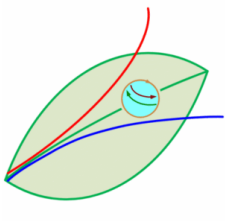
# CLES-CE 2022

## 1st INTERNATIONAL SCIENTIFIC CONFERENCE ON CLEANER ENERGY AND CHEMICAL ENGINEERING FOR SUSTAINABLE CIRCULAR ECONOMY



# Book of Abstracts

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Cleaner Energy Systems

Cleaner Chemical Engineering

BRNO UNIVERSITY OF TECHNOLOGY FACULTY OF MECHANICAL ENGINEERING

NETME Centre

SPIL

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## Organised by

- Institute of Chemical Engineering – Bulgarian Academy of Sciences, Sofia, Bulgaria
- Sustainable Process Integration Laboratory – SPIL, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology - VUT Brno, Brno, Czech Republic
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Book of Abstracts

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# PLENARY LECTURES

## Plenary Session PL-01

# Synthesis of Sustainable and Regenerative Systems to Achieve Carbon Neutrality

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**Abstract**

Our global system is currently facing severe problems related to population growth, depletion of non-renewable resources, and environmental and societal destruction. Along with the increasing competition, globalization alone has proven to be insufficient for fostering steady economics within the sustainable development of our global system. On the contrary, globalization based on unsustainable practices can only deepen and prolong the crisis. It is evident that the linear economy and linear production supply chains using non-renewable resources, should be upgraded to sustainable and regenerative systems based on a circular economy (CE) dealing with closed energy and material flows within production supply networks based mostly on renewable resources. Process Systems Engineering with its Sustainable Systems Synthesis can develop integrated methods and tools to provide engineers with a powerful enough tool to be able to shape sustainable development. The Mathematical Programming approach, especially combined with other approaches, e.g., Pinch Analysis, is a powerful and very efficient technology to solve large complex problems related to sustainable development. Several powerful concepts behind the synthesis of sustainable regenerative systems are discussed, and the use of the Mathematical Programming approach in the context of this synthesis is emphasized. It also discusses the impact of different objective functions on the solutions and the need to select the most appropriate function, as well as the need for considering the effect of solutions on the global GHG balance to achieve carbon neutrality and beyond. MIPSYN-Global, an interactive tool for the synthesis of sustainable regenerative systems, is briefly described. Several synthesis applications are shown to demonstrate the approach.

## Plenary Session PL-02

# Role and Significance of Mathematical Modeling in Environment Protection

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**Abstract**

The lecture focuses on the necessity, the opportunities, the benefits and the significance of mathematical modelling in environment protection. Ecosystems are large-scale and sophisticated objects for management. The assessment of their condition and the factors which it depends on, as well as diagnosing of existing or future problems cannot be based on a limited quantity of measurements at a limited number of points, but only on mathematical modelling. Different cases of mathematical modelling of objects and processes directly or indirectly related to environment protection such as: control of typical processes in crude oil refining – optimal management of crude oil storage, mixture design, optimal control of atmospheric crude oil distillation, development of short-cut distillation column mathematical model applicable for on-line control and optimization (energy saving); assessment and control of air quality; dispersion of oil and petroleum products in water basins; dissipation of gas pollutants in the atmosphere in particular meteorological conditions; evaluation of air pollutant emissions in highly urbanized areas are described. Some case studies are also discussed.

## Plenary Session PL-03

# Biogas, Biodiesel and Carbon Dioxide for Reduction of Carbon Emissions

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**Abstract**

The world economy is based mainly on oil as an energy source and raw material for chemical products. The extensive use of fossil fuels formed and stored underground for millions of years has made impossible for the present vegetation on Earth to treat the emitted carbon dioxide by photosynthesis. It leads to huge emissions of carbon dioxide and greenhouse effect on the planet climate. The present paper illustrates the options for reduction of carbon dioxide emissions by the use of biomass as a source of energy. This approach enables to close the carbon cycle at the present state. Examples for biogas and biodiesel production associated with utilization of waste glycerol as secondary feedstock for organic syntheses are given. The option of carbon dioxide recycling to useful organic products for reduction of its emission is demonstrated. Those products are formic acid, methanol, as well as methane. Thus there are multiple positive effects on environment: waste treatment with energy production, closing the natural carbon cycle, and reduced use of fossil fuels.

## Plenary Session PL-04

# Decarbonizing the Circular Economy

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**Abstract**

Circular economy and industrial decarbonization are two strategies for meeting sustainability goals. However, there has been limited work that has investigated how these two concepts interact and complement each other. Circular economy strategies do not necessarily result in the reduction of greenhouse gas emissions, particularly when technologies that transform waste streams require more energy inputs. Similarly, greenhouse gas mitigation strategies do not necessarily improve material circularity, as evidenced by increased use of finite mineral resources for renewable energy technologies. Despite the potentially conflicting goals, there are technologies that allow for synergies between circular economy and decarbonization goals. Alkaline industrial waste, for example, can be used to sequester atmospheric $CO_2$ either as solid carbonate minerals or dissolved bicarbonate ions. Large scale implementation of such systems will require integrated models which can account for trade-offs, identify optimal pathways for waste stream utilization, and define conditions which will maximize both decarbonization and circularity potential. We consider here the case of decarbonizing the primary aluminum supply chain by utilizing red mud waste from alumina production to sequester carbon. This strategy concurrently contributes to both waste management and climate change mitigation.

## Plenary Session PL-05

# Environmental Footprint of Electric Vehicles and the Underemphasise Spatiotemporal Effect of Charging

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**Abstract**

Electrification is one of the effective solutions to reduce the environmental burden of the transportation sector. Studies have suggested that the increasing share of renewable energy could not keep up with the rise in energy consumption, leading to an increase in overall eco-cost or GHG emission from the power sector. This issue is relatively less severe in Europe, with a comparatively higher renewable energy share, less significant increment in energy demand, and a notable expansion of charging infrastructure despite inequalities that persist across countries. However, to ensure a sustainable proliferation of electric vehicles (EVs) in Europe, it is essential to further assess the power generation across different countries in Europe, including the hourly pattern and the potential for GHG minimisation to a greater extent through optimal charging management. The environmental sustainability of EV usage is not undisputable better than the other alternatives and with room for further improvement. Prior research has frequently used theoretical assumptions and has not adequately considered the spatial-temporal heterogeneity (charging location, timing) of the power generation in EV charging events. The environmental footprint of electric vehicles at different stages, including the user phase, are discussed in this lecture. The GHG saving that could be achieved by changing the charging behaviour, as well as delayed charging, smart charging and vehicle to x (x= grid, building or home) technology, are also suggested. The presentation has in view to facilitate the EVs implementation in reaching the full potential contribution to sustainability.

# Plenary Session PL-06

## Integrated $CO_2$ capture and utilisation for nanoparticles production

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**Abstract**

Solvent-based $CO_2$ capture is an efficient process with high potential for large-scale implementation for the mitigation of climate change due to fossil fuel use. Several challenges need ingenious solutions in order to make $CO_2$ capture energetically competitive, environmentally benign and address the key issue of $CO_2$ utilisation. This presentation aims to bring a holistic approach to the entire chain of process development, optimisation for improved performance, and implementation in pilot-scale level novel concepts for $CO_2$ capture and subsequent utilisation for the production of high-valued materials. Novel new solvents that exhibit a superior performance from the current state-of-the-art have been identified through a systematic and rigorous procedure based on computer-aided molecular design that enumerates and assesses millions of solvents and solvent blends. The resulting solvent blend exploits the thermodynamic behaviour of the mixture upon reaction with $CO_2$ associated with the formation of a second liquid phase so that both the energy requirements for the solvent regeneration are greatly reduced and the cyclic capacity of the solvent mixture is substantially increased compared to the best available conventional solvents. Sustainability properties of the solvent mixture are explicitly considered enabling a low environmental impact. The computationally identified solvent blends are tested in phase-equilibria experiments to verify the predicted thermodynamic behaviour for the range of conditions pertained in the $CO_2$ absorption process. Further improvements are possible through the process flowsheet optimisation for the novel solvents. To this end, detailed and accurate process models are employed in a modular fashion so that physical and chemical phenomena in the $CO_2$ absorption are accounted for and the necessary flowsheet flexibility is enabled. Process economics drive the process system to high competitive design solutions satisfying product quality, process, safety, and environmental specifications and constraints. A pilot-plant setting tests the operational performance of the novel solvent mixture and the functionality of the liquid phases separation equipment and operational policies determined by the model-based optimisation procedure. The estimation of the energetic savings in $CO_2$ capture in the pilot-scale unit verified the predicted values and further provided useful insights in process equipment construction and process implementation features. The captured pure $CO_2$ is subsequently utilised for the production of nanoparticles of inorganic salts. In particular, a dilute solution of either calcium or magnesium hydroxide is contacted with the $CO_2$ stream in a rotating packed bed unit. The liquid stream enters the rotating disk through its center with the aid of a distributor and is accelerated radially by the high rotational speed of the disk. Simultaneously, $CO_2$ gas penetrates the disk from the outer diameter and flows counter-currently to the liquid. The reaction of $CO_2$ with the suspended particles generates particles organic salts with a large percentage of them with diameters in the nano-scale level. The process concept is tested on a pilot-scale unit under various operating

conditions, where electronic microscopy verified the production of high quality nanoparticles. In conclusion, a holistic approach to high performance solvent-based $CO_2$ capture and utilisations is proposed with innovative solvents, flowsheet configurations and equipment verified in pilot-scale experiments. The investigation sets the ground for an industrial-scale employment of the developed technology.

# SESSION

# CONCEPTUAL DEVELOPMENT AND MODELLING

# CDM-01

## A New Approach to Modeling and Simulation of Industrial Processes

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**Abstract**

This paper presents a theoretical analysis of methods for modeling of the industrial processes kinetics. The main problems in the industry are the optimal design of new devices and the optimal control of active processes, i.e., minimization of the investment and operating costs. These problems are solved by modeling methods. Thermodynamic, hydrodynamic, and Boltzmann approximations for a mathematical description of the kinetics of industrial processes are described. A new approach to modeling of industrial processes with unknown mechanism is presented. The kinetics of processes with an unknown mechanism, typical example of this are the complex chemical reactions, can be modeled on the basis of an axiom. The axiom "A mathematical structure of real (industrial) process does not depend on the measuring system of the quantities involved in them" is used for the formulation of the theorem "A mathematical structure of a quantitative description of real systems can be presented as a power function complex".

