

## Polymerization of Acrylic Acid co Acrylamide Hydrogel by Ultrasound

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### Abstract

High frequency sound wave, ultrasound, is widely used to facilitate chemical reactions, especially in the polymerization reactions. This paper reports a study which synthesized acrylic hydrogel in the presence of ultrasonic irradiation (20-kHz, power 80%, pulse 8) in a water/glycerol medium. Acrylic acid (AA) and acrylamide (AAM) were used as acrylic monomers, and methylene bisacrylamide (MBA) as the crosslinker. The experiments were performed at a constant temperature of 37 °C. It was found that hydrogel formation is faster in the presence of ultrasound than in its absence. In addition, FT-IR, UV-Vis, and SEM spectroscopy showed that the hydrogel synthesized ultrasonically has a higher swelling capacity and a more uniform and porous structure. It was also discovered that hydrogel formation speeds up at higher quantities of glycerol. However, an increase in crosslinker concentration proved ineffective, although it changed the appearance of the hydrogel. The method proposed in this research can be used in the synthesis of biomedical materials and in the development of drug delivery systems.

**Keywords:** Polymerization, Hydrogels, Ultrasound, Microscopic Structure, Drugs Delivery

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## Optimization of Biosurfactant Production for Cleaning of Floating Crude Oil

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### Abstract

In this research, the ability of *Pseudomonas aeruginosa* NP2 to produce rhamnolipid biosurfactant was investigated. Rhamnolipid has various applications in oil industry including cleaning oil sludge filters, cleaning oil storage tanks and biological treatment of oil wastes. The purpose of this paper was optimization of biosurfactant production for reduction of costs using taguchi experimental design methods. Source of carbon, salt concentration, phosphorus concentration and nitrogen concentration at three levels were investigated. The best condition for biosurfactant production was observed when sucrose was used as carbon source, 50 g/l NaCl as salt source, 6.75 g/l  $\text{NaH}_2\text{PO}_4$  as phosphorus source, and 1g/l  $(\text{NH}_4)_2\text{SO}_4$  as nitrogen source. The highest rhamnoliopd production among different experiments was 2.8 g/l. Also the evaluation of emulsification index (E24) of the produced rhamnolipid was studied and the emulsification index value of 80% was reached for crude oil (API=34).

**Keywords:** Biosurfactant, Taguchi, Rhamnolipid, Fermentation, Emulsion index

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## **Sediment as New Source of Clean Energy for Bioelectricity Production**

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### **Abstract**

Sediment microbial fuel cells (SMFCs) are new technologies for production of clean energy. SMFCs are able to convert a wide range of organic matter contained in the sediment to bioelectricity. In this study, four different ecosystems (sea, hatchery, river and spring) was evaluated to assess their potential to generate electricity. Graphites were used as anode and cathode electrode. The lowest produced voltage was around 310 mV and produced from hatchery. Compared to other ecosystems, rivers generate the highest maximum generated power density of 37.09 mw/m<sup>2</sup>. The maximum generated voltage was 740 mV and it was completely stable for 12 days.

**Keywords:** Sediment microbial fuel cell; Clean energy; Electrical current; Power density

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## Comparision between CER.M-PAN and H.C.F.C-PAN in Separation Cesium Radioactive in Water Flow

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### Abstract

In the present Research, in order to access new technologies eliminate radioactive contamination have been carried out. The construction and use of exchange resins with high efficiency and efficacy, as a new approach in research and practical method of separation is introduced. This project is one of the most important pieces of  $^{137}\text{Cs}$  radioactive decontamination nuclear fission, two new composite entitled as CER.M-PAN (cerium molybdate-poly acrylonitrile) and HCFC-PAN (Cu Hegzacyanoferrat II- poly acrylonitrile) was prepared and their performance was evaluated in terms of continuous and discontinuous. To identify the structure of the synthesized compound, infrared spectroscopy techniques were used. Surface Area and Porosity of adsorbent beads were assayed. In order to increase the efficiency of these two composites, combining them with the PAN and their stability in different environmental conditions assessed and evaluated. The results suggest that the same efficiency than HCFC-PAN composite composite is CER.M-PAN.

