainable industrial growth necessitate unprecedented precision in understanding and optimizing complex chemical and electrochemical reactors. Traditional modelling approaches, while foundational, often face limitations in comprehensively capturing the intricate, multi-scale phenomena governing these highly dynamic systems. This talk posits that a truly transformative leap in reactor engineering, particularly for multiphase systems, could be achieved through the “synergistic integration of Computational Fluid Dynamics (CFD), advanced Machine Learning (ML) techniques, and high-fidelity experimental data, exemplified by methods such as Radioactive Particle Tracking (RPT)”. This powerful combination enables the development of robust, predictive models that are able to tide over some of the limitations of classical multiphase CFD, the uncertainties in experimentation, and also utilise meaningfully the vast body of data on multiphase reactors that are available in the public domain, and indeed in confidential databases within organisations. Ultimately, such improved predictability and understanding can drive both efficiency and sustainability in hard-to-abate sectors. As an illustration of this philosophy, in this talk, some recent work on the modelling of bubble columns and slurry bubble columns will be presented.

Industrial processes frequently rely on gas-liquid and gas-liquid-solid bubble columns, whose intricate hydrodynamics present persistent challenges for accurate design and scalable operation. While CFD methods and experimental techniques are indispensable for assessing flow dynamics, their application typically demands significant computational resources and time, hindering rapid iterative design. To address this, this research has explored fundamentally lowering time scales and computational expenses through the innovative integration of artificial intelligence and data science into the study of bubble column hydrodynamics, aiming for superior flow behavior prediction.

First, a detailed CFD simulation was established for benchmark air-water flow within a rectangular bubble column reactor. This work meticulously examined the impact of various interfacial forces, such as drag and lift, on predicting time-averaged axial liquid velocity and gas volume fraction. Crucially, these foundational CFD findings were rigorously validated against high-precision experimental data acquired using Radioactive Particle Tracking (RPT), demonstrating the critical role of empirical validation in refining computational models. Furthermore, a CFD-coupled Population Balance Model (PBM) simulation was employed for the same column to identify optimal breakage and coalescence kernel combinations governing air bubble diameter evolution, utilizing three distinct kernel combinations within the PBM transport equation. The CFD-PBM work is further enhanced with CFD data-driven Deep Neural Network (DNN) models. These DNN models were adeptly utilised to rapidly predict key time-averaged hydrodynamic parameters, including axial gas and liquid velocity, gas and liquid volume fraction, and the mean air bubble diameter. The study also elucidated the influence of categorical variables, such as interfacial force combinations, on phasic velocities through the developed DNN framework. A significant outcome was the creation of a Graphical User Interface (GUI) powered by these DNN models, enabling real-time hydrodynamic prediction.

Extending beyond CFD-derived data, the work concurrently proposed “experimental data-driven Machine Learning (ML) algorithms” for crucial design parameters like estimating the overall gas holdup in Slurry Bubble Column Reactors (SBCR). Leveraging approximately 2000 data points from existing open literature, various ML models (including Boosting, Bagging, Support Vector Regression (SVR), and DNN) were developed, culminating in another intuitive GUI for instant gas holdup prediction under specified operating conditions. These ML models' robustness was further assessed under unknown operating conditions in cold-flow gas-to-liquid processes, complemented by a sensitivity analysis.

The investigation concluded with a focused exploration of local hydrodynamics in SBCRs, integrating CFD and DNN modelling. A 3D transient Euler-Euler-Euler CFD simulation was developed for cold-flow gas-to-liquid processes, employing a modified drag coefficient for gas-liquid interaction to enhance the accuracy of time-averaged phasic volume fractions. The impact of solids loading, operating pressure, and superficial gas velocity on phasic volume fraction was rigorously assessed, with validation against existing experimental results. A CFD data-driven DNN model, complete with a dedicated GUI, was also proposed for real-time prediction of time-averaged gas, liquid, and solid volume fractions in these slurry systems.

This talk will underscore how the precise integration of high-fidelity experimental data (including RPT), advanced CFD, and the predictive power of Machine Learning is paramount to truly mastering multiphase dynamics for precision reactor engineering. This quantitative, interdisciplinary approach is vital not only for optimizing existing industrial processes but also for accelerating the design and deployment of next-generation, sustainable chemical transformations, pushing the boundaries of efficiency and driving the journey towards a decarbonized and circular economy in the chemical and biochemical engineering landscape.

FOOD MaCKiE KEYNOTE 1**INTERNET OF THINGS (IOT) NONTHERMAL EXTRACTION OF PROTEINS FROM PLANT BY-PRODUCTS: PROCESS OPTIMISATION AND SUSTAINABILITY ASPECTS**

Anet Režek Jambrak^{1*}, Antonio Petošić², Janko Diminić¹, Igor Erceg², Josipa Dukić¹, Mojca Čakić Semenčić¹, Anita Slavica¹, Filip Jukić², Dražen Kubatović², Marko Jurčević²

¹University of Zagreb, Faculty of Food Technology and Biotechnology

²University of Zagreb, Faculty of Electrical Engineering and Computing

Corresponding Author: Anet Režek Jambrak (anet.rezek.jambrak@pbf.unizg.hr)

Abstract

Nonthermal processing (NTP) has been investigated for food preservation and several applications, among which are extractions of valuable compounds from plant matrices. Most of nonthermal technologies have not yet reach technology readiness level (TRL), to be applied in the food industry. Pulsed electric fields (PEF) and high-pressure processing (HPP) are two technologies that are already in use in food industry having TRL level of more than 7. As current state of the art for Industry 4.0, and smart factories accordingly, there are new opportunities to implement elements of industry 4.0 in nonthermal processing. Industry 4.0 includes automation and data exchange in manufacturing technologies and includes cyber-physical system, Internet of things (IoT), advanced connectivity and cloud-computing to transform production units into “smart factories”. Moreover, with application of IoT, collection of in-line data, smart control of the process, big data optimization, as well as sustainable production and monitoring, there is possibility to develop a new era of Internet of nonthermal food processing technologies (IoNTP). The internet of things is a system of interrelated computing devices, mechanical and digital machines, objects, or people that are provided with unique identifiers (UIDs) and the ability to transfer data over a network without requiring human-to-human or human-to-computer interaction.

The application of NTP technologies, specifically high-power ultrasound (US) equipped with different sensors and transformed to IoT device, has been optimised for extraction of proteins. IoNTP - ultrasound extraction has been done on residue leaves in beetroot processing (*Beta vulgaris* L.) and leaves from faba bean (*Vicia faba* L.) processing. The goal is to use digitalisation in the NTP set-up (with sensors - for temperature, electrical conductivity, humidity, energy consumption, pressure etc. and IoT), to monitor and optimise extraction process of proteins. Green extraction of RuBisCO (Ribulose-1,5-bisphosphate carboxylase/oxygenase) protein from residues (from leaves, as they are usually discarded in the factory) has been successfully optimised.

As very important aspect of current research and future application in food industry is sustainability, it is necessary to implement Sustainable Development Goals (SDGs) in research activities. Waste, energy, economy, and environment are major pillar that need to be managed in terms of Agenda 2030 and SDGs. Energy conservation is vital for the sustainable development of the food industry. The three pillars of sustainability refer to environmental, economic, and social impacts of nonthermal technologies (i.e., energy balances, life cycle assessment (LCA), waste production/reduction, cost of production, impact to society) as well to set novel approach to introduce nonthermal technologies as smart systems in food industries. To determine sustainability, quantitative data must be acquired, with the most common method of an LCA.

FOOD MaCKiE KEYNOTE 2

DESIGN AND MODELING OF RADIOFREQUENCY TREATMENTS FOR FOODS

Maria Elena Sosa-Morales
Universidad de Guanajuato, Mexico.

Corresponding Author: Maria Elena Sosa-Morales (mariae.sosam@gmail.com)

Abstract

Radiofrequency (RF) application for foods is considered a thermal emerging technology. RF treatments result in fast and volumetric heating in foods, getting shorter times than the conventional processes. Also, RF waves exhibit higher penetration depth into food materials than microwaves. However, the main challenge for RF commercial application is the non-uniform temperature during the treatments. RF technology is applied with different purposes, such as pasteurization, sterilization, drying and disinfestation. Dielectric properties are key factors to design properly an RF treatment. Once different food properties and process parameters are established, modeling may be a useful tool to predict final conditions in foods. COMSOL and other software have been reported to accomplish the modeling taking account the electromagnetic behavior and the heat transfer during the process. This talk will show equipment, conditions for foods and modeling results reported for RF treatments recently. RF technology has potential to reach more stable foods and make them available and safe for consumers in different parts of the world.

FOOD MaCKiE KEYNOTE 3**HIGH PRESSURE FOR NONTHERMAL PROCESSING AND
HYPERBARIC STORAGE OF FOODS**

Jorge A. Saraiva
LAQV-REQUIMTE, Department of Chemistry
University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

Corresponding Author: Jorge A. Saraiva (jorgesaraiva@ua.pt)

Abstract

High pressure processing (HPP) is being increasingly used industries worldwide as a nonthermal food pasteurization method for several types of foods, having given many proofs that it can be used as a reliable and safe alternative to the conventional heat-based pasteurization methods. The fact that HPP takes place at room-like temperatures (or below) results in pasteurized foods with higher quality compared to those pasteurized by heat.

In addition to the success of nonthermal HPP, pressure-assisted thermal sterilization (PATS) was also approved by the United States Food and Drug Administration (FDA) as an alternative to the current commercial conventional food sterilization, allowing to obtain shelf-stable foods with improved quality due to the lower thermal impact of PATS. In fact, PATS takes advantage of the adiabatic heating/cooling phenomenon to quicker and homogeneously heat up/cool down foods, allowing for a shorter sterilization process.

Another application of high pressure regards hyperbaric storage (HS) for food preservation as an alternative/complement to the conventional refrigeration processes, especially when performed at naturally variable/uncontrolled room temperatures. HS makes use of low pressures (up to 100 MPa) at room-like temperatures or slightly below to hurdle microbial development. The major advantages of HS regard the considerable shelf-life extensions of foods compared to refrigeration, due to the gradual microbial inactivation that occurs during HS. This methodology has proven to be feasible not only against vegetative microorganisms (including pathogenic ones) but also allowed to inhibit the development of bacterial spores, in some cases even causing their inactivation (at room temperature) without the application of heat. The microbial inactivation observed during HS was reported to be possible to achieve at least 5-log vegetative pathogens and is being so additionally explored as a new pasteurization method, tentatively called moderate pressure pasteurization (MPP) by hyperbaric inactivation (HI), to distinguish it from the current HPP pasteurization. This methodology makes use of moderate pressures (100-250 MPa) for slow pasteurization at room temperature, at the same time food is being preserved with no need of refrigeration, being this particularly interesting for pressure-sensitive foods, such as raw meat and fish, for which HPP pasteurization causes considerable color changes, while MPP achieves 5-log inactivation (pasteurization status) with minimal colour changes. In this presentation, an overview on how HPP can be used to inactivate vegetative pathogenic bacteria and spores (when combined with moderate to high temperatures) will be given, as well for future applications, such as HS and MPP.

FOOD MaCKiE KEYNOTE 4

ASSESSMENT OF THE COLD CHAIN FOOD PRESERVATION PERFORMANCE AND THE T-TAP COLD CHAIN MANAGEMENT PLATFORM

J. Antonio Torres

School of Engineering and Sciences, Tecnológico de Monterrey, Mexico

Chief Editor, CYTA Journal of Food, Taylor & Francis

Editor, Innovative Food Science and Emerging Technologies (IFSET), Elsevier

Corresponding Author: J. Antonio Torres (dr.j.antonio.torres@gmail.com)

Abstract

A major reduction in food waste is critically important because at present agriculture uses half of habitable land, 70% of freshwater, and generates 26% of greenhouse gas emissions. Currently, the design and operation of refrigeration systems focuses on energy use. However, improved energy efficiency has not helped in reducing food losses currently estimated at 30%. A key reason is the lack of science-based tools to assess food preservation performance when designing and operating cold chain units. To fill this need, Tecnológico de Monterrey developed a Refrigeration Performance Indicator (RPI) calculated using product time-temperature data and validate predictive microbiology models. We will briefly review published RPI applications assessing the impact on microbial preservation performance of refrigeration technology (single and variable speed compressors), door openings, ambient temperature, refrigerator load, food location (drawer w/independent T control, body shelf, door shelf) and food matrix/microflora (dairy, meats, seafood, etc.). Also presented in this Webinar will be RPI values calculated as the ratio of the microbial degradation at temperatures observed during transportation over the one that would have occurred under a constant recommended temperature for the handling of fresh-cut mango (4C). By definition, values of $RPI \leq 1$, $=1$, and >1 indicate excellent, good and poor refrigerated preservation performance, whereas values $\gg 1$ indicate situations requiring urgent attention.

Products with short shelf-life such as fresh-cut mango are produced and shipped immediately to customers. Product spoilage begins when microorganisms complete an adaptation phase during which they undergo intracellular changes allowing them to grow under refrigeration. This consideration led to a second indicator of cold chain performance, extent of lag phase completion (LPC) with values beginning at 0 and reaching 1 when microorganisms begin growth. In this talk, we will present the T-TAP platform to assess the refrigerated transport preservation performance considering LPC and RPI values. If the lag phase is incomplete ($LPC < 1$), the microbial degradation has not begun. Consequently, T-TAP accepts the shipment. If the lag phase is completed ($LPP \geq 1$), T-TAP calculates the RPI. If the $RPI \leq 1$, T-TAP accepts the shipment, otherwise it is rejected. Data collected during commercial shipping will be used for illustration.

FOOD MaCKiE KEYNOTE 5**VIRTUALIZATION IN FOOD ENGINEERING WITH MECHANISTIC MODELING APPROACH FOR FOOD INDUSTRY BEYOND X.0**

Ferruh Erdogdu
Department of Food Engineering, Ankara University, Ankara, Türkiye

Corresponding Author: Ferruh Erdogdu (ferruh.erdogdu@ankara.edu.tr)

Abstract

One of the current challenges in food manufacturing industry is to design a novel process in the view of sustainability with three pillars: providing safety and quality, being economically efficient and having a resource efficiency. In this framework, it is essential to determine the interactions among transport phenomena (mass, heat, and momentum) and any other relevant physics with a mechanistic mathematical modeling approach for the optimal design and innovation. Virtualization represents a sophisticated strategic tool to design and to innovate a process with the presence of a mechanistic mathematical model describing the transport phenomena governing the process. With this background, the objective of this presentation is to introduce the virtualization and mathematical modeling for design and optimization for the food manufacturing industry.

For this purpose, motivation and needs for virtualization in processing are focused, mathematical modeling background and various approaches for modeling are introduced for industry-oriented novel innovative approaches. Virtualization with mathematical modelling-based simulation schemes supported with artificial intelligence and machine learning applications (besides IoT and big data) are also presented as key components of designing a sustainable process with computational control.

With the introduction of Industry 5.0 and beyond industry x.0, combining the digitalization with virtualization will be more significant for improved smarter sustainable approaches to innovate the food manufacturing industry specifically in the view of quality, safety, and efficiency.

BIG DATA-DRIVEN MICROBIAL RISK IDENTIFICATION AND ASSESSMENT IN THE FOOD SUPPLY CHAIN

Runrun Zhang¹, Jinsong Feng^{1,2}, and Tian Ding^{1,2*}

¹ College of Biosystems Engineering and Food Science, Zhejiang University, Hangzhou, Zhejiang 310058, China

² Future Food Laboratory, Innovation Center of Yangtze River Delta, Zhejiang University, Jiaxing, Zhejiang 314100, China

Corresponding Author: Tian Ding (tding@zju.edu.cn)

Abstract

Food safety represents a major global public health challenge, with microbial contaminations being the primary cause of foodborne illnesses. Traditional microbial risk analysis suffers from apparent limitations, including inherent latency, narrow coverage, and difficulty in traceability, rendering them inadequate for managing risks within modern complex food supply chains. This study innovatively constructs a big data-driven framework for microbial risk identification and prediction, aiming to achieve a strategic shift in risk management from “passive response” to “active prevention”. Specifically designed to support new product development, the platform systematically evaluates microbial safety throughout the entire chain. This includes identifying high-risk pathogens in raw materials, assessing the effectiveness of sterilization processes, and predicting product shelf life. The integrated approach enables active warning, precise localization, and rapid response to microbial risks. The framework significantly enhances the accuracy and timeliness of risk prediction and optimizes the allocation of testing resources. By facilitating big data-driven collaborative decision-making and emergency management between R&D and production teams, this approach provides core technical support for building an intelligent modern food safety governance system, which is of great significance for safeguarding public health and promoting industrial upgrading

ORAL PRESENTATIONS

ABSTRACT #1

MaCKiE ABSTRACT REFERENCE NUMBER: G002

DEVELOPMENT OF A RATIONAL KINETIC MODEL FOR THE STEADY-STATE CONVERSION OF DIMETHYL ETHER OVER ZSM-5 CATALYSTS

Toyin Omojola

Department of Chemical Engineering, Claverton Down, University of Bath, BA2 7AY. Bath. UK

Corresponding Author: Toyin Omojola (toyin.omojola@bath.edu)

Abstract

The conversion of methanol-to-olefins is industrially mature, although fundamental challenges exist in the description of the mechanism governing the formation of the first C-C bond and primary olefins. Until now, there is no kinetic evidence for any of the intermediates in the archived literature. In this work, we use two rational kinetic models that allow for the formation of intermediates (surface methoxy species, adsorbed ethylene, adsorbed water) with kinetic, spectroscopic, and theoretical evidence. These rational kinetic models were independently embedded in a plug flow reactor model that describes the evolution of dimethyl ether to ethylene and propylene in a temporal analysis of products (TAP) reactor. Scheme 1 can predict several transient features of dimethyl ether conversion, although there is poor agreement with the experimental induction period and steady-state behaviour. Scheme 2 can predict the steady-state features of dimethyl ether conversion and gives a better agreement with the induction period of propylene formation, although the transient features are not reproduced. Further work will focus on the description of the transient features of dimethyl ether conversion using the 2nd rational kinetic scheme.

ABSTRACT #2

MaCKiE ABSTRACT REFERENCE NUMBER: G003

MATHEMATICAL MODELING AND SIMULATION OF STEAM CRACKING OF PLASTIC-WASTE PYROLYSIS OILS: OVERCOMING KINETIC AND COMPUTATIONAL CHALLENGES

Tamás Buzogány¹, Ismaël Amghizar², Guy B. Marin², Geraldine J. Heynderickx¹ and Kevin M. Van Geem^{1*}

¹Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

²AVGI BV, Ghent, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

Chemical recycling of plastic waste is expected to become an important chemical process in the coming decade, with thermal pyrolysis followed by steam cracking playing a key role. However, plastic-waste pyrolysis oils present challenges for conventional steam crackers, affecting both operational stability and product yields. To address these challenges, simulation tools will play a crucial role. Therefore, a dedicated reaction model for modeling steam cracking of such oils is developed, starting from the fossil-based COILSIM1D simulation tool. Mathematical challenges that need to be overcome are integrating the large number of differential equations resulting from the very extensive CRACKSIM kinetic model in COILSIM1D. This required specific adaptations for pyrolysis oils by incorporating additional species for their representation, various novel reaction families, and adapted lumping techniques, while still ending up with CPU simulation times of less than a second. Essential is the distinction between the β network, modeling C_5^- reactivity, and the μ network, describing radical decomposition of C_5^+ species while applying the Pseudo-Steady-State Assumption (PSSA) to reduce computational time. A priori, in situ, and a posteriori lumping techniques are applied to manage the vast number of species while ensuring accurate representation. The final reaction network enables, for the first time, the simulation of plastic-waste pyrolysis oils in steam crackers. Comparative COILSIM1D simulations highlight the differences between pyrolysis oils and fossil feedstocks, providing insights for optimizing cracker operations with alternative feedstocks.

ABSTRACT #3

MaCKiE ABSTRACT REFERENCE NUMBER: G004

MULTI-OBJECTIVE OPTIMIZATION OF ELECTRIFIED SHOCKWAVE TURBOREACTOR FOR ENHANCED HEAT TRANSFER AND SELECTIVITY

Rejish Lal Johnson^{1,2}, Mike Bonheure¹, Mohamed H. Aissa², Tom Verstraete² and Kevin M. Van Geem^{1*}

¹ Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

² Turbomachinery and Propulsion Department (TU), von Karman Institute for Fluid Dynamics, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

Steam cracking and gas heating for chemical processes significantly contribute to CO₂ emissions in the chemical industry. The novel Power-to-Heat electrified shockwave turboreactors mitigate these emissions. This study presents a meta-model-assisted active learning optimization framework for electrified shockwave turboreactor technologies to improve heat transfer and selectivity. The in-house Computer-Aided Design Optimization (CADO) tool employs a Metamodel-Assisted Evolutionary Algorithm (MAEA) integrated with Kriging meta-models for multi-objective optimization to obtain a Pareto front that maximizes temperature rise across the turboreactor while minimizing the required mass flow. Additive Manufacturing (AM) constraints are imposed to ensure a feasible design. A validated Computational Fluid Dynamics (CFD) solver is utilized to evaluate each design iteration. The optimized reactor, tailored to the laboratory pilot unit, achieves a 38.57% increase in temperature rise and a 2% reduction in mass flow relative to the baseline. The reactive modelling indicates a higher temperature rise, leading to improved turboreactor selectivity. This framework demonstrates significant potential for advancing turboreactor performance and is scalable for industrial-scale implementation in the electrification of the energy-intensive process industry.

Acknowledgements

Rejish Lal Johnson acknowledges the Moonshot cSBO project P2O; HBC.2020.2620. The research leading to these results has received funding from the European Research Council - ERC Grant No. 101142065 and No. 818607.

ABSTRACT #4

MaCKiE ABSTRACT REFERENCE NUMBER: G005

PARTICLE-SCALE MODELING OF JOULE HEATING IN ELECTRIFIED FLUIDIZED BEDS

Hamed Hoorijani¹, Yi Ouyang^{1*}, Patrice Perreault² and Kevin M. Van Geem¹

¹ Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

² Laboratory for the Electrification of Chemical Processes and Hydrogen (ElectrifHy), University of Antwerp, Antwerp, Belgium

Corresponding Author: Yi Ouyang (yi.ouyang@ugent.be)

Abstract

With the growing interest in electrified chemical processes, this study presents the first multi-scale framework for modeling an electrified gas-solid fluidized bed reactor (e-bed) using fundamental principles. The framework models direct resistive heating by capturing electrical conduction and Joule heating at the particle scale. Graph theory concepts were employed to dynamically identify conductive particle chains as electrical pathways. By applying conservation of electric current density and Ohm's law, particle potentials, electric current, and Joule heat flux were numerically determined. Given the high heating rates in e-beds, radiative heat transfer was incorporated using the Monte Carlo ray-tracing method. The approach was validated against electrified fixed-bed reactor data from the literature. A pseudo-2D e-bed study showed that higher input voltage increases both particle and gas-phase temperatures. However, thermal resistance at the particle-gas interface limits the gas-phase temperature rise, highlighting the potential of electrified reactors in minimizing unwanted gas-phase reactions. Temperature rise profiles differed at various voltages because increased temperature changed the physical properties of the gas, impacting flow patterns that affect the amount of joule heating in the reactor.