# CDM-02

# Integrating Hydrogen to the Local Energy Systems: a Case Study of an Island

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**Abstract**

Hydrogen energy is a promising energy carrier that has been developed by many countries in recent years. Some renewable energy sources can be transferred to hydrogen for use, transportation, and storage. The problem of integrating hydrogen in the existing local energy systems has been focused. This paper studies the planning of integrating hydrogen energy in the local energy system on an island. The power and heating demand of various processes should be satisfied, and the energy storage plan is proposed. This is done by proposing a mathematical programming model to find the optimal solution. The performance of the original energy system and the new energy system with hydrogen are compared. The integration plan for hydrogen energy under different scenarios are studied. An illustrative case was studied to show how is the economic and environmental benefits can be achieved by integrating hydrogen in the energy system.

# CDM-03

# Convective Type Models of Industrial Processes in Column Apparatuses. 1. Chemical Reactions

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**Abstract**

A new approach for the chemical processes modeling and simulation in column apparatuses is presented in industrial column apparatuses. This approach is based on the physical approximations of the mechanics of continua, where the mathematical point (in the phase volume or on the surface between the phases) is equivalent to a small (elementary) physical volume, which is sufficiently small with respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes in the medium. A hydrodynamic model is used, where the velocity components are equal to zero on the column wall. As a result, the effect of the column wall on the volume mass transfer is obtained. The use of experimental data, for the average concentration at the column end, for a concrete process and column, permits to be obtained the model parameters, related with the velocity distribution in the column volume. These parameter values permit to be used the average-concentration model for modeling of chemical processes with different reaction rates.

***Acknowledgement:*** *This work has received funding from the National Research Fund project No KP-06-N 37/11/06.12.2019 "Integrated absorption-adsorption process for waste free decontamination of gases from sulfur dioxide".*

# CDM-04

# Modeling, Estimation and Methods for Reducing Large-Scale Liquid Phase Maldistribution in Columns with Open-Structure Packings

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**Abstract**

This study is a summary of the theoretical model research and the results obtained under Activities 1.2 ÷ 1.4 of the project "Sustainable processes, sustainable systems, sustainable environment", contract with BNSF № DN 07-14/15.12.2016, which ended at the end of 2020. The possibilities of the dispersion model for the modeling of the radial distribution of the liquid phase after a layer of packing with open structure in a packed column are presented. The parameters of the model are analyzed and new methods for their determination in different situations are proposed, depending on the available experimental data and the conditions under which they are obtained. The estimation of the non-uniformity of the liquid phase is quantified by the integral characteristic - the maldistribution factor. The problem areas (with large-scale maldistribution of liquid phase) in a pilot column installation (own data) have been identified, which are the reason for reducing the efficiency of the processes in it: the irrigation device (above the packing layer) and the collecting device (below the packing layer). Structural changes have been proposed in their design, which significantly reduces the maldistribution effects in the installation. A theoretical methodology for determining the optimal geometric configurations of these devices in the problem areas is proposed. The verifications of the model and of the methods for identification of its parameters, as well as the verification of the methodology for optimal geometric configuration of the collecting devices were performed successfully with own and other literature data in columns of semi-industrial and industrial size (0.47m, 0.6 m and 1.2 m) and random open structure packings (RSRM 0.7, 1.5 and 3 ′ ′, 25 mm metal Pall rings (Yin, 1999); RMSR 70-5 and Raflux rings 50-5) (Hanusch et al., 2018, 2019).

# CDM-05

# Design and Fabrication of a Bubble-Cap Tray for an Absorption-Adsorption Column Using CFD and Additive Technologies

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**Abstract**

Modern design and manufacturing capabilities make it possible to shorten the time, resources and effort to develop, make and test new materials, devices and goods from different areas of consumption. Streamlining the development and manufacturing process of a specific part, by optimizing it with computer technology and digital skills, cuts the cost of making it and also reduces its carbon footprint. The present work offers an approach for the research design of a bubble-cap-tray absorption-adsorption column. The hydrodynamic characteristics of the tray were preliminarily tested in relation to its geometrical dimensions. The study was performed using a computational fluid dynamics (CFD) simulation software. After selecting the tray's appropriate parameters, a digital model of the object was made and processed to be handed to a three-dimensional printer for further production. Using the free form fabrication additive technology with three-dimensional printer, the necessary bubble-cap tray was made. The successful implementation of modern technologies allows scientific teams to work efficiently, qualitatively and in a more time-efficient workflow.

***Acknowledgement:*** *This work is supported by the National Science Fund under Contract KP-06-N37/11/ 06.12.2019*

# CDM-06

# Plastic Waste Supply Chain Optimisation with Data-Driven Approach

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**Abstract**

The worldwide plastic waste accumulation has posed irreversible harm to the environment. Resources quality is the main driving force for resources recycling development. The main dilemma of the issue is: How to define the waste quality grading system to maximise plastic recyclability? This work reports a machine learning approach in evaluating the recyclability of plastic waste by categorising the quality trends of the contained polymers with auxiliary materials. The results could reveal the hierarchical resource quality grades predictors that restrict the mapping of the waste sources to the demands. This provides physical insights into the recycling potential of plastic waste. As the quality categories have been defined for plastic waste, a proper regional resource allocation network can be synthesised within each quality cluster. The trade-off between energy requirements for the recycling or treatment technologies and the waste recycling rate can be explored while setting different objectives such as cost, environmental footprint and waste discharge.

***Acknowledgement:*** *The research was supported by the GACR (Grant Agency of the Czech Republic) under No. 21-45726L and from the Slovenian Research Agency for project No. J7-3149.*

# CDM-07

# Predictive and Optimization Modelling for Operational Strategy of Renewable Energy Sources and Heat Storage in a District Heating Substation

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**Abstract**

To fulfil decarbonisation policy commitments, the heating sector needs new and efficient solutions that foster the growth of renewable energy ratio in heat production share. Smooth integration with current infrastructure is essential to ease the energy transition of heat suppliers, making it more attainable and in line with strategies for climate change mitigation. Seasonal variations in district heating network conditions, an intermittent character of some renewable heat sources and limited obtainable urban areas pose a challenge to the reliable deployment of renewable heat sources. Distributed heat production from renewable energy sources coupled with efficient heat storage systems in district heating substations could be an attractive solution due to lower required operational temperatures onsite. In this study, in order to formulate an efficient operational strategy for substations, algorithms for obtaining the day-ahead demand and renewable energy production forecasts have been deployed. Moreover, a steady state mathematical model of a substation has been created. Additionally, based on predicted values and a developed substation model, an optimization algorithm has been implemented to find near-optimal heat storage control strategy within a 24-hour horizon. Lastly, analysis results have been evaluated to gain quantitative insight on implemented control strategy scenarios.

# CDM-08

# A Multi-Objective Approach Toward Improving Energy Efficiency of Biodiesel Supply Chain Using Dairy Waste Scum as a Feedstock

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**Abstract**

The gradual depletion of natural resources and the complex economic and political situations in different parts of the world pose global challenges to the scientific community in improving energy efficiency and sustainability. This provokes the work in two main directions - search for alternative energy sources and development of approaches for optimal use of energy resources. High production costs are one of the main difficulties hindering the economic feasibility of alternative energy sources. However, liquid biofuels provide one of the few opportunities to replace fossil fuels in the short and medium term. They are recommended by the European Union as a transport fuel, as they are able to reduce energy dependence, emissions of $CO_2$ and other harmful substances in the atmosphere, contributing to global warming. Biodiesel, as an environmentally friendly fuel obtained from a practically inexhaustible raw material (biomass), can be considered as an analogue of traditional energy carriers. The quality indicators of biodiesel are measurable with those of mineral diesel, which makes it suitable for stand-alone use or as an additive to conventional diesel fuel. Biodiesel can be obtained from various sources such as waste oil, vegetable oil, animal fats, dairy waste and others. The focus in this work is on the development of a multi-objective approach toward Improving energy efficiency of biodiesel supply Chain using Dairy Waste Scum as a feedstock. The developed toolbox is formulated in the terms of a mixed integer linear programming. The purpose of the mathematical model shown in the article is multiplied to minimize the total annual costs including the total annual capital costs, the annual operating costs, the annual government incentives and the $CO_2$ emission costs. The optimization criterion is defined in terms of economic sustainability, and environmental assessment data are implemented as part of it. As a result of the application of the multi-objective approach optimal operating conditions of the considered supply chain, which includes: dairy farms portfolios, dairy plants portfolios, production capacity and location of biorefineries that should be built, performance of biorefineries and transportation routes are obtained. The proposed approach is implemented on a real case study from Bulgaria. The results of the toolbox implementation may be used as a tool for decision-making.

***Acknowledgement:*** *This study was carried out with the financial support of National Science Fund, Ministry of Education and Science of the Republic of Bulgaria, Contract No. КП-06-Н37/5/06.12.19.*

# CDM-09

# CFD Modelling and Simulation of Liquid Distribution in Packed Columns

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**Abstract**

The efficiency of separation processes like absorption and distillation in packed columns depends strongly on regular distribution of the phases. The present study aims at investigation of the liquid phase distribution in order to fill in the missing data on liquid spreading in modern packings and to offer a reliable model for prediction of the liquid distribution using the tools of the Computational fluid dynamics (CFD). The CFD is chosen as a modern well-proven tool for predicting gas and liquid distribution in packings. Despite of the great number of solutions in literature, a new approach and model assumptions are needed for describing the liquid spreading in web-like, open-structure random packing types. The attempt of employing CFD for the packings under consideration has faced difficulties on one side due to the packing geometry and on the other, connected with the poor radial distribution properties of these packings leading to radial maldistribution of the liquid phase especially in industrial scale. The suggested CFD model is demonstrated for simulation of liquid spreading from a point source. Experimental data are used for model validation. The experiment has employed a liquid collecting method with a multisectional liquid collector under the packing layer. The model is intended for further development and application for regular initial distribution of the liquid in modern random and structured packings.

