

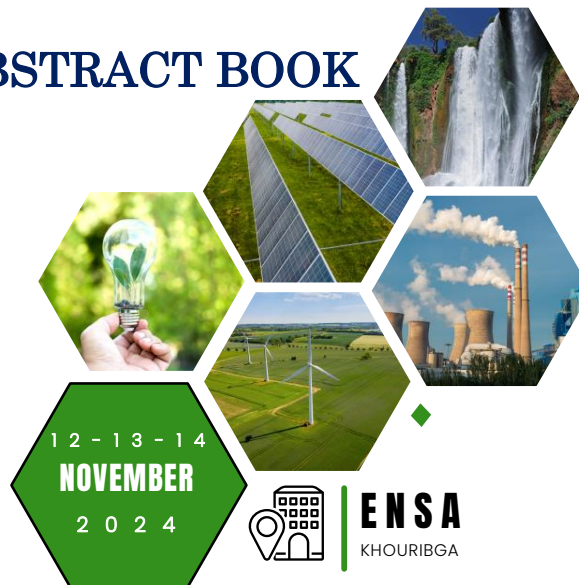


# 4<sup>EDITION</sup> International Conference

## Industrial Systems and Processes *SPIn 2024*

GREEN AND SUSTAINABLE ENERGY  
WATER-FOOD NEXUS AND CHALLENGES

ABSTRACT BOOK



**EDITORS:**  
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RECONNUE PAR L'ÉTAT

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# **PLENARY SPEAKERS**



### **Keynote 1**



Mohamed AZAROUAL obtained his Ph.D. in Reactive Geochemistry from the Institute of Earth Physics of Paris - University René Diderot, Paris 7, in 1993, focusing on Enhanced Geothermal Systems (EGS) technologies. He successfully defended his HDR (Habilitation à Diriger des Recherches) in December 2014 on "Multiphase Reactive Transport Processes in Hydrogeosystems for Geo-Resources and Environmental Challenges" at the University of Orléans (France).

Currently, he serves as the Deputy Director of ISTO (Institute of Earth Sciences of Orléans) at the Orléans University. His scientific interests encompass aspects of reactive transport modeling and mass and heat transfers between phases (water -gas-rock-microorganisms) in complex hydrogeological systems, including high temperature, high pressure, and high salinity conditions, for geo-resources (water, energy, etc.), underground uses (CO<sub>2</sub> storage, energy vectors), as well as environmental challenges. He has authored more than 60 A-ranked articles and delivered over 250 presentations at international conferences. He is a faculty member at INSA - Bourges Engineering School (National Institute of Applied Sciences) and has (co)supervised over than 20 doctoral theses.

Mohamed Azaroual has developed and managed R&D projects for the ANR (National Research Agency) in Europe, with active international scientific collaborations (USA, China, Morocco, Japan, Australia, etc.). He has initiated research projects in partnership with industrial and private companies (e.g., TOTAL, ENGIE, VEOLIA, SUEZ, VATTENFAL, OCP, Mitsubishi, BP, Shell, etc.). Since 2007, he has been the scientific coordinator of the BRGM - LBNL partnership, marked by the signing of four successive Memoranda of Understanding.

Currently, Mohamed Azaroual is the scientific coordinator of the O-ZNS Observatory (<https://plateformes-pivots.eu/o-zns/?lang=en>), focusing on reactive transfers in the unsaturated zone of carbonate aquifers in the Beauce aquifer (Centre Val de Loire, France).

## Predictive geosciences for georesources exploration/management – soil and underground exploitation and environmental issues

Mohamed AZAROUAL

BRGM (French Geological Survey) – 3 av. C. Guillemin, BP 36009, 45060 Orléans, France  
ISTO – Université d'Orléans - CNRS/INSU - BRGM, UMR 7327 Institut des Sciences de la Terre d'Orléans (ISTO), 45071 Orléans, France.

### Abstract:

Constant growth in world population and intense industrial development inevitably cause degradation of the environment and induce scarcity, and vulnerability. Predictive geosciences gather knowledge from different domains such as mathematics, physics and chemistry, biology and material sciences in order to develop geo-technologies based on big data assessment and predictive/inverse numerical simulations. Also necessary is the development of theoretical concepts and continuously improving methods of application based on recent scientific and technological innovations.

Land surface and subsurface are increasingly solicited for different uses including exploitation of water resources for farming, agriculture, and other uses. Exploration and exploitation of energy resources, useful substances, and storage of undesirable substances in the underground require knowledge of the dynamics of multiphase hydrosystems. The transfer of mass and heat between phases (water - rock - gas - "microorganisms") on different scales of time and space, from soil to groundwater and deep aquifers could induce biogeochemical reactions and redox processes, catalyzed by microbiological activity, seek to use electron end acceptors (TEAs) such as oxygen, nitrates, oxides / hydroxides of manganese and ferric iron, and sulphates which act sequentially.

Such applications demand multidisciplinary skills and complementary methods to enrich and extend both theoretical approaches and databases to build advanced concepts as well as revised predictive numerical models. These models must be continuously fed, updated, improved, tested, and validated models. The results can be used as guides to explore and manage geosystems to exploit resources (water, oil, gas, heat, recyclable materials, etc.) as well as to store some resources temporarily (water, heat, gas, etc.) and store undesirable substances permanently (CO<sub>2</sub>, industrial water, acid gases, radioactive waste, etc.).

A global overview of the state of development of these approaches for renewable energy, water management, mineral resources and environment issues for ecological transition and sustainable development will be presented.

## **Keynote 2**



Dr. Jamal Chaouki is a full professor at Polytechnique, Montréal, Canada. He is also the director of the Biorefinery Center and a member of the Canadian Academy of Engineering. He has supervised more than 120 researchers. He published more than 400 reviewed articles in refereed journals and in different reviewed proceedings, and more than 450 other scientific articles as well as edited 6 books. He has more than 22 patents on different processes. He is now editor of the Chemical Product and Process Modeling Journal. He is also the director of the Biorefinery Center and a member of the Canadian Academy of Engineering. He has co-chaired 10 International Conferences including the 8th World Congress of Chemical Engineering 2009, where he has acted as technical director. He is also a member of the 10th World CChE 2017, and he was the president of the Fluidization 15th Int. Conf. He is now supervising 30 researchers (15 Ph.Ds, 5 PDFs, 5 MScA, 4 research associates and 1 researcher). He is a member of the Board of the Ecole Polytechnique and several companies. He is a world-renowned consultant for at least 20 national and international companies. He has created 6 start-ups with his students: Formmat Tech. Inc., Shopmedia Inc., Pyrowave Inc, Ecolomondo, RMTech and GoldRecyc. He is Principal Chair Holder of NSREC-Total Group in hydrodynamic modeling of multiphase processes at extreme conditions. His work is mainly dedicated to develop processes from waste, biomass and complex feedstocks to heat & power, fuels and chemicals.

## Pourquoi les universités doivent-elles investir dans l'extrapolation des Procédés ?

Jamal CHAOUKI

Polytechnique Montréal, Canada & UM6P Benguéir

### Abstract :

Dans un premier temps, nous allons montrer que les compagnies d'engineering sont actuellement incapables de faire l'extrapolation de nouveaux procédés et nous allons montrer pourquoi. Ainsi, au lieu de laisser les découvertes des chercheurs dans les placards de nos universités, il est temps d'en faire de la richesse. Pour cela, il faut apprendre comment extrapoler ces procédés à l'échelle industrielle en investissant dans ce nouveau savoir dans nos universités.

Dans notre Livre intitulé « Scale-Up Processes : Iterative Methods for the Chemical, Mineral and Biochemical Industries » publié récemment, nous avons développé une nouvelle méthodologie de conception de procédés basée sur une méthode itérative. Dans cette méthode, on passe directement de l'échelle laboratoire à l'échelle industrielle désirée mais sur papier en utilisant toutes les potentialités numériques : bilans de matières et de chaleur, simulation des procédés, analyse numérique (CFD, DEM...) et le design de toutes les unités. De plus, il faut faire une Analyse de Cycle de Vie (ACV) et des estimations des CAPEX et OPEX. Enfin, il est crucial de déterminer soigneusement tous les risques technologiques et économiques, ce qui demande de l'expérience dans l'extrapolation des procédés. C'est un exercice difficile à mener par une équipe multidisciplinaire. Si l'ACV ainsi que les CAPEX et OPEX ne sont pas satisfaisants, il faut réitérer jusqu'à ce qu'ils soient acceptables. S'ils le sont, c'est à ce moment seulement qu'il faut commencer à réfléchir à l'unité pilote (taille, le sous-ensemble à « piloter », les analyses à planifier, les mesures à réaliser ...) car le but de celle-ci est de lever les indéterminations, les risques technologiques et économiques soulevés lors du passage de laboratoire à l'échelle industrielle.

La taille de l'unité pilote et sa capacité doivent donc permettre de trouver des réponses adéquates aux risques technologiques et économiques soulevés lors de la conception de l'unité industrielle. Ainsi, si un procédé est simple ou avec seulement des incertitudes limitées (le reste du procédé est maîtrisé), la taille du pilote serait petite, à la limite le passage direct du labo à l'industrielle pourrait être possible et inversement plus un procédé est complexe et pas maîtrisé, plus la taille du pilote est grande. La taille de l'unité pilote dépend donc aussi de l'expertise de la compagnie dans le domaine considéré. Dans certains cas, la taille qui répondrait aux risques technologiques ne peut pas répondre aux risques économiques (par exemple, la production est trop faible pour analyser l'acceptabilité du produit par des clients), il faut alors choisir un pilote d'une plus grande taille de manière à répondre aussi bien aux risques technologiques et économiques. De plus, on ne pilote presque jamais les parties déjà connues du procédé industriel à moins d'une production à faire accepter par des clients.

### **Keynote 3**



Abdelghafour Zaabout is an Associate Professor at University Mohamed 6 Polytechnic (UM6P). He has over a decade of expertise in decarbonization and energy transition, developing highly efficient and cost-effective technologies for decarbonization of the industrial, energy, and hydrogen sectors. Prior to joining UM6P, he worked jointly as a Senior Scientist at SINTEF Industry in Norway, and as an affiliate Prof. at UM6P. He received his Ph.D. from Aix Marseille University before starting a two-year Postdoctoral Fellowship at the Eindhoven University of Technology. Throughout the last decade, he served as a key driver in the demonstration of several CO<sub>2</sub> capture and low carbon hydrogen production technologies, in the framework of different Norwegian, EU funded, and direct industrial projects. Prof. Zaabout co-authored nearly 60 peer-reviewed journal papers & several patents, as well as co-supervised dozens of students combining Ph.D. students, postdocs, and graduates. He participated as a panelist at COP27 in Sharm El Sheikh in a UN official session on CCUS for Africa, he chaired key sessions in several international conferences (e.g., GHGT 16, Int. Conference on Fluidization), and lectured in many decarbonization-related events.

## Carbon Capture, Utilization, and Sequestration in the Process Industry

Abdelghafour Zaabout

Associate Professor of Process Engineering (Decarbonization), ACER CoE, Mohammed 6 Polytechnic University, Benguérir - Morocco

### Abstract:

Carbon capture, utilization, and sequestration (CCUS) is an emerging knowledge-based industry incentivized by the need to cut 60 Gt-CO<sub>2</sub> from current emissions to maintain the 1.5 °C global warming targets. Cheap renewable energy is key to enabling the massive deployment of such an industry. In this aspect, Morocco is well positioned for accommodating the different value chains of the CCUS industry, given the large renewable energy potential, sequestration and mineralization resource availability, long coastal areas, as well as the complementarity with the national priorities of the green hydrogen economy, biogenic energy, and water management. CCUS can boost those national priorities, both as an enabler (e.g., use of the captured CO<sub>2</sub> from hard-to-abate industry to produce renewable methanol, jet fuel, green chemicals & fertilizers) and for waste handling (e.g., fixing CO<sub>2</sub> in desalination brine, mineral & phosphate waste). Carbon-negative pathways are also on the rise worldwide, driven by the need to suck CO<sub>2</sub> from the atmosphere, bringing large opportunities in the carbon credit market. Cheap renewable energy and high storage capacity are the limiting factors for implementing such a strategic carbon-negative industry, where Morocco and Africa are well positioned to play a major role.

This talk will highlight the research activities under the program CaNCUS at UM6P targeting decarbonization of the process industry using CCUS value chain within the Moroccan context driven by its large renewable energy potential and waste valorization ambitions.

#### **Keynote 4**



Prof. Abdelilah Benyoussef received his "Doctorat d'état" degree from the Paris-Sud University in 1983. He is a permanent member of the Moroccan Hassan II Academy of Science and Technology, since 2006. He has been visiting professor in many research centers, laboratories and Universities in Belgium, Canada, Egypt, France, Germany, Japan, Spain, Tunisia, and United states. The main interest topics of Abdelilah Benyoussef are Ab initio calculation and Monte carlo method in modeling and simulation of new materials for renewable energy; Magnetism and phase transition in condensed matter; complex systems and critical self-organization in statistical physics. He is a co-author of more than 400 research publications and book chapters and about 100 conference presentations including numerous invited papers and talks. He has co-chaired or co-organized several international conferences. He holds a number of patents and supervised 40 postgraduate research candidates.

## Green hydrogen as an energy carrier: Production and Storage

Abdelilah Benyoussef

Hassan II Academy of Sciences and Technology, Rabat, Morocco  
LaMCSci, Faculty of Sciences, Mohammed V University, Rabat, Morocco

### Abstract:

Modeling and simulation are very effective and valuable approaches to understand, interpret and predict the behavior of systems. They are complementary to the experience and can even guide it, to study and investigate materials and devices which might be expensive and time consuming to fabricate.

The simulation cover a large scale; from the microscopic scale with ab initio calculation and density functional theory, to the mesoscopic scale with molecular dynamics and Monte Carlo simulation, to the scale of continuous media with the Finite elements methods.

Modeling and simulation are used extensively in science and engineering. They play a very important role in materials science, in particular for the design of new materials and nanomaterials for application in a wide variety of fields ; In energy conversion and storage, in magnetic and electrical refrigeration, in spintronics and valleytronics, etc. The majority of these themes are studied in different laboratories of Moroccan universities.

In this presentation I will focus on the conversion and storage of energy. In particular, on hydrogen as energy carrier. The mainly used method, for the design of new materials and nanomaterials, is the density functional theory which is a powerful method based on quantum mechanics. Molecular dynamics and Monte Carlo Simulation, are used to calculate the properties of these materials and nanomaterials under their operating conditions.

For hydrogen to be a clean energy vector, it must be produced from renewable energies by processes that do not release greenhouse gases. These processes include: - electrolysis by photovoltaic, by thermal solar concentrating (CSP) and by wind turbine - Thermolysis and thermochemistry by concentrated solar energy - or photo-electrolysis by photovoltaic and solar thermal with concentration. Photocatalysis is one of the most promising processes for the hydrogen production from renewable energies.

The main process in solid state hydrogen storage is the interaction between the hydrogen and the surface of the storage medium. Because of their enormous surface area, nanostructured materials can enhance the efficiency of this process and hence improve the storage capabilities. Various efforts have been made to enhance the hydrogen storage properties.

In this presentation, particular attention will be paid to the design of new nanomaterials for the two applications mentioned above; hydrogen production and storage. In particular, two-dimensional materials like phosphorene the phosphorus-based graphene analogue, siligraphene, borographene, 2D magnesium hydride, Beryllium Carbide and other nanomaterials.



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# Theme 1: Hydrogen – Renewable energy - Bioenergy

# Techno-Economic Analysis of Biochar Production Pathways Using Biomass Waste Pyrolysis

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Population growth accompanied with lifestyle change result on a notable increase in energy consumption and waste generation. Most of the global energy requirement is supplied from fossil fuel which leads to a substantial rise in CO<sub>2</sub> emissions, moreover the fact that those resources are finite push toward the conversion of renewable resources. Biochar from biomass waste gain a wide attention as a promising carbon-rich substance for energy generation and carbon sequestration in many application, while each application required specific characteristics of the biochar obtained ,for that many parameters can be controlled in slow pyrolysis process as the common technique for biochar production, fixing specific temperature and time required specific equipment size, additionally for each combination of time and temperature different bioproducts (electricity, bio-oil and heat) are collected, this variation in process sizing (CAPEX) and utilities (byproducts) affect significantly the cost of the obtained biochar. Having an economical and energy efficient process targeting the production of biochar with specific characterisation, necessitate the selection of the optimal feedstock and operating conditions, this can be covered with a detailed technoeconomic study considering different scenarios.

**Keywords:** Pyrolysis, Biochar, Technoeconomic study, CAPEX, Cost of biochar

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# Energy System Simulation Model to Assess Energy Transition Policies in Tanzania

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Strategic planning of an energy system is a complex political task, subject to significant technical and socio-economic uncertainties. This issue is particularly challenging in developing countries, where a rapid increase in energy demand is expected due to economic and population growth. Moreover, the number of variables to consider increases when energy expansion is planned in the context of a transition to renewable energies. To assist in decision-making regarding energy planning, a System Dynamics model has been developed to simulate the energy system applied to the electricity sector in Tanzania. This model can evaluate expansion policies by studying their impact on Energy Security. Aspects such as the need for firm capacity to cover peak demand, greenhouse gas emissions, aerosol PM2.5 emissions, investment requirements, capacity utilization and dependency on water resources during droughts are analysed, comparing scenarios of energy transition and fossil fuel expansion according to the energy policy outlined in the Ministry of Energy of Tanzania's Power System Master Plan 2020.

**Keywords:** Energy Transition, Energy Security, Energy Planning Model, Systems Dynamics, Tanzania

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# Improving NaBH<sub>4</sub> Stability and Dehydrogenation with 3d Transition Metal Enhancements

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The present study explores the structural stability and dehydrogenation properties of NaBH<sub>4</sub> doped with various 3d transition metals, employing first-principles density functional theory (DFT) calculations. Our findings indicate that doping NaBH<sub>4</sub> with transition metals significantly alters the crystal structure, primarily by weakening the B-H bond strength, thus leading to destabilization of the NaBH<sub>4</sub> lattice. Specifically, the introduction of Sc, Ti, Ni, V, Co, Mn, and Fe into the NaBH<sub>4</sub> matrix reduces the hydrogen desorption enthalpy, enhancing its hydrogen release characteristics. A detailed analysis of the electronic structure reveals that the presence of 3d transition metals modifies the total density of states (DOS), notably shifting both the conduction and valence bands. This shift results in changes to the electronic distribution near the Fermi level, which directly influences the bonding interactions and the thermodynamic properties. The decrease in hydrogen desorption enthalpy is directly correlated with the partial occupation of metal d-orbitals, which facilitates easier hydrogen release, thereby improving the overall hydrogen storage capacity of NaBH<sub>4</sub>. These results highlight the potential of transition metal doping as a strategy to optimize NaBH<sub>4</sub> for practical hydrogen storage applications.