Acknowledgments

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ABSTRACT #5

MaCKiE ABSTRACT REFERENCE NUMBER: G006

ARTIFICIAL NEURAL NETWORK-BASED MODELING AND OPTIMIZATION OF NANOFILTRATION MEMBRANES FOR LITHIUM/MAGNESIUM SEPARATION

Elif Gungormus* and Hasan Sildir
Department of Chemical Engineering
Izmir Institute of Technology, Izmir, Turkiye

Corresponding Author: Elif Gungormus (elifgungormus@iyte.edu.tr)

Abstract

With the increasing global demand for lithium, the significance of its extraction from salt-brine lakes, which offer advantages of low cost and abundant reserves, is becoming increasingly prominent. However, the high magnesium content in these sources necessitates the development of selective and efficient separation strategies to enable effective lithium recovery. Nanofiltration membranes present a promising alternative for lithium recovery due to their low energy consumption, absence of chemical requirements, and environmentally sustainable nature. Nevertheless, achieving a high Li/Mg separation efficiency requires a comprehensive optimization of membrane properties and filtration conditions. This study proposes an artificial neural networks (ANNs)-based data driven modeling approach to enhance the efficiency of this separation process. Given its capability to represent complex, nonlinear relationships among variables and generate high-accuracy predictions, ANN is a promising methodology for process optimization. Through this modeling approach, the relative significance of input variables will be determined, their impact on key performance metrics will be analyzed, and the optimum membrane characteristics and operating conditions will be predicted. The optimization facilitated by the developed model is expected to minimize the time and cost constraints associated with experimental trials, thereby enabling a more systematic and efficient approach to the development of high-performance membranes.

Acknowledgments

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ABSTRACT #6

MaCKiE ABSTRACT REFERENCE NUMBER: G007

A REACTION-ADVECTION-DIFFUSION MODEL TO DESCRIBE NON-UNIFORMITIES IN COLORIMETRIC SENSING USING μ PADS

N. Kulkarni and S. Pushpavanam
Department of Chemical Engineering
Indian Institute of Technology, Madras, India

Corresponding Authors: N Kulkarni (kulkarninamratha1207@gmail.com), S Pushpavanam (spush@iitm.ac.in)

Abstract

Non-uniform product (color) distribution in colorimetric μ PADs affects accuracy and reliability of measurements. The underlying mechanisms responsible for this remain unclear. We model a typical colorimetric sensor to investigate the influence of mass transport and reaction dynamics on product distribution in porous paper substrate. We consider an analyte (which needs to be measured), initially uniformly distributed in the porous substrate, reacting with a reagent imbibed from a sessile droplet. The intensity of the colored product is used to quantify the analyte. The model includes species mobility to capture washout and precipitation effects. The process is modelled in two stages. In Stage 1, the droplet imbibition creates two flow domains, forming a moving boundary problem. Stage 2 begins after droplet penetrates completely. We analyzed the effect of different parameters on product distribution. A monotonic, radially increasing distribution occurs for slow reactions with excess reagent, with a steeper gradient at higher reagent concentrations. An immobile product leads to non-monotonic distribution. This mimics ring-like patterns observed in experiments. A more uniform distribution is achieved in thicker, more porous substrates but with reduced color intensity. Immobilizing the analyte further enhances uniformity.

ABSTRACT #7

MaCKiE ABSTRACT REFERENCE NUMBER: G009

CONSISTENCY-REGULARIZED DUAL-STAGE SEMI-SUPERVISED LEARNING FOR PREDICTION OF ATTRIBUTES IN CHEMICAL PROCESSES WITH INCOMPLETE DATASETS

Xiaochen Liu, Minglei Yang* and Wenli Du
School of Information Science and Engineering
Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China
University of Science and Technology, Shanghai, China

Corresponding Author: Minglei Yang (mlyang@ecust.edu.cn)

Abstract

In chemical processes, the prediction of product attributes is crucial for real-time optimization and control, however, incomplete datasets, due to various sampling frequencies, strongly affect the accuracy and efficiency of data-driven models. To address this, this paper proposes a semi-supervised learning method based on such datasets, namely Consistency-Regularized Dual-Stage Learning (CRDL). The method subdivides the dataset into high-frequency and low-frequency parts and identifies relationships between different types of output data. A two-stage model was designed. The first stage uses high-frequency data, and the second uses data reclassified based on low-frequency and output relationships. The method performance is evaluated by considering the error accumulation, the number of labeled data, the impact of the noise scale and the unsupervised loss coefficient. The effectiveness of CRDL on accuracy improvement is validated through the case study on Continuous Catalytic Reformer (CCR) process.

Acknowledgments

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ABSTRACT #8

MaCKiE ABSTRACT REFERENCE NUMBER: G010

A CRITICAL EVALUATION OF THE CRITICAL LINES OF WATER HYDROCARBON SYSTEMS

Gust Popelier¹, Maarten Sabbe¹, Florence Vermeire², and Kevin Van Geem^{1*}

¹Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

²Department of Chemical Engineering, KU Leuven, Leuven, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

Recycling plastic waste through pyrolysis in combination with supercritical water has promised to result in a lighter and cleaner oil than standard pyrolysis. Predicting the behavior of a mixture of water and hydrocarbons at these conditions is fundamental to understanding this process. The basis of such predictions is usually an Equation of State, a model that predicts the thermodynamic state of the system, allowing for the determination of vapor-liquid, liquid-liquid and vapor-liquid-liquid equilibria. Validation of an Equation of State at these conditions is done by predicting critical points, as these are the most commonly available experimental datapoints at these conditions. This work presents a modified methodology to predict these critical points tailored to water-hydrocarbon systems. A new evaluation function is proposed to grade the performance of the Equation of State.

Acknowledgments

Gust Popelier acknowledges the Fund for Scientific Research Flanders (FWO) for financial support via doctoral fellowship grant 1S58323N.

ABSTRACT #9

MaCKiE ABSTRACT REFERENCE NUMBER: G011

CHEMINFORMATICS-DRIVEN AUTOMATED KINETIC MODELING WITH GENESYS-PY

Lowie Tomme¹, Ruben Van de Vijver¹, Yannick Ureel¹, Maarten R. Dobbelaere¹, Christian V. Stevens² and
Kevin M. Van Geem^{1*}

¹Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

²Department of Green Chemistry and Technology, Ghent University, Ghent, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

Kinetic models are essential to gain insights into chemical processes. First-principle models can provide valuable information on the followed reaction pathways. In this context, we have created Genesys-Py, an automatic detailed kinetic model generator that distinguishes itself by its high flexibility. For example, this software tool allows the user to model gas-phase and catalytic processes. Furthermore, the flexible thermodynamics and kinetics assignment allows users to easily include their own property estimation method, which is especially useful for catalytic processes. Also, the symmetry calculation method applies to all molecules and transition states. Overall, this software tool enables users to generate detailed kinetic models of tens of thousands of reactions flexibly.

ABSTRACT #10

MaCKiE ABSTRACT REFERENCE NUMBER: G012

MULTI-SCALE MODELING OF CALCIUM-LOOPING IN SUPER-DRY REFORMING

Robin Vercauteren*, Michiel W.F. Van Cauwelaert, Lukas C. Buelens, Kevin M. Van Geem and Vladimir V. Galvita
Laboratory of Chemical Technology (LCT)
Ghent University, Belgium

Corresponding Author: Robin Vercauteren (robin.vercauteren@ugent.be)

Abstract

This study explores super-dry reforming (SDR) of methane for intensified CO₂ utilization, focusing on modeling the carbonation-decarbonation of a CO₂-sorbent prepared through industrial methods. Solving the reactor model equations for the SDR process requires a trustworthy kinetic model governing the effect of operating conditions on the performance of this material. Kinetic parameters from existing models will be optimized based on experimental kinetic data. Additionally, the impact of internal mass transfer limitations in upscaled material extrudates will be assessed. Future work will include a detailed energy balance to account for the exo- and endothermicity of the process, aiming to obtain a model to assist in process optimization for pilot-scale super-dry reforming of methane.

Acknowledgments

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ABSTRACT #11

MaCKiE ABSTRACT REFERENCE NUMBER: G013

KINETIC ANALYSIS IN REACTION NETWORKS: ELUCIDATION OF REACTION MECHANISMS IN ASYMMETRIC AUTOCATALYSIS

Oliver Trapp
Department of Chemistry
Ludwig-Maximilians-University Munich, Germany

Corresponding Author: Oliver Trapp (oliver.trapp@cup.uni-muenchen.de)

Abstract

Chemical reactions that lead to a spontaneous symmetry breaking or amplification of the enantiomeric excess are of fundamental interest in explaining the formation of a homochiral world. An outstanding example is Soai's asymmetric autocatalysis, in which small enantiomeric excesses of the added product alcohol are amplified in the reaction of diisopropylzinc and pyrimidine-5-carbaldehydes. Comprehensive kinetic experiments and modelling of the hemiacetal formation in the Soai reaction allow the precise prediction of the reaction progress, the enantiomeric excess as well as the enantiomeric excess dependent time shift in the induction period of this autocatalytic reaction. New software tools will be presented for detailed and precise kinetic analysis.

ABSTRACT #12

MaCKiE ABSTRACT REFERENCE NUMBER: G014

REGULATION OF MICRO-ENVIRONMENTS BY MULTI-METAL PROMOTERS: A THEORETICAL STUDY ON CO₂ ACTIVATION OVER IRON CARBIDE CATALYSTS

Xingxing Li, Nan Song*, Xuezhi Duan, Xinggui Zhou and De Chen
State Key Laboratory of Chemical Engineering
East China University of Science and Technology, China

Corresponding Author: Nan Song (cuiky@ecust.edu.cn)

Abstract

Essentially developing and regulating the unique electronic property of iron carbide catalysts involving multi-metal promoters to understand structure–activity relationship of CO₂ activation process is still a great challenge. Here, metals and transition metals were introduced as strategies for electronic structure regulation to theoretically understand the underlying nature of CO₂ adsorption and activation behaviors over Fe₃C catalysts. The distinctive micro-environment on Fe₃C surface made it more conducive to CO₂ adsorption and activation, which could be further enhanced by the addition of multi-metal promoters. The electronic properties of promoters well explained their influence on CO₂ adsorption behavior, while the binding energy of promoters had a good linear relationship with the CO₂ activation barrier. Specifically, there existed a distance effect by the doped multi-metals. When the doped metals were adjacent to each other, it would be more beneficial for CO₂ dissociation, and when they were far away from each other, the effect of single metal near CO₂ became more pronounced. Moreover, there existed an extreme point in the Bader charge values to make CO₂ adsorption the most stable on the surface of catalysts.

Acknowledgments

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ABSTRACT #13

MaCKiE ABSTRACT REFERENCE NUMBER: G016

OPTIMAL MICROGRID PLANNING: INTEGRATING MIXED-INTEGER PROGRAMMING AND MONTE CARLO SIMULATIONS FOR RELIABLE AND COST-EFFECTIVE ENERGY SYSTEMS

Mohammadreza Jahanbakhsh, Can Erkey and Erdal Aydın*
Koç University, Chemical and Biological Engineering Department, Rumelifeneri Yolu, Istanbul, 34450,
Türkiye
Koç University, KUHyTech, Rumelifeneri Yolu, Istanbul, 34450, Türkiye

Corresponding Author: Erdal Aydın (eyaydin@ku.edu.tr)

Abstract

This paper presents a microgrid planning framework that combines mixed-integer linear programming with Monte Carlo reliability simulation to optimize system design under economic and technical constraints. Key components—diesel generators, fuel cells, batteries, and solar PV—are modeled using piecewise linear approximations to capture costs and reliability metrics. Implemented in Pyomo and solved with Gurobi, the model optimizes generation and storage capacities while providing visual insights. A case study yields an optimal system with 1500 kW diesel, 500 kW fuel cells, 1300 kW/1300 kWh batteries, and 6000 kW solar PV, achieving a \$31.1M total cost, \$0.0983/kWh LCOE, 0.53 MWh/year unmet energy, and 14.4 hours/year load loss. Sensitivity analyses confirm design robustness.

Acknowledgments

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ABSTRACT #14

MaCKiE ABSTRACT REFERENCE NUMBER: G017

PILOT-SCALE VORTEX REACTOR FOR EFFICIENT THERMAL PYROLYSIS OF POLYSTYRENE AND POLYETHYLENE

Rohit Kumar, Yihan Wang, Parviz Yazdani, Oğuzhan Akin, Bahman Goshayeshi,
Robin John Varghese and Kevin M. Van Geem*
Laboratory for Chemical Technology
Ghent University, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

The efficacy of polystyrene (PS) and polyethylene (PE) thermal pyrolysis in a pilot-scale vortex reactor was investigated at different temperatures. Sophisticated analytical techniques like comprehensive two-dimensional gas chromatography and a refinery gas analysis (RGA) system were employed to analyze the products. Styrene recoveries of 74 wt.%, 86 wt.%, and 88 wt.%, respectively, at 500 °C, 600 °C, and 700 °C temperatures exceed the yields of classical continuous reactors such as stirred tanks or fluidized bed reactors. PIONA analysis of the pyrolysis products of PE pyrolysis indicates ~73 wt. % primary olefins are formed. The quantified pyrolysis products indicate the reactor dynamics and lower residence time promote primary decomposition while minimizing significant secondary reactions, such as hydrogen transfer and cyclization.

Acknowledgments

We acknowledge financial support from C-PlaNeT, the ERC Grant OPTIMA (818607), and the China Scholarship Council (CSC).

ABSTRACT #15

MaCKiE ABSTRACT REFERENCE NUMBER: G018

KINETICS AND SIMULATION OF POLYETHYLENE LIQUEFACTION IN SUPERCRITICAL WATER

Sphurti P. Kulkarni, Gust Popelier, Gilles Dossche, Friso Versteeg, Miloš Auersvald, Marvin Kusenber and Kevin M. Van Geem*

Laboratory for Chemical Technology (LCT), Ghent University,
Technologiepark 125, Ghent B-9052, Belgium

Corresponding Author: Kevin M. Van Geem (Kevin.VanGeem@UGent.be)

Abstract

Supercritical water (SCW) liquefaction of Polyethylene (PE), a major component of waste plastic, has gained interest as a sustainable method for converting it into valuable liquid hydrocarbon products. This study combines experiments, advanced analysis, simplified kinetic modeling, and process simulations for a comprehensive investigation of SCW liquefaction of PE. The reactions were conducted using a batch reactor over a range of temperatures (360 to 430 °C) and time (30 to 120 min) under autogenic pressure (>22 MPa). A highest oil yield (~ 90 %) was obtained at 430 °C in 120 min, with only liquid and gaseous products formed. An advanced GC x GC analysis of oil revealed a broad hydrocarbon distribution with naphthene as dominant fraction. The hydrocarbon formation rates were estimated by developing a lumped kinetic model by grouping the hydrocarbons based on the carbon number and structure. Further, the batch process was simulated in Aspen Plus by coupling the lumped kinetic model. While simulations predicted yields of lumps accurately over wide range of conditions, the accuracy was highly dependent on the defined thermophysical properties of lumps. Overall, the mechanistic insights, kinetic model and simulation were developed providing a basis for design of large scale recycling process.

ABSTRACT #16**MaCKiE ABSTRACT REFERENCE NUMBER: G019****MULTI-STAGE GAS-LIQUID VORTEX REACTOR WITH A
CYCLONE FOR PROCESS INTENSIFICATION: CFD-BASED DESIGN
FOR MASS TRANSFER AND SEPARATION**

Siyuan Chen¹, Afroditi Kourou¹, Qingang Xiong², Geraldine J. Heynderickx¹, Kevin M. Van Geem¹ and Yi Ouyang^{1*}

¹Ghent University, Laboratory for Chemical Technology, Technologiepark 125, 9052 Gent, Belgium.

²South China University of Technology, Guangzhou, Guangdong, School of Light Industry and Engineering, 510641 Guangdong, China

Corresponding Author: Yi Ouyang (Yi.Ouyang@UGent.be)

Abstract

Carbon capture is a key approach for achieving net-zero emissions and mitigating climate change. Among various capture methods, chemical absorption is widely used in industrial settings due to its proven effectiveness. To enhance CO₂ absorption and desorption while lowering construction and operational costs, process-intensification equipment such as gas-liquid vortex reactors (GLVRs) has garnered increasing attention. However, the design and scale-up of these intensified reactors are particularly challenging because of complex multiphase transport and separation phenomena. In this study, a multi-stage gas-liquid vortex reactor (GLVR) is proposed that combines several vortex stages with a gas-liquid cyclone located at the central section of the chamber. A computational fluid dynamics (CFD) model, validated against experimental data, is employed to evaluate how varying the number of vortex stages and adjusting cyclone geometry influence pressure drop, CO₂ absorption efficiency, and gas-liquid separation. The validated multi-stage GLVR with an integrated cyclone demonstrated a marked increase in CO₂ capture, achieving nearly complete gas-liquid separation at the reactor outlet. These findings highlight the importance of optimizing both the multi-stage setup and cyclone parameters to enable robust scale-up, ensuring high separation efficiency and favorable energy usage in larger reactors.

Acknowledgments

We gratefully acknowledge the financial support of Francqui Start-Up Grant (365N05623) from Fondation Francqui-Stichting. The presented research is funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program / ERC grant agreement no. 818607 (OPTIMA). The computational resources (Stevin Supercomputer Infrastructure) and services used in this work are provided by the VSC (Flemish Supercomputer Center), funded by Ghent University, FWO and the Flemish Government – department EWI

ABSTRACT #17

MaCKiE ABSTRACT REFERENCE NUMBER: G020

CATALYTIC PYROLYSIS OF LDPE USING GALLIUM DOPED AND STRUCTURAL MODIFIED ZEOLITE

Qing He, Oguzhan Akin, Robin John Varghese, Parviz Yazdani and Kevin M. Van Geem*
Laboratory for Chemical Technology (LCT),
Department of Materials, Textiles and Chemical Engineering, Faculty of Engineering & Architecture, Ghent University,

Corresponding Author: Kevin M. Van Geem (Kevin.VanGeem@UGent.be)

Abstract

Converting plastic waste into high-value chemicals is crucial for achieving a carbon-neutral future. We investigated the catalytic pyrolysis of LDPE for the production of aromatics using modified zeolites. Commercial HZSM-5 zeolite (HZ5) was altered to HZ5@s1 (shell structure), HZ5-hol (hollow structure), and HZ5-meso (mesoporous structure), with Ga loaded via an impregnation-coupled reduction-reoxidation procedure. The catalysts were characterized in terms of their physicochemical properties, including pore structure, acidity, and metal sites. Ga loading reduced the specific surface area of the zeolite, decreased the number of strong acid sites, and increased the number of medium acid sites, leading to a higher overall acidity. Ga-HZ5 exhibited the best Ga dispersion. Py-GC×GC-FID/MS analysis indicates that Ga can promote aromatic yields while decreasing the yield of C₂-C₄ light olefins, with almost no C₄=. The yield of mono-aromatics (MA) followed this decreasing trend: Ga-HZ5 (63%) > Ga-HZ5-meso (62%) > Ga-HZ5@s1 (60%) > Ga-HZ5-hol (54%). However, an increase in the cumulative plastics-to-catalyst ratio, yields of C₂-C₄ olefins and C₅+ aliphatic hydrocarbons were higher, whereas aromatic yields declined. Regeneration of Ga-HZ5 restored MA yields to 60%. This research provides a foundation for using metal-loaded zeolite catalysts to recover aromatics from waste plastics selectively.

Acknowledgments

We gratefully acknowledge the financial support of the Flemish Government and Flanders Innovation and Entrepreneurship (VLAIO) through the Moonshot project PREFER (HBC.2020.2609), Catalisti clusterSBO project WATCH (HBC.2019.0001), the European Research Council (ERC) under the European Union's Horizon 2020 Programme (P8/2007–2013)/ERC grant agreement no. 818607 (OPTIMA). Qing He acknowledges the Research Fund of Ghent University (BOF; 01P04022).

ABSTRACT #18

MaCKiE ABSTRACT REFERENCE NUMBER: G022

MODELING OF MOMENTUM TRANSFER AT COMPLEX SPATIOTEMPORAL SCALES IN SIEMENS REACTOR

Fanzheng Meng, Yuan Zong*, Ling Zhao and Zhong Xin
School of Chemical Engineering
East China University of Science and Technology, China

Corresponding Author: Yuan Zong (zongyuan@ecust.edu.cn)

AbstractS

Siemens reactor is the core reactor for producing rod-like polysilicon. The surface morphology of silicon rods often exhibits both poor popcorn growth and excellent homogeneous growth. And during the growth of polysilicon rods, the free volume of the reactor is reduced, so that the flow phenomenon changes instantaneously. Moreover, the scale-up of Siemens reactor includes both the number increasing of silicon rods and the size scale-up of reactor, while the flow phenomenon has changed. Hence, the development of Siemens reactors must face the chemical reaction engineering problem, as well as the momentum transfer problem with complex spatiotemporal scale. This work utilizes experiment, CFD, and data-driven methods for research. In order to model turbulence reasonably, the flow visualization experimental method was employed. Then, two CFD flow characteristic models were established, corresponding flow pattern evolution laws have been summarized, and a dimensionless number has been proposed. And a classical reactor CFD model was established, by using dimensionless number, the changes of the flow structure in the reactor and the reactor scale-up have been explained. Finally, using data-driven technology (DMD method), the relationship between the transient flow and the quality of the silicon rod has been analyzed.

ABSTRACT #19

MaCKiE ABSTRACT REFERENCE NUMBER: G023

METHOXY INTERMEDIATES: KEY TO XYLENE FORMATION IN BENZENE-ETHYLENE ALKYLATION

Jundi Wang, Yueqiang Cao and Xinggui Zhou*

State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai
200237, China

Corresponding Author: Xinggui Zhou (xgzhou@ecust.edu.cn)

Abstract

Styrene is an important chemical intermediate widely used in polymer production. The alkylation of benzene with ethylene over acidic catalysts is a key industrial method for ethylbenzene production, but it generates xylene by products that complicate separation and increase costs. This study systematically investigates the main and side reaction pathways of benzene and ethylene alkylation over H-ZSM-5 catalysts using co-feeding experiments, density functional theory (DFT) calculations, and microkinetic analysis. The result reveals that methoxy species, formed via methyl transfer from rearranged xylene, are critical intermediates in xylene formation. Co-feeding toluene significantly enhances xylene production, while DFT calculations show that methoxy species react with toluene to form xylene isomers. These findings provide crucial insights for optimizing catalyst design, improving ethylbenzene selectivity, and reducing byproduct generation.

ABSTRACT #20

MaCKiE ABSTRACT REFERENCE NUMBER: G025

EXPLOITING A MASS TRANSFER PARADOX FOR OPTIMAL SCALE-UP OF A PHARMACEUTICAL DEBENZYLATION REACTION

Wout Callewaert¹, Jeroen Lauwaert², Mairtin McNamara³ and Joris W. Thybaut^{1*}

¹ Laboratory for Chemical Technology (LCT)

Ghent University, Belgium

² Industrial Catalysis and Adsorption Technology (INCAT)

Ghent University, Belgium

³ Pharmaceutical Research and Development,

Division of Janssen Pharmaceutica, Johnson & Johnson, Belgium

Corresponding Author: Joris W. Thybaut (joris.thybaut@ugent.be)

Abstract

Developing and optimizing multiphase processes is frequently complicated by the intricate interaction between kinetic and mass transfer effects. This work investigates the optimization of an industrial-scale pharmaceutical debenylation reaction of an amine-containing precursor. The kinetic model, derived from lab-scale experiments, identified the competitive adsorption between hydrogen and the precursor as the cause of inhibition at high hydrogen pressures. When transitioning to pilot and industrial scales, model simulations reveal that moderate mass transfer limitations could counterintuitively enhance the reaction rate by reducing hydrogen-induced inhibition. Optimizing operating conditions, particularly pressure and stirring speed, can enhance process performance by balancing the beneficial and detrimental effects of the gas-liquid mass transfer on the reaction kinetics. This highlights the importance of accounting for mass transfer effects and demonstrates the leveraging of lab- and pilot-scale data for accurate industrial-scale modeling and process optimization.

Acknowledgments

The authors gratefully acknowledge Janssen Pharmaceuticals (Belgium) for funding this project. We also gratefully acknowledge the financial support of the Flemish Government and Flanders Innovation & Entrepreneurship (VLAIO) (HBC.2021.0186).

