



Modeling batch and column phosphate removal by hydrated ferric oxide-based nanocomposite using response surface methodology and artificial neural network



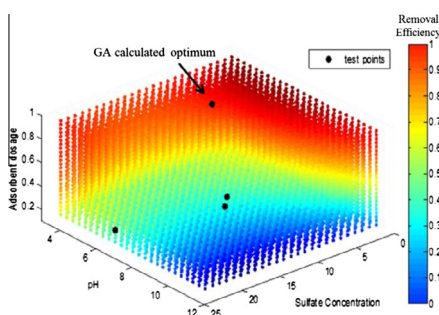
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HIGHLIGHTS

- Trace phosphate removal was realized by HFO-based nanocomposite.
- RSM and ANN model was developed to model phosphate removal.
- Four variables of temperature, pH, sulfate and solid dosage was involved.
- Genetic algorithm was employed to yield optimum conditions.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 8 January 2014
Received in revised form 16 March 2014
Accepted 20 March 2014
Available online 29 March 2014

Keywords:

Nanocomposite adsorbent
Phosphate removal
Artificial neural network
Response surface methodology

ABSTRACT

Batch and column phosphate removal was conducted by a commercially available nano-hydrated ferric oxide composite HFO-201 under varying conditions, and the performance was modeled and predicted with the aid of artificial neural network (ANN) model and response surface methodology (RSM). Initial pH, sulfate concentration, operating temperature, and adsorbent dosage were chosen as four variables for the batch study, while the removal efficiency was considered as the output. A central composite design (CCD) was referred to design 33 sets of batch experiments, and a RSM model was developed to compare with the ANN model. The three-layer feed-forward back-propagation network was established in MATLAB to estimate the phosphate removal efficiency. The positive behavior of both models was verified by Pearson and Spearman coefficient and mean squared error (MSE). Analysis of variance (ANOVA) tests and sensitivity analysis were performed on the models to find relative influence of four variables. Temperature was deemed as the least influential whereas the other three variables were considered significant to the output. Genetic Algorithm (GA) was employed to find optimum dosages for a desired removal efficiency under given conditions. ANN modeling was further attempted to estimate the breakthrough curves of fixed-bed adsorption, where pH, sulfate, temperature, flow rate (BV/h) and bed volume was considered as variables. Predictions made by the developed models were in reasonably good agreement with the test runs. This study suggested that ANN and RSM be considered as effective tools to model and predict trace pollutants removal by nanocomposite adsorbents.

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1. Introduction

Environmental nanotechnology has attracted increasing interest in water purification and remediation in recent years [1]. Till

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now a variety of nanomaterials has been reported to serve as catalysts, membranes and adsorbents for water decontamination. Such nanomaterials possess desirable properties not limited to large specific surface area, high activity and microbial restraining effect [2–4]. Recently, increasing studies have been performed to remove toxins from aqueous systems such as toxic metals [5–9], arsenic [10] and phosphate [11,12] by nanosized adsorbents. For instance, arsenic and phosphate removal by nanosized hydrous ferric oxide (HFO) have been extensively explored [13–15]. Nevertheless, most of the related references were based on laboratory scale experiments, and application of nano-adsorbent in field application has been scarcely reported. This is because direct use of nanosized adsorbents faces unavoidable challenges such as activity loss as a consequence of aggregation in aqueous solution and costly separation [16]. Additionally, great concerns regarding the potential environmental and health risks of released nanomaterials were also raised [17].

In response to the technical challenges of nanoparticle adsorbents for practical application, in the past decade, nanocomposite adsorbents has been developed by immobilizing or encapsulating target nanoparticles inside solid host of porous structure and large size. The resultant nanocomposites combine high activity of target nanoparticles for decontamination with readily separation and satisfactory mechanical strength of the solid hosts, thus exhibiting improved applicability and great potential in water treatment. Currently, some nanocomposite adsorbents are commercially available for field application in removal of arsenic, phosphate, and toxic metals from water [18–22]. Particularly, these adsorbents are capable of removing trace pollutants to meet the stringent standard of water and wastewater with exceptionally high treatable volume. Several studies were also carried out in our group using synthesized nanocomposite adsorbent to eliminate various ionic pollutants from wastewaters [23–26]. For instance, a patented nanocomposite adsorbent HFO-201 has been proved to be a specific phosphate adsorbent from bio-treated effluent [12,25].