**Keywords:** Hydrogen storage, sodium borohydride, 3d transition metal, electronic density, dehydrogenation, DFT study.

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\*Speaker

# Molecular Dynamics Simulations of the Solvation, Dynamics, and dielectric Properties of {NaBF<sub>4</sub> – Dimethyl sulfoxide} Electrolytic System for Sodium-Ion Batteries at various Temperatures

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Sodium-ion batteries (SIBs) have garnered significant attention as promising alternatives to lithium-ion batteries due to the abundance and low cost of sodium resources. The electrolyte composition plays a crucial role in determining the performance and stability of SIBs. In this study, we employed molecular dynamics (MD) simulations to determine the structural, dynamic, and dielectric properties of an electrolytic system consisting of sodium tetrafluoroborate (NaBF<sub>4</sub>) dissolved in a highly versatile and widely used polar aprotic organic solvent, dimethyl sulfoxide (DMSO), which is employed in various industrial sectors, particularly in rechargeable battery technology. Our molecular simulations were performed using the GRO-MOS force field in a microcanonical ensemble with a salt concentration of 0.75 mol/L in a cubic simulation box. Specifically, the structural behavior was analyzed through the calculation and analysis of the radial distribution function (RDF) for different ion pairs, providing microscopic information such as the coordination number (NC) and interatomic distances. Furthermore, the dynamic and dielectric behaviors of the energy storage system were evaluated by simulating the self-diffusion coefficient (D) and the dielectric constant over a broad temperature range from 278.15 to 373.15 K. Generally, the molecular dynamics approach provides valuable information for the design and optimization of SIB electrolytes, thus contributing to the advancement of sodium-based rechargeable battery technology.

**Keywords:** Molecular dynamics, Sodium, Ion Battery, Sodium Tetrafluoroborate, Dimethyl sulfoxide, Solvation phenomenon, Self, diffusion coefficient, Dielectric constant.

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# Large-scale bio-desulfurization of biogas from anaerobic digestion of WWTP sludge: performance and stabilization

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The main focus of this study is to analyze and control the operation of the biogas bio-desulfurization plant derived from the treatment of wastewater treatment plant (WWTP) of Kenitra (Morocco). The plant is designed to reduce the hydrogen sulfide (H<sub>2</sub>S) content of the biogas produced in the anaerobic phase of the sewage treatment plant. Various bacteria are capable of transforming H<sub>2</sub>S by adding oxygen - via the intermediate phase of elemental sulfur - into sulfate. The action of bacteria in highly acidic conditions to eliminate sulfur is produced on a large scale with the Full-Biological Trickling Bed (FBTB) was investigated in this study. The effect of the pH of the microorganism suspension (inoculation culture, pure culture) on the operation of the bio-desulfurization plant has also conducted through four experimental approaches. The obtained results show that the best performance removal of H<sub>2</sub>S was observed at a pH value of 1.6 and an oxygen injection rate of around 10%.

**Keywords:** wastewater treatment plant, Population Equivalents, Bio, Trickling Filter, Sulfur, Oxidizing Bacteria, Full, Biological Trickling Bed.

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# A review of artificial intelligence to predict energy consumption in buildings

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Improving energy efficiency and reducing costs in the construction sector, with the aim of minimizing carbon emissions, is a universal objective. To achieve this goal, a variety of solutions are used, including improved HVAC systems, efficient lighting and the integration of renewable energy sources. Thermal insulation is the most effective of these solutions. However, it is essential to know the building's energy consumption first. Predicting the energy usage of structures can be categorized into three primary classifications: hybrid, AI, and engineering methodologies. This study focuses on the second category. The AI-driven approach leverages historical data to forecast forthcoming consumption within defined boundaries. Emphasis is placed on contemporary developments in AI-driven methodologies for projecting energy usage in buildings. This review takes an in-depth look at the methodologies of linear regression, decision trees, logistic regression, random forests, neural networks and support vector machines (SVMs), as well as the ensemble prediction method. The article describes the principles, applications, advantages and limitations of these techniques, and concludes with an overview of potential research areas related to AI-driven building energy prediction.

**Keywords:** Artificial intelligence, Energy efficiency, Neural network, Building energy use prediction, Ensemble model, Support vector regression.

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# Advancing Sodium-Ion Battery Technology with High-Performance Hard Carbon Derived from Alfa Plant

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The quest for efficient and economically viable energy storage technologies has increasingly turned toward sodium-ion batteries (SIBs), driven by the abundant and cost-effective nature of sodium resources. Achieving high-performance SIBs, however, requires overcoming significant challenges, especially in optimizing anode materials. This study offers a novel solution by exploring hard carbon (HC) derived from Alfa plant derivatives through a controlled carbonization process. By varying the carbonization temperatures, this research reveals that hard carbon carbonized at 1300°C outperforms that produced at 800°C in several key performance metrics. The HC material obtained at 1300°C exhibits markedly superior reversible capacity, exceptional rate capability, and outstanding cycle stability, surpassing the lower temperature counterpart. These advancements are attributed to the refined microstructure and optimized electrochemical characteristics achieved through higher temperature carbonization. Moreover, the inherent properties of Alfa plant derivatives, including their crystalline structure and functional group composition, significantly influence the HC's performance. This study not only underscores the potential of utilizing renewable, plant-based resources but also paves the way for developing high-performance, sustainable anode materials for the next generation of sodium-ion batteries.

**Keywords:** Alfa plant, Cellulose, Hard carbon, Anode, Sodium, ion batteries

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\*Speaker



# Simulation of ten samples of biomass gasification in bubbling fluidized bed reactor using ASPEN PLUS-Electricity production

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A detailed process model was created to simulate the air-steam gasification of ten different biomass samples in a bubbling fluidized bed reactor using coal ash as the bed material. The aim was to produce useful syngas that would serve as fuel for vapor turbines- along with H<sub>2</sub>, CO, and CH<sub>4</sub> components- so that electricity could be generated during gasification at varying temperatures (700, 800, and 900 °C). These different temperature levels were tested under varying steam-to-air ratios (S/A = 10/90, 25/75, 50/50, and 70/30) and stoichiometric ratios (SR = 0.13 and 0.25). Results showed that both biomass conversion to gaseous increased with temperature; moreover, any increase of steam concentration in the gasifying agent led also to higher biomass conversion. The physical properties of related gas and solid substances were estimated via the Peng-Robinson equation which formed part of a kinetic model used in these calculations based on data obtained from simulation results. The model validation is carried out using a Palm Kernell shell. Later, nine different biomass samples of various origins were gasified under similar experimental conditions. In all the experiments, the total inlet gas flow rate is maintained constant to keep space residence time similar and fluidization conditions alike. High heat value prediction with cold gas efficiency predictions and producer gas yield from the model agrees well with experimental data based on nitrogen-free dry composition at gas composition level.

**Keywords:** Biomass, Gasification, Bubbling Fluidized bed, Simulation and ASPEN PLUS

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# Balancing Competition Between Energy, Food, and Forests with the New Integrated Assessment Model "WILIAM"

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The sustainable energy and food supply is a challenge for humanity in this century due to the increasing demand for food from an expanding population, the need for energy from biological resources to achieve the energy transition, efforts to decarbonize the energy system and tackle climate change, and the depletion of high-quality fossil fuel resources. Sustainability requires innovations from engineers and researchers in industrial processes, energy production and storage, and transport logistics. It also requires systemic and holistic perspectives to analyse the feedbacks and interactions that occur in complex, top-down real-world problems. Modelling and simulation are tools used in engineering to forecast, analyse, and control systems. They can also be used to analyse and manage human-nature-technology interactions, as demonstrated in the field of System Dynamics. System Dynamics, rooted in the fields of engineering but applied to a wide variety of scientific and social fields, is one of the best tools to analyse the challenges of sustainability as demonstrated in the seminal work of World3 by Meadows et al. (1)).

In this paper, the System Dynamics model WILIAM-TERRAE, which is part of WILIAM IAM (2), is presented. WILIAM-TERRAE model is designed to analyse the trade-offs and opportunities in the ecological transition of the food system, including dietary changes, the shift to regenerative ecological agriculture, and/or high-input industrialized cultivation. Furthermore, to demonstrate the potential and novel insights of the model, four scenarios were conducted. These scenarios explore the trade-offs among biofuel demand, dietary changes, and forest protection. Our findings reveal the significant impact that biofuels, dietary shifts, and forest protection can have on global food availability, highlighting our model's ability to navigate this complex competition.

(1) Meadows, D.H., Meadows, D.L., Randers, J., & Behrens, W.W. (1972). The limits to growth.

(2) WILIAM Model Description (Online). Available: [https://github.com/LOCOMOTION-h2020/WILIAM\\_model\\_VENSIM/wiki](https://github.com/LOCOMOTION-h2020/WILIAM_model_VENSIM/wiki).

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**Keywords:** WILLIAM Model, IAM, Biofuels, Food, Forests, Land Use Changes, Climate Change Impacts

# Towards a Comprehensive Database for Circular Economy Initiatives: Challenges, and Opportunities

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The Circular Economy (CE) model represents a paradigm shift towards sustainability by emphasizing resource efficiency, waste minimization, and the extension of product lifecycles. In contrast to the traditional linear 'take-make-dispose' model, CE seeks to create a closed-loop system where resources are continually reused, reducing environmental impact and generating ongoing value. For organizations to effectively transition to a circular economy, it is crucial to gather and analyze a wide array of data, including technical, economic, regulatory, and financial information. This need for diverse and comprehensive data is highlighted by our bibliographic study, which reveals the heterogeneity of required information. To address these challenges, we propose the Circular Economy Database (CED), a pioneering tool designed to facilitate the structured collection and management of CE-related data. The CED provides a user-friendly interface for accessing and analyzing various aspects of global CE concepts. By categorizing data into Quality Control, Technological domains, Social and environmental Indicators and Finance & Behavioral Change, the CED supports informed decision-making and aids companies in adopting and optimizing circular economy practices. This database represents a significant advancement in the field, aiming to revolutionize sustainability efforts and drive progress across industries.

**Keywords:** Circular economy, Database, Frameworks, Sustainability, IOT, Artificial intelligence

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# Optimized ANFIS Based MPPT Controller in PV-BES system for EV charging using PSO algorithm under various conditions

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Photovoltaic (PV) systems have emerged as one of the most promising renewable energy sources due to their potential for clean, sustainable, and abundant power generation. However, the efficiency of PV systems is highly dependent on their ability to operate at the maximum power point (MPP) under varying environmental conditions such as changes in solar irradiance and temperature. To overcome these limitations, advanced MPPT techniques leveraging artificial intelligence (AI) and optimization algorithms have been introduced. In this study, we present the development of a Particle Swarm Optimization-Adaptive Neuro-Fuzzy Inference System (PSO-ANFIS) based Maximum Power Point Tracking (MPPT) controller for photovoltaic (PV) systems aimed at enhancing the charging efficiency of Energy Storage Systems (ESS) and Electric Vehicles (EV). The PSO-ANFIS MPPT controller integrates the global optimization capability of PSO with the learning and adaptive capabilities of ANFIS to effectively track the maximum power point (MPP) under varying environmental conditions. The proposed system was tested under dynamic weather scenarios. The results demonstrate the robustness and efficiency of the PSO-ANFIS MPPT controller, where the MSE values were maintained at low levels, with  $MSE = 3.4712 \cdot 10^{-27}$  and  $RMSE = 5.891 \cdot 10^{-14}$ , confirming the high precision of the system in maintaining optimal power output. The simulation results highlight the superiority of the PSO-ANFIS MPPT controller in optimizing PV power extraction, thereby effectively meeting the energy requirements of EVs charging.

**Keywords:** Photovoltaic Energy (PV), Maximum Power Point Tracking (MPPT), Particle Swarm Optimization (PSO), Adaptive NeuroFuzzy Inference System (ANFIS), Electric Vehicle (EV), Battery Energy Storage System (BESS).

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# Effect Of Cu-Water-Based Nanofluid On Thermal Performances Of Coaxial Heat Exchangers

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Nanofluids are new coolants composed of suspensions of nanoparticles dispersed in base fluids, with typical sizes that can reach a size equal to 100 nanometers. Their remarkable thermal properties have made these fluids the subject of much research, particularly in heat transfer and improving the thermal performances of heat exchangers. The aim of this study is to evaluate the thermal performance of a coaxial tube heat exchanger using a nanofluid based on copper (Cu) suspended in water. The work carried out in the present study was based mainly on the effect of the nanoparticle volume fraction on the heat exchanger's operating parameters. The results show that increasing the volume fraction of Cu nanoparticles leads to an increase in these parameters, underlining the role of nanofluids in increasing heat exchange and improving heat exchanger performance.

**Keywords:** heat exchanger, nanofluid, heat transfert, Thermal performances, Water based nanofluid

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\*Speaker

# Optimization of Sugar Production from Acid Hydrolysis of *Opuntia ficus-indica* Fruit Wastes

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This study focuses on optimizing the acid hydrolysis process of *Opuntia ficus-indica* fruit juice waste to maximize the production of fermentable sugars, particularly total reducing sugars (TRS) and saccharose. Using Response Surface Methodology (RSM) with a Central Composite Design (CCD), the effects of varying sulfuric acid concentrations (1% to 5%) and reaction times (5 to 30 minutes) were systematically explored. The optimal conditions were identified as a 3% acid concentration and a 17.5-minute reaction time, yielding the highest concentrations of TRS (0.13 mol/L) and saccharose (1.42 mol/L). The study also introduced the Combined Severity Factor (R<sup>0</sup>), identifying an optimal range of 3.5-4.0, which balances effective sugar release and minimal inhibitor formation. The TRS model demonstrated high reliability with an adjusted R<sup>2</sup> of 0.9788, while the saccharose model showed potential overfitting issues. These findings are significant for improving biofuel production efficiency from *Opuntia ficus-indica* fruit waste, particularly in regions where this feedstock is abundant. Further research is needed to refine the saccharose model and validate these results on a larger scale.

**Keywords:** Acid Hydrolysis, Lignocellulosic Biomass, *Opuntia ficus, indica*, Response Surface Methodology, Sugar Optimization.

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# Optimized Photovoltaic/Thermal Hybrid System with D-Shaped Tubing for Enhanced Heat Dissipation

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The primary reason for the inefficiency of photovoltaic panels lies in the temperature rise of the photovoltaic cells. This increase in temperature affects the efficiency of the photovoltaic cells, leading to energy loss. Nevertheless, the addition of a D-shaped tube as a cooling agent lowers the temperature of the photovoltaic cells while simultaneously heating water. This study focuses on conducting a thermal evaluation to assess the efficiency of the Photovoltaic/Thermal system, with the aim of optimizing the electrical energy production. The influence of flow modification was evaluated up to 7.5 L/min. The numerical results revealed a considerable 30 % decrease of heat in system, down to 42 °C. As a result, the recommended photovoltaic/thermal system presents excellent electrical performance. The D-shaped tube delivers optimized heated water of 55.6°C, at lower water consumption. Assuming that water enters the system at a temperature of 20°C. The proposed system was introduced in this work with the aim of optimizing the efficiency of the photovoltaic cells while reducing their operating temperature.

**Keywords:** PV/T hybrid system, D, shaped tube, flow rate, electrical efficiency, thermal efficiency.

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\*Speaker



# Optimization Strategies for Used Cooking Oil Collection via the Green Vehicle Routing Problem

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Used cooking oil presents significant environmental issues, including pollution and blockages in sewage systems. This paper offers a systematic literature review on applying the Green Vehicle Routing Problem (GVRP) to enhance the collection of used cooking oil, highlighting the urgent need for efficient and eco-friendly waste management solutions in the food service industry. The GVRP is a robust optimization framework designed to improve route planning while considering constraints such as vehicle capacity, time windows, and environmental impact. By employing the GVRP for used cooking oil collection, routes can be optimized to reduce vehicle emissions, lower transportation costs, and ensure timely pickups from restaurants. This review compiles and analyzes existing research that applies GVRP techniques to the collection of used cooking oil. It explores various strategies, algorithms, and optimization methods used in these studies. Additionally, it assesses the practical effectiveness of these approaches in tackling challenges such as fleet management, route efficiency, and environmental impact reduction. By detailing recent advancements and identifying research gaps, this paper aims to provide a thorough understanding of how GVRP can be leveraged to address the complexities of used cooking oil collection.

**Keywords:** green vehicle routing problem, used cooking oil, optimization, transport

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# Harnessing renewable energies: towards a hybrid method to evaluate wind variability

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Recently, the growing presence of wind energy in national power systems has led to substantial interest in wind power potential evaluation and forecasting techniques. Assessing wind variability is crucial due to its potential to disrupt electric grids with high wind energy penetration, causing issues such as flicker, voltage changes, and equipment wear. These variability-induced grid integration challenges present significant barriers to the expanded use of wind energy. Therefore, developing metrics to classify and quantify variability accurately with minimal on-site data collection is essential for cost and time efficiency.

This study presents a novel methodology to assess wind variability by leveraging Fast Fourier Transform (FFT) for the decomposition of wind speed and direction time series data into distinct frequency components, revealing dominant periodic patterns and fluctuations. We introduce the Wind Variability Index (WVI) and the Global Variability Gradient (GVG) as comprehensive and complementary tools that captures the complex dynamics of wind behavior. These parameters are instrumental in characterizing the temporal variability of wind resources, thereby improving decision-making processes in wind energy projects and grid management.

*Keywords- Wind variability, Fast Fourier Transform (FFT), Wind Variability Index, Wind energy integration, Renewable energy planning, Time series analysis, Power systems, Wind resource assessment, Grid management.*

**Keywords:** Wind variability, Fast Fourier Transform (FFT), Wind Variability Index, Wind energy integration, Renewable energy planning, Time series analysis, Power systems, Wind resource assessment, Grid management

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\*Speaker

# Techno-economic assessment of algae-based waste Hydrochar production via HTC technologies.

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Addressing the global climate crisis requires significant decarbonization in the fuel and energy sectors. BECCS is expected to be crucial. However, a significant portion of biogenic waste is highly moist, making it challenging to convert using standard thermochemical procedures, which call for an energy-intensive drying pretreatment. Using a heated, compressed aqueous solvent, hydrothermal carbonization is a process that turns carbonaceous materials into solid hydrochar, condensable gas (bio-oil), and non-condensable gas (mostly CO<sub>2</sub>) without any drying step. With the use of HTC-based technologies, this study seeks to identify the best process schemes and operating conditions for hydrochar production from local algae waste. Acidic bio-oil and gas are combusted for electricity generation along with hydrochar main product. Process simulations were combined with economic calculations using a cash flow analysis over the lifetime of the plant to estimate the Levelized Cost of Hydrochar production (LCOHC). A sensitivity analysis was completed to assess the effect of the selling cost of byproducts such as electricity.

