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Artificial neural network for modeling the size of silver nanoparticles' prepared in montmorillonite/starch bionanocomposites

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ABSTRACT

In this study, artificial neural network (ANN) was used to develop an approach for evaluation of silver nanoparticles (Ag–NPs) size in the bionanocomposites substrate. A multi-layer feed forward ANN was applied to correlate the output as size of Ag–NPs, with four inputs include of $AgNO_3$ concentration, temperature of reaction, weight percentage of starch, and MMT amount. The results of proposed methodology were compared for its predictive capabilities in terms of coefficient determination (R^2) and mean square error (MSE) based on the validation data set. The model finding revealed that $AgNO_3$ concentration content has significant effect on size of Ag–NPs.

Introduction

The field of nanotechnology is one of the most active areas of research in recent materials science. Nanoparticles are attractive materials for basic researches and for various technical applications because of dependence on their physical and chemical features to the size and high surface areas. Utilizing pure nanoparticles alone have many problems, such as agglomeration between particles in nanoscale [1].

To remove or decrease the agglomeration, one of the appropriate solutions is to synthesis of nanoparticles in clay matrices, that nanoparticles are locates into the interlayers of clay and/or on the surface of clay structure [2,3].

Nanoparticles can be synthesized by physical, chemical and biological methods. These methods of nanoparticle synthesis used to cause accumulation of toxic and non-eco-friendly by-products. The development of green approaches for the synthesis of nanoparticles by sugars reduction is essential for the production of ecofriendly and non-toxic nanoparticles. Several biological systems, including plants, bacteria, fungi and algae have been used for the synthesis of nanoparticles.

Silver nanoparticles (Ag–NPs) have definite properties. This may perhaps have numerous applications in the fields of dentistry, clothing, catalysis, mirrors, optics, photography, electronics and food industries [4]. Because of such broad variety of applications, wide ranges of different preparation methods have been developed. However, the developing methods of Ag–NPs preparation, must give preference to control the size of Ag–NPs. Therefore, nanosilver with small particle size and devoid of aggregation between particles is favorable in this purpose.

There are several ways to reduce Ag^+ for instance, application of physical methods using of γ-rays, UV-irradiation, ultrasonic irradiation, microwave irradiation, heating and electrochemical reduction [5–7], application of reducing chemicals, such as hydrazine, sodium borohydride [8–12], polyethylene glycerol [13], *N,N*-dimethyl formamide [14], glucose [15], ethylene glycol [16], formaldehyde [17], sodium in liquid ammonia, etc. [18].

Bionanocomposites, a novel invention of nanocomposite materials, indicate a promising field in the frontiers of nanotechnology, materials and life sciences. Bionanocomposites are composed of a natural polymer matrix and organic/inorganic filler with at least one dimension on the nanometer scale [19]. Among natural polymers, starch is one of the most promising biocompatible and biodegradable materials because it is a renewable resource that is universally available and of low cost. A number of researchers have presented work in the field of starch-based

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bionanocomposites which can be obtained by filling a thermoplastic starch matrix with nanofillers such as layer silicates like montmorillonite and kaolinite are the usual layer silicates used in starch-based bionanocomposites [20].

The artificial neural networks (ANN) have been used for representing non-linear functional relationships between variables. The ability of an ANN to learn and generalize the behavior of any complex and non-linear process makes it a powerful modeling tool [21]. Solving and modeling the complex relation between input and output variable can be simply performed by an ANN model imitated by biological neuron processing. ANNs have been used to study a wide variety of chemical problems such as spectral analysis [22], prediction of dielectric constants [23], and mass spectral search [24]. In recent years, ANN has been introduced in nanotechnology applications as techniques to model data showing non-linear relationships and our estimation of particle size in variety nanoparticle samples [25,26].

Hence, the main motivation behind this study is to develop and predict the relationship between the experimental variables and the response variable for the evaluation of size of Ag–NPs produced by using green technique. The relationships between multi-input variables include $AgNO_3$molar concentration, reaction temperature, percentage of Stc, and amount of MMT help the researchers to design an efficient and ecofriendly process for the preparation of Ag–NPs in BNCs matrix.

The other parts of the paper are organized as follows. The experimental procedure has been presented in the 'Experimental section', analysis of the experimental data has been given in the 'Modeling section', and finally conclusion and suggestion have been presented.

Experimental Section

Materials

In this research silver nitrate, MMT, soluble starch and β-D-glucose powder were used for the production of Ag–NPs in montmorillonite/starch bionanocomposites. All reagents were of analytical grades and were used as received without further purification. The aqueous solutions were prepared with double distilled water (DD-water).