As generally known, adsorption is usually conducted in the form of fixed bed in practical application. The performance of an adsorption process is a function of solution chemistry (pH, ionic strength, temperature, other coexisting substances) and adsorbent structure. Optimum operational design of an adsorption system could be based on the experimental study involving all the above factors, but it is a time consuming process. Comparatively, prediction could help to allow maximum capacity of adsorbent in a much simpler way. The conventional way to predict the adsorption process is originated from deep understanding of adsorption mechanisms. Some mechanistic models such as surface complexation model and MUSIC model were developed to address on these issues [27,28]. During the development of mechanistic models, the unavoidable simplifications and assumptions would compensate the lack of knowledge of some unrevealed mechanisms. Unluckily, they could lead to inaccurate predictions [29,30]. In the past decade, alternative modeling tools such as response surface methodology (RSM) and artificial neural networks (ANN) have received increasing attentions and acceptance in the field of engineering and process study [31–36]. Both empirical models or statistical models take full advantage of the known data due to their inherent ability to extract knowledge from operating conditions and reproduce complex relationships in engineering without knowing the sophisticated underlying mechanism of the process [29,32]. RSM model is known for its strength in understanding environmental engineering process [37]. ANN was inspired by biological neurons [38] and was derived from artificial intelligence (AI) research. ANN can describe multivariate nonlinear problem well with suitable amount of data and appropriate training algorithm applied, in a way, it mimics human learning behavior [32]. A number of works using ANN as a modeling tool were reported in the field of

environmental engineering, including adsorption [39–41], AOPs [42], bio-reaction [43,44] and electrocoagulation [45]. Several papers took advantages of the genetic algorithm coupled with ANN to generate optimum operating variables for the studied process [45–47].

The objective of this study is to explore the potential of artificial neural network and response surface methodology to model phosphate removal from water by the nanocomposite adsorbent HFO-201. We first employed response surface methodology (RSM) and artificial neural network (ANN) to model the phosphate removal characteristics of HFO-201 in batch experiments. Initial pH, sulfate concentration (sulfate), temperature (temp) and dosage of the adsorbent (dosage) were chosen as the variables, and the removal efficiency was chosen as the target parameter. Afterwards, ANN was used to describe the phosphate adsorption characteristic in a fixed-bed column packed with HFO-201. The performance of both models was evaluated and sensitivity analysis was conducted to explore the relative importance of the variables. Then, genetic algorithm combined with the ANN was employed to yield the optimum conditions for desired removal efficiency. Additionally, the individual and combined effect of the variables of concern was analyzed on the basis of the established models.

2. Materials and methods

2.1. Materials

All the chemicals used in the study are of analytical grade from Shanghai Reagent Station (Shanghai, China) and used without further purification. The stock solution containing 100 mM orthophosphate (in *P*) was prepared by dissolving KH_2PO_4 into de-ionized water. The hybrid nanocomposite adsorbent HFO-201 was obtained from Jiangsu NJU Environmental Technology Co., Ltd. Essentially, HFO-201 comprises of two basic units, the host poly(styrene–divinylbenzene) anion exchanger beads binding $\text{R-N}^+(\text{CH}_3)_3$ groups, and the immobilized nanosized hydrated ferric oxide therein of ~10% Fe in mass. The BET surface area of HFO-201 is 27.5 m^2/g and the average pore diameter is 20.3 nm [25]. Prior to use, HFO-201 was subjected to cleanse with ethanol and de-ionized water to remove any possible impurities.

2.2. Batch and column experiments

Batch adsorption experiments were carried out using a traditional bottle-point method to study the effect of solution pH (3–11), temperature (20–40 °C), sulfate concentration (sulfate, 0–2.0 mM) and adsorbent dosage (dosage, 0.1–0.9 g/L) on the removal efficiency of phosphate (initial concentration 0.1 mM). Multiple experiments were conducted in 250 mL flasks containing 100 mL solution with different phosphate and sulfate levels. Appropriate amount of 0.10 M HCl or NaOH solutions were used for pH adjustment. After addition of the HFO-201 beads, the flasks were sealed immediately, placed in the thermostatic shakers, and shaken at preset agitation speed and temperature. The flasks were shaken for 24 h to achieve equilibrium, as indicated by our early study [25,48]. Then, the samples were filtered through 0.45- μm syringe filter for phosphate determination. A number of small Pyrex glass columns (12.0 mm in diameter and 130.0 mm in length) were used to implement fixed-bed experiments. These columns were equipped with a water bath to maintain a constant temperature. Five milliliter of HFO-201 was packed within the columns. Ten-liter synthetic solutions with different phosphate and sulfate levels and different pH values were applied as the feeding solutions. The lange-850 variable speed peristaltic pumps were employed to control the volumetric flow rate, and the feed

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