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# CDM-10

# Cleaner and Faster Chemometrics for Determination of Ingredients in Biscuit Doughs from Near Infrared Spectroscopy (Nirs) Spectra Based on Pls and Variable Selection Methods

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**Abstract**

The use of Process Analytical Technology (PAT) has been a tested concept in the industry for many years. The non-invasive identification of ingredients in food industry using PAT and chemometrics is used to evaluate and ensure food quality control. On-line monitoring systems for dough mixing process and extended applications has a crucial importance in laboratory or industrial conditions. The changes in dough properties during mixing come from chemical modifications that can be assessed through spectroscopic investigations. The use of NIRS to provide quantitative or qualitative measurements on dough, biscuit doughs or even proprietary mixes is not new, and its prevalence in the industry is a consequence of the technique's very fast measurement times that simultaneously deliver critical sample properties like moisture, sucrose, fat and flour. The main advantages of NIR was to monitor the mixing process directly with a fiber optic probe. In the present study was investigated the ability of the FT-NIR spectroscopy method to monitor the real biscuit doughs mixing process over the whole NIR wavelength range (1100–2500 nm). The main objective was to compare effect of variable selection algorithms on Partial Least-Squares (PLS) model performance for predicting fat, sucrose, flour and moisture from NIR reflectance spectra. Variable selection was important step in chemometrics for providing right candidate wavelengths for every component and to reduce the model complexity and risks of overfitting. It was compared two single points and two interval methods for variable selection to find the most informative spectral bands. This is motivated by the fact that functional groups absorb within relatively short wavelength bands. The selection of wavelength intervals instead of single spectral points makes more sense and should lead to more stable predictions. The performance of four variable selection approaches: successive projection algorithm (SPA), competitive adaptive reweighted sampling (CARS), interval PLS (iPLS) and interval variable iterative space shrinkage approach (iVISSA) was shown. The obtained results are compared and discussed.

# CDM-11

# The Use of Numerical Simulation in Modern Crop Production in Kazakhstan

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**Abstract**

The results of modeling the process of growth and development of barley in various soil and climatic conditions of Kazakhstan based on the processing and interpretation of data from satellite images of the Earth. To obtain information about NDVI, algorithms for processing satellite data obtained using the Leaflet API and the Sentinelhub API were used. Normalized NDVI values for a calendar week were obtained, calculated as averages over 5 years of observations. We considered seven-day (weekly) values of the NDVI index (cloudless composites Sentinel-2, Landsat 8) for a calendar year, calculated using an arable land mask. In total, 10 time series of normalized indicators were formed corresponding to 2017-2021. The maximum value of NDVI was reached on the 25th-30th calendar week, which corresponds to the end of July - the beginning of August. The determination of the maximum NDVI for early forecasting of yields was carried out by searching for the parameters of the approximating non-linear function corresponding to the distribution of the normalized NDVI values of past years. The calculations were carried out in the Python programming environment using additional scientific packages matplotlib, pandas, numpy. To calculate the yield, the annual values of the gross harvest of barley and harvested crop areas were used. In the case of heterogeneity of the time series, the initial data were filtered by statistical methods.

# CDM-12

# Thermodynamic Optimisation of Rankine Cycle System by Comparing Different Working Fluids and Integrating Different Renewable and Waste Heat Sources

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**Abstract**

The utilisation of renewable and alternative energy sources has attracted considerable interest due to fossil energy shortages, the depletion of fossil fuels, and global warming. The Rankine cycle has emerged as a promising heat recovery technology for converting thermal energy into useful work, as it can be applied to a variety of heat sources and a wide range of temperatures. Based on Rankine cycle technology, this study utilises multiple heat sources, including biomass, geothermal, solar and waste heat. In order to efficiently match the wide temperature, range of the heat sources, different working fluids are considered, for which a pre-selection is performed including thermodynamic, environmental and safety criteria. In addition to selecting the appropriate working fluids, the operating conditions of the Rankine cycle system are optimised to obtain maximum power output. To achieve the best exploitation of thermal energy contained in the heat sources while producing the highest power output, certain system configurations are investigated that include individual layout and cascade design.

# CDM-13

# Bi-Level Mixed Integer Linear Programming Model for Emissions Reduction Technology Selection

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**Abstract**

Governments can calibrate policy instruments to induce industry investment in clean technologies. The resulting interaction is a non-cooperative leader-follower game that can be formulated as a bi-level mathematical programming model. In this work, a novel bi-level mixed integer linear programming (MILP) model is developed for emissions reduction technology selection. The problem involves a set of technologies characterized by cost and emissions reduction performance. In the upper-level problem, the leader (government) seeks to minimize total social cost and controls the emissions limit as well as technology-specific subsidy rates. The leader's objective function includes the external cost of pollution and the actual cost of subsidies. In the lower-level problem, the follower (industry) seeks to minimize corporate costs and controls the choice of emissions reduction technologies. An economic penalty also needs to be paid if the emissions limit is exceeded. Government is seeking a Stackelberg strategy which induces industry decisions that are favorable to the general public. The model is demonstrated with a case study on greenhouse gas emissions reduction technologies and is solved using a fuzzy heuristic algorithm.

# CDM-14

# Optimization Models for Planning Plastics Recycling Networks

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**Abstract**

Plastic pollution is now recognized as a major environmental issue of global scope. The problem can be brought under control by using reverse logistics to recover economically valuable products from waste plastic under a Circular Economy (CE) framework. For example, incineration with energy recovery can be used to generate electricity, and thermochemical processes (gasification or pyrolysis) can be used to produce chemicals. Many of these technologies have commercial or near-commercial maturity level. However, contamination of waste plastic streams can hinder recycling efforts; even polymer cross-contamination in mixed waste plastic stream creates problems and often necessitates an additional sorting step at extra cost. In this work, Mathematical Programming (MP) models based on Process Integration (PI) are developed for planning Plastics Recycling Networks. The problem involves matching waste plastic sources with recycling facilities, while accounting for both quantity (flowrate) and quality (purity). Linear Programming (LP) and Mixed Integer LP (MILP) model variants are proposed and illustrated with a case study.

# CDM-15

## Integration of Renewable Fuels into Combined Heat and Power Plants

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**Abstract**

Combined Heat and Power (CHP) plants are significant for process industries to satisfy the varying demands of steam and power. However, most utility systems still use the fossil fuels and natural gas as the energy sources with the costs of a numerous climate and ecological problems. With the significant advances on renewable energy resources, it is crucial to introduce the renewable energy sources into the CHP system. This work will explore the Bioethanol, Biogas and Renewable Hydrogen as greener alternatives to natural gas for use in CHP plants with the considerations of availability, sustainability, blends perform of each of these fuels, and the implementation in CHP systems. Traditional CHP optimization for energy efficiency improvement has been developed greatly in recent decades. However, the integration of the renewable fuels into the CHP and the interaction between the utility systems and the production processes result in complex total site system modelling and optimization. This project will develop a holistic and integrated approach and use a case study to illustrate a systematic optimization method in a CHP design to reduce both the fossil fuels consumption and $CO_2$ emission.

# CDM-16

# Sustainable Design of Dairy Supply Chain Considering Uncertainties Regarding the Prices of Raw Materials and Products

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**Abstract**

Dairy production has a significant environmental impact related with wastewater and air pollution. In addition, it is a large consumer of water and energy. The most effective way to improve its sustainability is through analysis of the food-water-energy nexus, which can be done by optimizing all activities in the supply chain from the raw materials to the end user while meeting environmental, economic and social criteria. However, the presence of uncertainties regarding the main parameters of the supply chain would lead to problems related to the implementation of processes and the operating the system as a whole. To solve these problems an implementation of models for optimal design of dairy supply chains that take into account these uncertainties is needed. The present study proposes a mixed integer non-linear modeling (MINLP) approach to the optimal design of a sustainable supply chain for the production of two types of dairy products with a choice of technology, which includes models of economic and environmental impact as well as the dairy production. The latter take into account uncertainties regarding raw material and products prices. The approach is applied to a real case from Bulgaria, which includes suppliers of two types of milk, dairy plants for production of two types of dairy products and markets. The environmental impact is assessed in terms wastewater and $CO_2$ emissions related with the processes along the supply chain.

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# CDM-17

# Limits to Economic Restructuring as a Decarbonization Strategy: the Philippine Case

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**Abstract**

COP26 discussions in 2021 reiterated the need for nations to meet reductions in greenhouse gas (GHG) emissions committed as part of the Paris Agreement. Deep cuts leading to the ultimate goal of carbon neutrality can only be achieved through a portfolio of decarbonization strategies, including enhancing energy efficiency, increasing renewable energy penetration, and commercializing negative emissions technologies. Softer strategies such as economic restructuring can also be done at the national or regional scale, by predicating development on differentiated economic growth with a preference for low-intensity sectors. In this work, we develop a fuzzy linear programming input-output (FLP-IO) model to aid in planning such economic restructuring activities. We then apply this model to the case of the Philippines to identify the maximum GHG cuts that can be achieved with this strategy, and discuss the decarbonization policy implications of the model solution.

# CDM-18

# Using the Process Systems Approach (Mathematical Programming/optimization) for 'non-Process' Applications

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**Abstract**

The process systems approach based on mathematical programming (optimization) is well established in chemical engineering for process synthesis and optimization. It enables a systematic and comprehensive view of the entire plant or production network and the generation of optimal, feasible and integrated solutions. On the other hand, there are many socio-economic systems that are extremely important to society, but decision making is mostly done on individual segments without interrelationships. The lack of a holistic top-down view means that the management of such systems is not integrated, which does not lead to the best possible solutions. In this work, a systematic systems approach based on mixed integer linear mathematical programming (MILP) was used to model and optimize the food supply chain in Slovenia. The following steps were used: 1. collecting a plethora of available data on the object of study, 2. aggregating the data into an appropriate number of relevant groups, 3. obtaining and calculating factors for converting commodities into products, 4. preliminary calculations, sensitivity analyses, visualization, 5. modeling (optimization variables, mass balances, conversion equations), 6. definition of conditions and constraints resulting from European and national directives, 7. definition of objective functions, 8. definition of scenarios, 9. running the model for different scenarios and objective functions. The above approach was applied to food supply chain optimization. 11 scenarios were defined covering different assumptions, such as population growth, reduction of mineral fertilizer consumption, increase of organic production, change of eating habits towards a healthier diet, increase of locally produced food, etc. The results obtained represent the target values that can be achieved under the given assumptions. If the additional economic and political conditions were included in the model, the results would likely deteriorate. The model thus allows for policy decisions related to the promotion of certain production methods, food types, food waste management, etc. that benefit society. This approach can also be applied in other areas to optimize the portfolio of technologies and secondary raw materials produced from waste, such as municipal and industrial waste, sludge treatment, etc.

