Artificial neural network simulations and experimental results: Removal of trichlorophenol from water using *Chromolaena odorata* stem

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ABSTRACT

A novel adsorbent for trichlorophenol (TCP) has been developed through the treatment of *Chromolaena odorata* (Odorata) with iodated table salt. Odorata is an abundant and problematic alien plant which we have found to be effective in removing TCP from aqueous solutions. Kinetic batch tests demonstrated that at pH 5, 99% of TCP could be removed from a solution given sufficient adsorbent loading rate and adsorption contact time with Odorata treated with table salt. Adsorption data were found to fit a 2-layer feed-forward artificial neural network (ANN) with 10 neurons using the Levenberg–Marquardt (trainlm) algorithm. The ability of Odorata to extract TCP from water was tested using equilibrium, kinetic and thermodynamic studies. Thermodynamic studies showed that the adsorption of TCP by the new adsorbent is thermally feasible and is governed by a chemical adsorption mechanism. It was established that the experimental data fit the selected adsorption isotherms in the following order: Langmuir > Freundlich > Temkin > Dubinin-Radushkevich (D-R). Kinetic modelling was done using intra-particle diffusion, liquid-film, pseudo-first order and pseudo-second order models. With the aid of the normalised standard deviation, the pseudo-second order was found to be the appropriate rate expression for the adsorption data. Liquid-film diffusion was the rate-determining stage of the adsorption process.

Keywords: *Chromolaena odorata*; TCP; adsorption; table salt; ANN

INTRODUCTION

The pollution of water by organic materials is inexorable. Trichlorophenol (TCP) is one of the problematic compounds that end up in water as a result of industrial and agricultural activities. The main pollution sources containing chlorinated phenols like TCP are the wastewaters from pesticide, paint, solvent, pharmaceutics, wood, paper and pulp industries as well as water-disinfecting process (Hameed et al., 2008). Removing TCP from water is crucial. TCP is highly toxic, carcinogenic, structurally stable and persistent in the environment (Hameed et al., 2008). According to Tan et al. (2009) the stable C-Cl bond and the position of chlorine atoms relative to the hydroxyl group are responsible for TCP's toxicity and persistence in the biological environment.

Unlike inorganic water pollutants (like heavy metals), the concentration of organic compounds like TCP in water can be reduced by photo-degradation. Another technique used for the removal of TCP from aqueous media is membrane filtration technology. The major disadvantages of the membrane processes are the costs, as membrane filtration processes use pressure and their lifetime is limited before fouling (Subramani et al., 2009; Hoek et al., 2011). In accordance with the abundant literature data (Pei et al., 2007; Fan et al., 2011; Puyol et al., 2011; Zaghouane-Boudiaf et al., 2011), adsorption is one of the most popular techniques for the uptake of TCP from water. In recent years, a lot of attention has focused on developing effective adsorbents which are able to remove the pollutants from the contaminated wastewater at low cost. Cost is actually an important parameter for comparing the suitability of adsorbent materials. According to Ahmaruzzaman (2008), an adsorbent can be categorised as low-cost if it requires little processing and is abundant in nature.

Most of the adsorbents that have been developed can be loosely classified as either inorganic or agricultural. One inorganic adsorbent that has been widely studied is clay. For example, Dlamini et al. used organo-montmorillonite (2012a) and Bentonite (2012b; 2012c) as filler in polymeric composites aimed at removing lead ions from water. Motsa et al. (2011) and Mthombo et al. (2011) used clinoptilolite as a filler material in the preparation of composites which were used for the removal of heavy metals from water. Such adsorbents (polymeric composites) are ideal for easy recovery and are stable in the water environment especially if the polymer used as a support is hydrophobic. The downside with composite adsorbents is that a lot of the filler needs to be used, while lower adsorption efficiency is recorded compared to powder adsorbents. The agricultural products that have been used as adsorbents for heavy metals and organic pollutants are *Acacia leucocephala* bark (Kumar et al., 2012), rice husk (Mahvi et al., 2004), sawdust (Shukla et al., 2002) and TiO_2 (Dutta et al., 2010), to mention but a few.

Agricultural adsorbents are also called biosorbents. These materials contain various organic compounds (lignin, cellulose and hemicellulose) with polyphenolic groups that might be useful for binding TCP through different mechanisms. Agricultural products have to undergo treatment before they can be used in water treatment to remove lignin-based colour materials. To this end, NaOH (Mthombo et al., (2011), KCl and NaCl have been commonly used for preparing biosorbents; however, for this study the iodated salt has been used.

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