ABSTRACT #21

MaCKiE ABSTRACT REFERENCE NUMBER: G027

DEACTIVATION OF OLIVINE-DERIVED CATALYST IN NON-OXIDATIVE METHANE COUPLING

Ali Cheshmeh Roshan, Vladimir Galvita*, Parviz Yazdani and Kevin M. Van Geem
Laboratory for Chemical Technology (LCT),
University of Ghent, Belgium

Corresponding Author: Vladimir Galvita (vladimir.galvita@ugent.be)

Abstract

Non-oxidative coupling of methane (NOCM) offers a promising direct route for producing value-added hydrocarbons from natural gas. A key challenge is to develop industrially viable catalysts that resist deactivation mechanisms such as coke deposition and sintering. This study evaluates the catalytic performance of catalysts, including natural olivine ore (5.5 wt.% Fe), silica gel, and a novel composite catalyst of 5 wt% Olivine-Silica gel, prepared by rotary ball milling and calcined at 1000 °C. Catalytic tests at 950 °C and 4.8 NL/gcat/h showed that the composite catalyst offers improved stability due to better dispersion of iron, which helps suppress coke formation. A hypothetical mechanism is proposed in which agglomerated iron sites contribute to excess carbon buildup via the dehydrogenation of C₂ intermediates, particularly acetylene. This study posits that coke formation is a major cause of catalyst deactivation, supported by thermogravimetric analysis (TGA) of spent catalysts, which confirms significant carbon deposition after reaction. Understanding this deactivation pathway is crucial for developing accurate kinetic models and process optimization for NOCM.

Acknowledgments

This work was performed in the framework of the Moonshot clusterSBO project CAMELEON (HBC.2023.0551 "Electrified catalytic non-oxidative methane coupling for separated hydrogen and ethylene production"), with the financial support of the European Recovery Fund and VLAIO (Flemish Agency for Innovation and Entrepreneurship) via the Flemish spearhead cluster Catalisti.

ABSTRACT #22

MaCKiE ABSTRACT REFERENCE NUMBER: G028

CRADLE-TO-GATE LIFE CYCLE ASSESSMENT OF LIGHT OLEFIN PRODUCTION USING STEEL MILL OFF-GASES FOR FEEDSTOCK

Oleksii Mynko*, Simon de Langhe, David J. Brown and Kevin M. Van Geem
Laboratory for Chemical Technology
Ghent University, Ghent, Belgium

Corresponding Author: Oleksii Mynko (oleksii.mynko@ugent.be)

Abstract

This study investigates the environmental and technical feasibility of producing light olefins through the Methanol-to-Olefins (MTO) route using steel mill off-gases as carbon feedstock. The research addresses the significant carbon footprint of both steel and chemical industries by developing an integrated process that converts Blast Furnace Gas (BFG), Basic Oxygen Furnace Gas (BOFG), and Coke Oven Gas (COG) into valuable olefins. Process simulations demonstrate that a 550 KTA plant capacity can be achieved with efficient feedstock utilization. Life cycle assessment comparing four hydrogen production pathways—Alkaline Electrolysis, Solid Oxide Electrolysis (SOEC), Methane Pyrolysis, and Steam Methane Reforming with CCS reveals that SOEC powered by renewable electricity offers the most substantial climate impact reduction (89% lower than conventional steam cracking). Methane pyrolysis shows promising results but faces scalability limitations due to carbon black market constraints, while blue hydrogen maintains significant fossil resource dependence. The integrated process successfully addresses key technical challenges including high inert fractions in feedstock gases, carbon separation requirements, and thermal self-sufficiency, providing a pathway toward more sustainable olefin production.

ABSTRACT #23

MaCKiE ABSTRACT REFERENCE NUMBER: G029

STOCHASTIC OPTIMIZATION OF WATER-ENERGY NETWORKS WITH RENEWABLE ENERGY INTEGRATION

Kaan Altaş, Başar Kaan Tekkeşin and Erdal Aydın*
Department of Chemical and Biological Engineering
Koç University, Türkiye

Corresponding Author: Erdal Aydın (eyaydin@ku.edu.tr)

Abstract

A stochastic optimization framework for the sustainable design and operation of water–energy networks integrating renewable energy sources is developed, focusing on electrification and decarbonization. The approach extends an existing deterministic model by incorporating uncertainties in solar irradiance and wind speeds, using scenario based stochastic programming specifically tailored to climatic conditions in Çorlu, Türkiye. Representative scenarios capturing seasonal variations were constructed from historical regional data, enabling robust investment and operational decision-making. The optimization simultaneously considers infrastructure investments (solar panels, wind turbines) and operational strategies, including wastewater recycling between three interconnected processes. The results emphasize solar energy adoption due to favorable local conditions, effectively reducing grid electricity dependency and operational costs. Activated wastewater recycling interconnections further enhance environmental sustainability and resource efficiency. Overall, the proposed model significantly contributes to the practical implementation of sustainable and resilient chemical processes. The model may be further extended to capture more complex process interactions and dynamic behavior within the water–energy network.

ABSTRACT #24

MaCKiE ABSTRACT REFERENCE NUMBER: G031

ENTROPY PRODUCTION EXTREMA FOR SYSTEMS CONSTRAINED TO OPERATE FAR FROM LOCAL EQUILIBRIUM (COFFE)

Elijah Thimsen
Energy, Environmental and Chemical Engineering
Washington University in Saint Louis, Saint Louis, Missouri, USA

Corresponding Author: Elijah Thimsen (elijah.thimsen@wustl.edu)

Abstract

There is a need for unambiguous experimental tests of proposed entropy production rate extremum principles that govern systems constrained to operate far from local equilibrium (COFFE). In this paper, an approach to addressing that challenge is presented.

Acknowledgments

The author acknowledges partial financial support from the Consortium for Clean Coal Utilization (CCCU) at WashU and Peabody Energy. The author also acknowledges Grigoriy Yablonsky at WashU and Juan Pablo Trelles at UMass Lowell for valuable discussions during the early development of this work.

ABSTRACT #25

MaCKiE ABSTRACT REFERENCE NUMBER: G032

OPTIMIZATION OF CATALYST DEACTIVATION BASED ON MECHANISTIC ANALYSIS: ALKANE DEHYDROGENATION AS AN EXAMPLE

Zoë J.G. Gromotka*, Vladimir V. Galvita and Gregory S. Yablonsky
Delft Institute of Applied Mathematics, Delft University of Technology, Netherlands
Laboratory for Chemical Technology, Ghent University, Belgium
Department of Energy, Environmental and Chemical Engineering, Washington University in St. Louis, USA

Corresponding Author: Zoë J.G. Gromotka (z.j.g.gromotka@tudelft.nl)

Abstract

This study explores catalyst deactivation mechanisms using a modified Michaelis-Menten-Temkin-Boudart framework, incorporating irreversible deactivation steps. Two pathways—deactivation from intermediate or adsorbed complex—are analyzed, revealing distinct rate behaviors and optimization strategies. Experimental validation in alkane dehydrogenation demonstrates that hydrogen addition significantly enhances catalytic performance, with an optimal H_2/C_3H_8 ratio improving activity tenfold. These findings provide a mechanistic basis for mitigating deactivation and extending catalyst lifespan.

ABSTRACT #26

MaCKiE ABSTRACT REFERENCE NUMBER: G033

LEARNING TO OPTIMIZE: APPLICATION TO TWO-STAGE STOCHASTIC POOLING PROBLEM

S.E. Çamurcu and E. Aydın*
Department of Chemical and Biological Engineering, Koç University, Türkiye

Corresponding Author: Erdal Aydın (eyaydin@ku.edu.tr)

Abstract

This study applies the Learning to Optimize (L2O) method to solve the two-stage stochastic pooling problem, demonstrating its potential in reducing computational complexity while maintaining solution quality. The L2O method approximates stochastic optimization patterns after learning from simulation data, eliminating the need for explicit solution of the optimization model. Compared to traditional stochastic mixed-integer type optimization models, L2O significantly reduces computational time while having comparable optimal results. On the other hand, its performance depends on the quality and variance of the training data. L2O provides a viable alternative for complex two-stage optimization problems under uncertainty in terms of generalization using heuristic solutions.

ABSTRACT #27

MaCKiE ABSTRACT REFERENCE NUMBER: G034

ADVANCED DIGITAL SOLUTIONS THROUGH OPERATIONAL EXCELLENCE

Ozgun Deliismail^{1*}, Alperen Guler¹, Basak Tuncer¹ and Hasan Sildir²

¹SOCAR Turkey R&D and Innovation Co., Izmir, 35800, Türkiye

²Izmir Institute of Technology, Izmir, 35433, Türkiye

Corresponding Author: O. Deliismail (ozgun.deliismail@socar.com.tr)

Abstract

Recent chemical plants employ high number of sensor which appear in various forms of technology including online measurements, advanced cameras, and many others. Processing of these enables the decision making in real-time and offline work packages to infer and operate a set of complex variables to serve a more complex task which considers both the economical and environmental aspects. As the related digitalisation tasks deliver significant potential for last edge developments, they call for sophisticated formulations and software integration to implement for digitalized process management. This study presents several industrial case studies where an integration of image processing, machine learning and process systems engineering tools have proven significant improvements in decision making. The first case study includes the development of a particle size analyzer device design and development to evaluate the particle size distribution of solid particles itself and in liquid at various shapes in accordance with particle theory. The second case study includes the development of artificial intelligence tools for the real time monitoring and detection of flare inspection. The last case includes the development of remote sensing software based on drone technologies to calculate the vibration frequency at certain locations where human reach is challenging for safety issues.

ABSTRACT #28

MaCKiE ABSTRACT REFERENCE NUMBER: G035

PREDICTING LIPID NANOPARTICLE SIZE DISTRIBUTION USING A CFD-PBM APPROACH

R.G. Fonseca* and F.P. Bernardo
Department of Chemical Engineering
University of Coimbra, Portugal

Corresponding Author: R. G. Fonseca (ruifo@sapo.pt)

Abstract

Lipid Nanoparticles (LNPs) are a state-of-the-art drug delivery system for RNA-based therapies. A major issue in process design for LNP production is to ensure the production of particles with the desired size distribution, as this is a critical attribute for drug delivery efficacy. In this paper, a Computational Fluid Dynamics - Population Balance Modelling (CFD - PBM) model is proposed to describe particle formation and track particle size in the production of LNPs inside a microfluidic mixer. The used bivariate PBM model considers nucleation, particle growth and aggregation phenomena. The model distribution data presents promising results when compared with Dynamic Light Scattering (DLS) data.

Acknowledgments

The authors thank financial support from Project “CiNTech - Technological Hub for Innovation, Translation and Industrialization of Complex Injectable Drugs” (reference: 7131), in the scope of PRR - Recovery and Resilience Plan and by the Next Generation EU European Funds, following NOTICE No. 02/C05-i01/2022, Component 5 - Capitalization and Business Innovation - Mobilizing Agendas for Business Innovation.

ABSTRACT #29

MaCKiE ABSTRACT REFERENCE NUMBER: G037

**POPULATION BALANCE MODEL (PBM) INCLUDING NUCLEATION
AND SIZE-CONCENTRATION DEPENDENT GROWTH FOR
CRYSTALLIZATION PROCESS**

Özkan Avit* and Zehra Pinar Izgi
Faculty of Arts and Science, Department of Mathematics
Tekirdağ Namık Kemal University, Türkiye

Corresponding Author: Özkan Avit (ozkanavit@gmail.com)

Abstract

Crystallization problem one of the popular problems in wide area of science. The first principles are not used to design a crystallizer in which complicated processes include nucleation, crystal growth, attrition and agglomeration of crystals. It is modeled by the population balance model, which is one of the important models of mathematical biology and engineering, is a nonlinear partial integro-differential equation and examines the exchange of particles and the production of new particles in a system of particles. For the crystallization problem, one-dimensional and multi-dimensional models are considered and semi-analytical solutions are obtained via the linear separation method.

ABSTRACT #30

MaCKiE ABSTRACT REFERENCE NUMBER: G038

HOLISTIC DESIGN AND ASSESSMENT OF E-FUELS MANUFACTURING: THE CASE OF E-METHANOL AND E- AMMONIA

Fabio Cameli^{1,3*}, Evangelos Delikonstantis², Afroditi Kourou³, Victor Rosa³, Kevin M. Van Geem³ and
Georgios D. Stefanidis^{1,3}

¹ School of Chemical Engineering, National Technical University of Athens, Greece

² AristEng S.à r.l., Luxembourg City, Luxembourg

³ Laboratory for Chemical Technology, Ghent University, Belgium

Corresponding Author: Fabio Cameli (fabio.cameli@ugent.be)

Abstract

The chemical industry is set for a radical transformation towards sustainable manufacturing, where electrification will play a central role. However, holistic techno-economic and environmental assessment of new processes should guide their industrial implementation. In this work, we conceptualize and design two electrified processes that lead to two of the most largely produced chemicals: methanol and ammonia. The former is produced via electrolytic H₂ and CO₂ from Direct Air Capture (DAC), whereas the latter is generated via electrolytic H₂ and N₂ from cryogenic distillation. The simulation of the entire plant-wide process allows to calculate the Levelized Cost of Production (LCOP) of the products in two temporal scenarios: 2019 and 2050. For both processes, electricity demand drives OPEX, whilst DAC is the main CAPEX contributor in e-methanol production. Thereby, the e-processes' LCOP is higher than the conventional counterparts (~3.3x for methanol and ~1.7x for ammonia). Nonetheless, the electrified routes can lead to significantly lower carbon footprint when sustained by renewable power. Importantly, e-methanol produced via wind power features negative CO₂ emissions, compared to the state-of-the-art process based on carbon-intensive Steam Methane Reforming (SMR) for H₂ production. Similarly, e-ammonia is 5x less carbon intensive than commercial ammonia based on H₂ from SMR.

Acknowledgments

The authors acknowledge funding from the Flemish government (Moonshot clusterSBO project P2O).

ABSTRACT #31

MaCKiE ABSTRACT REFERENCE NUMBER: G039

TWO TO JIVE: ACCELERATING NUMERICAL REACTIVE FLOWS IN TURBOREACTORS

Mike Bonheure^{1*}, Ismaël Amghizar², Tamás Buzogány¹, Rejish L. Johnson¹, Guy B. Marin^{1,2}, Elina Nauha³ and Kevin M. Van Geem¹

¹ Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

² AVGI bv, Technologiepark-Zwijnaarde 122, 9052, Ghent, Belgium

³ Coolbrook Oy, Pieni Roobertinkatu 9, 00130 Helsinki, Finland

Corresponding Author: Mike Bonheure (mike.bonheure@ugent.be)

Abstract

Turboreactors represent a breakthrough in (chemical) process electrification, eliminating fossil-fueled furnaces through RotoDynamic™ technology that generates thermal energy via high-speed rotor-stator interactions. These systems create complex reactive gas dynamics that conventional simulation methods struggle to capture efficiently in a timely manner. By integrating AVGI's CRACKSIM with Ansys Fluent and leveraging Pseudo-Steady-State Approximation and adaptive cell clustering techniques, a model to accurately resolve turbulence, heat transfer, and chemical kinetics while achieving >100× computational speed-ups has been established. Validation studies demonstrate good agreement with full kinetic simulations, preserving critical flow features including shock systems and vortex shedding. This framework provides a powerful tool for accelerating the design and optimization of turboreactors, reinforcing their potential as a scalable and efficient alternative for sustainable, high-yield hydrocarbon cracking and electrified process heating.

Acknowledgements

Mike Bonheure gratefully acknowledges financial support from the Fund for Scientific Research Flanders (FWO) through project 1SD7121N. The research leading to these results has received funding from the European Research Council - ERC Grant No. 101142065 and No. 818607 and financial support from the European Union HORIZON CL4-2021-TWIN-TRANSITION-01 under Grant Agreement no. 101058412 (eLECTRO Project).

ABSTRACT #32

MaCKiE ABSTRACT REFERENCE NUMBER: G044

STEAM CRACKING BEYOND THE PLUG FLOW ASSUMPTION

Ismaël Amghizar^{1*}, Mike Bonheure², Tamás Buzogány², Guy B. Marin¹ and Kevin M. Van Geem²

¹AVGI bv, Technologiepark-Zwijnaarde 122, 9052, Ghent, Belgium

²Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

Corresponding Author: Ismaël Amghizar (ismael.amghizar@avgibv.be)

Abstract

Emerging reactor technologies in steam cracking increasingly deviate from ideal plug flow behaviour, challenging conventional modelling approaches that rely on simplified flow assumptions. This work introduces a computationally efficient modelling strategy that decouples the detailed CRACKSIM reaction kinetics (the core of COILSIM1D) from any predefined flow model by embedding it in a pseudo-multiscale framework based on networks of interconnected Continuous Stirred-Tank Reactors (CSTRs). These networks are calibrated to approximate key features of non-ideal hydrodynamics, such as axial dispersion, recirculation, and bypassing, using residence time distributions derived from tracer response experiments or simulations. Once calibrated, the complete CRACKSIM mechanism is solved within the CSTR network. In this proof-of-concept work, comparative simulations show that even minor deviations from plug flow, such as limited bypass flows, can significantly reduce light olefins selectivity. Configurations minimizing such non-idealities yield the highest selectivity, highlighting the sensitivity of cracking performance to reactor flow patterns. By bridging the gap between kinetic detail and realistic flow representation without resorting to costly CFD, this approach offers a robust and versatile tool for assessing and optimizing next-generation steam cracking reactors.

Acknowledgements

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Tamás Buzogány gratefully acknowledges financial support from the Baekeland mandate HBC.2023.0159.

The research leading to these results has received funding from the European Research Council - ERC Grant No. 101142065 and No. 818607 and financial support from the European Union HORIZON CL4-2021-TWIN-TRANSITION-01 under Grant Agreement no. 101058412 (eLECTRO Project).

ABSTRACT #33

MaCKiE ABSTRACT REFERENCE NUMBER: G046

TRANSPORT ENHANCEMENT OF ACCESSIBLE POROUS CARBON IN PEMFCs: A MULTISCALE MODELLING APPROACH

Daoming Yang¹, Guanghua Ye¹ and Xinggui Zhou^{1*}
¹ School of Chemical Engineering
East China University of Science and Technology, China

Corresponding Author: Xinggui Zhou (xgzhou@ecust.edu.cn)

Abstract

The multiscale transport processes within the cathode catalyst layer play a crucial role in the overall performance of PEMFCs. In this study, a multiscale modeling framework has been developed to accurately describe the reaction and transport processes occurring on accessible porous carbon.

Acknowledgments

The project was financially supported by the National Key R&D Program of China (No. 2023YFB4006101). The authors also expressed deep gratitude to Prof. Li Ping for the invaluable assistance in the characterization of accessible porous carbon catalysts.

ABSTRACT #34

MaCKiE ABSTRACT REFERENCE NUMBER: G048

MODELLING OF MICROFLUID SIPHONS FOR HIGH-PERFORMANCE POINT-OF-CARE DIAGNOSTICS AND NEAR-THE-SOURCE DNA PURIFICATION

Crescenzo Ianniello^{1,2}, Kirandeep Gill³, Barbara Kasprzyk-Hordern² and Nuno M. Reis^{1,2,4*}

¹Centre for Bioengineering and Biomedical Technologies (CBio), University of Bath, UK

²Centre of Excellence in Water-Based Early-Warning Systems for Health Protection (CWBE), University of Bath, Bath UK.

³Massachusetts General Hospital, Boston, Massachusetts, USA

⁴Centre of Biological Engineering (CEB), University of Minho, Portugal

Corresponding Author: Nuno M. Reis (n.m.reis@bath.ac.uk)

Abstract

One of the biggest challenges in high-performance bioassays routinely used in point-of-care diagnostics and near-the-source environmental surveillance is the ability to handle a sequence of liquid reagents without the need of bulky equipment nor complex fluid handling. To address that engineering gap, we developed a microfluidic siphon concept able to start/stop flow, self-prime, and deliver a sequence of reagents. Pressure balance modelling and CFD simulations validated by an extensive experimental dataset confirmed flow rates in microfluidic siphon devices is entirely driven by gravity and molecular cohesion.

Acknowledgments

Authors are grateful to the University of Bath and ESPRC for funding PhD studentships to C.I. and K.K.G. and UKRI Research England for funding CWBE.

ABSTRACT #35

MaCKiE ABSTRACT REFERENCE NUMBER: G051

PYKINEMOD: A SOFTWARE TOOL FOR AUTOMATED MODELING OF REACTION SYSTEMS FROM DATA

Tirthankar Sengupta¹, Vignesh Kumar¹, V Manokaran¹, Sridharakumar Narasimhan^{1*}, Nirav Bhatt^{2*}
¹Department of Chemical Engineering, Indian Institute of Technology Madras, India ²Wadhvani School of Data Science and AI (WSAI), Indian Institute of Technology Madras, India

Corresponding Author: Sridharakumar Narasimhan (sridharkrn@iitm.ac.in), Nirav Bhatt (niravbhatt@iitm.ac.in)

Abstract

Pykinemod is a software tool for the identification of homogeneous reaction systems from concentration data. The incremental identification technique is employed for parameter estimation from a set of rate expression candidates for each reaction. This approach is much faster in comparison to the simultaneous identification and therefore expedites the parameter estimation process. The metric for evaluating rate laws can be selected by the user and include the Akaike Information Criterion (AIC), AICC (corrected Akaike Information Criterion) and RMSE (Root Mean Square Error). Further, the module allows the user to fine tune the predictions from the incremental identification step by simultaneous identification. The k best candidate rate laws (where the integer k can be selected by the user) for each reaction identified in the incremental identification step form the candidates in simultaneous identification. Also, parameter estimates in the incremental identification step are used as initial guesses. Overall, this dual strategy of employing both the identification strategies results in rapid and robust identification of reaction systems.

ABSTRACT #36

MaCKiE ABSTRACT REFERENCE NUMBER: G053

MODELING AND EXPERIMENTAL STUDY OF AN INTEGRATED POST-PLASMA CATALYST

Victor Rosa¹, Fabio Cameli², Kevin M. Van Geem¹, Georgios Sefanidis^{1,2*}

¹ Laboratory for Chemical Technology, Ghent University, Ghent, Belgium

² School of Chemical Engineering National Technical University of Athens, Greece

Corresponding Author: Victor Rosa (victor.rosa@ugent.be)

Abstract

The advancement of electrified chemical processes prompts interest in novel hydrocarbon valorization technologies. Nanosecond-pulsed discharges (NPD) coupled with downstream Pd-based catalysts have shown the best small-scale performance to date in a plasma process to convert CH₄ into ethylene (C₂H₄). A series of bimetallic Pd-Ag catalysts are hereby screened in wash coated configuration and integrated with NPD plasma. Remarkably, the best performance is achieved with a low wt. % Ag catalyst. The thermal behavior of the post-plasma catalytic reactor is analyzed, where a high concentration of C₂H₂ poses challenges to traditional packed bed reactors in terms of heat management. The use of conductive metallic (copper) substrates proves beneficial in this case, allowing near-isothermal operation of the catalyst in a highly exothermal catalytic run. Finally, the result is confirmed via fiber optic measurements.

ABSTRACT #37

MaCKiE ABSTRACT REFERENCE NUMBER: G054

KINETIC MODELLING OF ACETYLENE HYDROGENATION IN ETHYLENE PRODUCTION PROCESS

Gizem Pınar^{1*}, Mustafa Demircioğlu² and Canan Uraz³

¹Department of Chemical Engineering, Ege University, Türkiye

²Department of Chemical Engineering, Middle East Technical University, Northern Cyprus

³Department of Chemical Engineering, Ege University, Türkiye

Corresponding Author: Gizem Pınar (gizem.pnar@gmail.com)

Abstract

The aim of this study is to obtain kinetic modeling of the selective hydrogenation reaction of ethylene by optimizing the working parameters to obtain ethylene as a product of the hydrogenation reaction of acetylene and investigating the theoretical and practical aspects of the main and side reactions taking place in the reactor. The kinetic models of Langmuir Hinshelwood, Langmuir Hinshelwood Hougen Watson, Eley Rideal and Houriti Polanyi are discussed and analyzed in this study because of the scanning made considering the Pd/Al₂O₃ catalyst used in the ethylene production process. MATLAB codes are developed for these four different kinetic models by using Petkim ethylene plant data. The parameters obtained with the model are used in the simulation by ASPEN HYSYS program and the results are compared with the plant data. In addition to this, the effect of the change in hydrogen mole fraction in the stream fed to the first column on ethylene and ethane conversions are also analyzed.

