Chem Rev Lett 5 (2021) 141-152

Research Article

Chemical Review and Letters
journal homepage: www.chemrevlett.com
ISSN (online): 2645-4947 (print) 2676-7279

Artificial Neural Network (FFBP-ANN) Based Grey Relational Analysis for Modeling Dyestuff Solubility in Supercritical CO2 with Ethanol as the Co-Solvent

Srinidhi[a*]

[a]*Department of Biotechnology, Ramaiah Institute of Technology (MSRIT), Bangalore, Karnataka, India*

ARTICLE INFO

Article history:
Received 13 December 2020
Received in revised form 22 March 2021
Accepted 23 March 2021
Available online 28 May 2022

Keywords:
Artificial Neural Networks; Mathematical Modeling; Dyestuff Solubility; Multivariate Analysis.

ABSTRACT

The research on dye solubility modeling in supercritical carbon dioxide is gaining prominence over the past few decades. A simple and ubiquitous model that is capable of accurately predicting the solubility in supercritical carbon dioxide would be invaluable for industrial and research applications. In this study, we present such a model for predicting dye solubility in supercritical carbon dioxide with ethanol as the co-solvent for a qualitatively diverse sample of eight dyes. A feed forward back propagation - artificial neural network model based on Levenberg-Marquardt algorithm was constructed with seven input parameters for solubility prediction, the network architecture was optimized to be [7-7-1] with mean absolute error, mean square error, root mean square error and Nash-Sutcliffe coefficient to be 0.026, 0.0016, 0.04 and 0.9588 respectively. Further, Pearson- product moment correlation analysis was performed to assess the relative importance of the parameters considered in the ANN model. A total of twelve prevalent semi-empirical equations were also studied to analyze their efficiency in correlating to the solubility of the prepared sample. Mendez-Teja model was found to be relatively efficient with root mean square error and mean absolute error to be 0.094 and 0.0088 respectively. Furthermore, Grey relational analysis was performed and the optimum regime of temperature and pressure were identified with dye solubility as the higher the better performance characteristic. Finally, the dye specific crossover ranges were identified by analysis of isotherms and a strategy for class specific selective dye extraction using supercritical CO2 extraction process is proposed.

1. Introduction

Supercritical fluid extraction has been amassing prominence as an effective method to separate and purify a variety of substances from multi-component mixtures. Supercritical fluid extraction has been employed for the purification of a raft of different products ranging from petrochemicals [1] to phytochemicals [2] and from dyes [3] to radioactive elements [4]. Among the different solvents employed in the supercritical fluid extraction process, CO2 has been extensively used for many of its fitting and desirable attributes [5]. The diversity of product applications that use supercritical CO2 extraction calls for the need to model the process accurately. Experimentation of supercritical fluid extraction on high-value dyestuff just for the sake of modeling is resource consuming and costly. Therefore, research focused on modeling dyestuff solubility using supercritical fluid extraction process using empirical data is being pursued at an accelerating pace over the past few decades. Although cubic equations of state are widely used to calculate solubilities of solutes in supercritical CO2, they are highly disadvantageous for application in industries for the various reasons explained by Gharagheizi et al [6].

Correspondence: Email: msrinidhi2@gmail.com ; srinidhikashyap@outlook.in ; srinidh2@buffalo.edu USN:1MS15BT050