# CDM-19

# Deep pipe: Theory-guided LSTM based method for multi-product pipeline pressure monitoring after shutdown

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**Abstract**

The pressure changes dramatically during the shutdown process of the multi-product pipeline. When the pipeline pressure comes to decrease, it is often mistaken as pipeline leakage or other abnormal condition which increases the burden of operator on-site. At present, the method of pipeline shutdown pressure analysis is mainly based on numerical simulation which cannot monitor shutdown pressure in real-time. In this work, the time-series approximate ability of long short-term memory (LSTM) is taken advantage of to construct shutdown pressure prediction model. In order to overcome the drawback of this deep learning algorithm that is trained only by ample data, the scientific principle and theory are integrated into LSTM. Subsequently, the theory-guided long short-term memory (TG-LSTM) is proposed for pipeline shutdown pressure prediction. The proposed model is trained with available data and simultaneously guided by the theory (physical principle and engineering theory) of the underlying problem. In the training process, the data mismatch, as well as monotonicity constrains, and boundary constraints are coupled into loss function. After acquiring the parameters of the neural network, a TG-LSTM model is established which not only fits the data, but also follows the physical principle and the engineering theory. The proposed model is verified by three real-world multi-product pipelines. The results indicate that TG-LSTM achieves better accuracy than other prediction models, with MAPE being 0.246%, 0.186% and 0.143%, respectively. Finally, the sensitivity analysis of different hyper-parameter is conducted to illustrate the robustness of TG-LSTM in pipeline shutdown pressure prediction.

# CDM-20

# Deep pipe: A hybrid model for multi-product pipeline condition recognition based on process and data coupling

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**Abstract**

It is significant for field monitoring and management to identify the operating state of the pipeline and prevent an abnormal accident from occurring. Aiming at the few unsteady and abnormal conditions data samples, different condition switching duration, and strong time-space characteristics of multi-product pipeline condition recognition, a hybrid model for condition recognition based on process and data coupling is proposed. First, collecting the relevant parameters of the real multi-product pipeline system and using Stoner Pipeline Simulator (SPS) to establish a simulation model. Based on the simulation model, performing the simulation of unsteady conditions and abnormal conditions to obtain the corresponding simulated data. Second, the reliability of the simulation model is verified by calculating the distribution similarity between the simulated data and the real pipeline data. Third, the simulated data and real data are processed by variable-length series and input into the proposed hybrid model for training and verification. The results show that the proposed hybrid model has high accuracy, precision, recall, and F1 score of 93.1%, 93.1%, 87.2%, and 84.7%, respectively, which has essential guiding significance for monitoring and ensuring the safe and stable operation of multi-product pipelines.

# CDM-21

# Deep pipe: Theory-guided neural network method for predicting burst pressure of corroded Pipelines

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**Abstract**

Crude oil and natural gas are the primary energy sources, mainly transported by pipelines. Pipeline safety has to be seriously considered to ensure the continuous and stable transportation of these two types of energy sources. The burst pressure is an important indicator of pipeline safety. Accurate prediction of the burst pressure is of great significance to the design, construction, daily operation, and maintenance of the pipeline. This paper proposes a theory-guided neural network model-based method to predict burst pressure prediction of corroded pipelines, which can incorporate physical principles into the deep learning framework. First, higher-order features with physical meaning are constructed and coupled with the original features to form a new feature space. Then the traditional burst pressure prediction formula Pipeline Corrosion Criterion (PCORRC) is integrated into the model to make full use of the prior knowledge contained in the empirical formula. The designed loss function enables the network to have different weights for different samples and focuses on learning the PCORRC formula to predict samples with large deviations. Finally, the model was verified using a public dataset based on experiments and finite element simulations. The results show that the theory-guided neural network model proposed in this paper has the highest accuracy compared with other models. The correlation coefficient is 0.9945, the root mean square error is 0.562, and the mean absolute percentage error is 2.65%. Further tests have shown that the model is very robust and has good adaptability to different data. This work presented that integrating domain knowledge into the traditional neural network model can effectively improve the performance of burst pressure prediction of the corroded pipeline.

## SESSION

# TECHNOLOGICAL SOLUTIONS AND PROTOTYPING

# TSP-01

# Sustainable Industrial Ecology and Environmental Analysis: a Case of Melamine Etherified Resin Fibres

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**Abstract**

The growing global consumption of plastic and its related waste emissions are becoming a major threat to the environment, and current linear approaches to plastic management have shown to be insufficient. This paper utilizes the concept of industrial ecology to demonstrate a holistic evaluation of the entire life cycle of thermoset plastic materials, focusing on three key life cycle phases: i) sustainable production, ii) material recycling to obtain secondary products, and iii) end-of-life behaviour in natural environments. Industrial ecology concepts alongside Life Cycle Assessment (LCA) are applied to a case study of melamine etherified resin (MER) fibre, a high value-added product with numerous applications that is nevertheless difficult to recycle and could pose a threat to the environment if it is discharged at the end of its life cycle. The study firstly presents the potential to produce MER fibres exclusively from renewable or waste sources. Conversion of MER fibres into secondary products using hydrothermal processes are further investigated. Finally, impact assessment of discharging used MER fibre material into soil and water environments is carried out. All three life cycle phases are analysed in detail to capture the material's impact and close the loop on its manufacturing, recycling, and disposal phases.

# TSP-02

# An Overview of Hydrogen-Carbon Fuel Cells System for Simultaneous Production of fuels and Power

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**Abstract**

Although hydrogen fuel cells still receive the most attention, carbon fuel cells (CFC) are becoming increasingly attractive due to their even better performance, reaching efficiencies of up to 90 %. As opposed to most other fuel cell types, CFCs have distinct feed and product phases, allowing the fuel utilization to be almost 100 %. CFCs also takes advantage of the fact that carbon has a very high volumetric energy density of 19 kWhL−1, compared to 2.4 and 9.8 kWhL−1 for hydrogen and diesel, respectively. Another very important advantage when using CFC for electricity generation based on carbonaceous fuels is the fact that the $CO_2$ product phase is pure. This is of considerable importance for carbon capture and storage. In fossil fuel-based power plants on the other hand, up to 30 % of the electrical output is consumed for carbon sequestration. Finally, the entropy change and thus the reversible heat of the cell reaction is almost zero. This eliminates the need for cooling and heating in steady state operation. CFCs are characterized by operating temperatures between 500 and 1000 °C and fuel cell efficiencies ranging from 70 to 90 %. Recent research into CFCs has focused on identifying the prevalent reaction mechanisms for different types of cells, mostly focusing on H-CFCs and CE-CFCs, which are of interest because of their ability to harness the conduction of multiple ionic species, as well as generate additional three phase contact with the carbon fuel. Many studies have done routine tests on the effects of temperature, feed gas composition, and fuel type on the I-V curve characteristics and maximum power density. Regarding the types of carbon fuels tested, particular attention has been paid to different types of coals and biochar, both with and without different types of pre-treatment. This presentation provides an overview of this technology and challenges to make it commercilize.

# TSP-03

# Technology Roadmap for Production of Clean Energy Based on Plastic Waste Treatment Considering Life Cycle Assessment and Circular Economy for Medium Size City in Latin America

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**Abstract**

Bucaramanga is a city located in the Andean region with overall population of metropolitan area 1.2 million inhabitants, is a typical Latin-American city with problems related to plastic waste utilization and generation of clean energy. The increase in plastic waste due to the pandemic that comes from domestic, health, and sanatory activities has been a serious problem since 2019 [1]. It is necessary to control the impact of plastic [2] on the environment, to facilitate the design of waste treatment systems and the comparison of alternatives such as incineration, pyrolysis, gasification, and others. Studies have reported that a volume reduction of 80% to 95% can be achieved for waste generated using thermal conversion technologies [3]. It is possible that by implementing concepts of environmental footprints and LCA, in the decision-making process about the implementation of new technologies for treatment of plastic waste, it will allow to minimize environmental impacts and risks on human health, provided from plastic waste related to COVID-19, especially in developing countries such as Colombia. The main objective of this research is the development of a technology roadmap for production of clean energy based on plastic waste treatment considering Life Cycle Assessment and circular economy for a medium size city located in Colombia, Latin America.

# TSP-04

# Wollastonite Supported Praseodymium Oxide as an Efficient Catalyst for Transesterification

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**Abstract**

Praseodymium oxide ($Pr_6O_{11}$) heterogenized on wollastonite was investigated as a promising catalytic system ($Pr_6O_{11}/CaSiO_3$) for sunflower oil transesterification with methanol (biodiesel synthesis). For that purpose, instrumental techniques such as X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) were used for $Pr_6O_{11}/CaSiO_3$ characterization. In addition, some kinetic parameters (reaction rate constant, activation energy and pre-exponential factor) were evaluated via nonlinear least-squares method. XRD of the support revealed peaks related to two phases, wollastonite ($CaSiO_3$) and cristobalite ($SiO_2$). Registered cristobalite was due to the presence of free silica in the precursor ($Na_2SiO_3I_2SiO_2$) for the carrier synthesis. Analyzing the XRD profile of bulk $Pr_6O_{11}$, diffraction patterns assigned to $PrO_2$ and $Pr_2O_3$ were detected. It was found that the deposition of $Pr_6O_{11}$ of the support surface decreases the diffraction peaks of $CaSiO_3$ and $SiO_2$. On the other hand, dispersed $Pr_6O_{11}$ particles are noticed on the carrier surface. The phenomena were connected with a surface active phase-support interaction (SASI) in the form of Pr–O–Si, additionally confirmed by XPS. The following was observed: (i) a lower binding energy of $PrO_2$ in $Pr_6O_{11}/CaSiO_3$ compared to $PrO_2$ in $Pr_6O_{11}$, (ii) an increased $Pr_2O_3$ content after support modification and (iii) shift of Ca 2p and Si 2p components binding energy toward lower values due to Ca–O–Si bonds cleavage. A decreased surface atomic concentration (SAC) of Si is another conformation for the prominent contribution of Pr–O–Si bonds in SASI. The support surface covered by $Pr_6O_{11}$ particles was represented by SEM as well. It has been established that the support itself is not active in the reaction of biodiesel synthesis. However, the presence of surface $Pr_6O_{11}$ particles led to a biodiesel yield of 93.4% at 110°C. At lower temperatures biodiesel yield diminished, i.e. 73.4% at 100°C, 51.3% at 90°C and 30.3% at 80°C, due to a decreased kinetic energy of the reactants. The respective forward kinetic constants were as follows: $41.71 \times 10^{-2}$ l/mol.h (110°C), $24.19 \times 10^{-2}$ l/mol.h (100°C), $13.33 \times 10^{-2}$ l/mol.h (90°C) and $6.35 \times 10^{-2}$ l/mol.h (80°C). Based on these, the activation energy (59.6 kJ/mol) and pre-exponential factor (115.5 l/mol.h) for the reaction of sunflower oil transesterification with methanol were calculated.