Acknowledgments

The author also extends gratitude to SOCAR (Petkim) for providing the necessary resources and a conducive environment for conducting this research.

ABSTRACT #38

MaCKiE ABSTRACT REFERENCE NUMBER: G055

A REACTION EXTENT-BASED APPROACH TO KINETIC ANALYSIS OF REACTION NETWORKS – GLYCEROL OXIDATION AS A CASE STUDY

Akkihebbal K. Suresh* and Jainesh H Jhaveri
Department of Chemical Engineering
Indian Institute of Technology Bombay, Mumbai, India 400076

Corresponding Author: Akkihebbal K. Suresh (a.k.suresh@iitmb.ac.in)

Abstract

In multiple reaction networks, kinetic identification from experimental data is fraught with uncertainties, because multiple kinetic models can often fit the data equally well. It is usual to start with a kinetic formulation and carry out parameter estimation from concentration-time data from a batch reactor. Part of the challenge in such data-fitting exercises stems from the fact that concentrations of species are affected in general, by not one, but several reactions. Here we present an alternative procedure based on the concept of reaction extents. The extents of reactions in the network are calculated as functions of time from concentration-time data in a data-preprocessing step, and these are then used in model fitting. This approach is a reaction-centric (as opposed to a species-centric) one, and makes it possible to discern the effects of changes in operating conditions or presence of catalytic principles on individual reactions in the network, and also provides ways of reconciling data when redundancy is ensured through more than the minimum number of measurements needed. The methodology is illustrated using data on the alkaline oxidation of glycerol on Pd/Al₂O₃ catalyst, by investigating how different pretreatments of the catalyst influence different reactions in the network.

ABSTRACT #39

MaCKiE ABSTRACT REFERENCE NUMBER: G056

HYDROCONVERSION OF VEGETABLE- AND LIGNIN-BASED FEEDS: MODELING THE IMPACT OF CO-PROCESSING

Arij Ben Hassine^{1*}, M. Joana N. Correia,² Pedro S.F. Mendes¹

¹ Centro de Química Estrutural, Instituto Superior Técnico, ULisboa, Portugal

² Centro de Recursos Naturais e Ambiente, Instituto Superior Técnico, ULisboa, Portugal

Corresponding Author: Arij Ben Hassine (arij.ben.hassine@tecnico.ulisboa.pt)

Abstract

This study employs a kinetic and reactor model based on Langmuir-Hinshelwood surface kinetics to predict the conversion and product distribution of a fatty acid and an aromatic compound, representing Used Cooking Oil (UCO) and pyrolysis oil, respectively. The model simulates their individual processing as well as their co-processing in a continuous system. Predictions for single feeds aligned well with experimental data, though some deviations were observed for the aromatic compound at lower temperatures. In mixtures, the model captured the experimentally observed trend of higher fatty acid conversion and lower aromatic conversion due to competitive adsorption effects. The observed deviations in the aromatic compound conversion indicate a need for further investigation and suggest that additional influencing factors might need to be incorporated into the model. These findings highlight the importance of refining kinetic parameters and incorporating further experimental validation for improved accuracy in co-processing models.

Acknowledgments

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ABSTRACT #40

MaCKiE ABSTRACT REFERENCE NUMBER: G057

CONSERVATIVELY PERTURBED EQUILIBRIUM AND PERTURBATION (LINEAR CASE, FREE GIBBS ENERGY ANALYSIS)

Jonah M. Sachs^{1*}, John E. McCarthy² and Jiayu Hu³

Departments of Computer Science¹, Mathematics², and Chemical Engineering³, Washington University in St. Louis, Missouri, USA

Corresponding Author: Jonah M. Sachs (jonahmsachs@gmail.com)

Abstract

The phenomenon of “Conservatively Perturbed Equilibrium” (CPE) has been previously analyzed since its discovery in 2019. Derived generally and illustrated computationally, new properties have been found for linear mechanisms with degrees of freedom of one. The Gibbs Free Energy (G) has also been extensively analyzed with consideration to CPE, involving energy levels and trajectories. Although the total G will descend to a global minimum, extreme values found in individual components share characteristics to CPE time(s). For $n = 3$, it was found that the times of all CPE points across substances are equal. This does not hold for general n . For general n , we find: 1) time(s) of CPE-points do not depend on the magnitude of perturbations, 2) for the unperturbed substance, the deviation of the CPE-extremum value from the initial equilibrium concentration is proportional to the value of perturbation of the perturbed concentration, i.e. its initial deviation, and 3) for the unperturbed substance, the individual contribution to the G will experience extremum, and its derivative will experience inflection point(s), both occurring at these CPE time(s). These obtained properties can be used both for revealing the chemical mechanism structure and for industrial applications, e.g., the obtaining of the over-equilibria which have been found and studied computationally in industrial methane reforming reactions.

Acknowledgments

John McCarthy was partially supported by National Science Foundation grant DMS 2054199. Special thanks also go to Dr. Grigoriy Yablonsky for his guidance, help, and management of this project. We are very thankful for his guidance

ABSTRACT #41

MaCKiE ABSTRACT REFERENCE NUMBER: G058

LOW-ORDER MODELING OF A SHOCK WAVE TURBOREACTOR FOR STEAM CRACKING

Diego Castellanos¹, Rejish Lal Johnson^{1,2}, Mike Bonheure¹, Yi Ouyang¹, Kevin M. Van Geem^{1*}

¹ Laboratory for Chemical Technology (LCT), Ghent University, Ghent, Belgium

² Turbomachinery and Propulsion Department (TU), von Karman Institute for Fluid Dynamics, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

This work presents a low-order model (LOM) for predicting the performance of a shockwave turboreactor, composed of a single stator-rotor-diffuser arrangement with a vaneless space. The aim is to bridge the gap between low-fidelity models and shockwave turboreactor analysis in the preliminary design process, delivering results in minutes rather than hours or days, as required by higher-order models. The LOM consists of a one-dimensional (1D) meanline model for the stator and rotor, and a quasi-one-dimensional (quasi-1D) computational fluid dynamics (CFD) model for the diffuser and vaneless space, where the continuity, momentum, and energy equations are solved to simplify the complex three-dimensional (3D) phenomena associated with high energy conversion in these components. The model is extended across multiple blade spans, with radial equilibrium constraints, to ensure realistic spanwise flow behavior. Validation and calibration of the LOM are performed using 3D CFD simulations for various turboreactor sizes. Finally, the model is coupled with a chemical kinetics tool to assess selectivity under different operating conditions. The results demonstrate that the LOM accelerates decision-making by providing reliable predictions in a significantly shorter time frame compared to full 3D CFD simulations, making it suitable for turboreactor preliminary design, analysis, and optimization.

Acknowledgement

This work was supported by funding from the European Research Council (ERC) as part of the European Union's Horizon 2020 research and innovation programme (Grant Agreement No. 818607) and the Horizon Europe research and innovation programme (Grant Agreement No. 101142065 number).

ABSTRACT #42

MaCKiE ABSTRACT REFERENCE NUMBER: G059

A COMPUTATIONAL MODEL TO ANALYZE THE IMPACT OF ENDOTHELIAL DYSFUNCTION ON H₂O₂ BIOTRANSPORT

Saptarshi Kar
College of Engineering and Technology
American University of the Middle East, Kuwait

Corresponding Author: Saptarshi Kar (Kar.Saptarshi@aum.edu.kw)

Abstract

Hydrogen peroxide (H₂O₂) is a key redox signaling molecule that is reported to play a dual role in the regulation/disruption of vascular homeostasis. The regulation of vascular and perivascular H₂O₂ levels during endothelial dysfunction, by H₂O₂ generating (SOD) and scavenging (catalase, Gpx, and Prx) enzymes is an area of active investigation. Studies investigating the effects of endothelial dysfunction on the expression and activity of H₂O₂ generation and scavenging enzymes have yielded ambiguous results. We developed an arteriole-based computational biotransport model to quantitatively analyze the complex biochemical interactions between superoxide, H₂O₂, and the H₂O₂-generating/scavenging enzymes in the microcirculation and adjoining tissue regions. Our results showed that vascular H₂O₂ levels remain in the nanomolar range (1–30 nM) during moderate oxidative stress, supporting regular signaling functions. As oxidative stress worsens, H₂O₂ levels increase to the micromolar range (up to 0.5 μM), where they are likely to disrupt vascular homeostasis.

ABSTRACT #43

MaCKiE ABSTRACT REFERENCE NUMBER: G065

ROBUST FEW-SHOT TIME SERIES MODELING FOR SILICONE MONOMER SYNTHESIS VIA TASK-AWARE TEMPORAL FUSION

Qinhao Sun, Zhongmei Li*, Bing Zhang, Jionghao Lou, Shiming Wu, Enbo Feng and Wenli Du
Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China University of Science and Technology.

Corresponding Author: Zhongmei Li (lizhongmei@sina.cn)

Abstract

Data-driven modeling of silicone monomer synthesis process faces severe challenges due to intricate reaction mechanisms, operational variability, and extreme sparsity of critical quality measurements (e.g., Dimethyldichlorosilane (M2) selectivity). In this paper, a novel task-aware temporal fusion network (TaFT-Net) enhanced with robust meta-learning techniques is proposed, specifically designed for accurate time-series prediction in such data-scarce industrial settings. First, in order to overcome the single architecture unable to capture diverse temporal scales, a Multi-Scale Fusion Network integrates Bi-LSTM (core patterns) is constructed, in which Transformer encoders model long-term dependencies, dynamic multi-scale CNNs extract mid-term features, and temporal decay attention handles short-term dynamics. Then, we present a hierarchical fusion mechanism with channel attention and gating, which adaptively combines multi-branch features to reduce redundancy and prevent overfitting inherent in complex models trained on few-shot data. Besides, an Enhanced Model-Agnostic Meta-Learning (EnhancedMAML) framework is introduced to tackle the challenges of few-shot learning and cross-task generalization in data-scarce industrial settings. In specific, a task reweighting scheme guided by gradient similarity and dynamic time warping (DTW) distance is adopted to reduce the negative impact of biased tasks. Meanwhile, projecting conflicting gradients (PCGrad) optimization guarantees the convergence rate with the help of conflict-reduced gradient updates. Tests on 2023-2024 plant data show TaFT-Net outperforms existing methods in accuracy, convergence stability, and cross-task generalization under extreme data scarcity.

Acknowledgments

This work was supported by the Independent Research Project of the State Key Laboratory of Industrial Control Technology under Grant No. ICT2024A01, and Shanghai Rising-Star Program under Grant 24QA2706100.

ABSTRACT #44

MaCKiE ABSTRACT REFERENCE NUMBER: G066

GREEN SYNTHESIS OF Pd/CeO₂ NANOPARTICLES FOR DEHYDROGENATION OF ETHYLENEDIAMINE BISBORANE

Selma Türk¹, Büşra Dülger¹, Selin Gezgen², Hatice Begüm Murathan², Göksel Özkan², Gülay Özkan^{1*}

¹Ankara University, Department of Chemical Engineering, Ankara, 06100, Tandoğan, Türkiye

²Gazi University, Department of Chemical Engineering, Ankara, 06570 Maltepe, Türkiye

Corresponding Author: Gülay Özkan (gozkan@eng.ankara.edu.tr)

Abstract

Catalytic hydrolysis of Ethylenediamine Bisborane (EDAB) has garnered great concern in the production of hydrogen. In this work, nanocomposites based on CeO₂ doped with Pd were synthesized. CeO₂ obtained using two process, one is hydrothermal synthesis methods using cerium nitrate another is green synthesis method using cerium nitrate and the Aloe Vera extract. To make a comparative analysis of the structural characteristics, morphology, composition, FTIR, SEM-EDX, BET, XRD analysis were used. The prepared catalysts were found to be efficient catalysts in the EDAB hydrolysis/methanolysis process. A thorough kinetic analysis of the catalyzed methanolysis/hydrolysis reaction was investigated.

ABSTRACT #45

MaCKiE ABSTRACT REFERENCE NUMBER: G067

CONDITION RECOGNITION METHOD FOR ORGANOSILICON MONOMER SYNTHESIS PROCESS BASED ON AUTOENCODER AND NONLINEAR CLUSTERING

Jionghao Lou*, Zhongmei Li, Shiming Wu, Qin hao Sun, Bing Zhang, Wenli Du and Enbo Feng
Key Laboratory of Smart Manufacturing in Energy Chemical Process,
Ministry of Education, East China University of Science and Technology, China

Corresponding Author: Jionghao Lou (jlou@mail.ecust.edu.cn)

Abstract

In organosilicon production, operating conditions of the monomer synthesis process are critical for ensuring product quality and production efficiency. However, strong coupling among process variables, delayed fault detection, and difficulty in tracing low-yield causes hinder optimization and control. To address these challenges, this paper presents a condition recognition framework that integrates deep feature learning with intelligent diagnostics. The proposed method, named SAE-UMAP-K-Means, follows a two-stage structure: in the first stage, stacked autoencoders are employed to compress and decouple high-dimensional process data, and UMAP is then applied for nonlinear dimensionality reduction to retain essential process features. In the second stage, the latent features are clustered using K-Means to identify distinct operational states. To further interpret low-yield conditions, a Z-score-based dynamic attribution mechanism is employed to perform variance contribution analysis and identify the key contributing factors. Finally, a case study on organosilicon monomer synthesis demonstrates the proposed method's superiority over traditional PCA-K-Means and direct K-Means approaches, achieving higher Silhouette Coefficients and lower Davies-Bouldin Index values.

Acknowledgments

This work was supported by the Independent Research Project of the State Key Laboratory of Industrial Control Technology under Grant No. ICT2024A01, and Shanghai Rising-Star Program under Grant 24QA2706100.

ABSTRACT #46

MaCKiE ABSTRACT REFERENCE NUMBER: G068

APPLICATION OF SYMMETRY AND TOPOLOGY FOR ENGINEERING NEW CARBON MATERIALS

Alexey Ignatchenko*, Degraj Suberi and Charlie Illingworth
Chemistry Department,
St. John Fisher University, USA

Corresponding Author: Alexey Ignatchenko (aignatchenko@sjfc.edu)

Abstract

Schwarzites are a hypothetical allotrope form of carbon proposed for the construction of new materials with desired properties. Schwarzite P-surface design is explored in this work by using isolated sp^2 -hybridized carbon heptagons for the construction of P-chambers according to Euler's formula and by adding various length nanotubes as connectors between chambers. The proposed design guides the bottom-up synthesis of Schwarzites and offers a variation in DFT calculated electric and mechanical properties of materials - porosity, density, Young's modulus, and electric conductivity. Suggested nomenclature for the networks includes the symmetry of the chambers, topological index of the chamber neck, number of carbon atoms, and the length of the nanotube.

Acknowledgments

Support from the NSF grant 1955130 for the shared use of Materials Studio software and a high-performance computer is greatly acknowledged.

ABSTRACT #47

MaCKiE ABSTRACT REFERENCE NUMBER: G069

ASSESSING STABILITY AND HYDROGEN YIELD OF CARBON CATALYSTS FOR METHANE DECOMPOSITION

Spyridon Fragkiskatos, Simon De Langhe, Parviz Yazdani, Soroush Zareghorbaei, Lukas Buelens, Hilde Poelman, Joris W. Thybaut, and Kevin M. Van Geem*
Laboratory for Chemical Technology, Ghent University,
Technologiepark 125, 9052 Ghent, Belgium

Corresponding Author: Kevin M. Van Geem (Kevin.VanGeem@ugent.be)

Abstract

Turquoise hydrogen, produced via methane pyrolysis, presents a promising low-emission alternative to conventional hydrogen production. This process thermally decomposes methane into hydrogen and solid carbon, avoiding direct CO₂ emissions. Carbon-based catalysts, such as carbon black, are active for catalytic methane decomposition and electrically conductive for Joule heating. Moreover, the solid carbon byproduct can be valorized.

Electrothermal fluidized bed (ETFB) reactors offer several advantages, including precise temperature control and compatibility with renewable energy sources, which further contribute to decarbonizing the process. However, long-term catalyst stability remains a key challenge for commercial deployment. This study evaluated the performance of carbon black (CB) Pearls 2000 and soft-templated mesoporous carbon (SMC2) in a fixed bed reactor. CB Pearls 2000 remained stable with the hydrogen space-time yield (STY) of 33.8 $\mu\text{mol H}_2 \text{ g}_{\text{cat}}^{-1} \text{ s}^{-1}$ over 7 h. SMC2 also met the industrial productivity target of 1 ton H₂ per kg_{cat} despite a gradual decline in STY to 19.8 $\mu\text{mol H}_2 \text{ g}_{\text{cat}}^{-1} \text{ s}^{-1}$. These results confirm the suitability of durable carbon-based materials for scalable and low-emission hydrogen production.

Acknowledgments

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement number 818607.

ABSTRACT #48

MaCKiE ABSTRACT REFERENCE NUMBER: G071

AN ABSOLUTELY-CALIBRATED INTEGRATING CYLINDER FOR STUDYING PHOTOCHEMICAL REACTIONS

A. Hamza and N.B. Üner*
Chemical Engineering Department
Middle East Technical University, 06800, Türkiye

Corresponding Author: N.B. Üner (nuner@metu.edu.tr)

Abstract

Photochemistry can provide a promising way to degrade recalcitrant chemicals accumulating in water resources, including per- and polyfluoroalkyl substances (PFAS). However, evaluating energy efficiency for photochemical reaction systems remains a challenge, especially with commercial water treatment lamps. This work aims to develop a cylindrical photochemical reaction chamber that can accommodate large-aspect ratio lamps, in which quantum yields, and hence the energy efficiency, can be measured for various photochemical reactions. A mathematical model was used to predict the number flux of photons that fall into a reaction environment placed inside the chamber and the model was validated through pyridine photolysis under 254 nm light. The capability of the system for studying photochemical pathways was further illustrated with methylene blue photolysis and its associated reaction network under visible red light (632 nm).

ABSTRACT #49

MaCKiE ABSTRACT REFERENCE NUMBER: G072

SOLVENT-MEDIATED DEHYDROGENATION OF ETHYLENEDIAMINE BISBORANE USING Pd/rGO CATALYSTS: A COMPARATIVE STUDY OF HYDROLYSIS AND ETHANOLYSIS

Bensu Naz ÖRS^{1,2}, Burak Uygur Mert Yorgun², Göksel Özkan³ and Gülay Özkan^{2*}

¹Department of Chemical Engineering, Atılım University, Ankara TR-06830, Türkiye

²Ankara University, Department of Chemical Engineering, Ankara, 06100, Tandoğan, Türkiye

³Gazi University, Department of Chemical Engineering, Ankara, 06570 Maltepe, Türkiye

Corresponding Author: Gülay Özkan (gozkan@eng.ankara.edu.tr)

Abstract

Catalytic dehydrogenation of Ethylenediamine Bisborane (EDAB) has recently gained attention for efficient hydrogen production. This study explores the preparation and comparison of Pd/Reduced Graphene Oxide (Pd/rGO) catalysts synthesized through three distinct methods: hydrothermal synthesis, thermal reduction, and green synthesis using linden (*Tilia spp.*) leaf extract. The prepared catalysts' structural, morphological, and compositional characteristics were analyzed using FT-IR, XRD, SEM, TEM, BET, and XPS methods. The effects of the Pd/rGO catalysts on the EDAB hydrolysis/ethanolize process were investigated. Comprehensive kinetic analysis revealed a notably low activation energy, emphasizing the significance of the green synthesis method in achieving both catalytic efficiency and environmental sustainability.

ABSTRACT #50

MaCKiE ABSTRACT REFERENCE NUMBER: G073

INTERPRETABLE MACHINE LEARNING MODELS FOR QUANTITATIVE STRUCTURE–PROPERTY RELATIONSHIPS IN AVIATION FUELS

Xiaomeng Zhao^{1,2}, Pieter Janssens¹, César Pernalet Piña¹, Siyang Tang², Bin Liang² and Joris W. Thybaut^{1*}

¹ Laboratory for Chemical Technology, Ghent University, Technologiepark 125, 9052 Ghent, Belgium

² Low-Carbon Technology and Chemical Reaction Engineering Laboratory, School of Chemical Engineering, Sichuan University, Chengdu 610065, China

Corresponding Author: Joris W. Thybaut (Joris.Thybaut@UGent.be)

Abstract

Quantitative structure–property relationships (QSPRs) are crucial for the rapid development of new sustainable aviation fuels (SAFs). Machine learning models can be used for such purposes; however, the limited data availability and the lack of interpretability hinder their application in SAF research. In this work, a comprehensive dataset was compiled from experiments as well as literature sources. An artificial neural network (ANN) proved successful in establishing (QSPRs) for important fuel properties – e.g., viscosity and flash point – as high prediction accuracies (>90%) were obtained for all of the investigated properties. In addition, the contribution of each feature within each descriptor of the ANN models was interpreted via a SHAP analysis.

Acknowledgments

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ABSTRACT #51

MaCKiE ABSTRACT REFERENCE NUMBER: G074

PYTHON-BASED SEMI-AUTOMATED ANALYSIS OF TURBIDIMETRIC GROWTH DELAY DATA TO STUDY ANTIMICROBIAL ACTIVITY

Vahit K orođlu, ađatay Gence, Devrim B. Kaymak, Ahmet Sirkeciođlu and H. Enis Karahan*
Department of Chemical Engineering
İstanbul Technical University, T rkiye

Corresponding Author: H. Enis Karahan (karahanhe@itu.edu.tr)

Abstract

Under suitable environmental and biological conditions, microbial cells often exhibit “S-shaped” growth behavior when no inward/outward flow occurs in a fixed volume (batch culture). Such “S” curves are rich in information regarding the response of microorganisms to altering conditions. To judge antimicrobial susceptibility, though, even a simple comparison of growth delay, i.e., the duration required to reach a certain optical density (OD) with respect to reference, offers great utility. Here, using the data obtained for multiplate-reader-based growth monitoring of two model bacterial species exposed to graphene oxide (GO), we describe a Python-based code, Growth Delay Comp (GDC), for analyzing the microbial growth delay (MGD) values. Minimizing manual data handling by large, GDC takes the OD₆₀₀ values as input and computes the best linear fits to the linear-like region of the exponential phase in each growth curve using a subset of data. Circumventing the outlier elimination needs, this approach speeds up data analysis.

Acknowledgments

The previously published dataset was generated during the doctoral research of H.E.K. at Nanyang Technological Univ., in a lab headed by Yuan Chen (now, at The Univ. of Sydney). We thank Y.C. for his support and cooperation. H.E.K. acknowledges funding support through BİDEB-2232-B (122C339) and T BA-GEBİP programs.

ABSTRACT #52

MaCKiE ABSTRACT REFERENCE NUMBER: G075

CHARACTERIZATION AND OPERATION OF A GLIDING ARC PLASMA REACTOR FOR METHANE PYROLYSIS

H. Öztürk, A.Y. Kaya and N.B. Üner*
Chemical Engineering Department
Middle East Technical University, 06800, Ankara, Türkiye

Corresponding Author: N.B. Üner (nuner@metu.edu.tr)

Abstract

Methane pyrolysis enables hydrogen production directly from natural resources while generating solid carbon and eliminating CO₂ emissions. When conducted with a plasma, methane pyrolysis is attractive due to its electrified nature and operational flexibility. This study presents the characterization and operation of a unique two-dimensional gliding arc (GA) plasma reactor for methane pyrolysis.

