Chemometrics and Intelligent Laboratory Systems 135 (2014) 70–75

Contents lists available at ScienceDirect

Chemometrics and Intelligent Laboratory Systems

journal homepage: www.elsevier.com/locate/chemolab

Application of cuckoo optimization algorithm–artificial neural network method of zinc oxide nanoparticles–chitosan for extraction of uranium from water samples

Mostafa Khajeh *, Elham Jahanbin

Department of Chemistry, University of Zabol, P.O. Box 98615-538, Zabol, Iran

ARTICLE INFO

Article history:
Received 4 March 2014
Received in revised form 31 March 2014
Accepted 5 April 2014
Available online 16 April 2014

Keywords:
Uranium
Zinc oxide nanoparticles–chitosan
Artificial neural network–cuckoo optimization algorithm
Water samples

ABSTRACT

In this study, a solid phase extraction using the new sorbent (zinc oxide nanoparticles–chitosan) has been developed for preconcentration and determination of trace amount of uranium from water samples. Hybrid modeling of cuckoo optimization algorithm–artificial neural network (COA–ANN) has been employed to develop the model for simulation and optimization of this method. The 1-(2-pyridylazo)-2-naphthol (PAN) was used as chelating agent. The pH, volume of elution solvent, mass of zinc oxide nanoparticles–chitosan, concentration of PAN, flow rate of sample and elution solvent were the input variables, while recovery of uranium was the output. At the optimum conditions, the limit of detections and enrichment factor were 0.5 μg L^{-1} and 125, respectively for the uranium. The developed procedure was then applied to the extraction and determination of uranium from water samples.

1. Introduction

Uranium is extensively used in the nuclear industry and is highly radioactive. It is present in low quantities in wash streams coming out of nuclear reactors both in aqueous as well as non-aqueous medium and monitoring of these streams for the presence of U in high activity content is important [1–6].

In recent years, there is increasing interest in the application of nanoparticles as sorbents for extraction of target compound. Semiconductor nanoparticles have much attention because of their novel electrical, mechanical and optical properties. Among various semiconductor nanoparticles, zinc oxide nanoparticles are the most frequently studied due to their applied aspects. Due to the large specific area, nanoparticle sorbent has a higher efficiency for the extraction of target compounds [7,8]. Hybrid materials based on chitosan have been developed such as metal nanoparticles, due to good properties of individual components and outstanding synergistic influences simultaneously [8–10].

In recent years, as a mathematical representation of the neurological function of a brain, neural network (NN), which is capable to depict the interactive influence between variables, has been applied successfully in multivariate non-linear separation process as a powerful tool to construct modeling [11–14].

In this study, an evolutionary optimization algorithm was applied for the first time in chemical modeling, which was inspired by the lifestyle of a bird family called cuckoo. Specific egg laying and breeding of cuckoos are the basis of this novel optimization algorithm.

The aims of this work are: (i) to use of zinc oxide nanoparticles–chitosan as sorbent for preconcentration and determination of uranium ions from water samples, (ii) to obtain a predictive model based on ANN technique for prediction of the recovery of analyte, (iii) to optimize the recovery of analyte using combination of ANN and cuckoo optimization algorithm (COA) methods, and (iv) to develop a simple and cheap method for extraction of uranium. Finally, UV–Vis spectrophotometry was employed for analysis of uranium.

2. Materials and methods

2.1. Reagents and samples

The 1-(2-pyridylazo)-2-naphthol (PAN) and HPLC grade of solvent including acetonitrile, benzene, chloroform and ethanol were obtained from Merck (Darmstadt, Germany). Reagent grade zinc oxide was obtained from Merck. $UO_2(NO_3)_2 \cdot 6H_2O$ was obtained from Merck (Darmstadt, Germany). A stock solution of uranium was prepared by dissolving the proper amount of this salt in double distilled water. Dilute solutions were prepared by an appropriate dilution of the stock solution in double distilled water.

* Corresponding author. Fax: +98 542 2226765.
E-mail address: m_khajeh@uoz.ac.ir (M. Khajeh).

http://dx.doi.org/10.1016/j.chemolab.2014.04.003
0169-7439/

2.2. Apparatus

The measurements were carried out with a UV–Vis (UV-2100 RAY Leigh, Beijing, China) by monitoring the absorbance changes at a wavelength of maximum absorbance (560 nm). All experiments were performed in triplicate and the means of values were used for optimization. The pH was determined with a model 630 Metrohm pH meter with combined glass-calomel electrode.

2.3. Preparation of zinc oxide nanoparticles–chitosan

Zinc oxide (1 g) was dissolved in 100 mL of 1% acetic acid where it changed to zinc cations. Then, 1 g of chitosan was added to this solution and the mixture was sonicated for 30 min. After that, 1 mol L^{-1} NaOH drop by drop was added until the solution attained pH 10. This solution was heated in water bath at 60 °C for about 3 h. Finally, it was filtered and washed with deionized water several times and then dried in an oven at 50 °C for 1 h [15]. The representative scanning electron microscopy (SEM) image of chitosan–zinc oxide nanoparticles and transition electron microscopy (TEM) image of zinc oxide nanoparticles are shown in Fig. 1.

