Petroleum Research

Petroleum Research 2018 (December-January), Vol. 28, No. 102. 44-46

DOI: 10.22078/pr.2018.3020.2401

Optimization of Extractive Desulfurization of Model Oil With a Novel Green Deep Eutectic Solvent Using Genetic Algorithm-Artificial Neural Network

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DOI: 10.22078/pr.2018.3020.2401

INTRODUCTION

The increasing trend of respiratory, digestive, and dermatological problems which lead to substantial annual death is mostly the result of environmental exposure to toxic colorless sulfur dioxide (SO_2). Direct emission of SOx into the air is considered as an international concern, which caused legislative pressures of US and European Environmental Protection Agency. Hydrodesulfurization [1], extraction [2], oxidation [3], and adsorption [4] are the alternative processes used for desulfurization. Among the different kinds of the desulfurization techniques, extractive desulfurization (EDS) is simpler, more economical and more efficient. Deep eutectic solvents (DESs) were first presented in 2003 [5]. The DESs consist of a mixture of two or more components which forms a eutectic system, and the melting point of the obtained eutectic mixture is lower than both of the individual components. DESs are cheaper and more biodegradable than ILs. The application of mathematical and optimization methods is increasing in chemistry nowadays. Artificial neural network (ANN) is one of the most efficient mathematical models which are widely used in chemistry to predict the chemical processes. After using ANN to find the best relation between inputs and outputs, the genetic algorithm (GA) is used to find the best input values according to the results of ANN whichare applied in complex spaces of different scientific areas.

In the this work, extractive desulfurization of dibenzothiophene from n-hexane as model fuel using 1,10-phenantroline 2,9-dicarboxamide-FeCl3-based choline chloride as a green, novel and efficient deep eutectic solvent (DES) was presented.

EXPERIMENTAL PROCEDURES

EXTRACTION PROCEDURE

First, the DES was synthetized. Then, 10 mL of solution containing 500 mg L^{-1} dibenzothiophene in n-hexane was prepared, and DES with mass ratio of 33.5 (model fuel to DES) was added to the solution. Moreover, it was stirred for 15 min at ambient temperature. After that, the mixture was centrifuged for 3 min to completely separate the phases. The remaining dibenzothiophene in the upper phase was determined with GC-MS. The desulfurization percent was calculated based on the following equation:

Desulfurization (%)=$(C_i-C_e)/C_i \times 100$ (1)

where Ci and Ce are the initial and the equilibrium concentrations of DBT in n-hexane as model fuel.

RESULTS AND DISCUSSION

MODELING WITH GA-ANN

MATLAB R2015 was used for optimization and prediction of the proposed process. Genetic Algorithm is one of the most reputable and applicable optimization algorithms implemented based on the evolutionary strategies. In GAs, mutation is randomly implemented with little chance in the range of 0.01 and 0.1, and adjusts components in the chromosomes. The equation of tan-sigmoid transfer function is defined as follows:

F(x) =1/ (1+exp (-x)) (2)

t can be seen that artificial neural network with 10 neurons in hidden layer has the minimum value of mean square error (MSE). Eq. (5) represents MSE function as performance function:

$$MSE = \frac{1}{N}\sum_{i=1}^{N} (Y_{pre} - Y_{ex})^2 \quad (5)$$

Iwhere Y_{ex} is the experimental output, Y_{pre} is the network output and is the number of data points.

THE EFFECT OF VARIABLES

The effect of influential parameters was considered. The effect of mass ratio of DES to model fuel was studied, and the desulfurization (%) was maximum and constant in the range of 13.4-33.5 and then reduced (Fig. 1).

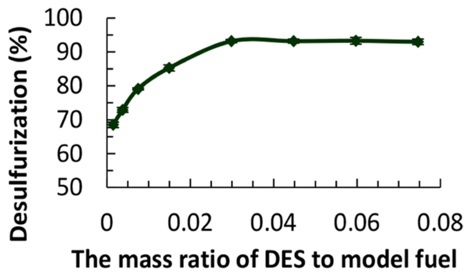

Figure 1: The effect of mass ratio of DES to model fuel on desulfurization (%).

The effect of time was considered in the range of 5-30 min, and the optimum time of 15 min was achieved (Fig. 2).

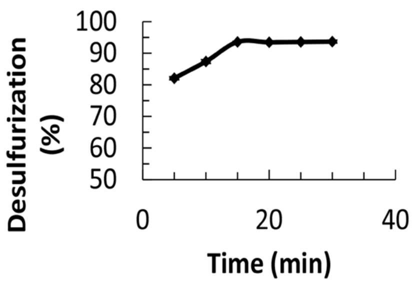

Figure2: The effect of time on desulfurization (%).

The effect of temperature in the range of 25-45 °C was investigated. By increasing the temperature, the desulfurization (%) decreased (Fig. 3).

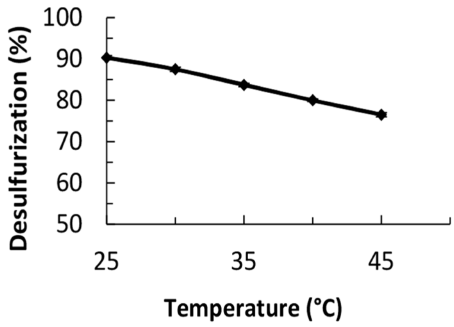

Figure 3: The effect of temperature on desulfurization (%).

CONCLUSION

In this study, a green solvent was introduced for extractive desulfurization of model fuel. GA-ANN was applied for prediction and optimization of the process for three parameters of temperature, time, and mass ratio of fuel to DES. Under optimum conditions of mass ratio of fuel to DES 33.5, temperature 25 °C, and time 15 min, the maximum sulfur removal percent of 93.5 ± 0.5 was achieved. Rapidity, short extraction time and the application of green process are the benefits of the proposed process.

Acknowledgement

The authors honorably appreciate University of Jiroft.

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