Acknowledgments

The authors acknowledge the support from METU Chemical Engineering Department workshop personnel and funding provided by SOCAR Research & Development.

ABSTRACT #53

MaCKiE ABSTRACT REFERENCE NUMBER: G076

QUANTIFYING DYE-SENSITIZED PHOTOCATALYSIS: A KINETIC STUDY WITH OXYGEN-DEFICIENT ZnO

Alireza Ranjbari¹ and Philippe M. Heynderickx^{1,2*}

¹ Center for Green Chemistry and Environmental Biotechnology, Ghent University Global Campus, Incheon, South Korea

² Department of Green Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, Ghent, Belgium

Corresponding Author: Philippe M. Heynderickx (Philippe.Heynderickx@Ghent.ac.kr)

Abstract

This study explores the photocatalytic behavior of dye-sensitized ZnO by dissecting the individual roles of the dye and the catalyst. Using a binary system of methylene blue (MB) and methyl orange (MO), we developed a kinetic model that tracks both adsorption and degradation processes across varying pH conditions (3–11). The model incorporates dye speciation and distinguishes between degradation in solution and on the catalyst surface, driven by radicals and electron-hole pairs respectively. Special attention was given to identifying whether MB sensitizer or ZnO initiates charge generation. To assess the impact of oxygen vacancies, ZnO was reduced at 500 °C by 10% H₂/Ar. Our findings offer new insight into the dual function of dye molecules as both pollutants and sensitizers in photocatalysis.

Acknowledgments

The authors gratefully acknowledge the support of the Research and Development Program at Ghent University Global Campus (GUGC), South Korea.

ABSTRACT #54

MaCKiE ABSTRACT REFERENCE NUMBER: G078

MODELING POLYETHYLENE PYROLYSIS: A COMPARISON BETWEEN KINETIC MONTE CARLO AND METHOD OF MOMENTS

Laura Pires Costa, Daniël Withoeck, Oğuzhan Akin, Robin John Varghese, Mackenzie Denton, Istvan Lengyel and Kevin M. Van Geem*
Laboratory for Chemical Technology (LCT), Faculty of Engineering & Architecture
Ghent University, Belgium

Corresponding Author: Kevin M. Van Geem (kevin.vangeem@ugent.be)

Abstract

Kinetic Monte Carlo (kMC) and Method of Moments (MoM) models were compared to simulate the pyrolysis of polyethylene. To account for the volatile behavior of products, the kinetic models were integrated with vapor–liquid equilibrium. The kMC model provided detailed molecular-level insights and accurate product yields, but was computationally intensive. The MoM model, while more efficient, requires practical simplifications in mass balance formulation and is less straightforward to integrate with volatilization, as more than average properties are needed to recover an accurate product distribution. Together, these models offer complementary strengths for mechanistic understanding and predictive modeling of the complex kinetics involved in polymer pyrolysis.

Acknowledgments

ERC grant agreement n° 818607.

ABSTRACT #55

MaCKiE ABSTRACT REFERENCE NUMBER: G082

MATHEMATICAL MODELLING AND MULTI-PARAMETER OPTIMIZATION OF PHOSPHATE REMOVAL FROM WATER USING POLYMER ENHANCED ULTRAFILTRATION

Yaşar Kemal Receptoğlu^{1*} and Özgür Arar²

¹Department of Chemical Engineering, Faculty of Engineering, Izmir Institute of Technology, Urla, 35430, İzmir, TÜRKİYE

²Department of Chemistry, Faculty of Science, Ege University, Bornova, 35040, İzmir, TÜRKİYE

Corresponding Author: Yaşar Kemal Receptoğlu (yasarrecepoglu@iyte.edu.tr)

Abstract

This study presents a systematic mathematical modelling and optimization framework for phosphate (PO_4^{3-}) removal from water using a water-soluble cationic polymer in a polymer-enhanced ultrafiltration hybrid process. A three-factor, three-level Central Composite Design (CCD) was employed to evaluate the effects of pH (A), polymer dose (B), and contact time (C) on removal efficiency as a model response. A second-order polynomial (quadratic) model was developed and statistically validated via ANOVA, revealing a highly significant effect of pH on the process ($p < 0.0001$), while other factors and interactions exhibited lesser influence. The model achieved an R^2 value (96%), indicating strong predictive power, and the analysis confirmed a statistically significant model fit. Optimization through response surface methodology (RSM) suggested that $>85\%$ PO_4^{3-} removal could be attained under alkali pH and optimal polymer dose conditions. These results promote data-driven water treatment by providing a robust, scalable model for optimizing PO_4^{3-} removal and guiding similar environmental remediation applications.

Acknowledgments

This study was funded by TUBITAK 1002-A (Project No: 125M246), with the polymer kindly supplied by Abaci Water and Environmental Technologies Co.

ABSTRACT #56

MaCKiE ABSTRACT REFERENCE NUMBER: G085

A FEATURE SELECTION METHODOLOGY FOR SCARCE DATA SCENARIOS

Flora Esposito¹, Ulderico Di Caprio¹, Florence Vermeire², Idelfonso B. R. Nogueira³ and M. Enis Leblebici^{1*}

¹Process Engineering for Sustainable Systems, Department of Chemical Engineering, KU Leuven, Agoralaan Building B, 3590 Diepenbeek, Belgium

²Department of Chemical Engineering, KU Leuven, Celestijnenlaan 200F-bus 2424, Leuven, 3001, Belgium

³Department of Chemical Engineering; Norwegian University of Science and Technology, Gløshaugen, Trondheim, 7034, Norway

Corresponding Author: Enis Leblebici (muminenis.leblebici@kuleuven.be)

Abstract

A feature selection methodology tailored for data-scarce scenarios in chemical engineering is presented. The approach combines domain knowledge, correlation filtering, and SHAP-based ranking to identify a compact, informative descriptor set. Designed to maximize predictive power while enhancing model interpretability, the method is demonstrated on surface tension data but is applicable to other low-data contexts.

ABSTRACT #57

MaCKiE ABSTRACT REFERENCE NUMBER: G086

BIOLOGICALLY INFORMED ARTIFICIAL INTELLIGENCE MODELS FOR PREDICTING HUMAN SENSORY PERCEPTION OF SCENTS AND FLAVOURS

Luana P. Queiroz^{1,2,3*}, Ana M. Ribeiro^{1,2}, Bernardo M. Aguilera-Mercado⁴ and Idelfonso B.R. Nogueira³

¹ LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

² ALiCE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

³ Chemical Engineering Department, Norwegian University of Science and Technology, Sem Sælandsvei 4, Kjemiblokk 5, Trondheim 793101, Norway

⁴ Corporate Fragrance R&D, The Procter & Gamble Company, Ivorydale Innovation Center, 5299 Spring Grove Ave. Cincinnati, Ohio 45140, United States of America

Corresponding Author: Luana P. Queiroz (luanaqu@stud.ntnu.no)

Abstract

This study presents biologically informed artificial intelligence models to predict human sensory perception of scents and flavours. By integrating molecular structures, psychophysical sensory data, and perceptual attributes (character and intensity), the models establish robust correlations that reflect the underlying biological mechanisms of sensory processing. Graph neural networks (GNNs), pretrained on odor character data, significantly enhance predictive accuracy when used to initialize intensity prediction models. Preliminary results demonstrate that this approach reliably captures complex relationships between chemical structure and perceived intensity. The resulting models provide valuable insights and practical tools for sensory innovation, facilitating product development tailored to consumer preferences in flavour and perfume engineering.

Acknowledgments

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ABSTRACT #58

MaCKiE ABSTRACT REFERENCE NUMBER: G087

ACCELERATING THE MOMENT INVERSION PROCEDURE IN QUADRATURE-BASED POPULATION BALANCE METHODS

Meltem Turan^{1,3}, Denis Constaes² and Abhishek Dutta^{3*}

¹ Simuligence UAB, Vilnius, 03203, Lithuania

² Ghent University, Department of Mathematical Analysis, Galglaan 2, B-9000 Gent, Belgium

³ Izmir Institute of Technology, Department of Chemical Engineering, Izmir, 35430, Türkiye

Corresponding Author: Abhishek Dutta (abhishek.dutta@iyte.edu.tr)

Abstract

The moment-inversion procedure currently used in EQMOM has been accelerated with Aitken's delta-squared process. In this study, the accelerated moment-inversion procedure has been used to solve pure aggregation with Brownian kernel and the results are compared with their self-similar solution.

ABSTRACT #59

MaCKiE ABSTRACT REFERENCE NUMBER: G089

AI-ENHANCED MODELING OF FLAVOR RELEASE AND SENSORY DYNAMICS IN COMPLEX (BIO)CHEMICAL SYSTEMS

Idelfonso Bessa dos Reis Nogueira
Department of Chemical Engineering
Norwegian University of Science and Technology, Norway

Corresponding Author: Idelfonso Bessa dos Reis Nogueira (idelfonso.nogueira@ntnu.no)

Abstract:

Flavor and aroma release in complex matrices is governed by a cascade of multiscale phenomena involving physicochemical transport, surface interactions, and human perception. Traditional modelling approaches often fall short in capturing the subtle interplay between material properties, environmental conditions, and psychophysical response. In this context, artificial intelligence (AI) together with mechanistic modelling, can offer a framework to uncover hidden relationships in high-dimensional data and to support the design of products with optimized sensory profiles.

This presentation introduces a set of hybrid mechanistic-AI methodologies for modelling the release and perception of volatile organic compounds (VOCs). In addition, it explores the use of these models within a generative AI framework to propose novel formulations of aromatic and flavored products. The goal is to identify alternative ingredients that preserve the sensory profile of existing formulations, offering viable replacements in response to regulatory, societal, or supply-chain constraints. This approach provides a decision-support tool for the industry, enabling innovation in formulation design while maintaining product identity and consumer acceptance.

We demonstrate the use of supervised learning approaches to model flavor retention and release, highlight the role of physicochemical descriptors in perceptual persistence, and illustrate how psychophysical factors (e.g., intensity decay and individual variability) can be captured and generalized across product categories.

Beyond formulation optimization, these approaches also support sustainability goals by enabling reduced reliance on trial-and-error experimentation and guiding the design of more efficient delivery systems for sensory-active compounds. This work bridges material science, transport phenomena, and AI to provide a scalable and transdisciplinary modelling strategy for (bio) chemical systems where human perception plays a critical role.

ABSTRACT #60

MaCKiE ABSTRACT REFERENCE NUMBER: G090

HYBRID MODELLING AND ITS AUTOMATION: A PARADIGM SHIFT IN CHEMICAL ENGINEERING

Mumin Enis Leblebici

KU Leuven, Process Engineering for Sustainable Systems, Department of Chemical Engineering, Agoralaan Building
B, Diepenbeek, 3590, Belgium

Corresponding Author: Mumin Enis Leblebici (Leblebici@kuleuven.be)

Abstract

The chemical industry is undergoing a transformative shift driven by the integration of digital technologies into process development and optimization. Among these, hybrid modelling (HM) has emerged as a powerful methodology that bridges the gap between traditional first principles models and modern data-driven approaches. By combining mechanistic knowledge—such as conservation laws, thermodynamics, and transport phenomena—with machine learning techniques, hybrid models offer a unique balance of physical interpretability, predictive accuracy, and data efficiency.

Hybrid modelling is particularly valuable in fine-chemical and pharmaceutical processes, where data scarcity, complex reaction mechanisms, and high regulatory standards pose significant challenges. Unlike purely data-driven models, hybrid models can extrapolate beyond the training domain, valorize prior knowledge, and maintain robustness under process variability. Applications range from CO₂ capture in spray columns and solvent-switch crystallization¹ to kinetic modelling of telescopic reactions² and activity coefficient prediction in multicomponent mixtures.³

To overcome the complexity and manual effort traditionally associated with hybrid model development, our Automatic HYbrid digital twins for PROcess modelling (HyPro) technology is pioneering the automation of hybrid modelling and digital twin generation for the chemical industry. While hybrid models have demonstrated exceptional potential, their construction typically requires deep interdisciplinary expertise and extensive manual tuning. HyPro addresses this bottleneck by introducing a systematic, algorithm-driven approach to model design and training. Leveraging deterministic and stochastic optimisation techniques - including mixed integer linear programming (MILP), differential evolution, and Bayesian optimisation—HyPro enables the automated identification, correction, and training of hybrid models.

A key innovation of the project is SINDybrid,⁴ an open-source algorithm that detects epistemic uncertainties in mechanistic models and augments them with interpretable, data-driven corrections. By framing model construction as a mixed-integer optimisation problem, SINDybrid autonomously selects which equations require refinement, identifies suitable surrogate expressions, and trains them efficiently—even with sparse or noisy data. This methodology has been validated across diverse dynamic systems, including reaction networks, bioreactors, and oscillatory processes, demonstrating strong generalization and robustness. HyPro also aims to extend these capabilities to a wide range of physical-chemical properties and unit operations, and to democratize access to hybrid modelling tools for domain experts without programming or machine learning backgrounds.

Hybrid modelling—especially when automated—is poised to become a cornerstone of smart chemical manufacturing. It enables faster, more reliable model development, reduces experimental burden, and opens new avenues for innovation and interdisciplinary collaboration in both industrial and academic settings.

ABSTRACT #61

MaCKiE ABSTRACT REFERENCE NUMBER: G091

KINETICS-INFORMED NEURAL NETWORKS FOR POST-EQUILIBRIUM DYNAMICS IN THERMODYNAMICALLY CONSTRAINED SYSTEMS

Bitan Mukerjee¹, Sk. Aftab Hosen¹, Abhishek Dutta^{2*}

¹Jadavpur University, Department of Chemical Engineering, Kolkata 70032 India

²Izmir Institute of Technology, Department of Chemical Engineering, Izmir, 35430, Türkiye

Corresponding Author: Abhishek Dutta (abhishekdutta@iyte.edu.tr)

Abstract

This study introduces Kinetics-Informed Neural Networks (KINNs) as a data-driven yet physics-constrained framework for modeling post-equilibrium dynamics in chemical systems governed by thermodynamic laws. Traditional equilibrium thermodynamics provides final states of reactions but often fails to capture the transient trajectories once systems are perturbed.

Classical kinetic modeling, while accurate, requires detailed rate constants and mechanistic assumptions that are frequently unavailable. To bridge this gap, KINNs integrate neural architectures with thermodynamically consistent kinetic constraints to learn dynamic responses beyond equilibrium. The methodology ensures conservation of mass, energy, and free-energy while approximating reaction fluxes from limited observational data. A conservatively perturbed equilibrium (CPE) approach is implemented, whereby small deviations from equilibrium states are propagated through both kinetic equations and neural surrogates. This allows the network to learn trajectories that respect detailed balance and second-law compliance. Benchmark case studies on reversible multi-species reactions highlight the framework's ability to reproduce non-linear transient responses. By embedding thermodynamic consistency directly into kinetic residuals, the model avoids spurious oscillations and unphysical steady states.

Overall, KINN represents a novel synergy between equilibrium thermodynamics, chemical kinetics, and machine learning. The framework offers new pathways for predictive modeling, control, and optimization of complex reaction networks in both academic and industrial domains.

ABSTRACT #62

MaCKiE ABSTRACT REFERENCE NUMBER: G092

ADVANCED POWER LAW MODELING OF BIO-BASED DRYING KINETICS

Robson Wilson Silva Pessoa^{1*}, Inara Oliveira do Carmo Nascimento², Luciano Matos Queiroz³, Luana de Pinho Queiroz¹ and Idelfonso Bessa dos Reis Nogueira¹

Chemical Engineering Department, Norwegian University of Science and Technology, Norway

² Chemical Engineering Department University of Virginia, USA

³Programa de Pós-Graduação em Energia e Ambiente (PGEAm), Escola Politécnica, Universidade Federal da Bahia (UFBA), Brazil

Corresponding Author: Robson Wilson Silva Pessoa (robson.w.s.pessoa@ntnu.no)

Abstract

The literature on drying kinetics has promoted various approaches to describe the behavior of the drying rate using analytical, empirical, and data-driven methods. In terms of empirical approaches, there is a lack of explanation of the structure of the drying process. We propose a generalization of a set drying kinetics equation inspired by the anomalous diffusion representation of Levy flights defined by Tsallis in terms of nonadditive statistical mechanics.

Acknowledgments

This work was done in the framework of Project 101119358, ‘PROSAFE’, funded by the Marie Skłodowska-Curie Actions programme, HORIZON-MSCA-2022-DN-01.

ABSTRACT #63

MaCKiE ABSTRACT REFERENCE NUMBER: G093

CORE-ANNULAR FLOW FOR BIOPROCESS PIPELINES: REDUCING PRESSURE DROP WITH AQUEOUS FILM LUBRICATION

Patrick Souza Lima* and Idelfonso B.R. Nogueira
Chemical Engineering Department, Norwegian University of Science and Technology, Sem Sælandsvei 4,
Kjemiblokk 5, Trondheim 793101, Norway

Corresponding Author: Patrick Souza Lima (patrick.lima@ntnu.no)

Abstract

We assess the use of core–annular flow (CAF) to transfer viscous bioprocess broths with lower hydraulic penalties. A 2D, interface-resolving CFD model (VOF; k–omega SST) represents the section downstream of an induction head by three coplanar inlets (water–broth–water) and is compared against single-phase broth at the same inlet velocity. The setup captures the formation of a lubricating water annulus. We report pressure drop per unit length, pumping power/energy, head, from start-up to a steady window. Results show that CAF consistently forms a lubricating layer and substantially reduces hydraulic losses and shear relative to single-phase transfer. The workflow provides a compact, reproducible “virtual plant” to support design decisions on CAF-style lubrication in sanitary pipelines.

ABSTRACT #64

MaCKiE ABSTRACT REFERENCE NUMBER: G094

SCENTS OF AI: UTILIZING GRAPH NEURAL NETWORKS AND OPTIMIZATION TO REPRODUCE AROMAS

Bruno C. L. Rodrigues^{1*}, Luana P. Queiroz^{1,2,3}, Mumin Enis Leblebici⁴, Matija Strlic⁵, Ana M. Ribeiro^{2,3}, Vinicius V. Santana¹ and Idelfonso B.R. Nogueira^{1,4}

¹ Chemical Engineering Department, Norwegian University of Science and Technology, Sem Sælandsvei 4, Kjemiblokk 5, Trondheim 793101, Norway

² LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

³ ALiCE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

⁴KU Leuven, Process Engineering for Sustainable Systems, Department of Chemical Engineering, Agoralaan Building B, Diepenbeek, 3590, Belgium

⁵Heritage Science Laboratory Ljubljana, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia

Corresponding Author: Bruno C. L. Rodrigues (bruno.rodrigues@ntnu.no)

Abstract

This work presents an AI-driven framework for reproducing a target fragrance profile by identifying cost-effective substitutes for key compounds. A mixture of limonene, geraniol, vanillin, and ethanol served as the target, with vanillin selected for replacement. Odor values were calculated from gas-phase concentrations predicted by a validated diffusion model and weighted using predicted fragrance note probabilities given chemical structure. Candidate molecules were generated with a Gated Graph Neural Network and selected based on similarity, cost, and availability, yielding 1,2-dimethoxybenzene as an effective substitute. Optimization via Covariance Matrix Adaptation Evolution Strategy yielded a new formulation with the substituted ingredient that closely matched the target sensory profile. This can accelerate innovation and reduce reliance on costly experimental trials.

Acknowledgments

This work was financially supported by the SCENTINEL project (UV101923100).

ABSTRACT #65**MaCKiE ABSTRACT REFERENCE NUMBER: E001****GUIDING ENERGY – SUPPORTING GREAT MINDS TO FLOURISH**

Christoph Sprung
Active-Sites, Training/Lecturing/Consulting

Corresponding Author: Christoph Sprung (kinetics@active-sites.de)

Abstract

Lecturers, supervisors and mentors have the unique privilege to support and shape individuals as well as society. Every thought, every idea is human energy, through which we create knowledge and experience. Our role as lecturers, supervisors and mentors is a highly responsible and deliberate action most appropriately desired. After decades of narrowing down the focus on leaning methodologies, structuring curricula, receiving grades and degrees and pushing people to reach others success, the time is right for a new vision for education, mentoring and support.

We humans want to create, understand and develop. When we do what love, we set off to seek for our worthy ideals becoming reality, which makes us successful. On that journey, we experience positive emotions and may even enter a state of enhanced capability when set challenges meet a high demand of our skills. We certainly need to enable in our learners, students and mentees the skill of being successful. For seeking our ideals to become reality, we might require more cognitive, more psychomotor or more affective skills, respectively, yet it all sources the same energy inside of us and just translated differently to the outside world. This might be one of the first learning goals to provide to everyone. Profound subject specific knowledge combined with the desire for collaboration and mutual cross-disciplinary understanding might be a worthy ideal for lecturers to offer their learners to acquire. We as lecturers, supervisors and mentors are role models, it starts with us. We can share our excitement for our subject, share our knowledge and expertise, and share our positive vision for the future. Hence, we need to provide our learners, students and mentees the freedom of choice where they want to go and support their development. They appreciate support way more than direction. Remember, we humans want to create, understand and develop, it is our nature.

The focus shall be on learners', students' and mentees' development to facilitate their inspiration, creativity and confidence. Time and energy are precious resources in any human being, the more we nourish it the better we (all) flourish!

ABSTRACT #66

MaCKiE ABSTRACT REFERENCE NUMBER: E002

INHERENT TRADEMARKS OF ACADEMIC CAREER

Mikhail V. Kurushkin
Faculty of Biotechnologies
ITMO University, Russia

Corresponding Author: Mikhail V. Kurushkin (kurushkin@scamt-itmo.ru)

Abstract

The three inherent trademarks of academic career (rather than just career in general) will be discussed: (1) accessibility, (2) reputation and (3) academic freedom.

While any general career has its own rules and milestones, ups and downs, the author of the present work argues that an academic career, a.k.a a career in science, does possess unique characteristic that are inherent to its very nature (Dietz and Bozeman, 2005).

The first trademark is accessibility. In the world of academia, the stars like Nobel prize winners and Clarivate Highly Cited Researchers are open for communication with beginners unlike, if you draw a parallel, the stars in Hollywood.

The second trademark is the importance of reputation, including adhering to research and publication ethics. Whereas in real life a person can eventually rehabilitate himself/herself after having committed something and continue a normal life, in the world of academia everything is etched in stone (Smaglik, 2006; Cyranoski, 2014; Chaplain, Kirschner and Iwasa, 2020).

The third trademark is academic freedom, including the ability to choose your own path, even being a freelance academician yet staying in the academia in broad sense of it.

The lecture will offer a rich discussion of academic career dos and don'ts, supplying the audience with colourful real-life examples of research ethics violations and the aftermaths, as well as inspiring stories behind groundbreaking scientific discoveries.