# TSP-05

# Assessment of Biomass Combustion with Pig Manure Biogas from Covered Lagoons

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**Abstract**

Pig farm manure is a problem in some regions with a high porcine population, such as in Catalonia region (Spain). However, instead of considering pig manure as a problem to eliminate, circular economy considers the waste streams as a profitable and useful source of secondary raw materials. Many pig farms are generating the required heat using the combustion of biomass from nearby forests instead of using fossil fuels. Methane emissions with high global warming potential from open lagoons would decrease when these lagoons are covered to produce biogas useful for heating. Unfortunately, the question if the biogas production from pig manure is profitable is not clearly addressed in the literature and many farms doubt about its implementation. Liquid manure has a low amount of carbon and therefore its anaerobic digestion would produce a rather moderate amount of biogas (8-12 $m^3$ biogas/$m^3$ aqueous manure), unable to fulfil the required heat consumption. The present study is based on literature and a real farm data. The $CO_2$ emissions from the biomass transport and losses by diffusion through the membrane covering the lagoon are negligible. The amount of biogas generated is estimated to be insufficient for the energy consumption. The combustion of biogas together with biomass allows improving the biomass combustion and a decrease of the excess of air from 100% to 8.6% reduces greatly the heat losses from the exhaust gases. Therefore, not only the global warming effect is decreased but also the amount of biomass required decreases to 41%, providing economic savings. Even without considering any $CO_2$ tax, the payback period is around 6 years due to the combustion improvement. Therefore, the results show that covering the lagoons is not only beneficial for the environment but also from the economic point of view. Therefore, the covering of the open lagoons is encouraged by the results of this study.

# TSP-06

# Prerequisites for Reducing the Carbon Footprint in Crop Production on the Example of the Experience of Farmers in East Kazakhstan

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**Abstract**

Traditional agriculture is a source of a significant amount of greenhouse gases emitted in the course of crop and livestock production and contributes to global warming. The introduction of elements of "carbon" farming in modern agriculture with the simultaneous active use of GIS technologies and remote sensing methods creates real prerequisites for reducing the carbon footprint in crop production. A review of domestic and foreign literature showed that digital mapping methods are actively developing and represent a wide range of approaches and tools for studying the soil cover. The main agricultural crops that are cultivated in East Kazakhstan are: cereals and leguminous crops on an area of 600 thousand hectares, of which spring and winter wheat occupy about 400 thousand hectares, oilseeds (sunflower, rapeseed, soybeans) - 580 thousand hectares and under fodder crops - 250 thousand hectares. Experimental farm - Limited liability partnership "Experimental farm of oilseeds" is represented by small hills and steep slopes of hills, as well as small valleys with heights of 200-400 m above sea level. Arable land is represented by six soil varieties: mainly leached and ordinary chernozems, as well as medium-thick typical and heavy loamy chernozems. The thickness of the humus horizon is 50-80 cm, according to the mechanical composition - fine loamy soils with a humus content of 5-17%. It is known, that the content of organic carbon in the soil is about 10 times greater than in the atmosphere. Various sources indicate that organic farming, including no-till technologies for growing crops, “No till”, as well as earthworms, can compensate for an annual excess of carbon of 4 Gt/year. In this regard, it is very important to develop technologies that allow you to bind soil carbon, accumulate it, preventing it from escaping into the atmosphere. The paper presents the results of experiments on the preservation of stubble on the soil surface, as well as part of the straw in the form of mulch for soil-forming processes.

# TSP-07

# Use of Alternative Minerals for Optimization of Existing Processes for Thermal Conversion of Renewable Fuels

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**Abstract**

Fluidized bed combustion and gasification are becoming two of the preferred processes for thermal conversion of heterogeneous fuels such as biomass and waste for electricity and heat production, as well as for production of synthetic natural gas (SNG) and syngas. In fluidized bed conversion even distribution of heat and oxygen throughout the reactor is accomplished by inert solid particles entrained by a gas flow. As an inert material quartz sand has been the common choice because this sand is considered as environmentally and economically sound inert material. The introduction of alternative to coal fuels such as biomass and waste has put new demands to the existing processes such as: 1) the need for a secondary gas stream; 2) the necessity to exchange the used bed material; 3) the requirement for downstream gas cleaning. These demands have increased the cost for the process, as well as the downtime due to unplanned stops for service. In order to meet the challenges imposed by the use of alternative fuels, minerals such as bauxite, feldspar, olivine, and ilmenite have been tested as alternative to sand candidates for bed materials. The tests were performed in a semi-industrial university unit, as well as in laboratory conditions. It was shown that the materials outperform sand as they add properties that improve the process efficiency. For example, olivine and feldspar decrease the tar levels in the produced gas during gasification, while ilmenite decreases the need for secondary air and the occurrence of corrosion in combustion units. As the use of quartz is becoming an environmental concern due to its scarcity, these new materials can lead to an increased process efficiency and therewith economic viability of the process, thereby helping the transition to fossil free energy system. The present study represents a review over results obtained for the three materials with process comparisons to sand and material characterization (SEM/EDX, TEM) showing the mechanism behind the observed material activity. The presented result shows in practice how alternative materials can be used for process optimization within energy conversion.

## TSP-08

# Cradle-to-Cradle: Transforming Waste and Integrating it as the Core of a 3D Printed Membraneless Fuel Cell for Wastewater Remediation

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**Abstract**

The "Cradle-to-cradle" design is shaping up to be the next step in technological evolution. It aims at mimicking the metabolism and life cycle of living beings (so called "biomimetic approach") in that the wastes from the previous cycle become resources for the next. In accordance with this approach our team focuses on reclaiming an organic waste – the paper cores (tubes) of various household foils and by processing it the former waste becomes the lynchpin of an innovative membraneless fuel cell (FC) for wastewater remediation, tackling yet another problem of the currently employed technological approach – the generation of vast quantities of wastewaters, contaminated with a wide array of pollutants. The cornerstone of the design is the pyrolysis of the paper tube and turning it into electricity conducting material. The process is performed by applying a patented technology with simultaneous activation, yielding tubes with high porosity and additionally, by employing a relatively simple pretreatment various types of catalysts can be incorporated as well. Thus prepared, the circular carbonized tube is affixed in a specially designed and produced circular 3D printed fuel cell (with the inner section of the carbonized tube being the cathodic compartment and the outer – the anodic one) where the tube acts as both a membrane and an electrode. Due to the simplistic design and absence of delicate components (membrane) the constructed FC can be employed with a wide range of organic and inorganic (or both) contaminated aqueous solutions at different conditions. The design also allows the use of the fuel cell as microbial fuel cell (MFC). For this particular study sulfide-contaminated and nitrate-contaminated fluxes are remediated in the anodic and cathodic compartments, respectively. Additionally, experiments with organic pollutants (wastewaters from pulp and paper industry) are performed as well. Power output, oxidation/reduction of pollutants and a comparison between FC and MFC are presented. Based on the results obtained the viability of the constructed fuel cell are evaluated. Future work would involve the construction, experimentation and evaluation of a stack of fuel cells in order to increase the power output and the remediation parameters of the presented FC design.

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# TSP-09

## Using of Kelex 100 Metals Reactive Extraction. Mechanisms

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**Abstract**

Metals, being chemical elements, are present in many areas of human life. On Earth, they are most often found in the form of ores, from which pure metal is extracted by pyro- or hydro-metallurgical methods. A significant advantage of hydrometallurgy, and more specifically liquid-liquid extraction as part of it, is the possibility for metals to be separated. The reactive extraction is a reversible reaction between the metals cations or metal-containing anions in the aqueous phase and the extractant in the organic phase by means of forming a metal-extractant complex. It follows the re-extraction of the metal from the organic phase, the regeneration of the extractant, and the return into recycle. Extractants, according to their extracting ability to extract metals from acidic or alkaline media, are generally divided into cation exchange and anion exchange. With the advance of extraction technologies and the development of new extractants, there is already an intermediate group of extractants, called bifunctional, which extract equally well in acidic and alkaline media. An example in point is the commercial extractant Kelex 100. Under conditions conducive to the existence of a protonated form of the extractant, metal-containing anion complexes can be extracted from highly acidic aqueous solutions through an anion-exchange mechanism. Given the existence of the deprotonated form of the extractant, metal anions get extracted from a base, neutral, and slightly acidic water medium through a cation-exchange mechanism. The present work shows the anion-exchange and cation-exchange mechanisms of the extraction process of metals with Kelex 100 as bifunctional extractants from both acidic and alkaline media.