HTC-based technologies are an efficient waste conversion process, with char efficiency of roughly 58% combined with net electrical, bringing an overall efficiency of 68.99%. Due to significant heat losses in the power unit, electrical output impact is little leading to 180 €/t of LCOHC assuming an electricity selling cost of even at 60 €/MWh. It should be noted that if the saving from the carbon tax (up to 100 €/ton-CO<sub>2</sub>) is applied to the electricity selling price, the HTC based hydrochar will become more attractive.

Nevertheless, hydrochar production remains costly within the current scenarios, compared to other technologies such as pyrolysis. Better feedstock pricing policies and appropriate carbon taxation may eventually result in lower final product costs, making the HTC technologies practical for use in the industry.

**Keywords:** Hydrothermal Carbonization (HTC), Process simulation, Techno, economic assessment, Algae valorization.

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# No Vacuum Monotube CPC Receiver for Linear Fresnel Concentrator: CFD Modelling and Simulation

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To improve the thermal performance of a **no vacuum monotube receiver** equipped with a **compound parabolic collector (CPC)**, a comprehensive investigation of **temperature distribution and heat losses** is crucial. Achieving accurate results necessitates the development of an accurate model that closely represents **real-world operating conditions**. In the present work, the modes of heat transfer conduction, convection, and radiation were simulated using the CFD method within ANSYS Fluent to thoroughly assess temperature profiles and heat loss. The analysis **identified critical temperature zones and heat loss points** within the receiver for a **target operational range of 130°C to 300°C**. The findings indicate that the majority of heat loss occurs through the glass cover, with conductive heat transfer from the secondary reflector to the glass cover being a dominant heat exchange. **The junction between these two components was identified as a critical point, with a high risk of glass failure, particularly at the extremities.** To assess the validity of neglecting solar radiation absorption by the glass cover and secondary reflector, a comparative analysis was conducted. Heat losses and temperature distributions were evaluated under three conditions: considering the absorbed flux by both the glass cover and the secondary reflector, considering only the absorbed flux by the glass cover, and neglecting absorption by both components.

**Keywords:** Linear Fresnel Collector, CPC monotube receiver, Free convection, Infra, red radiation, CFD simulation, Temperature, Heat loss.

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\*Speaker

# Numerical analysis of phase-change materials cooling with different fin configuration to enhance the Photovoltaic panel performance

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Photovoltaic technology is one of the most important components of the renewable energy sector, converting sunlight into electricity through semiconductor materials. The efficiency of PV panels typically ranges from 15% to 20%, which has led to extensive research to improve their performance. Surface temperature plays a crucial role in the efficiency of PV modules; For every 1°C increase in surface temperature, the efficiency decreases by 0.5%. This study used a 2D numerical model using computational fluid dynamics (CFD) to explore the integration of phase change materials (PCM RT25) in cooling systems with and without fins. The analysis revealed that most of the melting of the PCM occurred as a result of natural convective heat transfer on the back of the PV panel, while the PCM near the cooler channel side remained solid due to its low thermal conductivity. To enhance conductive heat transfer and thermal homogeneity, new fins with various configurations, such as the height and angle of the fin root, are evaluated and compared. The results indicated that heat exchange was driven by both conduction and convection, with natural convection playing a dominant role. It is worth noting that the innovative Y-shaped fins (5 fins) reduced temperatures by 2.8% compared to the finless PCM channel for 3 hours under a uniform heat flux of 300 W/m<sup>2</sup>, which greatly enhances the performance of the PV panel.

**Keywords:** Photovoltaic Panel, Phase change material, Fins, Heat sinks, Natural convection.

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# Measurements and Modeling of Thermophysical Properties of Binary Mixtures of DBE with Alcohol

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The economic and environmental problems caused by excessive fuel consumption have posed a threat all over the world. A strategy that has come into increasing focus recently is to exploit different sustainable energy sources to replace conventional petroleum fuels. Among these alternative fuel sources, biofuels are considered as the strongest contender because of their significant reduction in greenhouse gas emission and production cost. The reformulation of gasoline includes certain oxygenated compounds such as alcohols and ethers. These oxygenated compounds are added to improve the octane rating and pollution-reducing capability of gasoline. This work has been carried out as a part of the project to investigate the thermophysical behavior of liquid mixtures of the oxygenated compounds included in a hydrocarbon mixture. The main purpose of the present work is to investigate the thermophysical properties for binary system formed by two oxygenated compounds, such as dibutyl ether and 2-propanol. In this work, densities, viscosities, refractive indices, for binary mixture dibutyl ether + 2-propanol, are reported at  $T = (298.15 \text{ and } 313.15) \text{ K}$  and at atmospheric pressure. The experimental results are used to calculate some derivative properties such as: excess volumes, deviations in viscosity and deviations in refractive index. The derivative properties were fitted by using the Redlich-Kister equation. The Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) Equation of State was used to predict the experimental data of density for the studied binary mixture.

**Keywords:** Thermophysical Properties, Oxygenated Compounds, Ether, Alcohol, Modeling, PC SAFT EoS

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# Parametric Study of Polymer Electrolyte Membrane Fuel Cell Performance, challenges and opportunities

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Hydrogen has the potential to address energy and environmental concerns, and fuel cells are efficient devices that convert chemical energy into electrical power. Unlike traditional petroleum products, fuel cells produce low pollution and can be supplied by an abundant fuel source. Among the various fuel cell technologies, polymer electrolyte membrane fuel cells (PEMFC) are the most popular and widely used due to their benefits, including low operating temperature, rapid response, high efficiency, and high power density. PEMFCs are essential for hydrogen technology, which is the focus of our study. This paper presents a comprehensive numerical simulation of a PEMFC using MATLAB/Simulink software. The Simulink model was used to identify the impact of fuel flow rate on various parameters in a fuel cell stack, affecting the efficiency of the PEMFC. Meanwhile, MATLAB code generated two-dimensional and three-dimensional results based on an analytical model, revealing that activation losses, ohmic losses, and mass transport losses play significant roles in power generation. Our analysis of the electrical output of a PEMFC supplied with pure hydrogen and oxygen gas showed a strong dependence on the current density. Additionally, our examination of the impact of air and hydrogen pressure and temperature on PEMFC performance yielded important insights. This study contributes to a better understanding of PEMFCs and provides valuable insights for the practical application and optimization of PEMFC technology in various settings.

**Keywords:** Energy, Hydrogen, Fuel Cell, Proton Exchange Membrane.

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\*Speaker

# Flow topology of turbulent 2D natural convection within an enhanced air channel cooling attached behind photovoltaic panel

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The photovoltaic panel is a crucial renewable energy source, particularly important as fossil fuel reserves dwindle and greenhouse gas emissions rise. PV panels utilize semiconductor materials to convert solar irradiance into electricity. Despite advancements in PV technology, the electrical efficiency of PV panels remains around 15% to 20% (1), with the remainder of the energy being converted into heat. This heat surplus decreases PV panel efficiency by 0.5% for every 1°C increase in operating temperature (2). To address this issue, various cooling methods have been investigated and compared. This study analyzes the flow topology of turbulent 2D natural convection within an enhanced air channel cooling system attached behind a PV panel. Different cooling channel configurations were examined, including channel depth, fin height and inclination, and the size of secondary apertures. The results indicate that the optimal configuration for channels without fins has a depth of 15 mm, achieving a wall temperature of 359.68 K. For finned channels, a setup with 10 fins covering two-thirds (2b/3) of a 120 mm depth channel with 2 mm thickness reduced the average temperature by 5.9% compared to the standard channel without fins. Optimized configurations for the new channel design include 15 mm secondary apertures, 5° inclined fins, a fin height of 60 mm, and a channel depth of 15 mm. These parameters significantly enhance heat transfer and reduce heat accumulation by renewing the air through these openings, providing an effective solution for thermal management in vertical ducts. The new channel design achieves a temperature of 326.86 K, improving hot wall temperature by 4.31% compared to the channel with horizontal fins in the optimal configuration and by 9.12% compared to the vertical channel without fins at an optimal depth of 15 mm.

**Keywords:** Photovoltaic panel, Heat transfer, Turbulence model, Natural convection, Heat sink, Finned channel, CFD simulation

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\*Speaker



## **Theme 2: Phosphoric and nitrogen-based Fertilizer**

# A review on granulation process in the phosphate fertilizer production : Experiment studies and modeling by CFD approach

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The identification of hydrodynamic flow regimes and determination of behaviors are the important tasks in the design and scale-up of fertilizer granulation processes. This work reviews most hydrodynamic studies performed for flow regime identification in Drum granulator reactors. It begins with a brief introduction to the granulation process in phosphate fertilizer industries. The second section examines both various flow regimes and experimental methods for measurement of flow regime transition. A few experimental studies are presented in detail, followed by the effect of operating and design conditions on flow regime transition. A table summarizes the reported experimental studies, along with their operating and design conditions and significant conclusions. The next section deals with the current state of transition prediction, and includes purely empirical correlations, semi-empirical models, linear stability theory, and Computational Fluid Dynamics (CFD) based studies.

**Keywords:** Fertilizer, Granulation, Drum granulator, Flow regime, CFD approach, CFD, Modeling, hydrodynamic

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# Theme 3: Waste Water Treatment – Desalination – Brackish water treatment

# Desalination in Morocco: Past, Present, and Future – A Short Systematic Review

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This paper presents a systematic brief review of desalination technologies in Morocco, the country faces significant challenges related to water scarcity, a situation driven by a combination of climatic, demographic, and economic factors. focusing on the country's history and recent technological advancements. Desalination has been a significant part of Morocco's water supply system for decades, initially focusing on small-scale plants for coastal communities and agricultural activities. However, the country has expanded its capacity to meet rising freshwater demand and climate change challenges. Recent advancements in desalination technologies include advanced reverse osmosis systems, hybrid desalination systems, and the integration of renewable energy sources like solar and wind power. The country is also actively researching advanced membrane technologies, nanotechnology, and brine management solutions to address environmental and economic challenges associated with desalination. The review highlights Morocco's progress from traditional methods to advanced, sustainable technologies, positioning it as a global leader in water security.

**Keywords:** desalination in Morocco, recent advancement, systematic review.

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\*Speaker

# Design and filling of infiltration-percolation columns for Olive Mill Wastewater treatment with hydrodynamic flow study using sawdust and straw as adsorbents

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Olive Mill Wastewater (OMW) is an industrial by-product generated during the olive oil production process, presenting a significant environmental challenge for oil-producing nations. Its heightened acidity, conductivity, and substantial concentration of organic matter, predominantly composed of phenolic compounds, contribute to the toxicity and the characteristic red-brown to black color of OMW. To address this ecological concern, we conducted an experimental study focusing on its treatment using a sophisticated hybrid system. This system integrates innovative technologies, combining adsorption and infiltration-percolation. This study focuses on the second treatment, 'infiltration-percolation,' implemented through columns filled with alternating layers of permeable material (Pozzolan) and impermeable material (sand, natural adsorbent, activated charcoal, iron, natural adsorbent). To fill these columns, a preliminary study was conducted to select adsorbents that offer a high rate of COD and polyphenol elimination. An adsorption test was conducted under constant conditions using wheat bran, sawdust, peanut shells, pomegranate peels, straw, shrimp shells, and chicken feathers. Sawdust, straw, and chicken feathers were chosen as natural adsorbents due to their remarkable efficiency in remov-

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ing phenolic compounds, achieving percentages of up to 32%,19,3%, and 38% 19,3% respectively. The filling percentage relative to the impermeable layer was determined by testing various percentage combinations to identify the combination that provides significant elimination in terms of COD and polyphenols. These columns will be tested with OMW treated through adsorption and with OMW treated through adsorption and diluted with wastewater. Additionally, a small-scale hydrodynamic study was conducted by monitoring the content of KBr and the concentration of polyphenols to characterize the flow within the different proposed percentages.

**Keywords:** OMW, Infiltration, percolation, Adsorption, COD, Polyphenols, Hydrodynamic

# Multi-residue methods for the analysis of priority organic micropollutants in aqueous environmental matrices

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## Abstrait

Priority organic micropollutants (drug residues) present in the environment and the potential risks associated with them have become a matter of current concern. The knowledge and techniques for the analysis of these substances in human biological matrices such as blood plasma, urine and serum are well documented and mastered. On the other hand, awareness of the presence of these micropollutants in the environment is relatively recent, and the experimental challenges involved mean that this area remains largely unexplored. The analysis of aqueous environmental samples is constantly evolving, with increasingly selective extraction techniques.

The liquid-solid extraction method: Solid phase separation (SPE) involves preconcentrating the diluted sample and minimizing the loss of the analytes of interest, using different types of cartridges such as **Isolute**, **ENV+**, **Oasis HLB**, **Oasis MCX/ Oasis MAX**, depending on the physicochemical properties of the analytes. The separation, detection and quantification of these analytes requires a more powerful system, such as high performance liquid chromatography-ultraviolet coupled with mass spectrometry (**HPLC-UV/MS**), liquid chromatography coupled with tandem mass spectrometry (**HPLC-MS/MS**), to increase the number of analytes, The multiplication of the original analytical strategies for drug residues makes it possible to increase the sensitivity and to separate the matrix components to be studied, thus improving the specificity and the quality of the analyses.

The management of an environmental matrix is chronologically divided into pre-treatment, extraction, purification and concentration stages, designed to allow detection and quantification. This review describes these strategies.

**Keywords:** Priority organic micropollutants, drug residues, solid phase separation (SPE), cartridges, multi, residue methods

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# INTEGRATED PROCESS FOR ELECTROCHEMICALLY ASSISTED BATTERY MATERIAL RECOVERY: Modeling and Techno-Economic Assessment

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The increased use of Lithium-ion batteries in various applications including electric cars, portable equipment, and tools, creates a serious environmental challenge regarding their waste management. This study aims to develop a techno-economic model of the system to analyze the economic viability and different operating scenarios. Our system involves a hydrometallurgical process that is supported by electro dialysis for the regeneration of valuable compounds and proper management of waste liquid, the technique also uses the carbon capture unit (CCU) to enhance the sustainability of the system and use the electro dialysis by-product to close the system loop.

The system involves leaching the lithium cobalt oxide (LiCoO) cathode material using a sulfuric acid solution and hydrogen peroxide as leaching solution under defining parameters. Therefore, the leaching process provides us with complete efficiency for both lithium and cobalt recovery. Following leaching, a precipitation process recovers the solids, lithium carbonate, and cobalt oxalate. Finally, an electro dialysis system is employed to treat the remaining waste containing sulfate and sulfuric ions. This system effectively filters the waste and regenerates valuable components which are sulfuric acid and caustic soda. The system operates in a closed loop, where the regenerated components from the electro dialysis system are reused in the hydrometallurgy process and the CCU process, to reduce the consumption of these components.

The results indicate that this integrated process not only maximizes resource recovery but also significantly reduces environmental impact compared to conventional recycling methods. The findings suggest that scaling up this process could provide a viable industrial solution for the sustainable recycling of lithium-ion batteries, contributing to a circular economy in the energy storage sector

**Keywords:** LiB Recycling, CO2 Capture, Waste liquid valorisation, Hydrogen production, Closed loop.

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# Biosynthesis of iron oxide nanoparticles as efficient material for dyes degradation

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The world is facing a one of its biggest problems with water pollution, prompting ongoing scientific research into wastewater treatment solutions. Textile dyes present a significant hazard to human health and to environment, due to their resistance to biodegradation. Various conventional methods have been used to treat these organic pollutants. However, the heterogeneous Fenton process has emerged as one of the most efficient and effective alternatives, often resulting in near-complete degradation.

In this research, biosynthesized iron oxide nanoparticles were applied in the heterogeneous Fenton process to degrade tartrazine, as a mostly applied azo dye. The formed products were characterized using X-ray diffraction, Fourier transform infrared spectroscopy, scanning electron microscopy and energy dispersive X-ray.

The influence of degradation parameters chosen were examined using the Box Behnken design (BBD). The statistical results indicate that the biosynthesized iron oxide nanoparticles in a heterogeneous Fenton-like process are highly effective for advanced wastewater treatment.

**Keywords:** Biosynthesis, Iron oxide nanoparticles, Heterogeneous Fenton like process, tartrazine, Box Behnken design.

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# Investigating Erosion Dynamics in Straight Hydraulic Channels Under Applied Wave: Effects of Viscosity and Water Depth Using the Lattice Boltzmann Method

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In this study, the Lattice Boltzmann model for shallow water equations (LABSWE) was used to investigate the influence of viscosity and water depth on channel walls under wave action. The findings indicate that increased viscosity leads to higher shear stress and enhanced frictional forces at the fluid-solid interface, which increases the potential for channel erosion due to intensified mechanical wear. Additionally, the study reveals that lower water depths result in steeper velocity gradients near the walls, further elevating shear stress and erosion potential. These insights are crucial for predicting and mitigating erosion in hydraulic channels and similar structures, emphasising the importance of considering both viscosity and water depth in their design and management.

**Keywords:** LABSWE, viscosity, water depth, straight channel, shallow water flows

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# Valorization of olive mill wastewater as a potential green algaecide to control the potentially toxic cyanobacterium in aquatic ecosystems

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The anticyanobacterial raw effect of olive mill wastewater (OMW) was tested as a potentially sustainable solution to control the toxic cyanobacterium. In the present study, the effects of raw OMWW on cyanobacterial were assessed using microdilution and disc diffusion approaches. The growth and photosynthetic pigments of cyanobacterial in response to ROMW were investigated in an experimental bioassay. The potential allelochemicals were detected by High performance liquid chromatography (HPLC). The highest inhibition rates (IRs) reached 92 and 96% under the two highest concentrations of ROMW (3.125 and 6.25 mg L<sup>-1</sup>) only after 4 days (d) of experimentation. Then, it achieved 97% on 10d under both ROMWW treatments. The results of Chl-a and carotenoid contents significantly decreased following exposure of cyanobacterial to higher concentrations. Overall, the obtained results demonstrate that ROMWW might be proposed as eco-friendly alternative algaecides to control cyanobacterial harmful algal blooms (CyanoHabs) in aquatic ecosystems.