ABSTRACT #67

MaCKiE ABSTRACT REFERENCE NUMBER: F101

EXTRACTION OF CORN STARCH AND CORNCOB CELLULOSE AND THEIR APPLICATION IN FORMULATION OF FOOD EMULSION SYSTEM

Muhammad Bilal Sadiq* and Saeeda Fatima
KAM School of Life Sciences, Forman Christian College/University, Pakistan

Corresponding Author: Muhammad Bilal Sadiq (bilalsadiq@fccollege.edu.pk)

Abstract

The aims of this investigation were to extract starch from low grade corn, cellulose from corncob, and essential oil from sweet orange peel (SOP-EO) for the formulation of a pickering emulsion (PE) to inhibit fungal proliferation on peanuts. Ultrasonication assisted extraction (UAE) was used for corn starch extraction. The optimum starch yield was (54.3% db). Native starch (NS) was modified by annealing and autoclaving. NS and modified starch (MS) were characterized for various techno functional properties. SOP-EO was extracted by steam distillation and used to control the growth of *Aspergillus niger* (MIC 100µl/ml), *Penicillium griseofulvum* (MIC 50µl/ml), and *Botrytis cinerea* (MIC 50 µl/ml). Cellulose was extracted from corncob using an alkali-extraction method. Cellulose was characterized by field emission scanning electron microscopy, FT-IR, and TGA. PEs containing 5% and 10% EO were formulated by homogenization followed by ultrasonication. PE containing 0.5% cellulose remained equally stable as of those containing 0.5% tween 80 for up to 21 d at room temperature. The contamination index (CI%) in 10% PE coated peanuts was significantly less than the control group. PE based coatings are thus a promising strategy to enhance the shelf life of stored grain

ABSTRACT #68**MaCKiE ABSTRACT REFERENCE NUMBER: F102****KINETIC MODELING OF THE ANTIFUNGAL ACTIVITY OF SILVER NANOPARTICLES OBTAINED FROM A SHELF FUNGUS**S.I. Trujillo^{1*}, D. Sosa², J. Vielma³ and E. Vera¹¹Escuela Politécnica Nacional, Departamento de Ciencias de los Alimentos y Biotecnología, Ecuador²Facultad de Ciencias de la Vida-FCV, Centro de Investigaciones Biotecnológicas del Ecuador -CIBE, Escuela Superior Politécnica del Litoral, ESPOL, Campus Gustavo Galindo, Km 30.5 vía Perimetral, Guayaquil, 09092, Ecuador³Facultad de Ciencias Naturales y Matemáticas, Centro de Investigación y Desarrollo de Nanotecnología, Escuela Superior Politécnica del Litoral, ESPOL, Campus Gustavo Galindo, Km 30.5 vía Perimetral, Guayaquil, 09092, Ecuador*Corresponding Author:* S.I. Trujillo (sofi_1602t@hotmail.com)**Abstract**

The objective of this study was to model the kinetics of mycelial growth inhibition (PGI) of *Moniliophthora roreri* using silver nanoparticles (AgNPs) biosynthesized from a shelf fungus by evaluating their effect over time and across different concentrations. Microbial death models (Chick-Watson and Weibull) were applied to describe the kinetic behavior at concentrations of 50, 100, 200, and 400 ppm. The Weibull model showed a better overall fit, while the Chick-Watson model improved significantly when concentration was included as a variable. A median inhibitory concentration (IC₅₀) of 141.3 ppm was estimated on day 15. The Kruskal-Wallis test revealed significant differences between treatments ($p = 0.015$), and Dunn's post hoc test indicated greater antifungal efficacy at 200 and 400 ppm. The results confirm that AgNPs induce a dose-dependent inhibition of the pathogen and that their behavior can be described using robust kinetic models, representing a key step toward their potential application in the sustainable management of cacao diseases.

Acknowledgments

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ABSTRACT #69

MaCKiE ABSTRACT REFERENCE NUMBER: F103

THE LOGARITHMIC EQUATION FOR MODELING THE ENZYMATIC HYDROLYSIS OF BYPRODUCTS PROTEINS: EMPIRICAL OR THEORETICAL?

Pedro L. Valencia
School of Foods, Pontificia Universidad Católica de Valparaíso, Chile

Corresponding Author: Pedro L. Valencia (pedro.valencia@pucv.cl)

Abstract

The logarithmic equation is a very useful and simple model to describe the progress of the enzymatic hydrolysis of food byproduct proteins. The equation $P = 1/b * \ln(a * b * t + 1)$ describes the product concentration against time modulated by two kinetic constants, a and b. The use of the logarithmic equation was documented in the article of Marquez & Fernandez in 1993 to model the hydrolysis of bean proteins by Alcalase. The authors did not cite a reference article to sustain the use of this equation. An interesting approach was published by Qi & He in 2006 where the authors proposed a reaction mechanism and the deduction of the logarithmic equation. Unfortunately, the mechanism was not properly formulated. A possible source appeared from the hydrolysis of cellulose in the articles published by Ooshima and Ohmine. The mathematical analogy of Ooshima and Ohmine equation for the enzymatic hydrolysis of cellulose by cellulases and the logarithmic equation for the hydrolysis of proteins suggests that this is the origin although the lack of connection in the literature. In conclusion, the logarithmic equation is empirically based and does not need to be theoretical to justify its usefulness describing the hydrolysis of food byproducts proteins.

ABSTRACT #70**MaCKiE ABSTRACT REFERENCE NUMBER: F105****ALTERATION IN FATTY ACID PROFILE OF FRESHWATER CRAYFISH
PONTASTACUS LEPTODACTYLUS AFTER DIETARY SUBSTITUTION OF
FISH MEAL WITH INSECT MEAL**Maria V. Alvanou¹, Anastasia Kyriakoudi², Ioannis Mourtzinou², Ioannis T. Karapanagiotidis³ and Ioannis A. Giantsis^{1*}¹Laboratory of Ichthyology and Fisheries, Faculty of Agriculture
Aristotle University of Thessaloniki, Thessaloniki, Greece.²Laboratory of Food Chemistry and Biochemistry, Department of Food Science and
Technology, Faculty of Agriculture, Forestry and Natural Environment
Aristotle University of Thessaloniki, Thessaloniki, Greece³Department of Ichthyology and Aquatic Environment
University of Thessaly, Volos, Greece*Corresponding Author:* Ioannis A. Giantsis (giantsisg@gmail.com)**Abstract**

The rising demand for crayfish has led to population declines in several regions across their natural range. As a result, establishing optimal rearing conditions has become essential, with dietary optimization being a key factor. In this context, the present study conducted a 98-day feeding trial to assess the effects of fishmeal (FM) substitution with *Hermetia illucens* insect meal (HM) in the diet of *Pontastacus leptodactylus* juveniles. The inclusion of HM in the diet significantly altered the crayfish's whole-body chemical composition, indicating a distinct metabolic response compared to fishmeal-based diets. Fatty acid analysis showed that palmitic acid (16:0) was the dominant saturated fatty acid (SFA), oleic acid (18:1 ω 9) was the primary monounsaturated fatty acid (MUFA), and linoleic acid (18:2 ω 6) was the most abundant polyunsaturated fatty acid (PUFA), followed by cis-11,14,17-eicosatrienoate (C20:3 ω 3) and docosahexaenoic acid (C22:6 ω 3). Dietary HM inclusion significantly decreased the levels of SFAs, PUFAs, and ω 6 fatty acids, including C22:6 ω 3, while increasing the ω 6/ ω 3 ratio and the hypocholesterolemic-to-hypercholesterolemic ratio in the crayfish body. Alongside advancements in balanced diets and optimized culture conditions essential for rearing freshwater crayfish, this study offers new insights into the suitability of insect meals as a nutritional component for *P. leptodactylus*.

Acknowledgments

This research project was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the “2nd Call for H.F.R.I. Research Projects” to support Faculty Members & Researchers (Project Number: 3245).

ABSTRACT #71

MaCKiE ABSTRACT REFERENCE NUMBER: F106

DEEP LEARNING-BASED ESTIMATION OF CHICKEN FRESHNESS USING RGB IMAGE ANALYSIS

Serife Simsek, Aleyna Yigit and Sibel Uzuner*
Department of Food Engineering, Izmir Institute of Technology, Türkiye

Corresponding Author: Sibel Uzuner (sibeluzuner@iyte.edu.tr)

Abstract

Ensuring food safety and maintaining quality control is becoming more crucial, especially in the food industry, where chicken products are susceptible to spoilage and fraud. Properly identifying the freshness and species of chicken is vital to avoid foodborne illnesses, uphold consumer confidence, and minimize financial losses due to fraudulent activities. Traditional techniques for assessing meat quality, like visual inspection and manual labeling, are often slow, prone to mistakes, and inadequate for handling the high demands of large-scale food processing and distribution.

The system integrates image-based classification through a custom Convolutional Neural Network (CNN) with volatile organic compounds data to deliver a complete, real-time solution for determining the freshness of chicken. The custom CNN was trained on a dataset of 850 images, which were used to classify chicken freshness.

Additionally, the use of pre-trained deep learning models (SqueezeNet, AlexNet, ResNet50, VGG16, and GoogleNet) for evaluating chicken freshness resulted in an overall accuracy of 97.15%. It is worth mentioning that the same training and validation datasets were used for all models, ensuring a fair and consistent comparison of their performance. The custom CNN demonstrated a significant edge in processing complex image data.

ABSTRACT #72**MaCKiE ABSTRACT REFERENCE NUMBER: F108****THE EFFECTS OF NOVEL THAWING TECHNIQUES ON QUALITY OF FROZEN BEEF LIVER**

Nazlıcan Avsar and Sibel Uzuner*
¹Department of Food Engineering
Izmir Institute of Technology, Türkiye

Corresponding Author: Sibel Uzuner (sibeluzuner@iyte.edu.tr)

Abstract

Freezing is an effective method to preserve meat and retain its quality until it reaches consumers. However, freezing induces changes in meat, primarily due to the formation of ice crystals, which can affect tenderness and functionality. A more crucial step is the thawing prior to meat use because it has a large impact on the quality of frozen foods. Thawing often leads to protein oxidation and major physicochemical changes including ice crystals growth, all of which result in losses of quality and perceived value. This study aimed to evaluate the physicochemical and structural characteristics of beef liver freezing ($-18\pm 2^{\circ}\text{C}$, 20 h) and subsequently thawed using three methods: water immersion (WI), ultrasonication bath (UB) and air-fryer (AF). The objective was to assess the impact of these thawing methods on color attributes, drip loss, protein stability, and meat color stability of the frozen beef liver samples. Compared to WI and AFT, the drip loss of frozen beef liver treated with 40 kHz ultrasound was significantly higher ($p < 0.05$). The values of L^* , a^* , and b^* for the raw beef liver were significantly higher than those for the AF and UB samples ($P < 0.05$). The ΔE values of liver samples thawed in WI (8.08 ± 0.69) for prolonged periods were higher than those of other samples. In contrast, the color of liver samples thawed using UB showed ΔE value (6.32 ± 0.20) closet to that of the raw liver sample. Compared to raw beef liver (77.94°C) and WI (74.74°C), both air-fryer thawing (70.77°C) and ultrasonic bath thawing (71.14°C) lower the denaturation temperature of the beef liver, indicating a reduction in its thermal stability. The lowest MetMb content was observed in samples thawed using an UB (43.42%), followed by AF thawing (50.17%).

Acknowledgments

The authors would like to thank Prof. Dr. Ünver Ozkol for his help with construction of the thermal camera system, Yekta Gunay for assistance with FTIR analyses and Kjeldahl protein analysis at the Izmir Institute of Technology the Center of Biotechnology and Bioengineering Application and Research (IZTECH-CFB) Izmir, Turkey, Burcu Çağlar for assistance with DSC analyses at the Izmir Institute of Technology the Center for Materials Research, and Prof. Dr. Figen Korel for allowing us to use the chroma colorimeter (Konica Minolta).

ABSTRACT #73

MaCKiE ABSTRACT REFERENCE NUMBER: F113

MODELING AND EXPERIMENTAL VALIDATION OF FREQUENCY-DEPENDENT SOUND LEVEL DISTRIBUTION IN AIRBORNE ULTRASOUND

Ömer Faruk Çokgezme^{1*}, Naz Arsoy², Birkan Reyhanoğlu², Barış Oğuz Gürses³ and Filiz İçier¹

¹Ege University, Faculty of Engineering, Department of Food Engineering, Bornova, Izmir, Türkiye

²Ege University, Graduate School of Natural and Applied Sciences, Food Engineering Section, Bornova, Izmir, Türkiye

³Ege University, Faculty of Engineering, Department of Mechanical Engineering, Bornova, Izmir, Türkiye

Corresponding Author: Ömer Faruk Çokgezme (omer.faruk.cokgezme@ege.edu.tr)

Abstract

Airborne ultrasound (ABUS) is an emerging non-contact technology that transmits and receives ultrasonic waves through the air, offering promising applications in food processing where hygiene and non-destructive testing are critical. This study aims to simulate and experimentally evaluate the distribution of ultrasonic sound levels on the horn surface during ABUS treatments at different frequencies (20, 40, and 60 kHz). All treatments were performed at a constant power of 400 W, and sound level measurements were taken at five radial points along the horn surface using a sound level measurement device. Simulations were conducted using the finite element method in COMSOL Multiphysics (Version 6.3, Sweden) applying the Pressure Acoustics Model for air and Linear Elastic Shell Equations for the solid horn structure. Results revealed significant changes in sound levels from the center to the edge of the horn, with frequency-dependent interference patterns observed in both the experimental and simulated data. The predicted distributions closely matched the experimental measurements, demonstrating the model's accuracy in capturing radial variations in sound levels. The findings confirm the potential of finite element modeling as a reliable tool for predicting sound field behavior in ABUS systems operating at varying frequencies.

Acknowledgments

This study was financially supported by the Scientific and Technological Research Council of Turkey (TÜBİTAK), Project No: 122O951.

ABSTRACT #74

MaCKiE ABSTRACT REFERENCE NUMBER: F114

COUPLED THERMAL–MASS TRANSFER MODELING OF BIOACTIVE EXTRACTION FROM BERRY FRUIT: INTEGRATION OF COMSOL-BASED DIFFUSION KINETICS WITH BOX-BEHNKEN EXPERIMENTAL DESIGN

Ece Yildiz-Ozturk

Department of Food Processing, Food Technology Programme, Yasar University, 35100 Bornova- Izmir, Türkiye

Corresponding Author: Ece Yildiz-Ozturk (ece.yildizozturk@yasar.edu.tr)

Abstract

The aim of the study is to optimize pressurized water extraction, a sustainable and efficient technique for recovering bioactive compounds, under different temperature, pressure, and time conditions using Design Expert software. Additionally, to better understand the mass transfer mechanisms of the system, a multi-physics model combining heat transfer, laminar flow, and the transport of dilute species was developed in COMSOL Multiphysics®, and a simulation study was conducted to reveal diffusion profiles dependent on pressure and temperature. This integrative approach highlights the potential of physics-based modeling in the optimization of green extraction processes and supports the rational design of food-grade bioactive recovery systems.

Acknowledgments

This work was financially supported by the Yasar University Scientific Research Project Office grant numbers BAP-139. The author is thankful to the Chemistry Laboratory at Food Process Laboratory in Yasar University and Biomimetic Microsystems Laboratory at Bioengineering Department in Ege University for access to the facilities.

ABSTRACT #75

MaCKiE ABSTRACT REFERENCE NUMBER: F116

**INNOVATIVE AMBIENT TEMPERATURE HYPERBARIC
INACTIVATION OF *ALICYCLOBACILLUS ACIDOTERRESTRIS* SPORES
AND EFFECTS OF PASTEURIZATION PRE-TREATMENTS**

Carlos A. Pinto¹, Alireza Mousakhani Ganjeh¹, Maria J. Alegria² and Jorge A. Saraiva^{1*}

¹LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

²SUMOLCOMPAL Marcas, S.A. Estrada Nacional 118, 2080-023 Almeirim, Portugal

Corresponding Author: Jorge A. Saraiva (jorgesaraiva@ua.pt)

Abstract

This study investigated the hyperbaric inactivation (HI) of *Alicyclobacillus acidoterrestris* (ACB) spores in apple juice at pressures of 150, 200, and 250 MPa for up to 24 hours at ambient temperatures (18–23 °C). The impact of different pasteurization pre-treatments – thermal (90 °C, 30 s), high-pressure (600 MPa, 3 min, HPP), pulsed electric field (30 kV, 80 µs, 1400 Hz, PEF), and ultrasound (67 W, 20 kHz, 5 min, US) – on spore inactivation by HI was also evaluated. Inactivation data were fitted to non-linear kinetic models, including Biphasic, Log-logistic, and Weibull models.

Without pre-treatment, HI achieved approximately 4.56 log reductions in ACB spores after 24 hours across all pressure levels, starting from an initial load of ~6 log CFU/mL. Pre-treatments generally did not enhance HI effectiveness, with inactivation levels remaining around 4–5 log units after 24 hours, except for PEF, which resulted in a slightly lower inactivation of only about 3.5 log units. Phase contrast microscopy indicated that spores did not enter to vegetative cells state during HI, while this occurred for the control at ambient temperature and atmospheric pressure. When HI was performed at 5 °C, lower inactivation levels were observed, achieving 3.86, 2.54, and 1.77 log reductions at 150, 200, and 250 MPa, respectively, after 96 hours. The results of this work point to the possibility of using HI, before or after conventional thermal and other nonthermal technologies (HPP, PEF, and US) pasteurization to render apple juice free of ACB spores at room temperature and under refrigeration at moderate pressure (150-250 MPa) and with no thermal input. This novel ACB spores' inactivation process should be further studied in the context of ACB spores' high thermal stability and its industrial relevance and for other spores as well.

Acknowledgments

This work received support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006 – Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos. Thanks are also due to the FCT/MCTES for the PhD fellowships of Carlos A. Pinto (SFRH/BD/137036/2018). This study was funded by the PRR – Plano de Recuperação e Resiliência and by the NextGenerationEU funds at Universidade de Aveiro, through the scope of the Agenda for Business Innovation “Plataforma de Valorização, Industrialização e Inovação comercial para o AgroAlimentar (VIIAFOOD)” (Project no. 37 AAC nº 02/C05-i01/2022 with the application C644929456-00000040).

ABSTRACT #76**MaCKiE ABSTRACT REFERENCE NUMBER: F117****EFFECTS OF PULSED ELECTRIC FIELDS PROCESSING AND ULTRAVIOLET PROCESSING ON THE QUALITY, MICROBIAL INACTIVATION AND SHELF LIFE OF LICORICE SHERBET**Hakan Tanriverdi¹, Irem Demir¹, Sibel Uzuner^{2*} and Gulsun Akdemir Evrendilek³¹Bolu Abant İzzet Baysal University Faculty of Engineering Department of Food Engineering Bolu Türkiye²Izmir Institute of Technology Faculty of Engineering Department of Food Engineering Izmir Türkiye³University of Maine Cooperative Extension Orono Maine*Corresponding Author:* Sibel Uzuner (sibeluzuner@iyte.edu.tr)**Abstract**

Licorice drink, a traditional Turkish beverage, is produced and consumed in limited quantities due to its short shelf life. While heat processing extends shelf life, it negatively affects its physical, chemical, and sensory properties. This study investigated the use of pulsed electric fields (PEF) as a processing alternative. Licorice drink samples were treated under varying conditions of time (108, 432, 756 μ s), temperature (6, 18, 30 °C), and electric field strength (2, 4, 7 kV) based on a Box-Behnken design. PEF processing preserved the drink's quality while achieving ~ 3 log cfu/mL microbial inactivation. Response surface modeling identified optimum PEF conditions as 2 kV, 756 μ s, and 7.48 °C. Shelf-life studies showed that samples stored at 4 °C remained stable for up to 40 d, while those at 22 °C began deteriorating after 30 d. Overall, PEF proved effective for processing licorice drink without compromising quality.

Acknowledgements

This project was supported by General Directorate of Agricultural Research and Policies (TAGEM), Ministry of Agriculture and Forestry, Republic of Türkiye.

ABSTRACT #77

MaCKiE ABSTRACT REFERENCE NUMBER: F118

ENHANCING TOMATO SEED VIGOR AND MICROBIAL SAFETY THROUGH PULSED ELECTRIC FIELD (PEF) TECHNOLOGY: A SUSTAINABLE PRE-SOWING APPROACH

Bahar Yalcın^{1,2}, Gulsun Akdemir Evrendilek^{1,3*} and Sibel Uzuner⁴

¹Mardin Artuklu University, Center Research Laboratory Application and Research Center, Mardin Türkiye

²Bolu Abant İzzet Baysal University, Faculty of Engineering, Department of Food Engineering, Bolu, Türkiye

³The University of Maine, Cooperative Extension, Orono, ME USA

⁴İzmir Institute of Technology, Faculty of Engineering, Department of Food Engineering, Gülbahçe Campus İzmir, Türkiye

Corresponding Author: Gülsün Akdemir Evrendilek (gulsun.akdemir@maine.edu)

Abstract

Seed quality plays a pivotal role in ensuring crop performance, resilience, and productivity. This study explores the use of pulsed electric field (PEF) treatment as a sustainable, non-thermal technique to improve the physiological and microbial quality of tomato seeds. Seeds were subjected to PEF treatments delivering energy levels from 1.07 to 17.28 J. The treatment delivering 15.36 J resulted in the highest germination rate (72.81%) on day 7, while 17.28 J yielded the highest percentage of normal seedlings (94.62%) ($p \leq 0.05$). Under cold conditions (24 °C for 5 d), the greatest germination rate (46.67%) occurred at 1.92 and 10.88 J. Seeds exposed to 100 and 200 mM NaCl demonstrated markedly improved germination following PEF treatment, with the 17.28 J dose achieving $62.00 \pm 0.90\%$ and $50.00 \pm 0.60\%$ germination, respectively ($p \leq 0.05$). Electrical conductivity increased significantly with incubation time, independent of PEF intensity. Microbial analysis revealed a complete inactivation of aerobic bacteria and molds/yeasts at the highest treatment level, with microbial counts reduced from initial levels of 4.00 ± 0.03 and 3.06 ± 0.03 log cfu/g to below detectable limits. These results support the application of PEF as a practical seed enhancement strategy that fosters germination, improves stress resilience, and ensures microbial safety—contributing to more sustainable agricultural practices.

Acknowledgment

Financial support was provided by TUBITAK (217O068).

ABSTRACT #78

MaCKiE ABSTRACT REFERENCE NUMBER: F119

INFLUENCE OF RICE BRAN ON THE PHYSICOCHEMICAL AND FUNCTIONAL PROPERTIES OF LOW GLYCEMIC FOOD MODEL SYSTEM

Filiz Baser, Sukru Gulec and Cansu Ozel*
Department of Food Engineering
Izmir Institute of Technology, Türkiye

Corresponding Author: Cansu Özel (cansuozel@iyte.edu.tr)

Abstract

This study investigates the incorporation of rice bran (RB) as a functional ingredient in a low glyceemic pudding-like food model, focusing on its impact on physicochemical and functional properties. The compositional characteristics of RB were analyzed using attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR), while its microstructure was examined via scanning electron microscopy (SEM). RB was incorporated into rice starch (RS) pudding formulations at varying substitution ratios, and a factorial design approach was employed to optimize texture parameters resembling conventional RS pudding. The optimized RB:RS ratio was subsequently used to prepare the food model for further evaluation. An *in vitro* digestion protocol was applied to stimulate gastrointestinal conditions, and the release of glucose during digestion was quantified. The study further evaluates the impact of RB on glucose bioavailability using the Caco-2 intestinal cell model, highlighting its potential role in glyceemic control and enhanced functional food applications. This research aligns with growing interest in utilizing RB as a valuable ingredient to mitigate metabolic health risks.

Acknowledgments

The authors acknowledge Izmir Institute of Technology, Biotechnology and Bioengineering Research and Application Centre (IZTECH-BIOMER) for ATR-FTIR and SEM instruments.

ABSTRACT #79**MaCKiE ABSTRACT REFERENCE NUMBER: F121****HARNESSING CAROTENOIDS FROM SQUASH FOR CLEAN-LABEL FOOD INNOVATION: GREEN EXTRACTION, MICROENCAPSULATION, AND APPLICATION IN NUTRITIONALLY ENRICHED FOODS**

Carlos Alberto Fuenmayor^{1*}, Sandra Milena Ballesta¹, David Alejandro Garzón¹, Carlos Mario Zuluaga-Domínguez², Elizabeth Cristina Acevedo¹, Andrea Nieto-Veloza³ and Consuelo Díaz-Moreno¹

¹Institute of Food Science and Technology, Universidad Nacional de Colombia, Bogotá, Colombia

²Faculty of Agricultural Sciences, Universidad Nacional de Colombia, Bogotá, Colombia

³School of Food Engineering, Universidad del Valle, Cali, Colombia

Corresponding Author: Carlos Alberto Fuenmayor (cafuenmayorb@unal.edu.co)

Abstract

This study valorized carotenoids from *Cucurbita moschata* ("ahuyama" squash) through green extraction, spray-drying microencapsulation, and food application. Conventional extraction yielded the highest β -carotene content (1244 mg/kg), with ultrasound offering much faster, yet slightly lower yields and stability. Extracts were rich in β -carotene, lutein and α -carotene, and stable over storage. Microencapsulation using modified starch/maltodextrin achieved >84% efficiency under optimized conditions (~180 °C, 66% wall material). Both liquid and encapsulated extracts colored yogurt and crackers comparably to synthetic dyes (FD&C Yellow #5/6), with good consumer acceptance and added provitamin A value. This approach promotes clean-label innovations using a globally cultivated crop.

