Biological Removal of Nickel by *Virgibacillus* Isolated from Spring Badab Surt and Optimization and Adsorption Parameters

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Abstract

The basis of this research is based on sampling of different parts of Badab Surt Sari spring, including water, soil and sludge. The effect of parameters such as pH, contact time, amount of bacterial biomass and initial concentration of nickel metal ion on the sorption rate was investigated. The final equilibrium time in this experiment was eight hours, but in the first half hour the maximum absorption was made and the number eight is related to the optimal pH. The ion removal isotherm follows the Langmuir model equation and the maximum adsorption capacity of the metal ion was 0.51 mmol/g, Langmuir constant is 49.01, R^2 was about 0.994. The use of bacterial biomass without and with metal by means of FT-IR showed that the groups involved, including carboxyl, hydroxyl and the amine. The results indicate that this isolate of rod-shaped bacterium, medium gram-positive filament, containing catalase, methyl red positive, has no motility and belongs to the genus Virgibacillus based on 16 S rDNA gene analysis. The adsorption capacity of nickel metal is very significant in the initial minutes and therefore, the use of the studied bacteria is appropriate in industry and biotechnological processes. The ions studied were adsorbed in the early stages when they were inactive, then in the secondary stage they were actively adsorbed slowly. Therefore, this bacterium has the ability to absorb metal in both live and dead forms.

Keywords: Bacteria Virgibacillus, Nickel, Isotherms, Surface Groups, Biosorption.

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Modeling of Two Parameters Isotherm of CO_2 and H_2S Adsorption Using Metal Organic Frameworks (MOFs)

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Abstract

In this research, the adsorption potential of carbon dioxide and hydrogen sulfide storage in metal organic frameworks has been studied and modeled. Studying four different type of micro porous coordination polymer adsorbents metal organic frameworks including MOF-2 (Zn_2 (BDC)2), MOF-74 (Zn_2 (DHBDC)), IRMOF-1 (Zn_4O (BDC)3) and MOF-177 (Zn_4O (BTB)2) showed that the adsorbent have different structure caused different performance in gases adsorption. For adsorption isotherm modeling of these adsorbents used two parameters isotherm models. For calculation parameters of the models was used nonlinear regression technique. The results showed that the models have good agreements with experimental data. Hill model has high accuracy to compare with other models. The parameter values of D-R model for all adsorbents showed that the processes were physical adsorption and IRMOF-1 for H_2S and MOF-74 and MOF-2 for CO_2 adsorption were suitable.

Keywords: Gas Adsorption, Metal Organic Frameworks, Carbon Dioxide, Hydrogen Sulfide, Isotherm Modeling.

Optimization of Biodiesel Production from Waste Cooking Oil in Present of Polyoxometalate as Catalyst Via Electrolysis Method Based on Response Surface Methodology (RSM)

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Abstract

Today, due to emission of toxic and green gases from the combustion of fossil fuel, science look for renewable and eco-friendly fuels that biodiesel is kind of green fuel and has all properties. In these study, the biodiesel produced from waste cooking oil using phophomolybdic acid ($H_3PMo_{12}O_{40}$). In order to optimize esterification reaction via electrolysis method response surface methodology based on central composite (RSM-CCD) was used. The effect of three main factors of catalyst weight (wt%), methanol to oil molar ratio and time (h) was investigated and all experimental runs were performed at constant electric voltage (10 V) and room temperature. The highest biodiesel yield in the present of 3.58 wt% catalyst, 7.84:1 at 8.24 h were 94.42%. the produced biodiesel in accordance with the ASTM standard. A value of R^2=0.9933 indicates that the predicted model sufficient accuracy to estimate the parameters participating in the reaction. Also, the high activity of phosphomolybdic acid catalyst has made it a suitable option for biodiesel production on an industrial scale.

Keywords: Biodiesel, Phosphomolybdic Acid, Electrolysis Method, Response Surface Methodology (RSM).

