THESIS INFORMATION

Title: **STUDY MODIFY LIGNOCELLULOSE MATERIALS FOR THE REMOVAL OF HEAVY METAL IN WATER**

Major: **Organic Chemical Technology**

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PhD student: **Nguyen Thuong Dang**

Advisor: **Assoc.Prof. Dr. Pham Thanh Quan**

University: **University of Technology, Vietnam National University – Ho Chi Minh City**

Abstract

The selection in order to modify agricultural by-products to create materials replaced for cationite and anionite resins in the treatment of ground water and wastewater is considered "green" selection, environmentally friendly, taking advantage of the available natural resources and reduced water treatment costs but still achieve the desired effect. Lignocellulose materials have the advantages of low cost, renewable and their main components contain polymers modified easily and after modifying perform higher ability of adsorption and ion exchange, therefore studied more and more to apply in the removal of heavy metal ions in water.

Three kinds of lignocellulose materials are cotton, sawdust from acacia auriculiformis wood and coconut shell powder used to research in the thesis. The initial lignocellulose materials was delignified in NaOH 0.2 N/ ethanol 70^o aqueous solution, then modified with 4,5-dihydroxy-1,3-bis (methoxymethyl) imidazolidin-2-one (m-DMDHEU)/choline chloride mixture to create anionite lignocellulose materials and with acid citric to create cationite lignocellulose materials. Structural characterictics and physicochemical properties of materials were tested and dissected by some methods such as scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR), nuclear magnetic resonance spectroscopy-solid state ^{13}C (CP-MAS NMR ^{13}C solid state), BET surface area, pH_{PZC}, mass increase level and ability to ion exchange chromate (VI), iron (III).

Modification reaction mechanism was studied by Density Functional Theory (DFT) with computational method B3LYP/ Basis set 6-311g(d,p), combining experimental results and spectral analysis. Cationite lignocellulose materials were used to treat simulation solutions containing Fe(III),

Pb(II) ion in different conditions; together with reality wastewater samples of electronic printed circuit board and lead-acid battery plants.

The ability to adsorb and exchange ions of anionite lignocellulose materials were examined using solutions containing CrO_4^{2-} and $H_2AsO_4^-$ ions in different conditions. The results suggested that the ability to separate CrO_4^{2-} and $H_2AsO_4^-$ ions of modified materials were better than that of GA-13 anion exchange resin at pH = 7.0; the chromate adsorption capacity was the best in acidic condition. Lastly, the modified material was used to treat water samples containing a concentration of arsenate similar to groundwater in several arsenic-contaminated areas of Vietnam.

Furtheremore, anionite lignocellulose also are combined with cationite lignocellulose to treat hard water sample containing a mixture of Ca (II), Mg (II) and nitrate.

Contributions of this thesis

(1) Established succesful the synthesis process for three kinds of anionite lignocellulose materials modified with the mixture of new denaturation agents m-DMDHEU/ Choline chloride.

(2) Investigated and predicted reaction mechanisms of lignocellulose materials modified with mixture of m-DMDHEU/ Choline chloride and with citric acid based on the combination of evaluation, analysis with results of experimental, spectral analysis and quantum chemistry calculation.

(3) Anionite lignocellulose materials can separate chromate and arsenate ions better than strong anion exchange resin GA13; concentration of chrome and nitrate in outlet water meet the permissible drinking water standards according to **QCVN 01:2009/ BYT** and concentration of arsenic in outlet water meet the permissible clean water standards according to **QCVN 02:2009/ BYT.**

Advisor	**PhD student**
Assoc. Prof. Dr. Pham Thanh Quan	**Nguyen Thuong Dang**