Synthesis of Ag–NPs in MMT/Stc BNCs

Schematic illustration of the synthesis of the Ag–NPs on MMT/Stc is shown in Fig. 1. Starch solutions were prepared by soluble starch in the different temperature under constant stirring time. Then, different molar of $AgNO_3$ were added to the starch solutions under constant stirring for preparation of $AgNO_3$/Stc colloids. The $AgNO_3$/Stc colloids were added into the MMT suspension and the mixture was further vigorously stirred for more than 3 h at certain temperature to obtain $[Ag(MMT/Stc)]^+$ composites. Aqueous solutions of β-D-glucose were added to the $[Ag(MMT/Stc)]^+$ composites with molar ratio 2:1 from each. The mixtures were heated to a certain temperature and were maintained at each temperature for 24 h. The suspension turned of light brown to dark brown that indicating the initial formation of Ag–NPs. Then, obtained suspensions of Ag/MMT/Stc BNCs were separated by centrifugation, washed with double distilled water twice and dried under vacuum overnight. Unless stated otherwise, all experiments were conducted at ambient temperature [15]. The possible reaction between β-D-glucose, silver ions and starch in the MMT suspensions can be written as follows Equations [27].

$$Ag^+ + Stc + MMT \rightarrow [Ag(MMT/Stc)]^+ \tag{1}$$

$$R{-}CHO + 2[Ag(MMT/Stc)]^+ \rightarrow R{-}COOH + 2[Ag(MMT/Stc)]\downarrow \tag{2}$$

$$R = (CHOH)_4CH_2OH, Stc = Starch$$

In the suspension containing MMT/Stc, silver ions were reduced with glucose in two possible reactions. In Eq. (1), silver ions were compounded with starch in MMT firstly and complex ions were generated [Ag (MMT/Stc)]. In Eq. (2), glucose is changed to gluconic

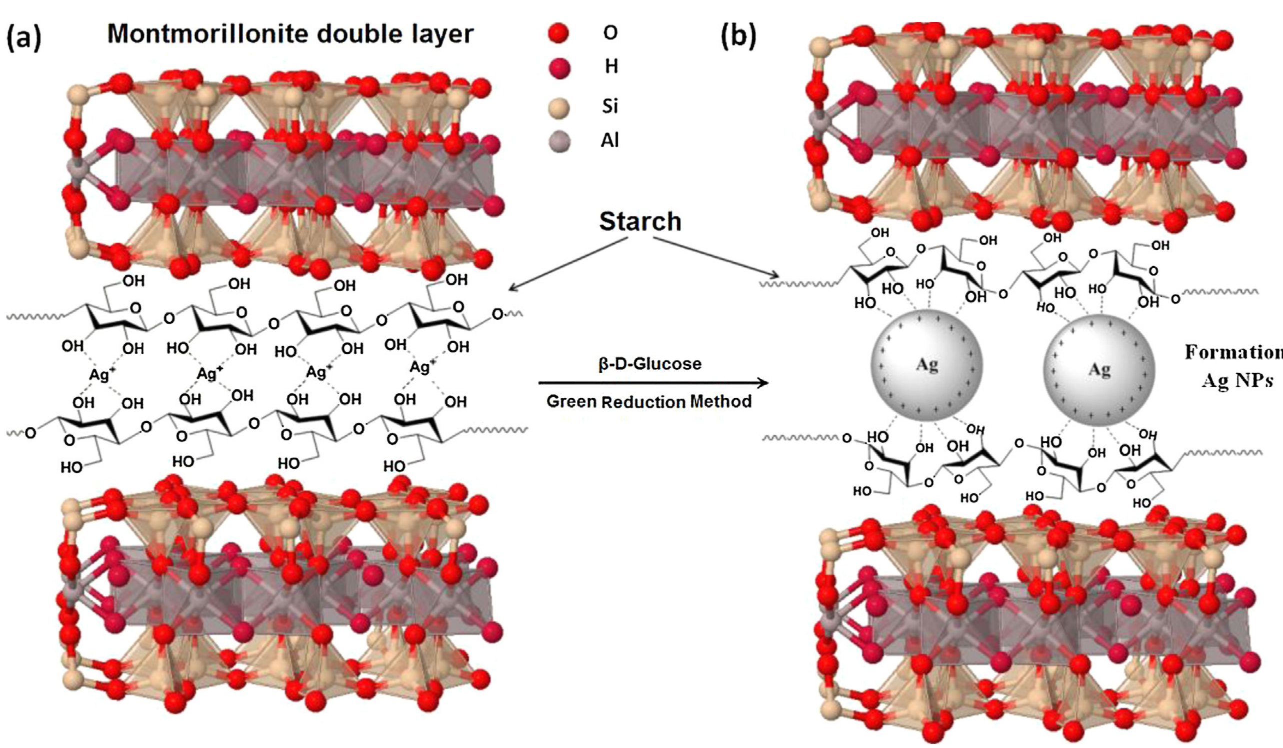

Fig. 1. Schematic illustration of the synthesis of the Ag–NPs in MMT/starch layers as bionanocomposites by green method.