**Keywords:** cyanobacterial, OMW, photosynthesis, control, growth, blooms

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\*Speaker

# Study of the Energy Efficiency of a Aerated Lagoon Wastewater Treatment Plant at Hattane - Morocco

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Aerated lagoon technology is an innovative extensive process that improves on the natural lagoon process initially recommended nationally for treating wastewater from small and medium-sized towns. However, like processes based on the use of energy to aerate biomass, this system requires greater consumption of electrical energy. The aim of this study is to investigate the energy efficiency, an important criterion in wastewater treatment, of this process at the Hattane wastewater treatment plant near the town of Khouribga in central Morocco.

The purification performance of this plant, which treats an average flow of 750 m<sup>3</sup>/d and was built in May 2018, was also evaluated by monitoring the principal purification parameters, in particular those subject to release limits into the natural environment, such as BOD<sub>5</sub>, COD and TSS. This analysis showed that the results were more than satisfactory, and much better than treatment by natural lagoon, while offering the possibility of reusing the purified water, which is much in demand considering the water stress that Morocco is currently suffering.

The analysis of the WWTP's energy efficiency made it possible to evaluate the plant's energy aspects and the measures designed to optimise the operation and maintenance of the electrical machines. This important feedback can help to improve the design and management of similar plants, in particular the importance of automated water quality analyses to control energy input and define the most reliable design rules.

**Keywords:** Wastewater treatment, Aerated lagooning, Performance assessment, Energy efficiency

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# Advanced material synthesized from straw for treatment of the OMW by adsorption

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The olive oil industry is an important socio-economic production in the Mediterranean country due to the beneficial proprieties on human health. The production process generates two residues as follows olive pomace (OP) and olive mill wastewater (OMW). This manufacturing is loaded with high-organic compounds characterized by negative effects on the environment, which is why several researchers have been interested in the treatment of these rejects, specifically OMW management because OP is simple to be valorized as combustible materials, livestock feed, and adsorbent. The focus of this work is to achieve the regulatory exigence of the OMW discharge as an effluent without any impact on the environment. Therefore, multiple treatment processes are proposed to reduce the acidity and the organic charge of the OMW precisely phenolic compounds that are responsible for the phytotoxic effect, such as membrane separation, coagulation-flocculation, advanced oxidation, biological degradation, and adsorption (1). The development of the adsorption efficiency was explored in this work, by using straw (SW) as a precursor material for carbon to produce activated carbon (AC), the synthesis was adopted by the combination of chemical and thermal treatment and using phosphoric acid H<sub>3</sub>PO<sub>4</sub> as an activating agent to favors more actives sites for the improvement of adsorbates-adsorbent interaction. The concentration variation for H<sub>3</sub>PO<sub>4</sub> at 63 and 85 % was studied. Also, the temperature influence on the porous structure at 400°C and 600°C was suggested. The treatment

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efficiency was determined by the measurement of the chemical demand of oxygen (COD) and polyphenols (2). The characterization of the SW and AC to compare the morphological surface difference by SEM, and functional group characteristics of both materials by FTIR analysis were used. This result demonstrated the elimination of 86 % and 63 % for polyphenols and COD, respectively. Hence, the adsorption isotherm, kinetics, and thermodynamics were adopted to explain the adsorption mechanism for AC.

**Keywords:** OMW, COD – Polyphenols – Adsorption – sawdust, activated carbon, Phosphoric acid

# Pollutant removal efficiency and antifouling enhanced by adding bentonite clay to the aerobic ceramic membrane bioreactor treating real wastewater from pharmaceutical industry.

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This research investigated the influence of incorporating bentonite clay, with concentrations ranging from 1.5 to 10 g/L, into a pilot-scale aerobic ceramic membrane bioreactor (AeCMBR) employed for the treatment of pharmaceutical wastewater (PhWW). The hydraulic retention time (HRT) was maintained at 24 hours, and dissolved oxygen levels ranged between 2 (during operation) and 4 (during idle periods). The study evaluated the rates of removal of organic pollutants, nitrogen compounds, and heavy metals (Cu, Ni, Pb, Zn). The efficiency of chemical oxygen demand (COD) removal surpassed 82%. The addition of bentonite enhanced the removal of ammonia (NH<sub>4</sub><sup>+</sup>) to 78%, with a notable 38% improvement observed with the addition of 5 g of bentonite compared to phases without its presence. The average nitrate concentration decreased from 169.69 mg/L to 43.72 mg/L. Removal rates for Cu, Ni, Pb, and Zn averaged 86%, 68.52%, 46.90%, and 56.76%, respectively. Incorporating 5 g/L of bentonite significantly mitigated membrane fouling. The combination of AeCMBR and bentonite adsorption demonstrates promising efficacy in treating high-strength wastewater.

**Keywords:** Keywords: Pharmaceutical wastewater, Bentonite, Membrane bioreactors, Nitrogen removal, Heavy metal, Adsorption, Fouling mitigation

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# Nitrate removal from water using adsorption and flocculation

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In the context of water stress in Morocco, it is an imperative to take advantage of all available water resources, including the resources that contain pollutants that are difficult to treat and require special technologies to do so.

Ground water contamination with nitrate is widespread in agricultural areas that misuse fertilizers and in the vicinity of raw wastewater effluents. As a result of that, precious water resources become unusable for the production of drinking water, especially around urban areas where drinking water consumption is higher.

Nitrate removal from water using reverse osmosis or ion exchange resins can be cost prohibitive and water resources that have become contaminated with nitrates are generally abandoned or used sparingly in combination with another resource that acts as a dilutant.

This work aims at exploring the use of a combination of technologies that are less costly (adsorption, coagulation/flocculation, bioflocculation), in order to lower nitrate concentrations and produce a water that conforms to the Moroccan drinking water guidelines.

**Keywords:** drinking water, nitrates, adsorption, coagulation, flocculation, bioflocculation

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# Towards Integrated Water Management at the Faculty of Sciences Ben M'Sick in Casablanca (Morocco): Experimental wastewater treatment using a pilot Biological Membrane Reactor (MBR)

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In Morocco, pursuant to the provisions of Framework Law 51.17 concerning the reform of the national training and education system and its strategy for 2030, universities are mandated to welcome and train students in sustainable campuses. Consequently, environmental considerations must be integral to the comprehensive management of water resources, liquid effluents, energy consumption and solid waste disposal.

In this context, with the objective of assessing the feasibility of implementing a "zero liquid discharge" approach at the Faculty of Sciences Ben M'sick (FSBM), laboratory-scale wastewater treatment experiments were conducted utilizing pilot Membrane BioReactor (MBR). This laboratory experiment employed a purifying biomass previously acclimated over a period of 28 days.

During this experimental treatment using the modular pilot system of Activated Sludge (AS) and MBR, the recorded purification performances were notably high, with reduction rate of 98% for Chemical Oxygen Demand (COD), 99% for Biochemical Oxygen Demand (BOD5), 98% for Total Suspended Solids (TSS), 95% for Total Kjeldahl Nitrogen (TKN), and 69% for Total Phosphorus (TP). The treated effluent met the standards for indirect discharge and irrigation water quality for all studied parameters (TSS, COD, BOD5, TKN, TP, HCO<sub>3</sub>, Electrical Conductivity (EC) and Fecal Coliforms), except for pH (6.4), Chloride (995 mg/L), and Nitrate (58 mg/L) in the AS treatment and pH (5.45), Chloride (1583 mg/L) and Nitrate (176mg/L) in MBR treatment.

These results underscore the promising potential for reuse of treated water within the FSBM campus. Nonetheless, a complete analysis of their trace metal element content and their salinity is imperative to accurately evaluate the efficacy and long-term sustainability of this reuse.

**Keywords:** Wastewater, Treatment, MBR, Reuse, University Campus, FSBM

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# Efficient removal of methylene blue and methyl red dyes using a novel adsorbent derived from *Saponaria officinalis* Root via H<sub>3</sub>PO<sub>4</sub>, H<sub>2</sub>SO<sub>4</sub>, and KOH-activation: Optimization, kinetics, and isotherm study

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In this study, a novel adsorbent, activated carbon derived from *Saponaria Officinalis* root, was prepared by optimizing the experimental factors influencing iodine adsorption. The effects of chemical agents, impregnation time, and activation temperature on iodine adsorption were examined. The findings revealed that chemical agents had the most significant impact on iodine adsorption. The novel adsorbent exhibited iodine adsorption capacities ranging from 336.42 to 1250.09 mg/g. The optimal conditions for preparing activated carbons with high iodine adsorption capacity were found to be an impregnation time of 24 hours, the use of H<sub>2</sub>SO<sub>4</sub> as the chemical agent, and a carbonization temperature of 650°C. The raw *Saponaria Officinalis* root was characterized using TG/DTG, and the optimal activated carbon was characterized using SEM, XRD, FTIR, BET, and pH Point Zero Charge. The optimal activated carbon was further utilized for adsorption studies involving methylene blue and methyl red. The experimental equilibrium data fitted to the Langmuir and Freundlich isotherm models demonstrated the suitability of the Langmuir model. Analysis of the experimental adsorption data using kinetic models, such as the pseudo-first-order and pseudo-second-order models, indicated the applicability of the second-order model. These results suggest that *Saponaria Officinalis* root is a promising precursor for producing highly mesoporous activated carbon.

**Keywords:** Adsorption Activated carbon, *Saponaria officinalis* root, Methylene blue, Methyl red, Experimental design

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# Optimizing constructed wetlands for agricultural irrigation: A Study on Locally available adsorbing materials in Morocco

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Constructed Wetlands (CWs) provide a sustainable, cost-effective, and energy-efficient approach to wastewater treatment and reuse, particularly in remote and rural areas. Recently, the use of adsorbing materials in CWs has garnered significant attention owing to their ability to improve treatment efficiency. These active media are highly effective at removing a wide range of contaminants, including heavy metals and emerging pollutants, through various processes such as adsorption, precipitation, complexation, and biofilm development.

The objective of the present study is to explore the adsorption capacity of several low-cost and locally available materials in Morocco and determine their feasibility as substrates for CWs. To achieve this, batch and column adsorption studies were conducted on different materials, namely: limestone (LS), mining residues (MR), clay (RC), and pozzolan (POZ), to evaluate their effectiveness in removing cadmium and copper. Afterwards, different combinations of selected materials were used in vertical constructed wetlands mesocosms supplied with domestic wastewater. The CW mesocosms were operated in batch feeding mode with varying hydraulic retention times (24 hours, 48 hours, 72 hours).

In the batch adsorption experiments, contact time and initial metal ion concentration were analyzed and modeled using kinetic and isotherm equations. The findings demonstrated a significant removal efficiency for copper, with all materials achieving up to 99% removal at an

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\*Speaker

initial concentration of 10 mg/l. Limestone and Mining residues exhibited the highest adsorption capacity for cadmium, achieving up to 98% removal, followed by pozzolan, and clay. These results indicate that these materials are highly effective as adsorbents and could be incorporated in constructed wetlands to enhance their performance.

**Keywords:** Adsorption, Constructed wetland, Wastewater treatment, Wastewater reuse.

# Production of a natural flocculant: Comparison of the effectiveness between cactus and nettle in water treatment.

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The thickening process is important in different industries especially those using water in their production, in order to increase the solid sludge concentration and to recover water that is as clear as possible. Recently, many advances have been achieved in the development of alternative green and sustainable technologies in chemical engineering (1,2).

The aim of our thesis is to propose a natural alternative to the chemical flocculants used in wastewater treatment, saving a large proportion of water that would be, then, recycled and reintroduced into the process.

Our alternative concerns the production of a bio-flocculant based on a plant resistant to arid and semi-arid climates, which is the "cactus". The process involves sourcing and storing the raw material, cleaning the rackets, grinding and filtering and finally centrifuging and extracting a flocculant juice that can be used directly or after the conservation and storage.

In this study, laboratory tests were carried out to evaluate and highlight the performance of cactus "Opuntia Ficus Indica" in water treatment and compare it's efficiency with other plants such us "Nettle".

**Keywords:** Flocculant, Cactus, Nettle, waste water treatment

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# Conservation of a Bio-Flocculant Produced from Cactus Paddles "Opuntia ficus indica" for Use in Water Treatment

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Wastewater treatment has become a crucial issue due to the increasing decline in water resources and the exploitation of this vital product at the individual and industrial levels. The bio-flocculant extracted from "Opuntia Ficus Indica" cactus rackets has demonstrated effectiveness comparable to synthetic flocculants that are used on the market. However, it remains a major challenge to maintain the produced bio-flocculant in good condition for prolonged use. This study aims to develop efficient methods for the conservation of bio-flocculant extracted from cactus and to evaluate its effectiveness in water treatment after storage.

The cactus rackets were harvested, cut, crushed and filtered to extract the juice. Different conservation methods have been tested in order to maintain the same flocculating effectiveness of the latter. These tests were accompanied by the measurement of some key parameters to better monitor the evolution of conservation over time.

Preliminary results show progress in maintaining the long-term efficacy of bio-flocculants. This research will have a significant effect on the field of industrial water treatment, since it will offer a sustainable and ecological solution in this aspect.

The conservation of bio-flocculant extracted from the "Opuntia Ficus Indica" cactus represents a great advance in the field of water treatment with bio-flocculants, because the advancement of work on this approach will contribute to eliminating the difference between the use of the latter and the use of chemical flocculants which already have a long shelf life.

**Keywords:** Bio, flocculant – Cactus – Opuntia Ficus Indica – Conservation

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# Application of machine learning techniques for improving the performance of water desalination systems in Morocco

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The most pressing global issue of the 21st century is water scarcity, with less than 3% of the Earth's water being potable, the rest is salt. In our Morocco, rising water demands and climate change-induced precipitation decline strain groundwater resources, necessitating unconventional solutions like brackish water and seawater desalination. However, desalination faces several challenges such as high energy consumption, environmental concerns over brine disposal, and substantial infrastructure costs. In our research and in response to these challenges, we aim to employ the machine learning techniques to analyze data and predict patterns, the machine learning models allows optimizing processes, enhancing efficiency, and reducing costs. They enable proactive maintenance, minimize downtime, and improve overall system performance. At this stage, the research is focusing on acquiring essential data on desalination plants in Morocco (city, technology used, water source, starting year, production capacity), water desalination policy in morocco, etc.

**Keywords:** water scarcity, brackish water, seawater, desalination, machine learning techniques

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\*Speaker

# Optimization of Reverse Osmosis demineralization: Prediction of silt density index using machine learning models machine learning models

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The efficient operation of reverse osmosis (RO) demineralization plants for brackish water treatment requires optimized monitoring strategies to minimize performance losses and membrane fouling. Monitoring RO parameters, which are nonlinear and complex, along with manual calculations and laboratory tests, are essential for this purpose. This study focuses on predicting the fouling indicator, Silt Density Index (SDI), using Machine Learning (ML) models. A dataset of RO feedwater physicochemical parameters, collected from January 24, 2020, to October 4, 2023 was used to train and validate five ML models: k-nearest Neighbor (kNN), Support Vector Regression (SVR), Random Forest (RF), and Artificial Neural Network (ANN). Evaluation measures, including correlation coefficient ( $r$ ), root mean square error (RMSE), and relative bias (RBIAS), were used to assess model performance. The results indicate that all models generated accurate predictions of SDI, with the RF model showing superior accuracy (the correlation coefficient de 98%). Additionally, the analysis revealed the significant influence of certain physical water parameters, such as electrical conductivity, turbidity, temperature, pH, iron, and RedOx potential, on SDI predictions. These results underline the importance of closely monitoring these parameters at the plant inlet to optimize system performance and demonstrate the potential of ML models in SDI prediction, offering valuable information to improve the management and efficiency of demineralization plants.

**Keywords:** Silt Density Index, Dataset, Prediction, Machine Learning, Demineralization, Reverse Osmosis.

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\*Speaker



# The adsorption of anionic and cationic dyes in aqueous solution on activated carbon produced from *Thapsia transtagana* stems: Insights from experimental, MD simulation, and DFT calculations

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This study aims to evaluate and understand the adsorption of methyl orange (MO) and methylene blue (MB) by activated carbon from *thapsia transtagana* stems (ACTTS) under different experimental conditions. Textural and structural properties of ACTTS adsorbent were observed by FTIR, XRD, SEM-EDX, potentiometric titrations and point of zero charge. Various initial values of the solution pH, adsorbent dose, temperature, reaction duration, and initial dye concentration were used in experiment series. The Langmuir and Freundlich models were used to assess the equilibrium isotherm data. Kinetic data were analyzed using pseudo-first order and pseudo-second order kinetic models. In order to obtain information regarding the electronic properties of dyes and its adsorption mechanism that has not been experimentally seen, we also used molecular dynamic (MD) simulation and DFT-based computational approaches. According to experimental findings, the pseudo-second order kinetic model and Langmuir model accurately describe the adsorption phenomenon. Maximum adsorption occurred at neutral to basic pH values for MB and neutral to acid pH for MO. The process was exothermic in nature and accompanied by a decrease in entropy. The Gaussian 09W program was used to assess the MO and MB structure at the B3LYP/LANL2DZ level. The analyzed quantum descriptors provided support for the study's experimental findings.

**Keywords:** *Thapsia Transtagana* Stems, Activated carbon, Synthetic dyes, thermodynamics, molecular dynamic, DFT calculations.

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# Recent advances and modification strategies of semiconductors for the photocatalytic remediation of water containing organic pollutants

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Synthetic organic dyes used in many industries present a major source of water contamination. The presence of these pollutants in water will produce negative effects on the aquatic organisms and ecological environment due to their resistance to natural degradation. In this context, numerous water treatment techniques methods including degradation by coagulation, ozonation, electro dialysis, electrochemical degradation and adsorption have been treated. Heterogeneous photocatalysis, an advanced oxidation process, has garnered extensive attention in environmental remediation for several reasons, including its simplicity, low cost, reproducibility, manageability, and efficiency. Various metal oxide (TiO<sub>2</sub>, WO<sub>3</sub>, SnO<sub>2</sub>, ZnO, Cu<sub>2</sub>O, CeO<sub>2</sub> and Fe<sub>2</sub>O<sub>3</sub>)-based semiconductors have been explored as excellent photocatalysts to degrade organic pollutants in wastewater. However, their photocatalytic performance is limited due to their high band gap (UV range) and recombination time of photogenerated electron-hole pairs. Different strategies for improving the performance of these metal oxides in the fields of photocatalysis are discussed. To improve their photocatalytic activity, researchers have investigated the concept of doping, semiconductor combinations and the formation of nanocomposites.