# TSP-10

# Novel Process for Aqueous Mea-$CO_2$ Hydrogenation to Methanol Using Reactive Distillation

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**Abstract**

Circular economy makes the maximum use of any atom before being discarded as waste. Waste streams are considered a source of secondary raw materials instead of being considered a problem to be eliminated. $CO_2$ released in exhaust gases is harmful for the environment due to its effect on nowadays climate emergency, but also is the raw material for the photosynthesis in the nature. Hence, the $CO_2$ reaction with hydrogen produced in excess by renewable energies leads to more valuable chemical products such as methane, methanol and formic acid or its derivatives. Intensive research is devoted to identify economically and ecologically viable routes for its exploitation. $CO_2$ capture is industrially performed by chemical absorption with aqueous MEA at 30 % wt. Nowadays, an energy consuming distillation recovers pure $CO_2$ and its hydrogenation to methanol is performed in a tubular catalytic reactor at 60 bar. Another distillation column is required to collect pure methanol product. The aim of the present study is the proposal of a novel process scheme: the $CO_2$ absorbed in MEA is fed to a 30-bar reactive distillation column where is hydrogenated to methanol. The MEA-absorbed $CO_2$ flows downwards the reactive column, and the hydrogen flows upwards achieving an effective counter current flow of reactants. ENRTL-HG thermodynamic model is used to determine the chemical equilibrium in each distillation stage, minimizing the Gibbs free energy; for the vapor phase the Redlich-Kwong equation of state is assumed. Aqueous MEA at 30 % wt useful for $CO_2$ capture is recovered at the column distillation bottoms. A partial condenser at the distillate generates a hydrogen stream which is recycled to the $H_2$ feed stream and an aqueous methanol stream that is further purified in a second distillation column that separates both reaction products: methanol and water. Further experimental research is required to determine the reaction kinetics and optimize the process. The proposed novel process scheme is proved feasible and provides novel opportunities to make the $CO_2$ hydrogenation to methanol more competitive and environmentally friendly.

# TSP-11

# Chemical Engineering Ni-63 Radionuclide Recovery of Spent Radioactive Sources

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**Abstract**

This paper highlights the chemical engineering of recovery from spent radioactive sources of radioactive elements such as Ni-63, and possible further applications of this radioactive recovered material. In the course of this work, the relationship between the ion flux density and the chemical activity of the deposited radionuclide in the production of radionuclide products was identified and demonstrated. As a consequence, the main focus of the research is on the practice developing of technology layer-by-layer elution of nickel covers from surface of radioisotope sources to obtain a reduced radionuclide preparation of nickel with the highest of possible specific activity. The revealed dependences of the material extraction rate on time in different chemical compositions of solvent mixtures and under different process conditions allowed to achieve high degrees of radionuclide extraction from spent radioisotope sources and to reduce the amount of radioactive waste generated multiple times.

# TSP-12

# Greene Approach for Synthesis and Application of Cost-Effective and Easy-to-Use Electrochemical Materials for Hydrogen Production from Seawater

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**Abstract**

In the present study microwave-assisted synthesis has been applied to the preparation of nanocomposites from natural zeolite and cellulose phosphate and alkali cellulose phosphate. Microwave irradiation conditions, such as irradiation power and time, required to optimize the synthesis of zeolite electrochemical materials were studied. This greener approach will open further research directions for the synthesis and application of cost-effective and easy-to-use electrochemical materials for hydrogen production from seawater based on natural zeolite impregnated with Cellulose phosphate and mercerized Cellulose phosphate by microwave-assisted synthesis. The growing interest in the use of zeolite modified electrodes results from the specific framework structure, containing the three-dimensional system of cages, channels with various shapes, sizes, and topologies. Their molecular sieve properties, as well as the ability to undergo the ion-exchange process with transition metals, result in their catalytic property. Cellulose-based materials also show interesting electrochemical properties and will be interesting to study their application of it for hydrogen production. The electrolytic model solution content 1 M KOH and 18 g.l-1 NaCl. The electrocatalysts were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and Brunauer-Emmett-Teller (BET). The electrodes are studied electrochemically by means of cyclic voltammetry, galvanostatic measurements, and Tafel slopes. The electrodes are designed and optimized in terms of the amount of catalyst. Acknowledgments: The authors thank the INFRAMAT project (part of the Bulgarian National Roadmap for Research Infrastructures, supported by the Bulgarian Ministry of Education and Science) for the research equipment that was used in this investigation.

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# TSP-13

# Effect of Direct Chemical Modification on the Surface Characteristics of Waste Egg Shells

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**Abstract**

Most of the reagents used for the treatment of waste egg shells reported are expensive, dangerous and require the application of relatively complex modification methods. Therefore, the aim of the present paper is to consider the possibility of using a simple economical method for efficient surface treatment of waste egg shells with suitable modifying reagents. Egg shell powders were subjected to a chemical surface modification by the direct method. The effect of chemical treatment on the surface characteristics of waste egg shells was studied. Standard Brunauer-Emmett-Teller (BET) method was employed to study porous characteristics of unmodified and modified egg shells, including pore size, pore distribution and specific surface area. The chemical structure of waste egg shells before and after treatment was characterized by Fourier Transform Infrared (FT-IR) analysis and compared to that of commercial calcium carbonate $CaCO_3$.

# TSP-14

# Are Greenhouse Gases Promising Feedstocks for Sustainable Chemical Industry?

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**Abstract**

As of 2022, fossil resources are still the main pillar of our global energy system, and common feedstocks for chemical synthesis of industrial and consumer products. The utilisation of non-renewable resources increases the concentration of greenhouse gases (GHG) in the atmosphere, contributing to anthropogenic global warming and air pollution. Being the products of combustion ($CO_2$, $SO_2$, $NO_x$) or organics decay ($CH_4$), GHG can technically be feedstocks to synthesise fuels and valuable materials, including bulk and commodity chemicals. Capturing and using GHG as alternative chemical materials offers a two-fold benefit where GHG emission could be mitigated and limit fossil resource depletion through resource recovery. Chemical synthesis GHG-based could play a part towards a circular economy. However, in some cases, this may be not entirely beneficial, and sustainability has to be assessed. GHG transformation into value-added products poses a great challenge, both technically, economically and environmentally. It is related to converting thermodynamically stable and kinetically inert GHG molecules to useful chemicals. These conversion processes require a large amount of energy and often use expensive reagents like hydrogen or costly and toxic catalysts. In this study, an overview is conducted, assessing various approaches that use GHG as the feedstock or precursor in chemical production. The advanced GHG conversion based technologies for chemical synthesis are compared to the conventional synthesis methods in the chemical industry. The ranges of energy requirements, material consumption and environmental footprint rates are summarised. Based on the results, the suitability of captured GHGs as feedstocks is evaluated, using as a criterion the potential to reduce the environmental footprints.

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# SESSION

# PRACTICAL IMPLEMENTATIONS AND MANAGEMENT

# PIM-01

# Presentation of a New Technology for Incineration of Municipal Solid Waste (MSW)

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**Abstract**

This article presents a technology for the incineration of MSW, the purpose of which is to avoid some problems and issues in the currently existing and applied technologies. The technical tasks meant to be solved by us are in the following directions: 1. To design a technology for the implementation of a plant for the incineration of MSW applicable for the generation of a small amount of domestic waste, namely - from 50 to 100 tons per day; 2. Maximum /almost complete/ energy recovery, namely – the generated heat to be supplied to the district heating network, and the electricity – to the electricity grid; 3. Residual ash after the incineration process may be used as a filler in concrete mixtures and as a base layer in road construction; 4. To reach high environmental standards.

# PIM-02

# Theoretical approach for integrated absorption-adsorption method for waste free decontamination of gases from $SO_2$ in a bubble tray column

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**Abstract**

In the paper a theoretical approach for integrated absorption-adsorption method for waste free decontamination of gases from $SO_2$ in a bubble tray column is presented. A new method for waste gas purification is realized in two steps: physical absorption of $SO_2$ with water and chemical adsorption of $HSO_3$ - from the water solution by synthetic anionite particles. The idea is to integrate those two steps in one absorption – adsorption apparatus - a bubble tray column. The adsorbent regeneration is made with $NH_4OH$ solution. The obtained $(NH_4)_2SO_3$ ($NH_4HSO_3$) is used (after reaction with $HNO_3$) for production of concentrated $SO_2$ (gas) and $NH_4NO_3$ (solution). Convection - diffusion and average concentration models of the absorption and adsorption processes are presented.

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# PIM-03

# Assessment of microbiologically influenced corrosion of structural metals by electrochemical methods

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**Abstract**

Microbiologically influenced corrosion (MIC) is a specific type of corrosion of metals and other materials resulting from the metabolic activity of microorganisms. The mechanisms of MIC are dependent both on the type of metals or alloys and the environments that can support the growth of microorganisms and formation of biofilms on their surface. It has been reported that MIC accounts for about 20% of the total cost of corrosion. In this study, we developed and tested a methodology for evaluation the contribution of MIC based on a set of electrochemical methods. Compounds of stainless steel, mild steel and copper were exposed to real wastewater inoculated with activated sludge from municipality Waste Water Treatment Plant. Identical samples of the three test materials were also exposed to the same wastewater, which was pre-autoclaved to eliminate the influence of microorganisms. Periodically, the corrosion behavior of all tested samples was explored by polarization resistance method, linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS) and the values of corrosion potential, polarization resistance and corrosion rate were evaluated. The corrosion tests with each material were performed for over a month. The comparison of results obtained in abiotic and biotic conditions shows different trends in the corrosion behavior of each material. Further analysis based on microbiological, biochemical and surface analytical methods are in a progress.

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# PIM-04

# Convectional Extraction of Phenolic Compounds from Red Fruits – Aronia and Elderberry

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**Abstract**

The red fruits are a source of many bioactive compounds with a wide spectrum of health-promoting properties. They are a good source of protein, free and conjugated forms of amino acids, unsaturated fatty acids, fibre fractions, vitamins, antioxidants and minerals. The aim of this study was to compare the quality, phenolic content and antioxidant capacity of Aronia and Elderberry plants. Characterisation of phenolic compounds was carried out by using spectroscopic methods (Folin–Ciocalteau method). Antioxidant activity of Aronia and Elderberry products were determined using 2,2-diphenyl-2-picrylhydrazyl (DPPH). All analyses were performed spectrophotometrically. All extraction runs were carried out at constant extractive parameters chosen previously - temperature, sample particle size, extraction manner. This study focuses on the convectional extraction of pre-dried Aronia and Elderberry. An investigation of total polyphenol contents (TPC) and total antioxidant capacity (TAC) was done. Extraction takes place at a pre-selected duration of 100 minutes. The effect of the solid-to-liquid ratio was examined with 2 solvents: ethanol solution (20%; 50%; 80% and 96%) and distilled water. The temperature was kept constant at 40 °C. The results showed higher total polyphenol content in Aronia compared to the Elderberry extracts. We established a correlation between antioxidant activity and total polyphenol content. Our results show that the highest concentrations for polyphenols and antioxidants were found in the case of extraction performed with 50% water solution of ethyl alcohol. It is also observed that ground fruits give better results. This study provided new data on the biological effects of red fruits. Our results have shown high antioxidant potential and opportunities for prerequisites for application in the pharmaceutical, cosmetics and food industries.

