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PREDICTION OF INTERACTION OF CITRIC ACID MODIFIED CELLULOSE WITH WATER REGION USING MOLECULAR MODELLING TECHNIQUE

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ABSTRACT

The discharge of toxic heavy metals in water bodies is a serious pollution problem affecting water quality, creating a direct hazard to human health if present in drinking water. In this study, metal of interest was ferric ion (Fe^{3+}) due to potential pollution impact on the aquatic environment. Ferrous ion (Fe^{2+}) which are dissolved in water will be converted into complexes ferric ion by bacteria activities and can be removed by citric acid modified cellulose (CAMC). The purpose of this research is to improve the method to remove heavy metal from a polluted water as the cellulose in nano-crystalline forms are less exploited for adsorption application. In this findings, chemically modified cellulose was used instead of cellulose because it has higher adsorption capacities, great chemical strength and good resistance to heat. As part of Phyto-Adsorption Remediation Method, CAMC was used to treat ferric ion. However, there is a large possibility that CAMC molecule might interact with water molecule that contain hydrogen and oxygen bond and hence pose as a competitor to ferric acid and reduces the efficiency of CAMC in ferric ion removal. Thus, the aim of this work is to identify the most stable hydrogen bond between CAMC and water, by using a computational technique. The interaction between the water molecules and CAMC was observed by varying the volume of water molecule with modified cellulose by an expansion in amorphous region. The simulation result showed that for water loading less than 20 molecules, the interaction between water molecules and CAMC is higher at temperature 311K, whilst for water loading higher than 20 molecules, the interaction weakens at higher temperature. This work proved that water molecules have the tendency to bind to hydroxyl group of glucose ring, to oxygen of ester and to oxygen of anhydride acid of the CAMC molecule. The calculation of coordination number has shown that the number of atoms present in the first hydration shell (of radius < 2.5Å) is more as the temperature increases from 298K to 311K. Whilst, at radius >2.5Å, cell temperature is not significant to the number of atoms present.

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TABLE OF CONTENT

vi

CHAPTER 1
INTRODUCTION

1.0 Research Background

Water pollution is a crucial problem in the worldwide context. Some industrial wastewater may contain heavy metals including the waste liquids especially produced from metal finishing or the mineral processing industries. Toxic metals apparently existing in high concentrations. If the wastewater were discharged into drainage system, it will give a great risk for the aquatic ecosystem, also the direct release into the sewage system can affect the biological wastewater treatment. Heavy metals are non-degradable metals. These metals are toxic and possess high density. Improper disposal of these heavy metals leads to pollution.

Heavy metals contamination in abandoned mines is a global environmental problem which several countries around the world are suffering from. In addition, contamination of aquatic environments by metals arising from both of mining processes, either underground or surface mine workings has received growing environmental concern worldwide. Hence, various studies showed that the mining activities have caused chemical and physical changes in their surrounding aquatic life. High concentrations of metal contamination have significant effect on the deterioration of the quality of ecosystem and increasing the phytotoxicity in sediments.

Plants is a key role in forming a fundamental part of the healthy structure of aquatic ecosystems. It can be considered as intermediate reservoirs of heavy metals from the sediments, water and air and digested by human and animal through the food chain (Kutty et al., 2016). In addition, Sanna et al. (2016) has mentioned that cellulosic materials was easy to obtain from natural sources and well known as cheap adsorbents. Cellulose is a natural bio-based materials that can be applied and modified in water treatment system.

Cellulose is an abundant polymer exist in nature that giving the plant rigidity and existed from variety of sources as microbes, woods and animals (Hongliang et al., 2015). Its molecular weight depends to its sources and extraction condition of purification. The adsorption capacities of cellulose for heavy metals and other toxic elements can be modified by chemical treatment. Hence, chemically modified cellulose shows great adsorption capacities for removal heavy metal