**Keywords:** Synthetic dyes, Heterogeneous photocatalysis, Semiconductors, Doping, Nanocomposites.

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# Storage post-harvest of opuntia ficus indica and its impact on the efficiency of bio-coagulants flocculants extracted.

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The use of bio-coagulants-flocculants derived from natural plants is currently a major concern for wastewater treatment. In this study, we evaluated the effectiveness of juices extracted from the cladodes of *Opuntia ficus-indica* (Cactaceae) for treating synthetic water rich in clay. We also examined the correlation between the storage conditions of the plants and the efficiency of the extracted bio-products. The findings of this study emphasize the importance of proper storage conditions for the effectiveness of bio-products in wastewater treatment. The study tracked the degradation of the cladodes over a period of 161 days in three different storage locations : open air, an anaerobic closed location, and a refrigerator at 0°C. The cladodes stored in the open air showed the highest resistance to microbial degradation, followed by those stored in the refrigerator. However, the cladodes kept in the closed location experienced complete degradation before 161 days were reached. The juice extracted from the cladodes that resisted during the storage study was compared to juice extracted from another pad stored in the open air in an area unprotected from the weather. The results of coagulation-flocculation and settling tests showed that cladodes stored in the open air with and without weather protection, as well as those stored in the refrigerator, provided a turbidity reduction of 99.5%, 99.43%, and 99.17%, and a settling rate of 27.5 cm/min, 14 cm/min, and 14 cm/min, respectively. The tests demonstrated a strong dependence between post-harvest storage conditions and the efficiency of the extracted flocculant bio-coagulants.

**Keywords:** *Opuntia ficus indica* – Storage – post, harvest – Coagulation – Flocculation – Settling – Turbidity, wastewater treatment.

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# Utilizing Yellow Nightshade (*Solanum elaeagnifolium*) as a Natural Adsorbent for Dye Removal in Wastewater Treatment

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Dye pollution poses a significant environmental challenge with detrimental effects on aquatic ecosystems and human health. The indiscriminate discharge of colored effluents from textile and dyeing industries leads to persistent pollutants in water bodies due to the resistance of synthetic dyes to conventional treatment methods. Consequently, there is a pressing need to explore effective strategies for dye removal from wastewater. This study aims to evaluate the potential of Yellow Nightshade (*Solanum elaeagnifolium*) as a natural adsorbent for colorant removal, contributing to eco-friendly solutions for wastewater treatment. Through a comprehensive analysis of the plant's phytochemical composition and physical properties, the active compounds responsible for the adsorption process will be identified. Understanding the mechanisms of colorant adsorption onto Yellow Nightshade will better assess its efficacy as a natural adsorbent and its integration potential into wastewater treatment systems. This research highlights the significance of exploring natural alternatives to conventional methods, emphasizing the advantages of using Yellow Nightshade, such as its widespread availability, biodegradability, and cost-effectiveness. Adsorption experiments were carried out under different solution pH and contact time. Experimental results indicate rapid adsorption process with maximum adsorption capacity occurred in basic medium. The maximum adsorption capacities were 279.79 and 32.24 mg/g, respectively for MB and MO samples.

**Keywords:** dye pollution, wastewater treatment, Yellow Nightshade, adsorption, phytochemical composition, sustainable technologies.

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\*Speaker

# Enhancing Water Recovery with Hybrid Solar-Powered Desalination: Integration of RO and Thermal Processes for Sustainable Freshwater Production

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To address the increasing water scarcity, recent innovations have focused on developing energy-efficient solar desalination systems. Solar desalination is categorized based on energy usage: (1) thermal solar processes like thermal vapor compression (TVC), multi-effect distillation (MED), multi-stage flash (MSF), solar stills (SS), and humidification-dehumidification (HDH); (2) photovoltaic (PV) electric-powered systems, including mechanical vapor compression (MVC), electro dialysis (ED), and reverse osmosis (RO); and (3) photovoltaic/thermal (PV/T) hybrid systems. In PV/T hybrid desalination, thermal energy recovered from PV cells powers low-grade thermal desalination processes, while electrical energy supports membrane-based methods. PV/T systems can integrate with processes such as direct desalination, HDH, SS/HDH hybrids, membrane and non-membrane technologies (MED, MSF), as well as methods like MVC and adsorption. HDH is appreciated for its simplicity and cost-effectiveness, while RO remains widely used due to its low specific energy requirements. Integrating HDH-RO desalination with concentrated photovoltaic/thermal (CPV/T) technology represents a promising approach for hybrid desalination.

A novel hybrid system combining a solar-powered RO unit and a thermal desalination unit aims to enhance water recovery rates through the integration of an adsorption cycle, ejectors, and an HDH process. Here, brine from the RO system feeds into the thermal desalination unit to produce additional freshwater. The concentrated brine is then repurposed for salt extraction in solar ponds, maximizing waste utilization.

Theoretical and economic models indicate that this hybrid system achieves a recovery rate of up to 84%, compared to 40.8% in standalone RO, with feed salinity of 32,500 ppm and brine thresholds up to 110,000 ppm. This approach reduces freshwater production costs by 23–27% compared to standalone RO at feed salinities of 40,000–50,000 ppm for a plant capacity of 10 m<sup>3</sup>/day.

**Keywords:** Hybrid desalination, solar desalination, Reverse osmosis, salt extraction

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\*Speaker

# Multi-Criteria Analysis for Integrated Management of Irrigation Water Resources in the Chtouka Region

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With climate change and successive years of drought, conventional water resources are becoming increasingly scarce and unable to meet farmers' water needs. These conditions result in the overexploitation of groundwater despite the presence of non-conventional water resources. Faced with this situation, sustainable and efficient resource management is necessary. The objective of this work is to develop a decision-making tool using a combination of two multi-criteria analysis methods, AHP and TOPSIS, for the sustainable and efficient management of various irrigation water resources in the Chtouka Ait Baha perimeter.

To achieve the objectives of this work, the adopted methodology includes bibliographic research to understand all aspects of the addressed problem. Then, we conducted surveys in the study area among different management actors to gather information for the application of multi-criteria analysis methods.

The developed tool aims to identify the most optimal alternatives according to experts, allowing for the sustainable management of irrigation water resources in the area by using the weights of 7 selected criteria.

We chose 7 management alternatives: Coupling Desalination Plants with Renewable Energy (A1); Financing through Subsidies and Public-Private Partnerships (A2); Reuse of Wastewater for Agricultural Purposes (A3); Modernization of the Irrigation Network (A4); Accelerated Management of the Aquifer by Quotas (A5); Utilization of Brine for Watering Halophyte Crops (A6); Development of Drought-Resistant Crops (A7).

After applying the two methods, which were mainly based on the judgment of several stakeholders, we concluded that cost and sustainability are the most important criteria in decision-making regarding water resources. We also determined that the best solutions to improve water resource management in the area are the modernization of irrigation networks, the development of drought-resistant crops, and the acceleration of quota-based management.

**Keywords:** Desalination, Groundwater, Surface water, Chtouka perimeter, AHP, TOPSIS

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\*Speaker

# Removal of a textile Azo Dye Yellow Bemacid on Zn-Al Layered Double Hydroxides in Aqueous Solutions: Structural, Kinetic, Equilibrium, and Thermodynamic Studies

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This study investigates the removal of a textile dye using a (Zn-Al-Cl) layered double hydroxide (LDH). The LDH was synthesized through the coprecipitation method at a constant pH. Structural and morphological properties of the synthesized LDH were characterized using techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA-DTG), and pH point of zero charge (pH pzc) determination. Several parameters were optimized, including the solution pH, the contact time, and the temperature. Maximum adsorption capacity occurred at pH values below 9. The adsorption kinetics followed a pseudo-second-order model, and the process was governed by Langmuir physisorption, indicating monolayer adsorption on a surface with a finite number of identical sites. Thermodynamic analysis confirmed that the adsorption was a physisorption spontaneous and endothermic process.

**Keywords:** Textile dye, LDH, Water pollution, Adsorption, physisorption.

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## **Theme 4: Materials: Conception, Elaboration and Valorization**



# Preparation and characterization of anti-insect capsules based on essential oil to combat *Tribolium castaneum*

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Global consumption of cereals is really crucial, as they provide carbohydrate protein, and essential nutrients to millions of people. However, this precious resource is often threatened by *Tribolium*, which is a pest that can cause great economic and food losses. And so finding an effective and environmentally friendly solution to combat *Tribolium*, has become a necessity that is why essential oils have been proposed as potential alternatives to synthetic insecticides. In addition, encapsulation methods using alginate and calcium can increase the effectiveness of essential oils by preserving them from deterioration and providing targeted release. In order to test and evaluate the performance of various repellent properties of free and encapsulated essential oil, an experiment was carried out in the biotechnology laboratory. We sought to test the effectiveness of free and encapsulated essential oil at various concentrations to combat the red weevil of flours in the laboratory. In addition, the results showed that the encapsulated essential oil has a higher repellent effect against *Tribolium* compared to free essential oils. This is due to the fact that encapsulation allows a prolonged and controlled release of the active compounds, which increases their effectiveness in the long term. Free essential oils, on the other hand, degrade and evaporate quickly, which decreases their effectiveness in the long term.

**Keywords:** Encapsulation, Essential oil, Tribolium

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\*Speaker

# Optical and Thermal Characterizations with DFT Calculations of ZnMgS Mixed Crystals

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II-VI wide bandgap semiconductors are promising materials due to their potential applications in the field of solid-state devices such as photodetectors, light-emitting diodes (LEDs), and solar cells (1). The ZnMgS mixed crystals investigated in this work were grown from the melt using the vertical Bridgman–Stockbarger method in the whole range of composition  $0 < x < 0.34$  (2).

The energy gap as a function of the composition was determined by both transmission spectroscopy and photoluminescence. The temperature-dependent absorption measurements to study the temperature dependence of band gap energy were also performed. Based on these analyses, the relationship between the band gap energies and the Mg content are verified and discussed. In this work, the systematical study of the thermal properties of ZnMgS alloys was undertaken for the first time. The thermal diffusivity and effusivity of the investigated crystals were derived from the experimental data and allowed the thermal conductivity to be calculated. Diagrams of the thermal conductivity versus composition were analyzed by applying the model for mixed semiconducting crystals given by Sadao Adachi.

DFT calculations were used to investigate the effects of structural disorder and alloying on the thermal properties. A detailed comparison between the experimental results and theoretical predictions for Mg substitution was discussed.

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**Keywords:** semiconductor alloys, ZnMgS crystals, crystal growth, thermal conductivity, gap energy,

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\*Speaker

DFT

# Study of the effectiveness of free and encapsulated essential oils against the rice weevil (*Sitophilus oryzae*).

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The contamination of food products, particularly cereals, is the subject of numerous studies because of its impact on human and animal health, but also on trade in raw materials and food. Insecticides nevertheless remain an essential means of controlling food infestation. They make it possible to minimize losses, preserve harvests and improve producers' income. Some synthetic insecticides have a persistence that can last for more than ten years. If this long persistence allows them to protect crops for a long time, it is also a source of nature contamination. With the aim of reducing post-harvest losses, while preserving the environment, several studies are now focused on the development of insecticides based on aromatic plants. Previous work on the effect of essential oils in biological control has proven, on the one hand, their effectiveness and, on the other hand, their vulnerability in the face of several criteria: release time, stability. In order to prolong the persistence of their effectiveness, the encapsulation of essential oils remains an effective alternative.

Encapsulation is defined as a process in which droplets of bioactive oils are coated or incorporated into a homogeneous or heterogeneous matrix, to yield small capsules containing numerous properties. The encapsulation of bioactives have a potential interest for the pharmaceutical, functional food, agricultural and cosmetic industries. Encapsulation of bioactive oils represents a feasible and effective approach to modulate their release, increase physical stability, protect them from oxidation reactions with the environment, decrease volatility, improve bioactivity, reduce toxicity and improve compliance and patient convenience.

The objective of this work is to study the effectiveness of essential oils, certain aromatic and medicinal plants, free and encapsulated at various concentrations against the rice weevil (*Sitophilus oryzae*).

The results showed that essential oil capsules have a lethal effect on weevils at different concentrations as well as a greater repellent effect than that of free essential oils.

**Keywords:** Encapsulation, Essential oil, Bioactive, *Sitophilus oryzae*

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\*Speaker

# Improvement of dielectric properties of CoAl layered double hydroxide by in-situ polymerization of intercalated Vinylbenzenesulfonate Anions: A study monitored by impedance spectroscopy

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Complex impedance spectroscopy (CIS) has become a powerful nondestructive tool for investigating the properties and the quality of materials in different fields. It is based on the modeling of the obtained electrical data by an equivalent electrical circuit, which gives an insight into the physical processes that occurs inside the material. Knowing that the electric and dielectric behavior of layered double hydroxide (LDH) strongly depends on the constitution of the interlayer space (nature and arrangement of interlayer anion, water content, etc.) (1), we demonstrate in this work that we can use the impedance spectroscopy to monitor the in-situ polymerization process of Vinylbenzenesulfonate monomers intercalated in layered double hydroxide. X-ray diffraction, Fourier transform-infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy have been carried out to confirm the crystallographic structure of the CoAl-LDH. The corresponding modelization of materials has been determined by equivalent electrical circuits, and electric and dielectric analysis has shown important results that can valorize these LDH in electric and dielectric fields, specially the effect of in-situ polymerization on the dielectric loss. This is significant because the search of materials with electric and/or dielectric properties is becoming increasingly interesting.

**Keywords:** Layered Double Hydroxide, In, situ polymerization, Impedance Spectroscopy, Dielectric Properties, Electrical Equivalent Circuit, Dielectric loss.

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# Nickel ferrite Micro- and Nanoparticles: A Study of Their Structural, Morphological, Optical, and Magnetic Properties in Thermoplastic Composites

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Soft magnetic ferrites, in general, possess useful properties such as significant saturation magnetization, a high electrical resistivity, low electrical losses, and mechanical hardness, making them an appealing class of magnetic materials appropriate for a wide range of uses. Nevertheless, their low corrosion resistance and their higher energy consumption during the processing, make them susceptible to degradation of the magnetic properties. One possible solution is the development of innovative polymeric composite magnetic materials. This composite material is a composition of particles with magnetic properties incorporated into an extended polymer thermoplastic matrix to create an integrated functional system with additional magnetic properties. Which allows to these materials to be used in different applications such as automotive and aeronautics fields. In addition to their magnetic properties, their corrosion resistance, cost effectiveness and their lower energy consumption during the processing, makes them the best substitute for current materials. In this sense and in order to obtain novel high-performance magnetic polymeric composite using injecting molding, NiFe<sub>2</sub>O<sub>4</sub> particles have been synthesized with two different methods and used as a filler in a polymeric matrix. X-ray Diffraction (XRD), Fourier Transform Infrared (FTIR), UV visible, Raman spectroscopy and Scanning Electron Microscopy (SEM) were used to study the structural and morphological characteristics of the magnetic particles as well as the composite materials, magnetic properties were investigated by using Vibrating Sample Magnetometer (VSM), and Thermogravimetric analysis (TGA) was used to examine thermal stabilities of magnetic composite materials.

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**Keywords:** Soft magnetic ferrite, Polymer magnetic composite materials, Extrusion modling, nanoparticles

# Innovative Strategies for Enhanced Piezoelectricity: Phosphate Particle Integration in PVDF (nano) composite Films for energy harvesting application.

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Energy harvesting, the process of capturing ambient energy and converting it into usable electrical power, has gained significant traction with the rise of wireless technology and low-power electronics. Poly (vinylidene fluoride) (PVDF) is a prominent material in this field due to its piezoelectric properties, particularly its  $\beta$ -phase, which is associated with enhanced piezoelectric behavior. This study investigates the incorporation of metal phosphate-based nanoparticles into PVDF to promote the nucleation of the  $\beta$ -phase, aiming to improve its piezoelectric performance for energy harvesting applications. Metal phosphate-based nanoparticles were selected for their natural abundance, cost-effectiveness, safety, and environmental compatibility. These nanoparticles were integrated into PVDF at concentrations of 3 wt% and 7 wt% using the solvent casting method. The resulting nanocomposite films underwent various characterizations to assess their structural, thermal, and dielectric properties. X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) analyses confirmed a significant increase in the  $\beta$ -phase content in the nanocomposites. Scanning electron microscopy (SEM) revealed a uniform dispersion of nanoparticles within the PVDF matrix, contributing to the enhanced properties observed. Thermogravimetric analysis (TGA) demonstrated improved thermal stability in the nanocomposites compared to pure PVDF, indicating the effectiveness of the nanoparticles in reinforcing the material. Furthermore, dielectric constant and dielectric loss have been studied. The ferroelectric behavior of PVDF nanocomposite films showed remarkable improvement in remnant polarization values as compared to bare PVDF. These findings suggest that the incorporation of metal phosphate-based nanoparticles not only promotes the  $\beta$ -phase in PVDF but also improves its overall performance in energy harvesting applications. In summary, this study successfully demonstrates that integrating metal phosphate-based nanoparticles into PVDF enhances the material's piezoelectric and dielectric properties, offering a promising approach for advanced energy harvesting devices.

**Keywords:** Energy harvesting, Polyvinylidene fluoride (PVDF), Metal phosphate, Piezoelectric films.

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# Architecture of a novel anode material for rechargeable lithium ion batteries

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Morocco has recently developed a national energy policy aimed at promoting the use of renewable energy sources. Notably, this initiative is aimed at meeting the country's energy needs in the context of continued growth. Moreover, this policy is intended to regulate the costs of future energy services, taking into account the gradual increase in the price of petroleum products and the country's overdependence on imported hydrocarbons, which hinder the development of sustainable energy sources. Electrochemical energy storage is essential for the use of renewable energy sources, which are limited by their intermittent nature. Among chemical energy storage systems, lithium-ion batteries have become the most widely used in the last decade due to their high energy density and relatively sufficient autonomy, while reducing mass and size. A new material has been synthesized using a solid-state reaction process. and is being studied as an cathode material for lithium-ion batteries. The Rietveld method was applied to refine the structural properties of this sample using X-ray diffraction data. The particle size and morphology will be studied by Scanning Electron Microscopy (SEM). Last but not the least, batteries performance, safety, lifetime and reliability test will be conducted to evaluate the new material in different application areas.