***Acknowledgements:*** *The investigations a partially financed by grant 12079 of the Research division of the University of Chemical technology and Metallurgy.*

# PIM-05

# The Electric System Cascade Analysis Method for the Optimal Design of Small Isolated Power Systems

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**Abstract**

Solar energy and wind energy are the two most viable renewable energy resources at the time. They are becoming very popular as renewable energy technologies are advancing. Therefore, it may be advantageous to consider both sources as a simultaneous option when designing an electrical supply system in remote sites. This paper's purpose is to present the new method to design and to minimize the system components, based on the Electric System Cascade Analysis and the Power Pinch Analysis. The algorithm takes the wind speed, solar irradiation, as well as data for the generations and storage facilities as inputs. Modified Electric System Cascade Analysis (MESCA) efficiency and the new results are demonstrated using a case study with two types of daily electrical energy demand. The goal of this study is to minimize the loss of power supply probability (LPSP), with the minimum of the used storage units and the annual cost of the system. As a result, the daily energy consumptions of the system are 33.9 kWh for DC load and 34.22 kWh for AC load, the optimal configuration is three wind turbines and 6 PVPs.

# PIM-06

# Exergy Assessment on the Circular Economy Processes of Pha Production from Municipal Organic Wastes Through Acidogenic Fermentation

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**Abstract**

Since the discovery of petrochemical subproducts, conventional plastics have been widely used in almost everywhere. This situation causes highly dependent on them due to their extensive usages. At the meantime, their average short lifetime accelerates the amount of waste generated. When conventional plastics are disposed, the environmental issues created have raised human´s awareness. Solutions have been proposed and among them, the replacement of biodegradable plastics could be the future. Recently, focus of studies has been put on the production of polyhydroxyalkanoates (PHA) as its central benefit of high biodegradability. However, the current trend of these so-called environmental green products, still having some imperfections especially in the PHA extraction methods. Existing studies regarding this step have shown some competitive results, instead of using dichloromethane/chloroform, carbonated based solvents such as dimethyl carbonate and propylene carbonated have been used. Moreover, a combination of bead milling and surfactant method seems to have promising results in terms of yield and purity of biopolymers. When it comes to optimization, Exergy footprint assessment acts as a unifying measurement to obtain some initial solutions. This assessment has been applied as footprint indicator in various industrial sectors. However, only few literatures are based on circular processes. In this study, the aim is to perform Exergy assessment on the circular economy process of PHA production using municipal organic wastes as feedstock. At the same time, a recent developed procedures of Exergy which based on a chemical recycling process, are applied to evaluate the entire process chain of PHA synthesis through acidogenic fermentation. Since there are many PHA extraction methods, several cases study are presented taking into account the existing research as data sources for the Exergy assets and liabilities calculation. The results of Exergy assessment provide an overall view of the circular processes of PHA and address some social aspects such as sustainability, feasibility, energy policy and ecology.

# PIM-07

# Capacity of Microalgae as a Supplement for Improved Bioactive Substances Production by Lactobacilli

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**Abstract**

Microalgae are available and renewable crop of rising biotechnological importance. Besides the fact that they are green factories for bioactive compounds with nutritional and pharmacological value, they have demonstrated its capacity to be used as supplements for lactobacilli for the production of lactic acid, as well. Reports show that they are a potential prebiotic for human colonic microbiota. In this respect, employed as a substrate, microalgae provide an alternative of the dairy products consumption, on the background of lactose and cholesterol intolerance, and the uncontrolled antibiotics intake. Moreover, the data show that there are cases of symbiotic action between lactobacilli and microalgae, as the latter act as enzyme enhancers. The beneficial properties of the two types of organisms would contribute a lot for improving the nutritional value of food and boosting the immune system at the same time. In addition, they are safe, widely available and relatively easy to grow.

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# PIM-08

## Potential Organic Extractants for Butyric Acid Separation

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**Abstract**

Organic acids have a variety of applications in the industry today. Some of them are obtained by bioprocessing of natural products instead of the general way from synthetic sources. Butyric acid can be produced via fermentation. For acid separation from fermentation broth liquid-liquid extraction could be applied. Thus, effective extractants are needed. In this study pure dodecane, 2 % v/v trioctylamine, 2 % v/v decanol in dodecane, 5 % v/v tributyl phosphate in dodecane and kerosene were investigated as potential organic solvents. Simultaneous extraction and stripping of butyric acid was successfully carried out in a three-liquid-phase rotating disc contactor. The four investigated organic extractants proved to be suitable for butyric acid separation. From the results obtained the following could be concluded: the highest rate of transport was achieved when 5 % v/v tributyl phosphate in dodecane was used, while the system with 2 % v/v trioctylamine 2 % v/v decanol in dodecane attained the most stable overall transfer process.

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# PIM-09

## Application of Biotechnology in Industry. Part 1

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**Abstract**

Biological methods are the best option compared to other methods, because are eco-friendlier and require low expenditures. Classical methods are useful but new methods are more effectively. Parts of new methods are: algal and enzymatic treatment; microbial fuel cell; immobilization techniques; nanoparticles in bioremediation; membrane bioreactor etc. Biological methods are applied extensively in some industries. Parts of them are: removal of pesticides, pharmaceutical industry, petroleum refinery, textile industry, alcohol distillery; olive removal; heavy metal removal, cyanide removal, mining industry and phosphorus removal. Biological treatment is divided into aerobic, anaerobic and anoxic treatments. Among pesticides, the dichlorinated pesticides are known to be digested by aerobic treatment. Pressurized activated sludge is a highly efficient treatment technique that does not demand large land area, it is less costly and more environmentally friendly when compared to chlorination. The pharmaceutical wastewater of different organic loads i.e. high (HSW) and low strength wastewater (LSW) were collected from the bulk pharmaceutical industry and subjected to different applications of Fenton's treatment followed by subsequent biological treatment with the aerobic activated sludge. Overall results indicated that among the utilized Fenton technologies, pre-treatment of pharmaceutical wastewater with solar driven photo-Fenton (PF) lead to better chemical oxygen demand (COD) and Total organic carbon (TOC) removal efficiency. Excessive sludge production is cost prohibitive and a major concern in biological treatment of petroleum refinery wastewater. Biological treatment of oily wastewater can be cost-effective, environmental friendly, and more compatible with existing plant facilities compared to other techniques. The three most important textile wastewater quality parameters (COD, total suspended solids (TSS) and color) were tested on the basis of the comparison of different treatment techniques. Other critical parameters such as treatment time, ease of operation and chemical cost employed were also considered. No single biological or physico-chemical treatment technique was found capable of removing up to 80% of the influent COD, TSS and color simultaneously from the textile wastewater. The treatment of distillery wastes is a priority area for the environmental sustenance. Anaerobic treatment can be done by using conventional digester, di-phasic digestion, upflow anaerobic sludge blanket reactor, fixed bed reactor, hybrid reactor. Recently, anaerobic filter of fixed-film digester is emerging with better performance than the other high-rate anaerobics reactors. The aerobic environment in the reactor is achieved by the use of diffused or mechanical aeration, which maintain the mixed liquor in a completely mixed regime. In general, bioremediation processes are categorized as bioaccumulation, biosorption, biotransformation and biomineralization using microorganisms, whereas phytoremediation techniques are carried out using plants and plant parts in a metal

containing environment. Among these, biosorption is a promising technology, which plays a central role in the removal of heavy metals. Biosorption is an emerging technology and a passive uptake process, which is mostly reversible and metabolism-independent involving adsorption on the cell surfaces of biological materials. Bioaccumulation is a complex process that involves the accumulation of heavy metals inside the cellular components. The major advantage of microbial biosorption is its low operational cost, simple, high effective and environmental friendly methodology. The cyanidation process has been, and still remains, a profitable and highly efficient process for the recovery of precious metals from ores. However, this process has contributed to environmental deterioration and potable water reserve contamination due to the discharge of poorly treated, or untreated, cyanide containing wastewater. A biological treatment process is found to be the most effective, robust, environmentally benign and cost effective method for the destruction of all cyanide related compounds. However, this process has been hindered by the use of cyanide sensitive microbial species in secondary stages that carry out the nitrification and denitrification processes, thus rendering the process ineffective, especially during cold seasons. Acid wastewater contaminated with Fe and Cu are remediated by microbial sulfate-reduction at high organic loading in a laboratory installation. The equipment design includes a fixed-bed anaerobic bioreactor for sulfate-reduction, a chemical reactor, a settler and a three-sectional bioreactor for residual organic compounds and hydrogen sulfide removal. Sulfate-reducing bacteria are immobilized on saturated zeolite in the fixed-bed bioreactor. Enhanced biological phosphorus removal (EBPR) is an inevitable need of sustainable waste water treatment systems (WWTS). In this regard for enhanced phosphorus removal was investigated the potential of an aerobic continuously stirred tank reactor (CSTR), enriched with selected bacterial consortium. The CSTR biomass was bioaugmented through addition of 12 distinct phosphorus accumulating and solubilizing strains.