**Keyword:** separation, H.C.F.C-PAN,  $^{137}\text{Cs}$ , Ion exchange, CER.M-PAN

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## Formic Acid Removal from Aqueous samples by Adsorption on Rice Bran

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### Abstract

The aim of this study is to investigate the possibility of the using rice bran as a natural and suitable adsorbent for the removal of formic acid, which is an organic acid from liquid solution, allow the effect of various parameters such as adsorbent dose, initial concentration adsorbate, temperature and time on the adsorption process and finally the adsorption isotherm constants in determined. Removal of organic acids from liquid solutions is an important environmental challenge. Batch adsorption experiments showed that the adsorption increased with the increasing of the amount of adsorbent, initial concentration of adsorbate and decreasing temperature and adsorption process is reached the equilibrium state after one hour. The adsorption data were analyzed using the various isotherm models. From these various isotherm models, the adsorption process obeys the Langmuir and Freundlich adsorption isotherms. The results show a good agreement with both methods. The average amount of adsorbate per 3 degrees of freedom and confidence 95%  $10.39 \pm 0.095$  was obtained.

**Keywords:** Organic acids, Adsorption isotherm, Adsorption, Rice bran

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## Investigating the Variation of Activated Carbon Adsorbents' Particle Size and Its Effect on Equilibrium Time and Nickel Ions' Removal Efficiency from Aqueous Solutions

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### Abstract

The environmental pollution of harmful toxic metals is one of the important issues in the world today. Nickel is one of the toxic heavy metals which if enters into the human body in high concentrations, it will cause skin allergy, heart disease and various cancers. Therefore, this is a pressing necessity to remove Nickel from industrial wastewater. The purpose of this study is firstly to remove nickel from aqueous solutions with synthesized activated carbon from carrot remains and secondly to investigate the effect of variations of the adsorbent particle sizes on the equilibrium time and the removal efficiency. To this end, adsorption of Ni (II) ions on the adsorbent was studied in a batch process. Firstly, the activated carbon was prepared from carrot remains with particle sizes between 37 and 300 micrometers. The results showed that the maximum absorption efficiency occurs (100%) at pH of 6. Moreover, it was shown that with decreasing the adsorbent size from 300 to 37  $\mu\text{m}$ , the equilibrium time will decrease from 130 to 20 min. Experimental data was best fitted onto pseudo-second order model. Langmuir and Freundlich isotherms equation were used to fit the adsorption isotherms. It is evident from this study that activated carbon is a suitable material for the uptake of Ni (II) from aqueous solutions.

**Keywords:** Activated Carbon, Nickel, particle size, Kinetic Models, Adsorption Isotherm

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# Theoretical Study of the Catalytic and Inhibition Mechanism of the $\beta$ -lactam Antibiotics by Metallo- $\beta$ -lactamases in the Different Solvents and Different Temperatures Using Quantum Mechanical Calculations

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## Abstract

The most prevalent and important mechanism of bacterial resistance to  $\beta$ -lactam antibiotics, is the production of  $\beta$ -lactamase enzymes which inactivate these drugs by the hydrolytic cleavage of the four-membered  $\beta$ -lactam ring during two steps which is including the nucleophilic attack of the bridging hydroxide ion on the substrate and eventual protonation of the leaving amine group. During this reaction, metal ions play an important role in the catalytic process. Despite the availability of  $\beta$ -lactamase crystallographic structures, their mechanism of action is still unclear and no clinically useful inhibitors of these enzymes have been reported.

Density functional theory (DFT) using B3LYP and 6-31G, 6-31G\* and 6-311G\*\* basis sets have been employed to calculate the details of electronic structure and electronic energy of catalytic reaction of CcrA enzyme active center from metallo- $\beta$ -lactamase enzymes (M $\beta$ LS), penicillin from  $\beta$ -lactam antibiotics, and the formed complexes including ES, ETS<sub>1</sub>, EI<sub>1</sub>, EI<sub>2</sub>, ETS<sub>2</sub> and EP respectively, has been used. Also all the thermodynamic functions including  $\Delta H^\circ$ ,  $\Delta S^\circ$  and  $\Delta G^\circ$  to form two transition states, ETS<sub>1</sub> and ETS<sub>2</sub>, and for the total reaction are evaluated at 25 °C, 31 °C, 37 °C and 40 °C and 1 atmosphere pressure. In all calculations solvent effects have been considered by using PCM method for water, ethanol, protein environment, nitro methane and carbon tetrachloride. Finally this reaction proceeds during an exothermic and spontaneous process, and the first step, the nucleophilic attack of the bridging hydroxide ion on the substrate, is the rate-limiting step.

**Keywords**  $\beta$ -Lactam antibiotics, Metallo- $\beta$ -lactamase enzymes (M $\beta$ LS), CcrA enzyme, Penicillin, Thermodynamic functions, QM calculations.

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