**Keywords:** Electrochemical energy storage, material, lithium, ion batteries

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# Enhancing NaBH Stability and Dehydrogenation Kinetics via 3d Transition Metal Modifications for hydrogen storage

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The investigation focused on the structure, stability, and dehydrogenation characteristics of NaBH<sub>4</sub> when infused with 3d transition metals, employing first principles calculations based on density functional theory (DFT). The outcomes suggest that the introduction of transition metals destabilizes the NaBH<sub>4</sub> crystal due to their impact on the strength of the B-H bonds. Additionally, doping with Sc, Ti, Ni, V, Co, Mn, and Fe was observed to decrease the hydrogen desorption enthalpy in the NaBH<sub>4</sub> structure. Furthermore, the analysis of the electronic structure revealed that 3d transition metals influence the total density of states, offering potential enhancements to the thermodynamic properties.

**Keywords:** Hydrogen storage, sodium borohydrid, 3d transition metal, electronic density, dehydrogenation, DFT study

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# Advancements in Synthesizing Zinc Nanoparticles for Catalytic Applications

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Zinc, copper, iron, and nickel, among others, are promising candidates for non-precious metal hydrosilylation catalysts due to their abundance on Earth, affordability, and low toxicity. This work focuses on the preparation of zinc nanoparticles using a simple and easily implementable method. The characteristics of these catalysts are studied using advanced techniques such as X-ray diffraction (XRD) and transmission electron microscopy (TEM), enabling the determination of their crystal structure and morphology. The catalytic efficiency of ZnO nanoparticles is evaluated in hydrosilylation reactions for the formation of silylated products. These results highlight the potential of ZnO-based nanocatalysts for developing efficient and selective catalysts for advanced chemical transformations, paving the way for practical applications in various industrial fields.

**Keywords:** catalysts, nanoparticles, hydrosilylation

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# Synthesis of Zinc-Incorporated Hydroxyapatite via Solid-State Reaction for Enhanced Electrochemical Detection of Amoxicillin Using Ultraviolet Radiation (UV) as Step Catalytic

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In this study, we developed a carbon paste electrode modified with zinc integrated into hydroxyapatite (Zn-NPh-CPE) for the electrochemical detection of amoxicillin (AMX). A key aspect of the method involved a UV radiation pre-activation step, enhancing AMX's electrochemical response before detection. The zinc-modified natural phosphate (Zn-NPh) was synthesized through a solid-state reaction at temperatures between 200°C and 900°C for 14 hours, using natural phosphate and zinc sulfate hexahydrate as precursors. The resulting material was characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX). Results showed that zinc was effectively integrated into the hexagonal structure of hydroxyapatite (HAP) at high temperatures. Additionally, the influence of UV radiation on the activation of AMX was investigated using various electrochemical techniques, such as differential pulse voltammetry (DPV), chronoamperometry (CA), and electrochemical impedance spectroscopy (EIS). The findings confirmed that applying UV radiation catalyzes the oxidation of AMX. A linear correlation was observed between the oxidation peak current and AMX concentration, with two linear ranges from  $4.0 \times 10^{-7}$  mol L<sup>-1</sup> to  $1.0 \times 10^{-5}$  mol L<sup>-1</sup> ( $R^2 = 0.99$ ) and  $1.0 \times 10^{-5}$  mol L<sup>-1</sup> to  $1.0 \times 10^{-4}$  mol L<sup>-1</sup> ( $R^2 = 0.989$ ). The detection limit (LOD) was determined to be  $1.58 \times 10^{-7}$  mol L<sup>-1</sup>, using the slope of the lowest concentrations. The designed sensing platform exhibited excellent repeatability, with a relative standard deviation (RSD) of 2.78% ( $n = 8$ ). This highly sensitive method was successfully applied to detect AMX in real water samples, including tap water and wastewater samples.

**Keywords:** Amoxicillin, Carbon paste electrode, Natural phosphate, Ultraviolet, Water, Zinc.

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# Influence of the type of activating agent on the performance of an activated carbon electrode made from Argan tree waste

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This study investigates the production of three types of activated carbons (AC) derived from Argan (*Argania spinosa*) shells, using different activation agents: phosphoric acid (PA), zinc chloride (ZC), and sodium hydroxide (SH). The activated carbons, designated ACPA, ACZC, and ACSH, were synthesized through a two-step process involving carbonization at 900°C for 2 hours, followed by chemical activation with the respective agents. Scanning electron microscopy (SEM) analysis revealed a varied pore size distribution across the samples, influenced by the type of activating agent used.

Subsequently, electrodes were fabricated from these activated carbons, referred to as ACPA-E, ACZC-E, and ACSH-E. The electrochemical performance of these electrodes was evaluated through cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. The findings showed that the specific capacitances for ACPA-E, ACZC-E, and ACSH-E electrodes were 138.26 F/g, 122.21 F/g, and 82.6 F/g, respectively. These capacitance values were closely related to the specific surface areas of the activated carbons, measured using the BET method: 476 m<sup>2</sup>/g for ACPA, 441 m<sup>2</sup>/g for ACZC, and 362 m<sup>2</sup>/g for ACSH.

The results demonstrate the behavior of electrochemical double-layer capacitors (EDLC) in an acidic aqueous electrolyte (1M HSO) and suggest that Argan shell waste materials hold significant potential for supercapacitor applications. Among the activation agents tested, phosphoric acid emerged as the most effective, yielding the highest specific capacitance.

**Keywords:** Activated carbon, Argan, electrode, supercapacitor, Activating agent

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# Walnut Shell Particles Employed in Development of Sustainable and High-Performance Reinforced Cement Composites

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The rapid increase in bio-waste from the food and agricultural sectors presents a significant environmental challenge. In this context, more recent research has focused on lignocellulosic materials for their potential to create environmentally friendly building materials, such as cement-bonded particle boards (CBPBs). Our study explores the use of walnut shell particles (WSP), derived from agricultural bio-waste, as a sustainable filler in CBPBs, aiming to reduce manufacturing costs while enhancing fracture strength, thermal insulation, and acoustic properties. Indeed, CBPBs were produced using Super White Cement (SWC) as a binder, with WSP content varying from 10% to 50%. The boards, designed with a target density of 1300 kg/m<sup>3</sup> and a thickness of 10 mm, were created by mixing the components at a water-to-SWC ratio of 0.6:1, and the mixture was cold-pressed at 25°C using a hydraulic press at a pressure of 3 N/mm<sup>2</sup> for 24 hours. After pressing, the boards were demolded and cured for 28 days under atmospheric conditions to ensure full cement hardening and prevent moisture loss. Notably, WSP was used without pre-treatment to examine its impact on board characteristics. Physical properties such as density (D), water absorption (WA), and thickness swelling (TS) were evaluated, while mechanical properties were assessed using flexural tests. Additionally, scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), and X-ray fluorescence (XRF) were used to analyze the fracture surface, internal microstructure, and cement composition. The results, supported by thermal (TGA and DSC) and FTIR analyses, clearly demonstrate that CBPBs with up to 30% WSP content exhibit satisfactory physical and mechanical properties for non-structural applications. This research highlights the potential of recycled bio-waste in enhancing the sustainability of construction materials, offering a pathway to more environmentally friendly and cost-effective building solutions.

**Keywords:** Particleboard, bio, waste, walnut shell particles, cement, bonded composite, mechanical properties, physical properties, cement hydration products.

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# A Novel Polymer Inclusion Membrane Containing an Organometallic Complex Carrier for The Extraction and Recovery of Chromium and Nickel from batteries lithium-ion.

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The relative recognition of transport and diffusion phenomena at the microscopic scale slows down the application of affinity membranes in industry. This results in the need to have sufficiently reliable tools and measurements to better understand the transport by diffusion of species across the membrane in the case of aqueous solutions. This thesis work was devoted to the study of the influence of different transport agents on the extraction and recovery of cobalt II and Nickel II ions through PIMs inclusion polymer membranes by applying the principle of transport processes To facilitate this, a kinetic model has been established which makes it possible to determine and quantify the macroscopic parameters; permeability P and initial flow J0 relating to the performance of each of the membranes adopted. Likewise; a thermodynamic model was established; and which is based on an interaction mechanism of each of the extracted substrates with each of the different extractive agents as well as the apparent diffusion coefficient D of this substrate. These two specific parameters allow; to explain the performance of each of the membranes adopted and to elucidate the nature of the mechanisms relating to the processes carried out the activation and thermodynamic parameters relating to the transition state of the stage of migration of the substrate through the membrane have been determined. these parameters make it possible to analyze the evolution of the specific values of the parameters K ass and D to confirm the nature of the mechanism of the facilitated extraction process through the adopted affinity membranes and thus give exact explanations to seek the best conditions operating procedures for good performance of each of the membranes prepared and which were adopted for the directed processes relating to the extraction and facilitated recovery of substrates; Co(II) and Ni(II) ions

**Keywords:** Extractive agents · Polymer inclusion membranes · Recovery of Nickel (II) ions · Li, ion battery waste

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# Thermal behaviour of double pipes heat exchanger using Ag-Cu hybrid nanofluid: Thermal analysis

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Improving heat exchangers' thermal and hydraulic performances has always been a major concern for researchers in fluid mechanics and heat transfer because of the many industrial applications they have adopted and used over the last few decades. The present work studies the thermal behaviour of hybrid nanofluids based on a suspension of Ag-Cu 50:50 hybrid nanoparticles in water within a double coaxial tube heat exchanger with counterflow fluids. The effect of the volume fraction and different flow rate values are tested and form the basis of our study. All this work was carried out over a wide range of concentrations from 0% to 10% for Ag and Cu-based nanofluids and their hybridisation mixture. The results show that adding hybrid nanoparticles improves heat transfer compared with conventional fluids due to the increased thermal conductivity, which improves heat transfer.

**Keywords:** Nanofluids, hybrid nanofluids, Ag, Cu, thermal performances, double pipes, heat exchanger.

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\*Speaker



# Innovative Valorization of Phosphogypsum into Calcium Oxalate and Ammonium Sulfate: A Sustainable Approach

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The phosphoric acid industry generates significant quantities of phosphogypsum, a byproduct with profound environmental and health challenges. For every ton of phosphoric acid produced, five tons of phosphogypsum are generated, accumulating and leading to ecosystem degradation, groundwater contamination, and increased risks of toxic exposure and respiratory health hazards for nearby communities. Despite limited use in construction, agriculture, and landfill cover, most phosphogypsum remains unutilized, necessitating alternative management strategies.

This research explores a novel approach to phosphogypsum valorization by converting it into high-value products—calcium oxalate and ammonium sulfate. The goal is to develop scalable processes that both mitigate environmental impacts and create economic opportunities. Calcium oxalate offers diverse applications, from ceramics to serving as an intermediate for producing oxalic acid and organic oxalates, while ammonium sulfate, a key fertilizer component, enhances agricultural productivity and reduces reliance on conventional mining sources.

The research focuses on key steps such as the characterization of phosphogypsum feedstock, optimization of reaction conditions, and evaluation of product purity and yield. Additionally, the economic and environmental feasibility of scaling up the conversion process is analyzed. By transforming phosphogypsum into valuable commodities, this work contributes to the circular economy, promoting sustainable practices within the phosphate industry. The presentation will highlight the potential of phosphogypsum conversion in addressing waste management challenges while fostering environmental responsibility and economic resilience.

**Keywords:** phosphogypsum, byproduct valorization, Phosphate industry, Fertilizer production, and sustainable processes.

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# Valorization of Natural Products via Catalytic Pathway Using Iron-based Waste Materials as Efficient Heterogeneous Catalyst

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Heterogeneous catalysis is recognized as sustainable alternative that is widely used for various processes in diverse fields of chemical industry (1). Among these processes, catalytic chlorination represents a convenient way to synthesize allylic and vinylic chloride derivatives (2). Indeed, these derivatives lead to high value-added compounds as building blocks for more complex atomic arrangements (3). The present work focuses on the study of industrial iron-based waste materials as efficient heterogeneous catalyst for catalytic chlorination reaction. The catalytic reaction is carried out in presence of sodium dichloroisocyanurate (NaDCC) as an eco-friendly and highly stable free available chlorine (FAC) agent. First, advanced characterization techniques were used to investigate the physicochemical properties of the studied iron-based waste materials. Thereafter, various influencing parameters of the catalytic reaction were optimized in presence of carvone as model substrate. The optimized conditions were subsequently used to study a variety of terpenic olefins towards high value-added allylic chlorides in good to excellent yields.

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**Keywords:** Heterogeneous catalysis, allylic chlorination, terpenic olefins, iron, based waste materials, chlorine donor, NaDCC.

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# Integrating Experimental Techniques and Theoretical Models for Optimizing Perovskite Solar Cells

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This study investigated the potential of all inorganic CsPbBr<sub>3</sub> perovskite solar cells through a combined experimental and theoretical approach. CsPbBr<sub>3</sub> thin films of 700 nm as thickness were successfully fabricated using physical vapor deposition (PVD), and their structural, optical, and optoelectronic properties were extensively characterized. Atomic force microscopy revealed smaller, sharper, and more uniformly distributed nanograins, impacting surface roughness which can influence device performance. Optical studies demonstrated high transparency in the visible/near-infrared regions and a suitable bandgap of  $\sim 2.3$  eV for efficient light absorption. Photoluminescence analyses unveiled the radiative recombination behavior and charge carrier dynamics within CsPbBr<sub>3</sub>, providing insights into its optoelectronic properties. Complementing experiments, SCAPS-1D simulations optimized the device structure by determining ideal thicknesses for charge transport layers, absorber layer, and metal work functions in order to enhance the power conversion efficiency. Based on optimized parameters, a CsPbBr<sub>3</sub> perovskite solar cell with ITO/SnO<sub>2</sub>/CsPbBr<sub>3</sub>/Spiro-OMeTAD/Au architecture was fabricated via PVD, exhibiting a promising 14.42 % efficiency. The agreement between experimental and simulated results validated the theoretical models, highlighting the synergy of combined experimental-theoretical approaches. This study advances understanding of CsPbBr<sub>3</sub> perovskites, paving the way for potential commercialization in renewable energy. Future research can focus on further improving efficiency, and stability, exploring alternative architectures, and addressing manufacturing scalability challenges to unlock the full potential of this photovoltaic technology.

**Keywords:** Perovskite, AFM, PL, Decay time, SCAPS numerical simulation, Efficiency.

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\*Speaker

# Compositional dependence of properties of $Pb(Yb_{1/2}Nb_{1/2})O_3$ - $Pb(Mg_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$ ternary ferroelectric crystals

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*A series of  $Pb(Yb_{1/2}Nb_{1/2})O_3$ - $Pb(Mg_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$  ternary ferroelectric crystals with different compositions have been grown by the top-seeded solution growth technique in order to investigate systemically this ternary system based on the single crystal form. The compositional segregation and the compositional dependence of electric properties have been studied for the selected compositions in the vicinity of the morphotropic phase boundary (MPB) region. All the samples exhibit perovskite structure with rhombohedral symmetry at room temperature. The lattice parameter ( $a$ ), coercive field  $E_c$ , Curie temperature  $T_C$ , the rhombohedral-tetragonal phase transition temperature  $Trh-te$  increase gradually with increasing PYN content. All the samples exhibit quite high piezoelectric performance. In particular, the crystal with composition  $0.20PYN-0.40PMN-0.40PT$  possesses excellent electric properties such as  $T_C = 180$  °C,  $Trh-te = 130$  °C,  $k_{33} = 90.9\%$ ,  $d_{33} = 2240-2580$  pC N<sup>-1</sup>,  $Pr = 28.4$  mC cm<sup>-2</sup> and  $E_c = 5.4$  kV cm<sup>-1</sup>, indicating that the PYN-PMN-PT ternary crystals will be a promising candidate for electromechanical applications.*

**Keywords:** PYN-PMN-PT, ferroelectric crystals, electric properties, morphotropic phase boundary and piezoelectric.

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# Optimization of Catalytic Graphitization for Enhanced Nano-Carbon Production from Lignin

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This study focuses on optimizing the catalytic conversion of amorphous biomass into crystalline carbon materials with potential applications in energy storage and electronic devices. By employing various catalytic systems, the research aims to identify the optimal conditions that facilitate high-yield and high-crystallinity transformations of lignin-derived carbon. Key reaction parameters, including catalyst type, temperature (ranging from 800 to 1000 °C), reaction duration (1-2 hours), and catalyst concentration, were systematically investigated to understand their impact on the structural and chemical characteristics of the resultant graphitized materials. Advanced characterization techniques, such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy, were employed to analyze the materials' crystallinity, morphology, and surface chemistry. The findings revealed that increasing the reaction temperature and duration improved the graphitization degree but also led to a trade-off with reduced yield under more extreme conditions. The research successfully established a set of optimal reaction parameters that enhance both the yield and crystallinity of the carbon materials. The synthesized crystalline carbon materials have a high potential for application in energy storage devices, offering improved electrical conductivity, thermal stability, and mechanical strength. Ongoing studies are exploring their integration into batteries and supercapacitors to harness their full potential in sustainable energy solutions.

**Keywords:** Biomass, Lignin, Catalyst, Carbon, Graphite, Crystallinity, Energy.

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\*Speaker

# Co-doping effect of Cerium concentration on MgAl<sub>2</sub>O<sub>4</sub>(Sm) properties for energy conversion

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Doped with rare earth elements, Magnesium alumina MgAl<sub>2</sub>O<sub>4</sub> can occur outstanding optical properties (1-3). In this work, undoped MgAl<sub>2</sub>O<sub>4</sub>, Samarium and Cerium as down converter rare earth couple codoped magnesium alumina nanoparticles are prepared by conventional solid-state method. Their structural, elemental and morphological properties are provided. These studies have been done using XRD, FTIR spectroscopy, MEB and MS-ICP measurements. XRD results show the formation of MgAl<sub>2</sub>O<sub>4</sub> and MgAl<sub>2</sub>O<sub>4</sub>(Sm,Ce) in cubic spinel phase (4-5) with crystalline size varying from 9 to 53 nm. The elemental composition determined by the ICP-MS indicates the presence of Sm and Ce in doped samples with desired composition. The IR-ATR spectra shows two fundamental absorptions peaks 665 and 456 cm<sup>-1</sup>.