2.4. Procedure

A plastic syringe was used as a cartridge and then, was filled with various amounts of dried synthesized chitosan–zinc oxide nanoparticles (according to experimental design). A filter was placed on top to avoid disturbance of the sorbent chitosan–zinc oxide nanoparticle during sample solution passage. The cartridge was treated with 5 mL nitric acid and methanol. Finally, the cartridge was washed with deionized water. A portion of aqueous sample solution containing 1 mg L^{-1} of uranium and different amounts of PAN (0.5, 2.5 mg L^{-1}) were prepared.

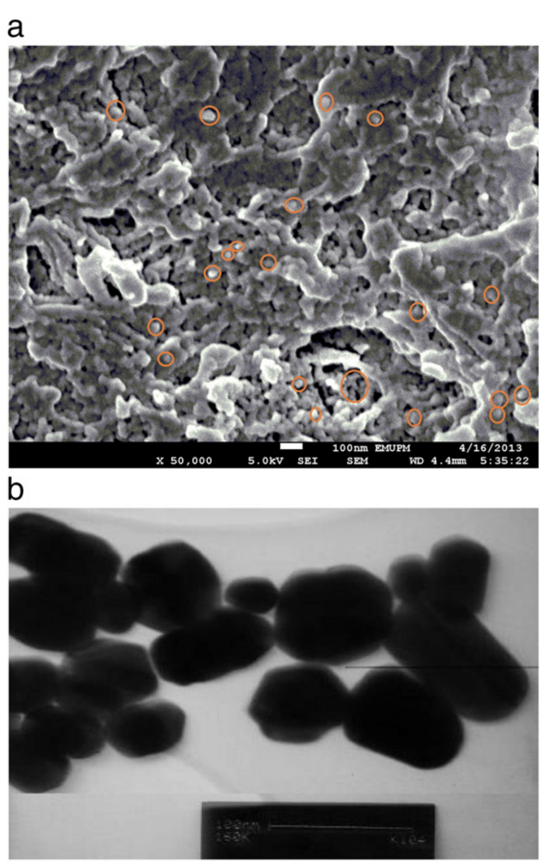

Fig. 1. (a) SEM image of chitosan–zinc oxide nanoparticle, (b) TEM image of zinc oxide nanoparticles.

After that, the pH was adjusted at 7.5 to 11.5 by the dropwise 0.1 mol L^{-1} NaOH and passed through the cartridge with a flow rate in the range from 2 to 6 mL min^{-1}. Subsequently, uranium retained on the sorbent, was eluted with 1 to 3 mL of eluent (benzene). The eluent was analyzed for the determination of uranium concentration.

2.5. Definition of the ANN model

In this research, Neural Network Toolbox V7.12 of MATLAB mathematical software was used to predict the recovery of analyte in water samples.

In this study, a feed forward neural network (FFNN) with back propagation (BP) algorithm was used [14]. The hyperbolic tangent sigmoid (*tansig*) was used as transfer function between input and hidden layer, while linear transfer function (*purelin*) was used as transfer function between hidden and output layer, shown by the following equations:

$$Purelin(sum) = sum \tag{1}$$

$$tansig(sum) = \frac{1-exp(-sum)}{1+exp(-sum)}. \tag{2}$$

Training of ANN by means of BP algorithm is an iterative optimization process where the *mean-squared-error* (MSE, below eq.), the error between the predicted and experimental data, is minimized by adjusting the *weight* and *bias* appropriately.

$$\mathrm{MSE} = \frac{\sum_{i=1}^{N} (Y_t - Y_N)^2}{N} \tag{3}$$

where Y_t is the target output, Y_N is the predicted output and N is the number of points.

The algorithm adjusts the weights in each layer to reduce the MSE. This process is repeated to the error between the predicted data and the experimental data that satisfies certain error criterion. There are many variations of BP algorithm for training neural networks (NNs). During training step the *weight* and *bias* are iterative updated by the Levenberg–Marquardt (LM) method until the convergence to the certain value is achieved.

To avoid over-fitting, input and output variables were normalized [14] within a uniform range of [0–1] according to the following relationship:

$$x_{norm} = \frac{(x - x_{min})}{x_{max} - x_{min}} \tag{4}$$

where x is the variable, x_{max} is the maximum value and x_{min} is the minimum value.

2.6. Cuckoo optimization algorithm (COA)

Similar to other evolutionary algorithms, COA starts with an initial population of cuckoos. They have some eggs to lay in host birds' nests. Some of the eggs which are more like to the host bird's eggs have the chance to grow up and become a mature cuckoo. But, others they are detected by host birds and will be killed. The eggs that grow reveal the suitability of the nests in that area. The more eggs survive in an area, the more profit is gained in that area. So the position where eggs survive will be the term that COA is going to optimize. Cuckoo search for the most appropriate area to lay eggs for maximum survival rate of eggs. After eggs remained to grow and turn into a cuckoo mature, they make some societies. Each society has its habit region to live in; the