Acknowledgments

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ABSTRACT #80

MaCKiE ABSTRACT REFERENCE NUMBER: F122

CFD DATASET GENERATION AND SURROGATE MODELING FOR TEMPERATURE DYNAMICS IN CHICORY STORAGE ROOMS

Abhishek Bhat K.N.¹, Pieter Verboven^{1*}, Klaar Elsen², Tim De Clercq² and Bart Nicolai^{1,3}

¹ KU Leuven, Department of Biosystems, Division MeBioS, Postharvest Group, Leuven, Flanders, Belgium

² Praktijkpunt Landbouw Vlaams-Brabant, Herent, Flanders, Belgium

³ Flanders Centre of Postharvest Technology, Leuven, Flanders, Belgium

Corresponding Author: Pieter Verboven (pieter.verboven@kuleuven.be)

Abstract

Chicory (Belgian endive) is a specialty crop and a prime export product of Belgium. Before production of the white leafed crop in specialized dark hydroponic systems, roots are harvested from fields and stored in cold rooms. Accurately predicting temperature dynamics in chicory storage rooms is critical for maintaining product quality and ensuring energy-efficient operations. This study focuses on generating comprehensive Computational Fluid Dynamics (CFD) datasets to capture the complex interplay of airflow, heat transfer, and dynamic thermal loads under multiple operational scenarios. The validated CFD model incorporates detailed room geometry, porous media for the bins, fan dynamics, and the cooling effect of the evaporator. Multiple transient CFD simulations were performed, each representing different dynamic load conditions, external influences, and control inputs. These simulations provided detailed snapshots of spatial and temporal temperature and velocity fields, forming a high-fidelity dataset for training a Time-Derivative Physics-Informed Neural Network (TD-PINN). The TD-PINN learned the dynamic operator of temperature evolution. This surrogate model aims to deliver accurate and rapid temperature predictions, supporting real-time scenario analysis and adaptive control in chicory storage facilities.

Acknowledgments

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ABSTRACT #81**MaCKiE ABSTRACT REFERENCE NUMBER: F123****ARTIFICIAL INTELLIGENCE (AI) IN FUNCTIONAL FOOD DEVELOPMENT**

Şükrü Güleç^{1,2*}, Ceren Daşkaya Dikmen³, Burcu Kahraman³, Gülay Özkan⁴, Esra Çapanoğlu⁴, Atalay Çelik⁵, Hasan Fatih Durkaya⁵ and Mehmet Gönen⁶

¹İzmir Institute of Technology, Faculty of Engineering, Department of Food Engineering, Molecular Nutrition and Human Physiology Laboratory, Urla, İzmir, Türkiye

²DynamisBio Functional Food Development Research A.Ş., Teknopark İzmir, Urla, İzmir Türkiye

³Ülker Bisküvi Topkapı R&D Center, İstanbul, Türkiye

⁴Department of Food Engineering, Faculty of Chemical and Metallurgical Engineering, Istanbul Technical University, Maslak, Istanbul, Türkiye

⁵Scientific and Technological Research Institution of Türkiye, Informatics and Information Security Research Center, Artificial Intelligence Institute, Gebze/Kocaeli, Türkiye

⁶Koç University İşBank Center for Infectious Diseases (KUISCID), Koç University Hospital, Istanbul, Türkiye, Department of Industrial Engineering, College of Engineering, Koç University, Istanbul, Türkiye

Corresponding Author: Şükrü Güleç (sukrugulec@iyte.edu.tr)

Abstract

The integration of artificial intelligence (AI) into functional food research and development is redefining traditional formulation strategies by introducing greater efficiency, precision, and adaptability. Functional food design typically involves multiple steps—such as ingredient selection, literature evaluation, biofunctionality assessment, and production—each of which requires extensive time and expertise. AI-driven approaches can streamline these processes by rapidly analyzing vast datasets, identifying patterns and relationships, and generating predictive insights that support more targeted nutritional solutions. A central strength of AI lies in its ability to process both unstructured and structured data sources. Unstructured data, including open-access scientific literature and clinical studies, provides broad insights into ingredient interactions, dosage efficacy, bioavailability, production technologies, and consumer demographics. Structured data, derived from proprietary databases and laboratory-generated results, offers more specific and higher-quality evidence, though it is often limited in scope. The integration of these complementary data streams allows AI systems to construct a holistic view of functional ingredients, enabling the design of formulations that are scientifically grounded and consumer-responsive. Equally important is the validation of AI-generated predictions through empirical studies. Preclinical and clinical trials not only confirm the safety and efficacy of proposed formulations but also feed back into AI models, refining their predictive power and enhancing trustworthiness. This iterative feedback loop strengthens regulatory credibility and supports substantiated health claims. Ultimately, the successful application of AI in functional food development depends on interdisciplinary collaboration. Partnerships among data scientists, nutritionists, food technologists, and manufacturers are essential for translating AI-driven insights into products that meet regulatory standards while addressing evolving consumer health expectations.

Acknowledgments

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ABSTRACT #82

MaCKiE ABSTRACT REFERENCE NUMBER: F124

FOODOMICS: AN EVOLVING HOLISTIC APPROACH IN FOOD QUALITY, FOOD SAFETY AND HUMAN HEALTH

Pinar Balkir*, Kemal Kemahlioglu and Ufuk Yucel
Ege Vocational School, Department of Food Technology, Ege University, Bornova, Izmir, Türkiye

Corresponding Author: Pinar Balkir (pinar.balkir@ege.edu.tr)

Abstract

The progress in the analytical methods in food science and technology brought about a novel and modern approach concerning food quality, food safety, human health and even environmental health. The constituent omics approaches have extensively been applied in biology and medical domains so far. Recently, food and nutrition scientists have also been interested in these omics studies.

Constituent omics technologies, which are increasingly evolving, are implied separately or in combination, not only in analyzing food constituents but also in food authentication, evaluation of food quality, food safety and human nutrition. It is evident that using advanced analytical techniques in omics research has empowered scientists looking into food and nutrition science at a broad perspective.

This review discusses the evolution of foodomics, and how foodomics approach elucidates the arguments concerning food quality, food safety, the origin of food, human nutrition, and relatedly human well-being.

ABSTRACT #83

MaCKiE ABSTRACT REFERENCE NUMBER: F125

PRODUCTION OF A HEALTHY SNACK ENRICHED WITH BEECH NUT (*FAGUS ORIENTALIS* L.) POWDER

Ahsen Rayman Ergün* and Kadriye Altay
Food Engineering Department, Engineering Faculty, Ege University, İzmir, Türkiye

Corresponding Author: Ahsen Rayman Ergün (ahsenrayman@gmail.com)

Abstract

European beech (*Fagus sylvatica* L.) stands out as the most widespread forest tree in Europe, extending from southern Sweden to Spain, Sicily, and northwestern Türkiye. Oriental beech (*Fagus orientalis*) is a straight-stemmed beech species from the Fagaceae family that can grow up to 40 meters tall and is native to Türkiye. Beech nuts consist of approximately 33% shell and 67% kernel. The protein yield was determined to be 19.4% which is comparable to the protein content of cashews, hazelnuts, and pistachios. In this research, the aim is to produce a functional grissini snack enriched with aroma and flavor components by roasting and grinding the fruit seed of the beech tree, known as beech nut, and adding olive paste. For this reason, the beech nuts were roasted traditionally then the formulation was made for the snack dough and with olive paste the functional product obtained. Some physical and chemical properties were investigated. As a result, color, textural and sensorial properties were determined and a healthy snack with beech nut powder was produced successfully.

Acknowledgments

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ABSTRACT #84

MaCKiE ABSTRACT REFERENCE NUMBER: F129

ENVIRONMENTALLY FRIENDLY PACKAGING SOLUTIONS FOR THE FOOD SYSTEM

Adnan Cenker Ege, Duygu Büyüktas and Figen Korel*
Food Engineering Department, Izmir Institute of Technology, Türkiye

Corresponding Author: Figen Korel (figenkorel@iyte.edu.tr)

Abstract

The increasing emphasis on sustainability within the global food system necessitates the development and implementation of environmentally friendly food packaging systems. These innovative packaging solutions, commonly referred to as green packaging, aim to reduce environmental impact while ensuring the preservation of food quality and safety throughout the supply chain. This review examines recent advancements in biodegradable and bio-based packaging materials and their functional roles within contemporary food systems, with particular focus on emerging active and intelligent packaging technologies. The integration of such environmentally sustainable packaging systems plays a pivotal role in minimizing food waste and reducing plastic pollution, thereby fostering more sustainable and resilient food systems. Despite significant progress, widespread adoption of these packaging solutions is impeded by challenges related to economic feasibility, material performance, regulatory compliance, consumer acceptance, and the establishment of adequate end-of-life infrastructure. By elucidating the multifaceted functions of environmentally friendly packaging within food systems, this study provides comprehensive insights and strategic approaches for their effective integration to enhance sustainability across the food value chain.

ABSTRACT #85

MaCKiE ABSTRACT REFERENCE NUMBER: F130

MODELING MICROBIAL SPOILAGE OF UNTREATED & OHMIC HEAT TREATED MANGO PIECES

Fernandez-Villanueva G¹, Martinez-Martinez E¹, Morales E², Welti-Chanes J¹ and Torres JA^{1*}
¹School of Engineering & Sciences, Monterrey, Tecnológico de Monterrey, NL, 64849, Mexico
²Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada
Instituto Politécnico Nacional, Querétaro, Qro 76090, Mexico

Corresponding Author: J. Antonio Torres (dr.j.antonio.torres@gmail.com)

Abstract

The need to refrigerate minimally processed products and waste of up to 30% in the cold chain demonstrate the need to develop tools that allow for efficient and low-cost evaluation of cold chain performance. Predictive microbiology was used to evaluate the growth of spoilage microorganisms in fresh-cut mango pieces stored at temperatures between 2 and 15°C using the Weibull-Peleg model and a power function to determine microbiological growth and lag phase duration, respectively. Ohmic heating not only reduced microbial loads but also extended the lag phase and reduced growth rates of psychotropic bacteria and mold and yeast. These models could be a valuable tool for shelf-life prediction of refrigerated mango pieces when handled under highly variable temperature such as those observed in refrigerated shipping.

Acknowledgments

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ABSTRACT #86

MaCKiE ABSTRACT REFERENCE NUMBER: F137

OPTIMIZATION AND VALIDATION OF ULTRASOUND-ASSISTED SOLVENT EXTRACTION OF OLIVE LEAF POLYPHENOLS USING BOX-BEHNKEN EXPERIMENTAL DESIGN

Semanur Yildiz^{1,2*}, Yaren Didem Esendemir^{1,2}, Abdil Özdemir³, Gözde Seval Sözbilen⁴ and Levent Yurdaer Aydemir⁵

¹ Department of Food Engineering, Sakarya University, Serdivan, Sakarya, Türkiye

² Sustainable Food Processing Laboratory (SuProLab), Sakarya University, 54050, Sakarya, Türkiye

³ Sakarya University, Faculty of Nature, Chemistry Department, Sakarya, Türkiye

⁴ Olive Research Institute, İzmir, Türkiye

⁵ Department of Food Engineering, Adana Alparslan Türkeş Science and Technology University, 01250 Adana, Türkiye

Corresponding Author: Semanur Yildiz (semanury@sakarya.edu.tr)

Abstract

Olive leaves, a major byproduct of olive oil production, are rich in polyphenolic compounds (especially oleuropein) with notable antioxidant and health-promoting properties. Ultrasound-assisted solvent extraction (UAE) can enhance the recovery of these phenolics compared to conventional methods. In this study, a Box–Behnken design (response surface methodology) was employed to optimize UAE conditions (ultrasonic amplitude, extraction time, and ethanol–water concentration) for maximizing total phenolic content (TPC) in olive leaf extracts. Three factors (amplitude 40–80%, time 2–18 min, EtOH 40–80% v/v) were varied, and a quadratic model was fitted to the experimental data. The model identified 68% amplitude, 18 min, and 59% ethanol concentration as the optimal conditions, which yielded the highest TPC. This optimum was experimentally validated, yielding notable higher TPC than extractions using water only or higher ethanol concentration. The optimized UAE process substantially improves polyphenol yield from olive leaves, supporting the valorization of olive leaf waste into value-added antioxidant extracts.

Acknowledgments

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ABSTRACT #87

MaCKiE ABSTRACT REFERENCE NUMBER: F138

FOOD MATRIX INTERACTIONS AND PHYTOCHEMICAL STABILITY: EXPERIMENTAL AND MODELLING APPROACHES TO PREDICT BIOACCESSIBILITY

Esra Capanoglu

Department of Food Engineering, Faculty of Chemical and Metallurgical Engineering, Istanbul Technical University, 34469 Maslak, Istanbul, Türkiye

Turkish Academy of Sciences (TUBA), Bayraktar Neighborhood, Vedat Dalokay St. No: 112 06670 Çankaya, Ankara, Türkiye.

Corresponding Author: Esra Capanoglu (capanogl@itu.edu.tr)

Abstract

The health effects of phytochemicals such as phenolics depend on their stability, bioaccessibility, and transport during gastrointestinal digestion. These factors are influenced by food processing methods and matrix interactions, which can enhance or inhibit compound release and absorption. This study aims to present the results of our current research on the impact of thermal and non-thermal processing (high-pressure, pulsed electric field) and matrix composition (e.g., milk proteins, dietary fibers) on the stability, bioaccessibility, and transepithelial transport of phenolics using in vitro simulated digestion coupled with Caco-2 cell models. On the other hand, examples of mathematical modelling framework developed to simulate phytochemical release, transformation, and transport kinetics during digestion, incorporating physicochemical properties, enzymatic reactions, and matrix–compound interactions will be covered. Model predictions aligned closely with experimental data, enabling the identification of conditions that optimize phytochemical retention and bioefficacy. In general, results demonstrate that certain non-thermal techniques and specific matrix compositions can improve phenolic transport, while others may reduce bioaccessibility. The integration of experimental and predictive modelling provides a powerful tool for designing functional foods with enhanced nutritional value and health benefits.

ABSTRACT #88

MaCKiE ABSTRACT REFERENCE NUMBER: F139

MECHANISTIC INSIGHTS INTO THE IMPACT OF MEDIUM CHAIN FATTY ACIDS ON BIOFILM FORMATION IN *SALMONELLA* TYPHIMURIUM

Runrun Zhang¹, Jinsong Feng^{1,2} and Tian Ding^{1,2*}

1. College of Biosystems Engineering and Food Science
Zhejiang University, Hangzhou, China

2. Future Food Laboratory, Innovation Center of Yangtze River Delta
Zhejiang University, Jiaxing, China

Corresponding Author: Tian Ding (tding@zju.edu.cn)

Abstract

Salmonella enterica is one of the main pathogens associated with the ingestion of contaminated food worldwide, with Typhimurium being the most frequent serotypes isolated from contaminated food. *S. Typhimurium* shows the capacity to develop biofilms, responsible for cross-contamination during the food processing. Despite differences in adaptation among different *S. Typhimurium* isolates, the underlying mechanism remains poorly understood. Therefore, this study investigated the responses of different *S. Typhimurium* isolates to medium-chain fatty acids (MCFAs). By analyzing physiological differences among *Salmonella* isolates, the impact of MCFAs on *S. Typhimurium* biofilm formation and colonization capabilities were clarified. Then, we identified key association of AceK function with response to MCFAs, revealing two distinct adaptation strategies. Furthermore, we confirmed the regulatory function AceK and the key gene site was verified. This study highlights the physiological variations among *S. Typhimurium* and demonstrates the crucial role of AceK in governing its metabolic adaptation. These findings provide new insights into understanding the ecological behavior of *S. Typhimurium* and shed light on potential control strategies.

Acknowledgments

This work was supported by the Zhejiang Province Natural Science Foundation (ZCLTGN24C2001).

ABSTRACT #89**MaCKiE ABSTRACT REFERENCE NUMBER: F147****BIOSYNTHESIZED SILVER NANOPARTICLES: A SUSTAINABLE ALTERNATIVE FOR *MONILIOPHTHORA RORERI* CONTROL IN CACAO**S.I. Trujillo^{1*}, D. Sosa², J. Vielma³ and E. Vera¹¹Escuela Politécnica Nacional, Ecuador²Facultad de Ciencias de la Vida-FCV, Centro de Investigaciones Biotecnológicas del Ecuador -CIBE, Escuela Superior Politécnica del Litoral, ESPOL, Campus Gustavo Galindo, Km 30.5 vía Perimetral, Guayaquil, 09092, Ecuador³Facultad de Ciencias Naturales y Matemáticas, Centro de Investigación y Desarrollo de Nanotecnología, Escuela Superior Politécnica del Litoral, ESPOL, Campus Gustavo Galindo, Km 30.5 vía Perimetral, Guayaquil, 09092, Ecuador*Corresponding Author:* S.I. Trujillo (sofi_1602t@hotmail.com)**Abstract**

Moniliasis, caused by *Moniliophthora roreri*, is one of the main threats to sustainable cacao production in Ecuador. Due to the limited effectiveness and negative impacts of chemical fungicides, biosynthesized silver nanoparticles (AgNPs) have emerged as a promising alternative. In this study, the antifungal activity of AgNPs obtained through green synthesis was evaluated *in vitro*. Four concentrations (50, 100, 200, and 400 ppm) were tested against three *M. roreri* strains, and the percentage of mycelial growth inhibition (PGI) was calculated. The AgNPs exhibited significant and dose-dependent inhibition, with values exceeding 90% at 400 ppm in two of the strains. Statistical analysis confirmed significant differences between concentrations and strains. These findings support the potential use of fungal-derived AgNPs as a sustainable plant disease control tool, with positive implications for food security and the reduction of agrochemical use in cacao production.

Acknowledgements

The authors gratefully acknowledge the support of the Department of Food Science and Biotechnology (DECAB) at the Escuela Politécnica Nacional (EPN), as well as the Biotechnological Research Center of Ecuador (CIBE) and the Faculty of Chemical Sciences at the Escuela Superior Politécnica del Litoral (ESPOL).

POSTER PRESENTATIONS

ABSTRACT #90

MaCKiE ABSTRACT REFERENCE NUMBER: G021

A DIFFUSION APPROACH TO KINETIC MODEL DISCRIMINATION IN HETEROGENEOUS CATALYSIS

Oleksii Zhokh*, Andrii Trypolskyi and Peter Strizhak
L.V. Pysarzhevskii Institute of Physical Chemistry
National Academy of Sciences of Ukraine, Ukraine

Corresponding Author: Oleksii Zhokh (al.zhokh@gmail.com)

Abstract

Several kinetic equations may simultaneously describe the rate of a heterogeneous catalytic process. In these circumstances, discrimination between the competing kinetic models is necessary. Herein, we introduce an approach to select the relevant kinetic model of a heterogeneous catalytic process by the transition from a reaction-rate-limited regime to an intraparticle-diffusion-limited regime. The effectiveness factor for the rival models may obey considerably different trends versus reactant concentration. Therefore, accounting for the effectiveness factor allows one to obtain an instrument for the discrimination between the kinetic models. The proof of concept is demonstrated using exemplary kinetics of the methanol dehydration over a commercially available activated γ -alumina catalyst.

ABSTRACT #91

MaCKiE ABSTRACT REFERENCE NUMBER: G042

COUPLED AND DE-COUPLED ACTIVE SITES IN CATALYTIC REACTIONS

Christoph Sprung
Stirnerstr. 12
12169 Berlin, Germany

Corresponding Author: kinetics@active-sites.de

Abstract

Kinetics in catalysis is often described by events on a single active site in simulations and calculations. It is assumed that all catalytic reactions take place on that site and selectivity is explained through multi-route concepts. Chemical logic, however, would suggest to look at it from a different angle. In this contribution the experimental evidence and simulations for the necessity of various active sites are presented, satisfying chemical logic. Furthermore, the view is extended to several reactions in order to support the more general validity of this concept, which states: For every product that is produced there has to be an individually shaped active site for the formation of this specific product. Therefore, every product appears with its own kinetic trend, which could be called a *kinetic fingerprint*.

ABSTRACT #92

MaCKiE ABSTRACT REFERENCE NUMBER: G047

USE OF SPECTROSCOPY, MACHINE LEARNING AND CHEMICAL SPECIATION MODELS TO DETERMINE CHROMIUM CONCENTRATION IN AQUEOUS SOLUTIONS

Divyang Deep Tiwari^{1*}, Ramkumar Kothandam², Sridharakumar Narasimhan^{1,2} and Shankar Narasimhan²

¹ Robert Bosch Center for Data Science and Artificial Intelligence, Bhupat and Jyoti Mehta School of Biosciences, Indian Institute Of Technology, Chennai, India

² Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India

Corresponding Author: Divyang Deep Tiwari (divyangdeeptiwari@gmail.com)

Abstract

Chromium exists in several valance states in nature of which Cr(VI) is carcinogenic. Chromium contamination in water is a widespread problem and determination of different oxidative states and concentrations, especially of Cr(VI) is very important. The aim of this work is to combine machine learning with chemical speciation models to determine Cr(VI) concentrations in aqueous solutions using spectroscopic data. The proposed approach first constructs a database of UV-vis spectra of different Cr (VI) species by combining machine learning with chemical speciation model. This is subsequently used to infer concentrations of various Cr(VI) ionic species and total Cr(VI) concentration directly from UV-vis spectra. We show that fairly accurate estimates of ppm level Cr(VI) concentrations in water over a wide range of pH can be obtained in a direct manner without use of any additional reagents.

ABSTRACT #93

MaCKiE ABSTRACT REFERENCE NUMBER: G060

UNCERTAINTIES IN NET ZERO ROADMAP USING MONTE CARLO TECHNIQUE

Srijita Bhattacharyya^{1*}, Miray Kaya² and Abhishek Dutta²

¹Department of Chemical Engineering, Jadavpur University, Kolkata 700032, India,

²Department of Chemical Engineering, Izmir Institute of Technology, Gülbahçe Campus, Izmir 35430, Türkiye

Corresponding Author: Srijita Bhattacharyya (srijitab.chemical.ug@jadavpuruniversity.in)

Abstract

This study employs Monte Carlo simulation to quantify uncertainties in national CO₂ emission trajectories for India, China, and Türkiye, focusing on technology adoption rates and emission coefficients in the steel sector—one of the most emission-intensive industries. Alongside probabilistic projections, deterministic Business-as-Usual (BAU) and Net-Zero (NZ) scenarios were constructed to evaluate emissions reduction potential. By quantifying the range of possible outcomes, this approach can provide policymakers with a robust framework to design flexible, risk-informed decarbonization strategies that remain effective under uncertainty.

ABSTRACT #94

MaCKiE ABSTRACT REFERENCE NUMBER: G061

PHYSICS-INFORMED NEURAL NETWORK (PINN) FOR A PARTICULATE AGGREGATION-BREAKAGE SYSTEM

Sk. Aftab Hosen^{1*}, Meltem Turan² and Abhishek Dutta³

^{1*} Department of Chemical Engineering, Jadavpur University, Kol-032, West Bengal, India

²Ege University, Department of Mathematics, Izmir 35180, Türkiye

³Izmir Institute of Technology, Department of Chemical Engineering, Gülbahçe Campus, Izmir 35430, Türkiye

Corresponding Author: Sk. Aftab Hosen (skhosen.chemical.ug@jadavpuruniversity.in)

Abstract

Population Balance Equation (PBE) is crucial for modeling particulate aggregation and fragmentation phenomena across chemical and allied industries. This study presents a novel Physics-Informed Neural Network (PINN) tailored for solving a simplistic aggregation-fragmentation problem using a classic case study with analytical solutions. The case of embedding the governing equations in the loss function enforces the underlying physics throughout training. Comparisons with analytical solution of PBE confirm the accuracy of PINN approach, validating its predictive capability. This approach significantly advances particulate system dynamics modeling, with potential applications in optimizing industrial particulate processes and addressing broader class of integro-differential equations.