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**Keywords:** Magnesium alumina, rare earth, structural and optical properties, energy conversion

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\*Speaker

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# Tailoring hydrophobic Paper for Water Repellency: Thermochemical Modification and Structural Insights

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Paper is a porous network of cellulose microfibrils, naturally hydrophilic due to free hydroxyl groups, this limits the paper's properties when exposed to wet environments. Here we have proposed a simple single-step method to prepare hydrophobic paper by introducing long-chain oleic acid (OA) through an esterification reaction using a hot press machine, with optimization of the thermochemical conditions for the esterification. The surface chemistry and morphology of the hydrophobic paper were thoroughly studied using FTIR, solid-state <sup>13</sup>C-NMR, XRD, scanning electron microscopy, and 3D nano-tomography. The hydrophobic paper exhibited strong hydrophobicity, with a water contact angle greater than 120°, primarily due to the low surface energy provided by OA. Compared to unmodified paper, the hydrophobic paper showed significantly reduced water uptake and lower moisture sensitivity, owing to the substitution of cellulose hydroxyl groups. Additionally, the hydrophobic paper demonstrated mechanical stability under wet conditions.

**Keywords:** Cellulosic paper, oleic acid, thermochemical pressing, hydrophobization, wettability

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\*Speaker

# Effect of friction stir welding parameters on microstructure and mechanical properties of the dissimilar alloys of AZ91D and AA7075

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*In advanced industries, particularly in automobile, and aerospace engineering, there is a considerable drive toward dissimilar material joining to achieve enhanced performance, cost and weight reduction. Dissimilar materials such as Al/Mg alloys are functional materials whose welding quality is being explored to enhance the material performance. The welding of Al and Mg alloys is complicated owing to the difference in their mechanical and physical properties. In this work, the metallurgical characterization of the friction stir welded joints of AZ91D and AA7075 was investigated. It was observed that the welding parameters enhanced the morphological characteristics and reduced the heat input of the brittle IMCs in the welded region. The primary Al and Mg diffraction peaks were present, and Al<sub>12</sub>Mg<sub>17</sub> and Al<sub>3</sub>Mg<sub>2</sub> were intermetallic in all the joints. This occurred due to the inter-diffusion behavior of Mg and Al atoms in the welding process and formed IMCs. The Al<sub>12</sub>Mg<sub>17</sub> phase mixed with the Mg phase has preferentially lowed to the weld surface where the AZ91D plate was placed, and constitutional liquation may occur and be observed in the eutectic microstructures. The maximum ultimate tensile strength (UTS) of 116.64 MPa was observed at rotational tool speed (RTS) of 800 rev/min with a Traverse speed (UTS) of 20 mm/min, and the lower UTS (68.32 MPa) was found at RTS of 400 rev/min with a TS of 20 mm/min. A thick layer of IMC (Al<sub>12</sub>Mg<sub>17</sub> and Mg+ Al<sub>12</sub>Mg<sub>17</sub>) was observed in the SZ with lower rotational and welding speeds. This may be attributed to inappropriate processing parameters, leading to the IMC's materialization in the SZ, resulting in reduced mechanical properties.*

**Keywords:** Friction stir welding, Microhardness, Microstructure, Tensile strength, intermetallic compounds

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\*Speaker



# Biobased phase change materials in energy storage and their applications: A State-of-art review of recent advancements

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The rapid increase in energy demand due to urbanization, population growth, and technological advancements has led to the depletion of fossil fuels and the associated environmental damage. Faced with these challenges, renewable energies appear to be an essential solution, with a particular focus on ecological and sustainable technologies. Phase change materials (PCMs) are at the heart of current research due to their exceptional ability to store and release thermal energy at constant temperatures, making them ideal for thermal energy storage (TES) applications.

This paper examines the use of bio-based PCMs, sustainable and environmentally friendly alternatives to conventional PCMs. Derived from renewable sources, these materials offer comparable performance while reducing the carbon footprint and conserving natural resources. The types of bio-based PCMs, their thermophysical properties and potential areas of application are analysed. Recent innovations in sustainable PCM technologies, such as improving thermal stability and thermal conductivity via the incorporation of nanomaterials, are also being explored.

In conclusion, bio-based PCMs represent a significant step forward towards more sustainable energy solutions. This review provides an overview of concepts and technological advances in this field, highlighting their potential for a green and sustainable energy transition.

**Keywords:** Phase Change Materials, Biobased, latent heat, Thermal energy storage, Stat of art, heat storage, Temperature.

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\*Speaker

# Study the inter-building effects on building energy balance and solar energy use: an application to the climate of Morocco.

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This study addresses the challenge of achieving Net Zero Energy Buildings (NZEB) in Morocco through the strategic deployment of building-integrated photovoltaic (BIPV) systems. The research acknowledges the critical impact of the Inter-Building Effect (IBE) on building energy performance and explores the optimization of BIPV system design to minimize energy consumption while maximizing cost-effectiveness.

Using a comprehensive optimization framework that incorporates various design variables, including insulation thickness, overhangs, and PV panel configuration, the study evaluates four different building scenarios in six distinct climatic zones in Morocco. The results demonstrate significant reductions in heating and cooling loads across all scenarios. Optimized designs incorporate PV systems that generate sufficient energy to meet the building's energy demand, achieving a near-zero energy balance.

The study highlights the importance of considering the IBE and the unique climatic conditions of each region when designing BIPV systems for NZEB.

**Keywords:** Inter, building, NZEB, Building energy balance, BIPV, Solar energy, jEPLUS +EA, Morocco.

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\*Speaker

# Whey Valorization Innovative Strategies for Sustainable Development and Value-Added Product Creation

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In recent years, the pursuit of sustainable practices and the efficient utilization of resources has become paramount in various industries, including the food and beverage sector. One such challenge faced by the dairy industry is the management of whey, a byproduct generated during cheese and yogurt production. Historically, whey has been perceived as a discarded waste product, leading to environmental concerns due to its high organic load and disposal challenges. However, with the increasing emphasis on sustainability, researchers and industry leaders have recognized the potential of developing innovative approaches to valorize whey, transforming it into valuable products while minimizing waste and environmental impact. Essentially turning it from "gutter-to-gold."

**Keywords:** Whey valorization strategies, circular economy, value added product

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\*Speaker

# Optimizing Perovskite Solar Cells Efficiency using Impedance Spectroscopy

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In this study, we utilize impedance spectroscopy to investigate the internal processes that affect the efficiency and performance of perovskite solar cells (PSCs). We employ SCAPS-1D software to simulate the FTO/ZnO/MASnI/NiOx/Au heterostructure solar cell. Our focus is on analyzing the complex impedance ( $Z^*$ ) and electric modulus ( $M^*$ ) to distinguish between bulk material and interface phenomena such as ion migration and charge transport. Using Nyquist and Bode plots, we identify three key relaxation processes linked to charge migration, interface polarization, and charge injection/extraction. Through this detailed analysis, we observe that these processes are critical to the device's overall performance. Additionally, we model the impedance and modulus spectra using an equivalent electrical circuit, which closely fits the experimental data. Our results indicate that as bias voltage increases, relaxation times for charge transport and interface effects lengthen, signaling a performance drop at higher operational voltages. This is likely due to increased resistive and recombination losses.

**Keywords:** Impedance spectroscopy, Perovskite solar cells, Relaxation processes, Efficiency

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\*Speaker

# **Theme 6: Supply Chain, Modelling, Simulation and Optimisation**

# Optimization of temperature during phosphoric acid process by Golden section method

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For all process industries, the optimization of operatory conditions is a central challenge and a key performance factor. Crystallization is the most common unit operation used in the chemical industry as a purification and separation method and is heavily influenced by the temperature effect, which is critical for end product quality and operational efficiency. In this sense, the aim of the present study was to implement a sequential Golden ratio search technique to optimize the temperature of the reactive crystallization during phosphoric acid manufacturing. The selected objective functions to be maximized were chemical and industrial yields, which were initially supposed to be unimodal within the specified interval (70–85 °C). A set of batches simulating industrial operating conditions were carried out. First, only two experiments were executed, and then several experiments were performed iteratively according to the golden ratio method by comparing various solutions until the optimal point was found. By initially choosing the tolerance and the number of iterations, and in order to verify the obtained experimental optimum values, a simulation via Matlab® using a fitted second-order function was performed. Interestingly, results conclude that chemical and industrial yields are very dependent and vary with the slightest variance of the phosphoric slurry temperature. In conclusion, the use of the golden section method has proven to be an effective way to accurately determine the optimal temperature, and the employed approach may also be applicable for the optimization of other process parameters and to a wide range of crystallization processes.

**Keywords:** Golden section, Optimization, Temperature, Reactive crystallization, Phosphoric acid process, Performance.

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\*Speaker

# A simulation model to schedule a remanufacturing system with returns of varying quality

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Recently, the matter of acquiring information about the quantity and quality of used items in reverse supply chains has gained substantial interest from both industry professionals and scholars. The classification of return items based on quality stands as the initial step in a sequence of essential processes preceding the validation of a used product's suitability for meeting the demand for remanufactured goods. Within this study, we address a lot scheduling problem with returns specific to remanufacturing, where returns are categorized into two quality grades. Both, manufacturing and remanufacturing activities are performed by a single machine. Demand is deterministic and is fulfilled without stock shortages. The research contrasts an independent remanufacturing process that schedule remanufacturing activities with a process where the remanufacturer does not implement scheduling. The aim of this study is to reduce the average total cost through the optimization of the acquisition lot size and planning the remanufacturing sequence.

**Keywords:** Remanufacturing, simulation, returns, Lot scheduling, quality grading.

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# Optimizing Vaccine Supply Chains through Advanced Modelling, Simulation, and Data Management

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*The COVID-19 pandemic has highlighted the critical importance of efficient and resilient vaccine supply chains for global public health. This research proposes a comprehensive framework for Vaccine Lifecycle Management (VLM) that integrates Product Lifecycle Management (PLM) principles with innovative digital solutions to optimize the vaccine lifecycle through advanced modelling, simulation, and data management techniques.*

*Our approach begins with an analysis of current challenges in vaccine supply chains, including data integration, quality control, and stakeholder coordination across various lifecycle stages. Key issues identified include data fragmentation, lack of standardization, and interoperability problems that hinder the seamless flow of information and materials.*

*To address these challenges, we propose a unified data management model. This model aims to leverage cutting-edge technologies to improve data integration and quality, enhancing supply chain efficiency and effectiveness. The proposed model will be validated through rigorous simulation and optimization techniques to ensure it can handle the complexities of modern vaccine supply chains.*

*This study seeks to highlight the benefits of a holistic approach to vaccine lifecycle management. By optimizing the entire supply chain, we aim to ensure timely and equitable access to vaccines, thereby contributing to the enhancement of global public health infrastructure.*

**Keywords:** Vaccine Supply Chain, Lifecycle Management, Data Integration, Simulation, Optimization

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# Experimental Study and Thermodynamic Modeling of Cadmium Behavior in the PO-SO-Ca-HO System

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*Cadmium (Cd) is a highly toxic heavy metal, initially found in phosphate rock and transferred directly to the phosphoric acid (PAC) produced during the leaching process. This study examines, the thermodynamic behavior of this impurity within the PO<sub>4</sub>-SO<sub>4</sub>-Ca-H<sub>2</sub>O system. To achieve this, we used the Debye-Hückel model to predict the thermodynamic saturation indices of the main minerals that can incorporate cadmium into their structures and are likely to form during the PAC manufacturing process, under conditions ranging from dilution to saturation and at temperatures between 298.15K and 353.15K. The chosen thermodynamic model has been validated and accurately describes the system, as evidenced by the strong agreement between its predictions and experimental measurements*

**Keywords:** Thermodynamics models, phosphate, Phosphoric acid, Cadmium, Saturation index, speciation

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# Improvement of NRTL Model for Accurate Vapor–Liquid Equilibrium Calculations of Binary Systems

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Modifications to the NRTL equation have been proposed to improve vapor-liquid equilibrium (VLE) prediction. The first method applies the NRTL equation to aqueous mixtures by calculating interaction parameters from the properties of pure compounds. The second method proposes a modification of the NRTL equation by adding a new term and using a modified geometric mean for the cross-interaction parameters. These approaches enable better prediction of VLE for complex systems, including those that are strongly associated or asymmetric.

**Keywords:** VLE, modified NRTL model, Excess Gibbs energy, activity coefficient, ternary interaction parameters

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\*Speaker

# Quantifying uncertainties related to reverse logistics implementation: state of the art.

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It's over six decades that Reverse logistics had appeared as a research area, and it is emerging again and again in the scientific fields. As reverse logistics presents real potential for value recovery and environmental impacts decrease, it's still necessary to extend this concept more in the industrial and commercial field especially in developing countries. The process of reverse logistics is a progression of steps beginning with the customer and finishing with the organization or even the customer, however the issue is that this cycle must be adjustable to the organization concerned, in addition of legislative, operational, financial and social obstacles. Literature had demonstrated that there are many other barriers and uncertainties while the implementation of this process that vary in function of the sector concerned and the kind of activity. Besides, even if literature is developing this topic over the last years, it's treated in specific sectors and not yet generalized in other areas due to these uncertainties. Our paper has the objective to decrease this gap, and carry out a state of the art to identify methods for uncertainties quantification related to reverse logistics process in order to help researchers to generate solutions for facilitating the implementation of reverse logistics. This paper presents also an explanation of Mixed Integer Linear Program (MILP).

**Keywords:** reverse logistics, uncertainties quantification, MILP

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\*Speaker

# FINITE ELEMENT MODELING OF THE HUMAN MIDDLE EAR USING MEDICAL IMAGING

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*In recent decades, many researchers have attempted to develop virtual models of the human ear using the finite element method. However, one of the main challenges they have encountered is the high degree of geometric complexity of the middle ear, which contains many intricate structures within a confined space. This complexity makes the geometric design of the model very difficult. To address this issue and approximate the actual geometry as closely as possible, we utilized Computed Tomography (CT) to develop an accurate and realistic geometric model of the human middle ear. In this study, we created a three-dimensional finite element model of the human ear using CT imaging. This model includes the external auditory canal, tympanic membrane, ossicular chain, ligaments, and muscle tendons, while the inner ear is modeled as a viscous damping applied to the stapes footplate. We used CT images of a human head to construct an anatomically accurate model of the middle ear. After developing the model geometry, all tissue domains were imported into COMSOL Multiphysics for finite element analysis. Material properties were assigned to the different parts of the model, and frequency domain analysis was performed to simulate the response of the tympanic membrane and stapes over a frequency range of 100 to 10 000 Hz. To validate our model, the obtained results were compared with experimental data and numerical results from previously collected models.*

**Keywords:** Finite element method, Middle ear, Medical imagin, Tympanic membrane

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\*Speaker

# Improving the NRTL Model for Liquid-Liquid Equilibrium Optimization and Calculating Plait Point Coordinates

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The purpose of the regression data for phase equilibrium is to describe how components behave in a system based on different factors, including the quality of experimental data, the robustness of the calculation algorithm, and the chosen thermodynamic model. Occasionally, even minor adjustments to these factors can yield highly satisfactory results. This work focuses on one of the most commonly used thermodynamic models, the NRTL model. We introduce a simple modification by incorporating a new parameter,  $F$ , termed the "distance parameter," which connects the aqueous phase to the organic phase. This modification is based on the Flory-Huggins equation and includes Hansen solubility parameters. The goal is to provide a more accurate explanation of the random phenomena resulting from collisions between different components in ternary type I systems within the immiscibility region, and to optimize the calculation of liquid-liquid equilibrium and the plait point for systems featuring the liquid phase.

**Keywords:** Modified NRTL model, plait point, liquid liquid equilibrium, thermodynamic modeling, Flory Huggins equation, Hansen solubility parameters

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# New Modeling Approaches for Ethylene Oxychlorination in Fluidized Bed Reactors

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1,2-dichloroethane used in the manufacture of thermoplastics, is produced by oxychlorination ( $C_2H_4 + 0.5O_2 + 2HCl \rightarrow CH_2CH_2Cl_2 + H_2O$ ). On an industrial scale, in the majority of cases, this gas-phase reaction takes place in a fluidized bed, in the presence of a solid catalyst based on copper chloride. To predict the behavior of this reactor under industrial conditions, several models have been developed. Among them, the Plug Bubble - Continuous Stirred Emulsion approach, which provides a good approximation of the behavior of these industrial converters. But this approach present certain mathematical difficulties. In fact, this model requires the resolution of a system comprising a number of non-linear equations, which is increasingly important if we take into account more and more concurrent reactions. The assumption that the reactor behaves as a single-phase continuous stirred reactor allows to have less and simpler equations. This assumption can be justified for industrial situations characterised by high flow rates. In fact, in turbulent regime, single-phase models can adequately describe the behavior of fluidized beds and many studies of other experimental fluidized bed reactors proves that (CSTR) hypothesis can approach the FBR . For this reason, a (CSTR) approach has been developed to predict the behavior of industrial FBR of ethylene oxychlorination. This approach showed good agreement both with results from industrial reactors and with those corresponding to the litterature approach (Plug Bubble - Continuous Stirred Emulsion). Since the modeling work carried out in many articles has only focused on conditions characterized by high flow rates, we have turned our attention to low-flow situations, as found in laboratory or pilot reactors, adopting the model (Simple two phases - Plug bubble - Plug emulsion) that is best suited to these conditions. This has enabled us to highlight the location and importance of undesirable thermal hotspots, and to propose actions to control them by acting on temperature and/or feed gas flow rates. Comparison of this model with the plug approach highlights the significant slowdown in ethylene conversion due to mass transfer resistance at low feed rates.

**Keywords:** Fluidized bed reactor, Bubble phase, Emulsion phase, Continuous Stirred Tank Reactor, Plug Reactor

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# Performance Modeling and Simulation for Water Distribution and Wastewater Collection Networks.

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**Water distribution** and **wastewater collection** networks are crucial for ensuring the supply of **drinking water** and the efficient management of wastewater in urban environments. However, these networks often face complex challenges related to their management and performance. This thesis focuses on developing an advanced **system dynamics model** for the **strategic asset management** of water and wastewater networks, using the city of **Taounate** as a case study.

In Taounate, although water resources such as the **Sahla** and **Bouhouda** dams and provincial wells are sufficient, the management of these networks faces significant challenges. Current **models** for managing water and wastewater networks have major **gaps**. They primarily focus on technical aspects, neglecting **financial** and **political** dimensions. This approach leads to inefficiencies in asset management and operational problems such as **leaks** and suboptimal performance. In 2023, the **performance** of the drinking water network fluctuated between **69.76%** and **75.41%**, highlighting significant losses and ineffective management.

Leak analysis shows that **74%** occur at the **service connections**, **25%** on the **pipelines**, and less than **1%** on **special fittings**. This distribution of leaks reveals considerable challenges in managing and maintaining the networks. In quantitative terms, this translates to approximately **852 leaks** at service connections, **282 leaks** on pipelines, and **12 leaks** on special fittings, totaling **1,146 leaks**.

