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Artificial neural network modeling for the oxidation kinetics of divalent manganese ions during chlorination and the role of arsenite ions in the binary/ternary systems

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ABSTRACT

This study investigated the coexistence and contamination of manganese (Mn(II)) and arsenite (As(III)) in groundwater and examined their oxidation behavior under different equilibrating parameters, including varying pH, bicarbonate (HCO_3^-) concentrations, and sodium hypochlorite (NaClO) oxidant concentrations. Results showed that if the molar ratio of NaClO: As(III) was >1, the oxidation of As(III) could be achieved within a minute with an extremely high oxidation rate of 99.7 %. In the binary system, the removal of As(III) prevailed over Mn(II). The As(III) oxidation efficiency increased from 59.8 ± 0.6 % to 70.8 ± 1.9 % when pH rose from 5.7 to 8.0. The oxidation reaction between As(III) and NaClO releases H^+ ions, decreasing the pH from 6.77 to 6.19 and reducing the removal efficiency of Mn(II). The presence of HCO_3^- reduced the oxidation rate of Mn(II) from 63.2 % to 13.9 % within four hours. Instead, the final oxidation rate of Mn(II) increased from 68.1 % to 87.7 %. This increase can be attributed to HCO_3^- ions competing with the free Mn(II) for the adsorption sites on the sediments, inhibiting the formation of H^+. Moreover, kinetic studies revealed that the oxidation reaction between Mn(II) and NaClO followed first-order kinetics based on their $\boldsymbol{R^2}$ values. The significant factors affecting the Mn (II) oxidation efficiency were the initial concentration of NaClO and pH. Applying an artificial neural network (ANN) model for data analysis proved to be an effective tool for predicting Mn(II) oxidation rates under different experimental conditions. The actual Mn(II) oxidation data and the predicted values obtained from the ANN model showed significant consistency. The training and validation data sets yielded $\boldsymbol{R^2}$ values of 0.995 and 0.992, respectively. Moreover, the ANN model highlights the importance of pH and NaClO concentrations in influencing the oxidation rate of Mn(II).

1. Introduction

Groundwater is the world's most important source of fresh water. It is used for agricultural, domestic, municipal, and industrial purposes. According to the United Nations Educational, Scientific and Cultural Organization (UNESCO) (Connor, 2015), over 2.5 billion people rely on groundwater as their primary water source (Siebert et al., 2010). The presence of arsenite (As(III)) and manganese (Mn(II)) contaminants in groundwater limits safe drinking water supplies in various parts of the world (Fendorf et al., 2010); Ying et al., 2017; McMahon et al., 2018; McArthur et al., 2018). Reportedly, over 250 million people worldwide experience long-term exposure to As(III) and Mn(II) contamination (Kapwata et al., 2023; Frisbie et al., 2012). Most importantly, As(III) and Mn(II) bioaccumulate in soft tissues and potentially the brain. Prolonged and extensive exposure can lead to various adverse effects on the human body, including the development of multiple cancers (Muzaffar et al., 2023; Fatoki and Badmus, 2022; Kuo et al., 2022; Kalimuthu et al., 2022). Therefore, the World Health Organization (WHO) and the United

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