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Verification of Experimental Design and Statistical Methods for Optimization of Dark Hydrogen Production

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Abstract

Hydrogen has high energy content known to date, which produces water vapor due to combustion and is converted to electricity by fuel cells with high efficiency, therefore is considered as a candidate of future energy source. Production of bio- hydrogen through dark fermentation can ferment sustainable renewable substances such as C_5 and C_6, wastewater and converted waste, compared to photosynthetic methods requires no light, has higher production rate and yields. Fermentative hydrogen production is a complex process and is influenced by several factors, statistical methods of optimization offer relatively understandable interaction among the factors. One of the approach to increase the rate and yield of reaction is to screen, model, and optimize factors which have strong influence on the response comprising inucolum, operating temperature, pH, type and concentration of substrates etc by employing appropriate method. For screening factors and performing regression ANOVA is used. The experimental design method used for screening and understanding the effect of factors are one-factor-at-a-time, full factorial, fractional factorial, Taguchi, Plackett–Burman,central composite and Box–Behnken design, steepest inclined or declined, neural network ANN, genetic algorithms and, for optimization response surface methodology is frequently applied. The overview, presents appropriate advantages and disadvantages of analyzing abilities of modeling of experiments and addresses few statistical methods of optimization to understand complex effect of factors on fermentative dark hydrogen production. Such deep knowldge leads in understanding more in details the interactions of complex reactions involved and to select sound statistical method of optimization, resulting in reasonable reduced number of experiments to achieve higher rate and yield of production at lower cost of operation.

Keywords: Biohydrogen Production by Dark Fermentation, Design of Experiments, Plackett–Burman Design, Response Surface Methodology, Neural Network.

A Novel Method to Simulation of Heterogeneous Fractured Oil Reservoirs with Eclipse

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Abstract

Fractured reservoirs form a major part of the country's hydrocarbon reservoirs. The proposed models for modeling fractured reservoirs, including dual porosity and dual permeability, consider the dispersion of the fractures in the reservoir to be homogeneous and consider their dimensions to be much smaller than the matrix dimensions. If there are large heterogeneous fractures in the reservoir, the use of these models does not provide acceptable results for reservoir simulation. In Eclipse 300 software, simulation of heterogeneous fractured reservoir with long fracture length is conducted by using CONDFRAC keyword to identify long permeable fractures which causes an error in the parts of the reservoir that have a curvature, due to the lack of correct detection of a specific plate perpendicular to the fracture plate and the overlap of the fractures, causes an error in the reservoir simulation results. In this study, in order to eliminate the existing shortcomings, a new method is presented by using the box definition of matrix and fractures network properties in Eclipse 100 software, which simplifies the reservoir simulation process and reduces the program execution time. The studied oil reservoir is carbonate type in the Arabian Formation, which includes heterogeneous fractures with long length. The simulation results are compared between the two methods presented in this study. Comparing the results of the single medium method with the new method for field oil in place (FOIP), revealed that the average difference between the two methods is less than 1.1% and reduces the simulation execution time by about 40%, which indicates the optimal performance of the new method.

Keywords: Novel Method, Simulation, Heterogeneous, Fractured Oil Reservoirs, Eclipse.

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Simulation of Silver Nanoparticles Green Synthesis Using *Aloe Vera* leaf Extract and Microwave Heating, and Evaluation of their Characteristics

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Abstract

Green synthesis of metal nanoparticles using plant extracts is an efficient, fast and low cost method. In order to synthesis of silver nanoparticles (AgNPs) using aqueous leaf extract of Aloe vera, due to its reducing and stabilizing agents, such as flavonoids and acetic acid which those were detected by FTIR analysis, and microwave heating, at different powers of 480, 640 and 800 W were used. Synthesized AgNPs were characterized by UV-Vis and DLS analysis, and results indicated that AgNPs with concentrations of 38.58, 61.52 and 91.35 ppm, as well as mean particle sizes of 94, 74 and 61 nm, were obtained, at different powers of microwave, respectively. After simulating the synthesis conditions of the AgNPs using COMSOL Multiphysics in different powers (800-480 W), in order to optimize the time, energy and temperature applied for synthesizing AgNPs, results indicated that AgNPs with desirable properties were fabricated at average temperature, power and processing time of 337 ºK, 800 W and 175 s, respectively.

Keywords: Aloe Vera Leaf Extract, Green Synthesis, Microwave Heating, Synthesis Conditions, Silver Nanoparticles, Simulation.