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# PIM-10

## Application of Biotechnology in Industry. Part 2

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**Abstract**

Biological methods are the best option for wastewater treatment because end products of the treatment are acceptable to the nature. Organic matter can be removed by using microorganisms (mostly bacteria, fungi, actinomycetes, etc). The most recent research has been focused on the development of enzyme processes for the treatment wastewater. A large number of enzymes from a variety of different plants and microorganisms to play an important role in an array of waste treatment applications. Enzymes can act on specific recalcitrant pollutants by precipitation or transformation to other products. They can also change the characteristics of a given waste to render it more amenable to treatment or aid in converting waste material to value-added products. Various oxidative enzymes such as peroxidases and/or phenoloxidases are mainly involved in biotransformation or bioremediation of recalcitrant compounds. Although the enzymatic system related with decolourization of melanoidins is yet to be completely understood, it seems greatly connected with fungal ligninolytic mechanisms. The white-rot fungi have a complex enzymatic system which is extracellular and non-specific, and under nutrient-limiting conditions is capable of degrading lignolytic compounds, melanoidins, and polyaromatic compounds that cannot be degraded by other microorganisms. Fungi especially the white-rot fungi produce enzymes laccase, Mn peroxidase, and lignin peroxidase, which are involved in degradation of lignin in their natural lignocellulosic substrates. Lignin peroxidase is able to oxidize various aromatic compounds, while manganese peroxidase oxidizes almost exclusively Mn(II) to Mn(III), which then degrades phenolic compounds. Laccases are coppercontaining oxidases. They reduce molecular oxygen to water and oxidize phenolic compounds. Membrane bioreactors are practically used for industrial and municipal wastewater treatment. Algae are the solution for global warming, water pollution and the next generation energy crisis. High efficiency can be achieved in a thermophilic microbial fuel cell, where electricity generation and wastewater treatment are carried out simultaneously. Immobilization of cells has been considered as an alternative technology for various environmental applications. Immobilized whole cells deem to be advantageous than freely suspended cells because of improved mechanical strengths, production of high biomass, effective biosorbent restoration, easy separation of solid-liquids and greater bacterial cell density. Immobilization process can be performed using various materials such as sodium alginate, polyacrylamide, polysulfone, cellulose, polyvinyl alcohol and carboxymethylcellulose. Recent years have witnessed a surge of nanotechnology in all walks of human life. Nanoparticles claim a higher surface to volume ratio and hence, have found wide applications in water treatment, catalysis, biosensing and pollutant degradation. In line with these advancements, scientists working on bioremediation have also reported various

combinatorial approaches that integrate nanotechnology with bioremediation to eventually enhance the bioremediation efficiency.

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# PIM-11

# Aquatic Weed Hydrolysate Nanofiltration for Separation of Saccharides from Phenolics

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**Abstract**

The current study deals with nanofiltration for separation of saccharides from phenolics. Experiments are carried out in concentration mode using two types of aqueous solutions. The one is a hydrolysate of Eurasian water milfoil (EWM), an invasive worldwide spread aquatic weed, which we previously found out that it is a potential source of bioenergy (monosugars) and valuable phenolics. The other one is a synthetic solution that simulated the carbohydrates (mono- and disaccharides) found in the real solution.

The study is conducted in a MaxiMem cross-flow filtration system (PS Prozesstechnik) equipped with Microdyn Nadir NP030P (MWCO 500 Da) flat-sheet nanofiltration membrane. The results show a linear increase in solute amounts which means that the permeate has constant mass density over time. Only the amount of Glucose (Glu) transferred from the model feed exceeds that one from EWM. This is expected because of the lower Glu rejection in the former case. The amounts of the other sugars permeated from EWM, however, are similar or greater compared with the model. The initial amounts of monosugars - Galactose, Mannose and Fructose, are substantially lower than the Glu one. This means that the sugar recovery from the hydrolysate is comparable to that one from the model, despite the presence of high molecular weight components like phenolics. However, the overall sugar amount transferred in concentration mode is not sufficient. In addition, high rejection of disaccharides from the membrane is observed, as well as of phenolics.

In order to achieve better permeation of sugars and potentially increase their separation from phenolics, the effect of diananofiltration is suggested for further investigation.

# PIM-12

## Electrocatalytic Oxidation of $H_2S$ by a $ZrO_2$ Catalyst on Biochar Carbon

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**Abstract**

The electrochemical properties of electrocatalysts from $ZrO_2$ incorporated into a bio char carbon matrix ZCSH ($ZrO_2$ deposit onto carbon sunflower husks) are studied. The catalyst synthesized is intended to be used in the oxidation of sulfide ions from electrolytic model solutions content 65 $mg.l^{-1}$ $S^{2-}$ and 18 $g.l^{-1}$ NaCl. The electrocatalysts were characterized by scanning electron microscopy, X-ray diffraction, XPS and BET. The electrodes were studied electrochemically by means of cyclic voltammetry, galvanostatic measurements and Tafel slopes. Polarization curves were recorded of electrodes preparation from different quantity catalytic mass of ZCSH. The electrodes are designed and optimized in terms of the amount of catalyst and binder (PTFE). The electrodes comprised of 40 $mg.cm^{-2}$ of catalytic mass within the electrode exhibit a lower overvoltage following the galvanostatic measurements.

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# PIM-13

## Using of Ionic Liquids for Organic Acids Reactive Extraction. Mechanisms

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**Abstract**

Organic acids are a large part of biochemical substances widespread in nature - they are found in plants, fruits and vegetables. The interest in organic acids is determined by their wide and varied applications in various fields of industry – food, pharmaceutical, chemical and many others. The reactive extraction is a reversible reaction between the acid molecule from the aqueous phase and the extractant in the organic phase by means of forming an acid-extractant complex. It follows the re-extraction of the acid from the organic phase, the regeneration of the extractant and the return into recycle. In the last decade aqueous two-phase systems (ATPS) based on ionic liquids (ILs) have been successfully applied in various extraction and separation processes, including and reactive extraction. Ionic liquids are salts, consisting of ions - usually a large asymmetric organic cation and an organic or inorganic anion. Typical cations are imidazolium, pyrrolidinium, ammonium or phosphonium. Various organic groups are usually attached to a cation. Anions may be small inorganic ions, e.g. chloride, bromide, sulfates, nitrates, etc., or large organic anions, such as ethyl-sulfate, trifluoroacetic trifluoromethyl-sulfonylamide and the like. In the extraction by means of ILs the essential factor is the interaction with the water molecules. The great importance of water in extraction processes through ILs is determined by the presence of water molecules in the complexes between the molecules of extracted components and ILs. In water saturated system, containing an IL as a solvent, one ion pair of IL and HA is hydrated with an almost constant amount of water and then the loading is independent of the IL concentration. So in the simultaneous extraction of acid and water there are formed stoichiometrically defined complexes and thus four mechanisms for simultaneous extraction of acid and water are defined. This research investigates and explains the mechanisms of extraction of organic acids through ammonium-based, imidazolium-based and phosphonium-based ionic liquids, which have recently been applied for the recovery of organic acids of industrial interest.

# PIM-14

# Problem Analysis of Implementing the Electric Tricycle Program in the Philippines

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**Abstract**

Electric vehicles could play an important role in reducing greenhouse gas emissions from the transport sector. The future of e-mobility in particular electrification of road transport is gaining some traction as more electric vehicles are being deployed across the world. For example, the Philippine government had entered a loan agreement with Asian Development Bank to introduce and implement the electric tricycle (e-trike) program. A tricycle, which is a motorized vehicle commonly used for public transportation, consists of a motorcycle with a passenger cab. Shifting from motorized tricycles to e-trike would need to consider multiple factors such as financial viability, environmental and economic benefits, and social acceptability. This study thus proposes a methodology that integrates the Analytic Hierarchy Process (AHP) and multi-criteria interactive decision-making method (TODIM) for problem analysis of implementing the e-trike program. An illustrative case study is presented based on the perspectives of multiple stakeholders.

# PIM-15

# Thermal Characterisation of Beeswax and Hydrogenated Palm Stearin Eutectic Mixture for Use as a Phase Change Material in Solar Thermal Energy Storage Systems

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**Abstract**

The development of solar thermal energy storage systems for hot water supply or space heating can contribute positively to the implementation of renewable energies while minimising dependence on fossil fuels. A general implementation of these systems requires, among other factors, the development of technically suitable and low-cost phase change materials. Among the phase change materials, the possible use of beeswax, which has suitable thermal characteristics at a relatively high cost, has been reported. In contrast, palm stearin, a by-product of palm oil refining, has suitable thermal characteristics for the application at a lower cost than beeswax, with the disadvantage of lower chemical stability due to the presence of free fatty acids. This work explores the preparation of beeswax and hydrogenated palm stearin eutectic mixture for obtaining phase change materials with suitable properties for application. Five binary mixtures were prepared by melting and mixing the components for 30 minutes. Weight ratios of 80/20, 65/35, 50/50, 35/65 and 20/80 were used. For both raw materials and mixtures, melting and solidification temperatures and enthalpies, and heat capacity were determined by DSC according to ASTME793-06(2018) and ASTME1269-11(2018). Thermal characterisation was carried out both for the freshly prepared materials and after being subjected to 180 cycles of melting and solidification. For all prepared mixtures, a relatively high heat of fusion above 190 J/g, melting temperatures between 50 °C and 68 °C and adequate thermal stability were observed. The results demonstrate the possibility of obtaining a phase change material with suitable thermal characteristics for solar energy storage that combines the advantages of beeswax and hydrogenated palm stearin.

# PIM-16

# Feasibility Study of a New Roof-Top Multipurpose Solar Thermal Cooking Device

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**Abstract**

Utilizing solar thermal energy for household drying, cooking, baking of food items is an attractive option in regions of the world where clear sunny weather is experienced for a significant part of the year. Besides defraying the cost of fuel, solar-driven food processing is advantageous from the viewpoint of low carbon footprint also. For this purpose, a compact roof-top multipurpose solar appliance was designed and fabricated. This versatile unit was tested for water warming, rice-cooking, baking of cake, and dehydration of food materials. In cooking mode, the plate stagnation temperature under no-load condition reached the highest 114.85ºC, and for cooking operation, the temperature of food inside the cooking pot approached 90.60ºC in 115 minutes of operation and touched the maximum of 99.33ºC in January at Bhavnagar (21.7645° N, 72.1519° E), situated at the western part of India. The values of figures of merit-F1 (stagnation test) and F2 (sensible heat test) were determined to be 0.11683ºC $m^2$/W and 0.61ºC l, respectively. In drying operation, the unit was tested for drying ginger under mixed-convection mode using a photovoltaic operated small fan. The maximum drying air temperature was 74ºC during a clear sunny day when the average solar radiation was 550 W/$m^2$, and the average surrounding air temperature was 31ºC. When converted into baking mode and the unit functioned as an oven, a cake could be baked with the maximum cake temperature of 87ºC. The conventional solar thermal devices, such as the solar dryer, cooker, oven, and water disinfector, are primarily single-purpose devices. Even if they have standard features such as mirrors for reflectors, thermally insulated bottom and sides, black absorber bases, etc., individually, they cannot meet different needs for diverse heating temperatures or different heating chamber sizes. Instead of going for single-purpose solar thermal devices for various applications, this versatile roof-top solar cooking device is capable of meeting all the food preparation and processing needs of a family.

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