ABSTRACT #95

MaCKiE ABSTRACT REFERENCE NUMBER: G062

A PHYSICS-INFORMED NEURAL NETWORK (PINN) APPROACH TO OVER-EQUILIBRIUM DYNAMICS IN CONSERVATIVELY PERTURBED EQUILIBRIUM SYSTEMS

Bitan Mukherjee^{1*} and Abhishek Dutta²

^{1*}Department of Chemical Engineering, Jadavpur University, Kolkata 700032, India

²Department of Chemical Engineering, Izmir Institute of Technology, Gülbahçe Campus, Izmir 35430, Türkiye

Corresponding Author: Bitan Mukherjee (bitanm.chem.ug@jadavpuruniversity.in)

Abstract

This study introduces a novel Physics-Informed Neural Network (PINN) framework for simulating hydrogen and carbon-monoxide over-equilibrium deviations under conservatively perturbed equilibrium (CPE) conditions in methane reforming. The method eliminates the need for dense solution data by enforcing complete compliance with chemical dynamics by directly integrating precise reforming kinetics and equilibrium boundary values into the PINN's loss function. The trained model accurately resolves transient extrema in product mole fractions—features often missed by conventional solvers—using substantially fewer collocation points. Superior accuracy in forecasting the timing and amplitude of CPE peaks is confirmed by validation against exact ODE integrations. These results demonstrate that PINN is a potent, mesh-free tool for uncertainty-quantified design, process optimization, and real-time reactor diagnostics in industrial reforming.

ABSTRACT #96

MaCKiE ABSTRACT REFERENCE NUMBER: G063

**A KINETIC MONTE CARLO SIMULATION ON FISCHER-TROPSCH
SYNTHESIS TO MODEL THE EFFECT OF HYDROGEN DYNAMICS
ON PRODUCT SELECTIVITY**

Ceren M. Uyhan, Necip B. Üner and Deniz Üner*
School of Chemical Engineering
Middle East Technical University of Ankara, Türkiye

Corresponding Author: Deniz Üner (uner@metu.edu.tr)

Abstract

Monte Carlo simulations of Fischer-Tropsch synthesis (FTS) conducted using a MATLAB-based surface model demonstrated that methane selectivity significantly decreased when hydrogen access to the surface was limited to defect-like sites or when (CO)₂ formation occurred, consistent with literature findings. These results emphasize the critical role of adsorbate distribution in steering FTS product selectivity and provide a computational framework for optimizing catalyst surface design.

ABSTRACT #97

MaCKiE ABSTRACT REFERENCE NUMBER: G077

KINETIC MODELING OF MALONDIALDEHYDE REACTIVITY: IS THIS A TRUE LIPID OXIDATION MARKER?

Philippe M. Heynderickx^{1,2*} and Bruno De Meulenaer³

¹ Center for Green Chemistry and Environmental Biotechnology, Ghent University Global Campus, Incheon, South Korea

² Department of Green Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, Ghent, Belgium

³ NutriFOODchem Unit, Department of Food Technology, Safety and Health, Faculty of Bioscience Engineering, Ghent University, Coupure Links 653, B-9000 Ghent, Belgium

Corresponding Author: Philippe M. Heynderickx (Philippe.Heynderickx@Ghent.ac.kr)

Abstract

The degradation of malondialdehyde (MDA) in saturated glycerol triheptanoate oil is studied in the temperature range 298.2 – 453.2 K. Given the non-ideality of the solution, activity coefficients are taken up in the kinetic model. The corresponding reactions in the kinetic model include the reversible MDA hydrolysis and irreversible MDA dimerization (self-condensation). Significant parameter estimates are obtained via nonlinear regression and an excellent correspondence with experimental data was found.

Simulations with (1) variation on initial water content and (2) variation in MDA production, via a general production rate using an Arrhenius relation mimicking the lipid oxidation reactions, demonstrate that the measured MDA, as well-known marker for lipid peroxidation processes, is no straightforward indication for its production via lipid oxidation processes as degradation might occur.

Acknowledgments

PMH gratefully acknowledges the support of the Research and Development Program at Ghent University Global Campus (GUGC), South Korea. The authors thank Dr. Angelique Vandemoortele and Ms. Ludivine Leloup for the experimental data.

ABSTRACT #98

MaCKiE ABSTRACT REFERENCE NUMBER: G080

PARTICLE-RESOLVED SIMULATIONS FOR THE CATALYTIC DEHYDROGENATION OF ETHANE TO PRODUCE ETHYLENE

Dalia N. Dorantes-Landa,¹ J. Fernando Durán-Pérez¹, J. Francisco Hernández-Ramírez¹, José G. Rivera de la Cruz¹ and Carlos O. Castillo-Araiza^{1*}

¹Laboratory of Catalytic Reactor Engineering, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, Col. Vicentina C.P, 09340, Ciudad de México, México.

Corresponding Author: Carlos O. Castillo-Araiza (coca@xanum.uam.mx)

Abstract

This work simulates the performance of selective oxidation within a representative volume of a wall-cooled packed-bed catalytic reactor using particle-resolved simulations. Transport phenomena are coupled with a microkinetic model developed through multiscale hierarchical methodologies, incorporating information from Density Functional Theory (DFT). The study reveals how fluid dynamics affect heat and mass transfer and, in turn, how these influence reaction kinetics, particularly by enhancing selectivity toward the compound of interest. These insights provide guidance on how to optimize, or even intensify, selective oxidation reactions of industrial relevance.

ABSTRACT #99

MaCKiE ABSTRACT REFERENCE NUMBER: G081

KINETICS OF CARBOXYLIC ACID ENOLIZATION ON METAL OXIDES IN VAPOR PHASE

Alexey V. Ignatchenko*, Reem Ibrahim, Jordan R. Kostera, Jordan D. Walker, Jared J. Jorolemon and Christian J. Leonardo,
St. John Fisher University, Rochester, NY 14618, United States

Corresponding Author: Alexey V. Ignatchenko (aignatchenko@sjfc.edu)

Abstract

A previously overlooked, reversible catalytic reaction—enolization—consistently occurs when carboxylic acid vapors contact metal oxide surfaces. The relatively strong acidity of the CO₂H group leads to formation of surface-bound carboxylate on Lewis acid sites. Although the α -C–H is much less acidic and invisible in direct observations, it participates in H/D isotopic exchange, revealing enolization. This enolized intermediate can condense with another surface carboxylate, forming ketones via decarboxylation—a key step in oxygen removal during biofuel upgrading. In this study, the rate of equilibrium H/D exchange at the α -carbon of isobutyric acid (in vapor with D₂O) and reverse D/H exchange (with α -deuterated acid and H₂O) was measured over monoclinic ZrO₂ and anatase TiO₂. Faster H/D vs. D/H exchange indicates α -deprotonation as rate-determining. Intrinsic enolization rates were obtained using the McKay equation, with activation parameters determined from temperature-dependent kinetics. KOH-doped ZrO₂ showed increased enolization rates and raised the H/D isotope effect from 1.4 to 8.3, due to transition state changes. In contrast, KOH had little effect on TiO₂, with rates slightly reduced and kH/kD stable at 2.7–2.8. These findings confirm that C–C coupling, not enolization, is the rate-limiting step in decarboxylative ketonization.

Acknowledgments

This work has been supported directly by the National Science Foundation under research Grants No. 1955139, and No 1828310.

ABSTRACT #100

MaCKiE ABSTRACT REFERENCE NUMBER: G083

SURROGATE SUPERSTRUCTURE OPTIMIZATION BASED ON MACHINE LEARNING AND MIXED INTEGER PROGRAMMING

Ibrahim Mert Kahraman¹, Alperen Guler², Basak Tuncer², Ozgun Deliismail² and Hasan Sildir^{1*}

¹ Department of Chemical Engineering, Izmir Institute of Technology, Türkiye

² SOCAR Türkiye R&D and Innovation Co., Izmir, 35800, Türkiye

Corresponding Author: Hasan Sildir (hasansildir@iyte.edu.tr)

Abstract

Chemical process optimization involves selecting unit operations and pathways to maximize profit while minimizing costs. This study develops a surrogate-based superstructure optimization methodology using artificial neural networks (ANN), mixed-integer nonlinear programming (MINLP), and chance-constrained programming. The cumene production process, which is an example process, is modelled in Aspen Plus, and a dataset is generated for ANN training. A superstructure is formulated with alternative pathways, and optimization is performed using Pyomo library via Python. Three case studies compare ANN training methods and constraint formulations. The proposed approach optimizes complex process flowsheets, identifying optimal process design variables and pathways while ensuring robust solutions through chance-constrained programming.

ABSTRACT #101

MaCKiE ABSTRACT REFERENCE NUMBER: G088

OPTIMAL OPERATION STRATEGY FOR KOÇ UNIVERSITY CAMPUS ENERGY SYSTEM: ENHANCING ENERGY EFFICIENCY

S. Sanyal and E. Aydın*

Department of Chemical and Biological Engineering, Koç University, Türkiye

Corresponding Author: Erdal Aydın (eyaydin@ku.edu.tr)

Abstract

As university campuses strive for carbon neutrality, deploying energy management tools that uphold long-term sustainability objectives while maximizing operational efficiency is essential. This study develops a mixed-integer linear programming (MILP) framework focused exclusively on maximizing the energy efficiency of an integrated on-campus energy system. Historical heating, cooling, and electricity demand measurements (originally recorded at irregular intervals) are transformed into continuous profiles by fitting cubic smoothing splines and enforcing total-energy consistency via integral matching to daily aggregates. These continuous demand functions are then discretized at hourly, half-hourly, and 15-minute resolutions, before being used in the MILP formulations. By comparing dispatch performance across these time-step granularities, the analysis will quantify the benefits of high-resolution control for improved tracking of load dynamics and enhanced storage utilization.

ABSTRACT #102

MaCKiE ABSTRACT REFERENCE NUMBER: F104

PREDICTIVE MICROBIAL MODELLING IN DRIED FRUIT PROCESSING: CURRENT APPROACHES AND FUTURE POTENTIAL

Ali Nalbant
K.F.C. GIDA R&D Center, Menemen Izmir Türkiye

Corresponding Author: Ali Nalbant (ali.n@kfc.com.tr)

Abstract

Dried fruits are widely consumed for their nutritional value and prolonged shelf life; however, they remain vulnerable to microbial contamination during processing, packaging, and storage (Guirguis, 2018). Predictive microbial modelling has become an essential tool in food safety management, allowing researchers and industry professionals to estimate microbial growth, survival, and inactivation under diverse environmental conditions (Tarlak, 2023). These models are generally classified into primary, secondary, and tertiary types, and are already extensively applied in dairy, meat, and fresh produce sectors (Tarlak, 2023; Meinert et al., 2023). Emerging techniques such as artificial neural networks (ANN), computational fluid dynamics (CFD), and multiscale modelling offer enhanced predictive accuracy with reduced dependence on experimental trials (Akter et al., 2022). Despite this progress, dried fruit applications remain underrepresented in current literature (Canakapalli, 2021). Given the distinctive properties of dried fruits—low water activity but high hygroscopicity—their microbial safety requires special attention (Canakapalli, 2021). This review highlights the relevance of modelling approaches such as Gompertz, Baranyi, and Ratkowsky models, and advocates for the adaptation of these tools to dried fruit systems. Expanding the use of predictive microbiology in this sector can improve risk assessment, support HACCP integration, and foster the development of safer and more sustainable drying and storage practices (Koseki, 2016; Tarlak, 2023).

ABSTRACT #103

MaCKiE ABSTRACT REFERENCE NUMBER: F131

MICROBIAL PRESERVATION PERFORMANCE OF A RESIDENTIAL REFRIGERATOR: A MULTIPLE PRODUCT, STORAGE LOCATION AND TEMPERATURE SETTING CASE STUDY

E. Martínez-Martínez, G. Fernández-Villanueva, J. Welti-Chanes and J.A. Torres*
School of Engineering and Sciences, Tecnológico de Monterrey, Eugenio Garza Sada 2501, Monterrey 64700, NL,
México

Corresponding Author: J. Antonio Torres (dr.j.antonio.torres@gmail.com)

Abstract

This study evaluated the microbial preservation performance of a residential refrigerator by integrating time-temperature data and predictive microbiology models to develop a Refrigerator Performance Indicator (RPI). Whole milk, Panela cheese and chicken breast meat samples were stored in different locations of a refrigerator operating with different ambient temperatures, food loads and temperature settings. Storage location and temperature setting had a statistically larger influence on preservation performance. Milk samples placed on the door shelf consistently showed poor performance, whereas excellent preservation performance was achieved for chicken breast samples stored in a closed cabinet with independently controlled temperature. Moreover, higher food loads buffered temperature increases during door openings but delayed food temperature recovery due to thermal inertia. This study suggests that changes in the temperature setting chosen by consumers and cold air distribution improvements can enhance the microbial preservation performance of a refrigerator and reduce foodborne illness risks and food waste.

Acknowledgments

Authors Gerardo Fernandez Villanueva and Enrique Martinez Martinez acknowledge the support from SECIHTI-Mexico for their support stipend scholarship and Tecnológico de Monterrey for their doctoral program tuition waiver. All authors acknowledge also the financial support received from EMBRACO, Apodaca, Mexico.

ABSTRACT #104

MaCKiE ABSTRACT REFERENCE NUMBER: F132

NOVEL TOOLS TO ASSESS THE PRESERVATION PERFORMANCE OF FRESH-CUT MANGO TRANSPORTED UNDER REFRIGERATION

G. Fernandez-Villanueva*, E. Martinez-Martinez, J. Welti-Chanes and J.A. Torres*
School of Engineering and Sciences, Tecnológico de Monterrey, Eugenio Garza Sada 2501, Monterrey 64700, NL,
México

Corresponding Author: G. Fernandez-Villanueva (gerardo.fer.villa@gmail.com)

Abstract

The preservation performance of fresh-cut mango shipments under the highly variable temperatures characterizing refrigerated transportation was assessed using indicators based on predictive microbiology and time-temperature data. After assessing the statistical variability of these indicators using Monte Carlo simulations, they could be used for the real-time monitoring of refrigerated transportation and of the entire cold chain for fresh-cut mango and other products.

Acknowledgments

Authors Gerardo Fernandez Villanueva and Enrique Martinez Martinez acknowledge the support from SECIHTI–Mexico for their support stipend scholarship and Tecnológico de Monterrey for their doctoral program tuition waiver. All authors acknowledge also the financial support received from the US National Mango Board.

ABSTRACT #105**MaCKiE ABSTRACT REFERENCE NUMBER: F133****DIELECTRIC PROPERTIES OF SHELLED WALNUT (*JUGLANS REGIA* L.) USING THE THRU-REFLECT-LINE METHOD**

R. Hernández-Nava¹, J.M. Meza-Arenas², D. Sarmiento-Narvaez², T. Kaur³, A. Corona-Chavez², R. Rojas-Laguna⁴, and M.E. Sosa-Morales^{5*}

¹ Department of Chemical, Food and Environmental Engineering, Universidad de las Américas Puebla, San Andrés Cholula, Mexico

² Department of Electronics, Instituto Nacional de Astrofísica, Óptica y Electrónica, Tonanzintla, Mexico

³ Department of Electronic and Telecommunications Systems, Universidad Autónoma de la Ciudad de México, Mexico City, Mexico

⁴ Department of Electronics Engineering, Division of Engineering, Irapuato-Salamanca Campus, Universidad de Guanajuato, Salamanca, Mexico

⁵ Department of Food Engineering, Division of Life Sciences, Irapuato-Salamanca Campus, Universidad de Guanajuato, Irapuato, Mexico

Corresponding Author: M.E. Sosa-Morales (mariae.sosam@gmail.com)

Abstract

Shelled walnut (*Juglans regia* L.) was characterized by its dielectric properties using the thru-reflect transmission line method, determining the permittivities of the air-nut mixture and the solid nut, bulk permittivity (ϵ_{bulk}) and particle permittivity (ϵ_{part}), respectively, at three temperatures (20, 40, 60°C) in the frequency range of 27 – 5000 MHz. The dielectric constant and loss factor decreased as the frequency increased, regardless of the type of permittivity used (ϵ_{bulk} or ϵ_{part}), whereas a decreasing trend with temperature was observed. Higher penetration depth (d_p) values were observed in the radiofrequency range. For example, at 40 °C and 27 MHz, the d_p was 5.27 m, whereas at the same temperature and 5000 MHz, the d_p was 1.35 m. Additionally, d_p values using ϵ_{bulk} were higher than with ϵ_{part} . DP are useful to design future radiofrequency and microwave treatment strategies for these nuts.

Acknowledgments

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ABSTRACT #106

MaCKiE ABSTRACT REFERENCE NUMBER: F134

IMPACT OF A RADIOFREQUENCY TREATMENT ON THE PHYSICOCHEMICAL PROPERTIES OF PINE NUTS (*PINUS CEMBROIDES*)

Mitzi G. Flores-Sánchez^{1*}, Flor M. Gutiérrez-Sánchez¹, Ruth Hernández-Nava², Tejinder Kaur³ and María Elena Sosa-Morales¹

¹ Department of Food Engineering, División de Ciencias de la Vida, Universidad de Guanajuato, Irapuato, Mexico

² Department of Chemical, Food and Environmental Engineering, Universidad de las Américas Puebla, San Andrés Cholula, Mexico

³ Department of Electronic and Telecommunications Systems, Universidad Autónoma de la Ciudad de México, Mexico City, Mexico

Corresponding Author: Mitzi G. Flores-Sánchez (mg.floressanchez@ugto.mx)

Abstract

The physicochemical quality of in-shell pine nuts was evaluated to analyze the impact of a radiofrequency (RF) heat treatment at 60°C for mold inactivation. An analysis of variance was performed with a 95% confidence level and a Tukey test to determine significant differences before and after radiofrequency heating. The results showed a significant reduction in water activity (a_w) from 0.659 ± 0.01 before treatment to 0.510 ± 0.01 reflecting a reduction in moisture content ($p < 0.05$). Color was not affected by the RF treatment ($p > 0.05$). Although the RF treatment lowers the moisture content, the a_w reduction of the in-shell pine nuts may be positive since the risk of being attacked by molds will be lower.

Acknowledgments

This research was funded by Consejo Nacional de Humanidades, Ciencias y Tecnologías (CONAHCYT, now SECIHTI), research project [CBF2023-2024-1220].

ABSTRACT #107

MaCKiE ABSTRACT REFERENCE NUMBER: F135

ADVANCED MACHINE LEARNING AND STATISTICAL MODELING FOR DRYING KINETICS AND ULTRASOUND-ASSISTED PROTEIN EXTRACTION FROM MOSAMBI (*CITRUS LIMETTA*) PEEL

Khwaja Osama* and Kaiser Younis
Department of Bioengineering, Integral University, Kursi Road, Lucknow, India

Corresponding Author: Khwaja Osama (osama@iul.ac.in)

Abstract

Mosambi (*Citrus limetta*) peel, an abundant agro-industrial by-product, was valorized through optimized drying and protein extraction, employing advanced modeling and optimization techniques. Drying kinetics were studied under varying temperature (50–90 °C), sodium chloride concentration (2–10%), and bed thickness (1–4 mm), modeled using Gaussian Process Regression (GPR), Artificial Neural Network (ANN), and Response Surface Methodology (RSM). GPR achieved superior predictive accuracy for unseen data ($R^2 = 0.82$, RMSE = 0.191), outperforming ANN and RSM. Ultrasound-assisted protein extraction using the pH-shift method was modeled via Support Vector Regression (SVR) and optimized with a Genetic Algorithm. Optimal conditions (187.5 μm particle size, 10.79 min, 53.15% amplitude) yielded 54.24% protein with 90.2% purity. Functional characterization revealed good emulsifying (26.3%), oil-holding (3.1 ml/g), and foaming (30%) capacities, with XRD indicating predominantly amorphous structure. The study demonstrates the potential of machine learning-based modeling for process control and optimization, enabling sustainable utilization of citrus peel waste in functional food applications.

Acknowledgments

The authors acknowledge Integral University, Lucknow for providing the necessary infrastructure and financial support to perform this research.

ABSTRACT #108

MaCKiE ABSTRACT REFERENCE NUMBER: F136

KINETIC MODELING AND MACHINE LEARNING OPTIMIZATION OF CITRUS LIMETTA PEEL PECTIN EXTRACTION FOR SUSTAINABLE FOOD APPLICATIONS

Alvina Farooqui*, Poonam Sharma, Khwaja Osama and Kaiser Younis
Department of Bioengineering, Integral University, Lucknow, India

Corresponding Author: Alvina Farooqui (alvina@iu.ac.in)

Abstract

Two independent studies investigated the extraction kinetics and process optimization of pectin from Citrus limetta peel using ultrasound-assisted extraction (UAE) and microwave-assisted extraction (MAE). Kinetic modeling through central composite design (CCD) in UAE revealed significant influences of pH and extraction time, achieving a maximum yield of 35.58%. MAE incorporated Support Vector Regression (SVR) coupled with a genetic algorithm to capture nonlinear microwave heating kinetics, predicting optimal conditions (600 W, pH 1, 180 s) with 32.75% yield ($R^2_{\text{train}} = 0.984$, $R^2_{\text{test}} = 0.993$). Both methods confirmed pseudo-second-order kinetics, with cavitation (UAE) and volumetric heating (MAE) as key mechanisms. Extracted pectins exhibited high equivalent weight (>790), methoxyl content (~8%), and desirable water/oil holding capacities, qualifying as high methoxyl pectins. Application trials in cookies demonstrated up to 30% butter replacement without compromising sensory quality. These results highlight the role of machine learning and kinetic modeling in sustainable valorization of citrus waste into functional food ingredients.

Acknowledgments

The authors are grateful to the Integral University, Lucknow for the providing the necessary infrastructure and financial support to perform this research.

ABSTRACT #109

MaCKiE ABSTRACT REFERENCE NUMBER: F148

DECODING HONEY ORIGINS: ML AND DL METHODS FOR BOTANICAL CLASSIFICATION

Nathan Mekuria Solomon*, Cansu Turan and Durmuş Özdemir
Department of Chemistry, Izmir Institute of Technology, Gülbahçe Campus, Izmir 35430, Türkiye

Corresponding Author: Nathan Mekuria Solomon (nathansolomon@std.iye.edu.tr)

Abstract

Accurate classification of honey by botanical origin is essential for authenticity verification and quality control. In this study, FTIR spectroscopy was combined with machine learning (ML) and deep learning (DL) approaches to classify honey samples from five botanical classes. Spectral data were normalized and evaluated using 5-fold cross-validation. Classical ML models (SVM, Decision Tree, Ensembles, and Logistic Regression) achieved accuracies ranging from 86% to 96%, with the Voting and Logistic classifiers reaching 96% ($F1 \approx 0.94$). A 1D Convolutional Neural Network (CNN) trained on the original dataset achieved perfect classification (Accuracy = 1.0, $F1 = 1.0$). To test dimensionality reduction, Principal Component Analysis (PCA, $n=10$) was applied before CNN training, yielding slightly lower but still robust results (Accuracy ≈ 0.96 , $F1 \approx 0.95$). Random Forest feature selection identified key spectral bands contributing to discrimination, while autoencoder-based t-SNE visualization revealed clustering of most classes with some overlap. The framework integrates predictive accuracy with interpretability, providing a rapid and reproducible approach for honey authentication and botanical classification.