Modeling temperature and reaction time impacts on hematite nanoparticle size during forced hydrolysis of ferric chloride

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Abstract

On the hypothesis that a mathematical relationship exists between synthesis conditions and hematite nanoparticle (NP) sizes, an empirical model was developed by synthesizing hematite NPs at different temperatures and hydrolysis times, and then correlating them with the obtained NP sizes. We found that the hematite NP sizes can be described by a simple relationship, $d_P = \frac{(0.49/T + 26.4) \times C_{176}}{a \times C_0}$. The predictive capabilities of the model were validated by synthesizing NPs at randomly selected experimental conditions and comparing them to the model predictions. The experimental findings suggested that the model may be limited to predicting NP sizes smaller than 50 nm because of a possible shift from a slow, hydrolysis-driven growth mechanism to a mechanism characterized by rapid aggregation of the existing NPs.

1. Introduction

Synthetic iron oxides have become a commonly engineered nanoparticles (NP) and widely used in commercial and industrial applications such as pigments, catalysts, adsorbents, and sensors [1–3]. The use of iron NPs as catalysts in advanced oxidation processes (AOPs) is a promising alternative to existing technologies for the decontamination of soil, groundwaters, sediments, and industrial effluents [4–6]. Once NPs enter the environment, they will inevitably come into contact with humans and other living organisms in the environment. The small size of NPs may induce various biological effects, including DNA damage [7–13].

It is well documented that the properties of nanomaterials, including their toxicity, strongly depend on particle size and its associated parameters [14–17]. The changes in the surface charge as particle size decreases will alter the adsorption affinity of NPs toward cells [14,18]. For example, the adsorption of small iron NPs (< 50 nm) onto Escherichia coli cells and human intestinal cells was faster than that of large NPs (> 75 nm) [14,18]. The impact of iron NP size on aggregation behavior and stability under environmentally relevant pH and ionic strength conditions has been investigated [19–22]. Other studies also have shown that smaller particles are more readily adsorbed, which influences the transport of NPs significantly. However, it can be difficult for researchers to prepare and use uniform dispersions of engineered NPs without modifying their surfaces with organic dispersants. These dispersants can alter the properties of the NPs and seriously impact...