This thesis proposes developing an advanced **system dynamics model** that integrates **physical**, **financial**, and **political** aspects to improve the management of water and wastewater networks. A key objective is to integrate the drinking water and wastewater networks, promoting more cohesive and integrated asset management. By creating a comprehensive analytical framework, the goal is to optimize resource management, reduce leaks, and enhance the **sustainability** of the networks. This model will provide tools to assess performance, identify issues, and propose strategic solutions, contributing to better overall efficiency and improved urban quality of life.

**Keywords:** Water distribution, wastewater collection, system dynamics model, strategic asset management, Taounate, financial, political, leaks, performance, sustainability.

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\*Speaker

# Optimising the dynamic placement of mobile units in a hybrid network under uncertainty

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Determining the optimal location for production facilities is crucial in supply chain management, allowing decision makers to strategically and tactically meet customer demand. In today's highly dynamic markets, incorporating uncertain parameters into the decision-making process can enhance robustness under unpredictable conditions. This paper introduces an optimization approach to address the dynamic location problem of mobile modular units in a hybrid network, accounting for stochastic demand. The model aims to minimize the total expected cost, reduce cost variability due to demand uncertainty, and mitigate penalties for unmet demand. Numerical results from a case study in the chemical industry demonstrate the model's efficiency and robustness. Furthermore, the study explores the trade-off between the model's robustness and solution robustness.

**Keywords:** Robust optimisation, Demand uncertainty, Modular mobile facilities, Hybrid network.

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# Enhancing Materials Procurement with Blockchain Technology

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The challenges posed by traditional materials procurement processes, characterized by inefficiencies and complexities, have long posed a significant obstacle for industries on a global scale. The emergence of blockchain technology provides an optimistic resolution to these challenges through the provision of a decentralized, transparent, and secure method for overseeing procurement operations. This scholarly article delves into the utilization of blockchain technology to enhance materials procurement, focusing on its key advantages such as improved traceability, heightened transparency, and decreased transactional hurdles. By conducting a thorough examination of existing literature and case studies, the research identifies crucial factors for success and essential strategies for implementing blockchain within procurement frameworks. Furthermore, the article evaluates the effects of blockchain technology on procurement performance indicators like cost minimization, accelerated delivery times, and bolstered supplier relationships. The findings point towards the potential of blockchain in significantly optimizing procurement processes, resulting in enhanced efficiency and dependability. In conclusion, this study underscores the promising directions for future research and practical applications, advocating for the incorporation of blockchain solutions to cultivate a more resilient and robust procurement environment.

**Keywords:** Materials procurement, blockchain technology, procurement ecosystem uncertainties

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# CFD Simulation for Wind Comfort and Safety in Urban Area: A Case Study of the Mohammed VI Tower

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The Mohammed VI Tower, a 250-meter-tall skyscraper in Rabat, Morocco, stands as the tallest building in Africa. Assessing wind loads on such a high-rise structure is essential for ensuring its structural safety and comfort for occupants and surrounding areas. This study employs Computational Fluid Dynamics (CFD) simulations using ANSYS Fluent to evaluate the wind loads and comfort around the Mohammed VI Tower. A detailed 3D model of the tower and its urban surroundings was developed, with a refined computational mesh and appropriate boundary conditions to capture accurate wind flow patterns. The RNG k- $\epsilon$  turbulence model was utilized to simulate turbulent effects around the tower's structure. The results provide insights into the velocity distribution, pressure profiles, and turbulence characteristics, informing areas of high wind pressure, recirculation, and flow separation. This analysis contributes to understanding the aerodynamic performance of the Mohammed VI Tower, enhancing structural safety and guiding improvements in urban wind comfort design around high-rise buildings.

**Keywords:** Computational Fluid Dynamics (CFD), wind comfort, structural safety, high, rise buildings, Mohammed VI Tower.

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\*Speaker

# Influence of temperature on the hydration, transport, and dielectric properties of the ternary aqueous system {NaF - Na<sub>2</sub>CO<sub>3</sub>} (aq) using a molecular dynamics approach and FTIR spectroscopy

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The dissolution of sodium fluoride and sodium carbonate electrolytes in the presence of water has several industrial applications, including water treatment, air pollution control, and industrial waste treatment, due to their unique chemical properties. In this context, we studied the influence of temperature on the ternary aqueous electrolyte mixture {NaF - Na<sub>2</sub>CO<sub>3</sub>} using two approaches: the first purely theoretical, involving molecular dynamics, and the second experimental, involving FTIR spectroscopy. Molecular dynamics simulations were conducted using the GROMOS force field combined with the SPC/E water model to evaluate the structural behavior induced by the hydration phenomenon, as well as the dynamic and dielectric behavior of ion pairs in the presence of water. Microscopic structural properties, such as interatomic distances and hydration numbers, were analyzed using the radial distribution function (RDF). Additionally, dynamic and dielectric properties were evaluated through calculations of the self-diffusion coefficient and dielectric constant over a wide temperature range from 278.15 to 353.15 K. Furthermore, the second part of this study focused on validating our structural data obtained from molecular dynamics simulations using the Fourier-transform infrared (FTIR) spectroscopy technique. The combination of both approaches allowed us to enhance our understanding of the various physicochemical mechanisms resulting from the dissolution of sodium fluoride and sodium carbonate in water. This comprehensive analysis provides valuable insights for fundamental research and its industrial applications.

**Keywords:** Molecular dynamics, FTIR Spectroscopy, Sodium fluoride, Carbonate fluoride, Hydration phenomenon, Self, diffusion coefficient, Dielectric constant.

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# Simulation and analysis of hybrid absorption-compression refrigeration system behavior

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Absorption refrigeration systems play a crucial role in the valorization of industrial thermal waste and the efficient utilization of renewable energy sources. The objective of this study is to simulate and analyze a hybrid absorption-compression refrigeration system using the water-lithium bromide pair. This system is designed to harness the thermodynamic properties of the water-lithium bromide solution for industrial applications. To achieve this, a detailed mathematical model is developed, incorporating the conservation equations of mass and energy, as well as the thermodynamic property correlations for the water-lithium bromide solution. This model enables a precise description of the system's thermodynamic behavior. The model has been implemented using the C programming language, following a modular programming approach with separate source and header files to enhance code readability and ease of maintenance, despite containing dozens of functions. The developed model is validated by comparison with previous studies on the energy analysis of absorption refrigeration cycles, and the results demonstrate good agreement with those prior works, confirming the accuracy of the model. Furthermore, a sensitivity analysis is conducted to identify the most influential parameters affecting the system's performance. This analysis highlights key factors that need to be optimized to improve the system's energy efficiency. The findings provide valuable insights for the future design of hybrid refrigeration systems, particularly those intended for applications involving renewable energy sources or the recovery of industrial thermal waste. This work contributes to advancing the understanding of hybrid absorption-compression systems and their potential in sustainable energy solutions.

**Keywords:** Absorption refrigeration system, Hybrid absorption, compression, Water, lithium bromide pair, Industrial thermal waste, Renewable energy utilization, Thermodynamic modeling, Energy conservation equations, Sensitivity analysis, Energy efficiency

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# Modelling the behaviour of pharmaceutical powders in compression

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Numerical simulation has become an increasingly important means of investigation among industrialists, as it avoids the high costs of conventional and traditional experimental approaches. In the pharmaceutical industry, the production of a tablet involves several phenomena and requires the consideration of the particular characteristics related to the powders exploited (coefficient of friction, cohesive character, mechanical behaviour, modulus of elasticity, fish coefficient, etc.). In compression, the pressure on the powder mixture increases under the effect of the displacement imposed by the upper punch, resulting in a decrease in volume according to elastic and plastic deformations sustained by the particles. Nevertheless, and based on the results from the literature, the densification mechanism considered is elasto-plastic behaviour. Thus, numerical simulation occupies a prominent place in the optimization of this manufacturing process. However, there are several ways to model compact compression: simulation by the discrete approach or by the continuous approach. Under both approaches, a number of simulation models have been developed. It is for this purpose that the various modelling methods developed so far will be introduced in this press release. The aim is to identify the principle and approach followed by each method, in order to highlight the advantages and limitations of each of them to have a good starting point.

**Keywords:** Matrix Compression, Modeling Method, Cold Powder Compression, Elastic Properties, Elasto, Plastic Properties, Finite Element Method, Multi, particle Finite Element Method, Discrete Element Method, Mesh, Free Method

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# Study of the elasto-plastique densification mechanism for pharmaceutical powders: numerical modeling by the continuous approach.

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Tablets are widely used in the pharmaceutical industry due to their numerous advantages in terms of manufacturing and patient usage. The quality of tablets is typically assessed based on their appearance, such as the presence or absence of cracks, as well as their functional properties like strength, dryness, and dissolution. Creating a high-quality tablet requires considering various factors, including the formulation's pharmacological properties, pharmacokinetic parameters, process control parameters (such as production speed, temperature, and humidity changes, and maintenance status), and powder properties (such as coefficient of friction, mechanical behavior, and modulus of elasticity). To optimize the compaction process and predict the final product's quality and properties, numerical simulation is a valuable tool. However, the process of numerically characterizing the densification mechanism of pharmaceutical powders during compression starts with choosing the appropriate analysis scale, whether microscopic or macroscopic. Since direct compression is a common method for tablet manufacturing due to its stability, robustness, performance, and cost-effectiveness, the behavior of the powder mixture under pressure can be understood through the classical theory of elasto-plasticity. Continuum constitutive models offer a coherent mathematical and numerical framework for this purpose, as they can be established using mathematical formalisms based on the analytical solution of partial differential equations. In this research, we aim to model the behavior of pharmaceutical powders during compression using numerical methods such as the finite element method (FEM) and mesh-less methods (MSM). These approaches enable us to perform numerical simulations that provide insights into the density and stress distribution inside the tablet. Furthermore, we will conduct experimental validation to ensure that the numerical results accurately reproduce the observed behavior of the powder.

**Keywords:** Die compaction, Pharmaceutical powder compaction, Tablets, Modelling, Numerical Simulation, Meshless Methods, Finite Element Method

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# Improving the fidelity of measurement system through preventive maintenance and standardisation: a case study

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Measurement System analysis (MSA) is an effective method that seeks to confirm the measurement system's degrees of precision and accuracy using various techniques. This research highlights three distinct approaches to gage R&R analysis, the first one known as the Average and Range (Xbar/R) method is the most established technique. The second is the Analysis of Variance (ANOVA) method, which shows a remarkable advancement in gage R&R analysis. The third one known as the Evaluation Measurement Process (EMP III) introduced by D.J.Weeler and differs from the other two with a unique methodology for assessing the measurement system. A comparative analysis of the three methods reveals commonalities in computations and distinctions in the interpretation of outcomes in addition to acceptance requirements. This is understandable given that the Automotive Industry Action Group (AIAG) recommends the Xbar/R and ANOVA methods, while D.J.Weeler declares that the EMP III goes beyond the AIAG's acceptability limitations. Using the previously indicated techniques, a preliminary gage R&R study is conducted, indicating that the measurement system is not acceptable according to AIAG but still a first-class monitor based on EMP III rules. In order to increase the accuracy and precision of the measurement system, an improvement plan is established in this regard. This plan emphasizes the critical role that preventive maintenance scheduling plays for the measuring instrument, as well as the efficacy of standardizing the measuring methods and training the operators. The final gage R&R results demonstrate a great improvement in the measurement system performance.

**Keywords:** Measurement System Analysis MSA, gage R&R, preventive maintenance, standardization, Xbar/R, ANOVA, EMP III

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# Ability of Retail Stores to Meet Increased Demand during the Pandemic Period

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The retail sector experienced unstable and increasing demand during the pandemic, resulting in successive stock-outs. Although stock-outs have been a persistent problem for many years, they consistently result in lost sales and lower customer satisfaction. This problem became evident as retailers struggled to meet increased demand during the pandemic period, particularly for basic necessities and convenience goods. It was therefore necessary to analyze sales of these products during this period. To this end, we conducted an empirical study in five retail stores specializing in the sale of convenience goods. We compared sales between stores for all products, then by category. The results revealed that, due to common factors in all stores, sales were maintained at a certain level and were relatively stable throughout the months, without being able to meet the increase in demand. In addition, our case study provides a comparison of the sales distribution of six major product categories during the pandemic period.

**Keywords:** Demand, Stock, Pandemic, Convenience Good, Retail Store, Case study

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# Supply Chain Demand Distortion: The Unexpected Increase in Consumption

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Today's businesses are undergoing an unusual transformation, imposed by an unstable environment and a competitive international market. This dynamic context, marked by the pandemic of recent years, is forcing companies to rethink their strategies and manage their supply chain more effectively. Indeed, supply chain management relies on systemic and strategic coordination and collaboration, both within the company and with other partners in the chain. This involvement results in considerable gains in productivity and efficiency. However, while some factors affecting management are under control, others are beyond the control, such as the unexpected increase in demand variation during the pandemic period. Indeed, an unusual amplification of the demand variation over several successive months is one of the key factors of the bullwhip effect, which can lead to considerable losses for upstream partners, and therefore have an impact on the entire supply chain performance. In this sense, through an empirical study conducted in large-scale retail stores specializing in the sale of convenience goods, we examine the demand for products that experienced the most significant changes in sales during this period, namely the fast-moving consumer goods. Thus, on the basis of historical sales data collected in the various points of sale, we determine whether the amplification of the demand variation experienced by retailers is statistically significant and over several successive months. The analysis covers the entire pandemic year, equivalent to twelve months from the date of the containment announcement, in order to determine whether the variation persists throughout the whole year or depends on the evolution of restrictive measures taken. The results of our research serve as a basis for further studies to analyze management methods that will enable retail stores to take into account a potential increase in demand and mitigate the amplification generated throughout the chain.

**Keywords:** Supply Chain Management, Bullwhip Effect, Pandemic, Consumer Good, Large, scale Distribution

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# **Theme 7: Management of Industrial Organizations and CSR**

# Workplace Safety as a Core CSR Commitment: Upholding Employee Well-being and Safety in the Mining Industry

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the mining industry remains one of the most challenging sectors regarding workplace safety due to its inherently hazardous nature. Despite significant technological advancements and regulatory measures, miners are still exposed to numerous risks, including harmful gases, hazardous substances, dust generated during operations, excessive noise from blasting or rock breaking, rock falls, machinery accidents, and the physically demanding ergonomic postures required in many tasks. These risks can lead to serious consequences such as work-related diseases, injuries, disabilities, or even fatalities.

In light of these challenges, workplace safety is increasingly recognized as a crucial component of Corporate Social Responsibility (CSR) for mining companies. In its broadest sense, CSR entails a company's commitment to ethical, sustainable, and socially responsible business practices. In the mining sector, this responsibility encompasses environmental stewardship and protecting employee health and well-being.

This article explores the critical role of safety in CSR strategies, emphasizing its importance in the mining sector, which is inherently hazardous. Through an analysis of industry practices, regulatory frameworks, and case studies, the article highlights the benefits of integrating robust safety protocols into CSR initiatives and their impact on employee well-being, operational efficiency, and corporate reputation.

Furthermore, the article investigates the unique safety challenges miners face daily and how proactive CSR efforts can mitigate these risks.

Finally, the article looks ahead to the future of mining safety, examining how technological innovations such as automation, artificial intelligence (AI), and Internet of Things (IoT) technologies can further reduce risks and support CSR initiatives. By prioritizing safety as a core aspect of CSR, mining companies can play a pivotal role in safeguarding their workforce while contributing to sustainable industry practices. The intersection of safety and CSR in the mining sector is thus not only a moral obligation but also a strategic imperative for long-term viability and success.

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**Keywords:** mining industry, mining risks, occupational health and safety, CSR, technology

# How the regions of Morocco are performing from an economic-entrepreneurship perspective ? A comparative study using the TOPSIS method

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The present paper aims to describe the performance of the twelve regions of Morocco from a dual economic-entrepreneurship perspective using the TOPSIS method for a seven successive periods under the new administrative structure from 2015 to 2021 based on ten various macroeconomic aggregates. Findings show a quite stagnation of the regions final ranking over the period of study, in which three observations can be mainly concluded:

Casablanca-Settat is all long placed on the top twelve, which consolidates its position as an economic capital of the country, followed by two regions in an alternative rank; Tanger- Tétouan- Al Hoceima and Rabat-Salé- Kénitra, while the southern regions are remaining at the bottom.

The disturbance observed in 2020 is due to the effects of Covid19 crisis, especially for the region of Marrakech- Safi which was brutally affected because of the rupture of touristic cash-flows, but soon as this stressful conjecture was faded, a return to the original pattern is observed.

The region of Béni Mellal-Khénifra is actually in a noticeable progression and it is recently well performing.

**Keywords:** Morocco, regions, economic, entrepreneurship, Covid19, TOPSIS

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\*Speaker

# Renewable energy impact on inward industrial foreign direct investment in Morocco

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<sup>1</sup>, Elmehdi Ferrouhi \*

1

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This paper investigates the role of renewable energy production in the location choice of multinational enterprises (MNE) in the Moroccan industrial sector. In particular, we analyze the impact of the production of hydraulic and wind energies on the attractiveness of industrial foreign direct investments (FDI) in Morocco. Using the robust weighted least squares (RWLS) estimation method for a 25-year series for the period 1997-2021, the results show that the higher the domestic hydroelectric and wind energy production, the more industrial FDI is attracted to Morocco, which means that renewable energy is a determining factor for industrial FDI. The implications of the study are resorting to renewable energy instead of importing fossil fuels that its dependency affects negatively the inward FDI.

**Keywords:** Renewable energy, Industrial FDI, Foreign direct investment, Energy transition, Morocco.

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\*Speaker

# Le management du développement durable comme levier de compétitivité pour les entreprises : une approche stratégique de rupture

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## Abstract

Ecological and social concerns are increasingly taking center stage in corporate management, but not all companies embrace sustainable development with the same level of commitment. Becoming a "responsible company" is a complex reality. Sustainable development can be simply integrated into managerial practices without disrupting them, or it can lead to a change in decision-making logic within the company.

The integration of sustainable development as a disruptive strategy in the field of management is a major challenge for companies. In the face of growing environmental, social, and economic challenges, more and more companies are seeking to rethink their practices and adopt innovative approaches to ensure their sustainability and competitiveness. This approach goes beyond mere compliance with existing standards and regulations; it involves a profound transformation of business models and organizational mindsets.

This article aims to explore the practical implications and potential benefits for companies that adopt sustainable development as a disruptive lever in their management strategy. To do this, we will first present the different responsible strategies of the company, and then explain how sustainable development can create a true disruptive strategy.

**Keywords:** sustainable development, disruptive strategy, responsible company

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