Application of optimal RBF neural networks for optimization and characterization of porous materials

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Abstract

Optimization and characterization of porous materials have been extensively studied by various surface phenomena researchers. Efficient methods are required to predict the optimum values of operating parameters in different stages of material preparation and characterization processes. A novel method based on the application of a special class of radial basis function neural network known as Regularization network is presented in this article. A reliable procedure is introduced for efficient training of the optimal isotropic Gaussian Regularization network using experimental data sets. Two different practical case studies on optimization and characterization of carbon molecular sieves and activated carbons were employed to compare the performances of properly trained Regularization networks with the optimal conventional methods. It is clearly demonstrated that a Regularization network with optimum value of isotropic spread and optimum level of regularization can efficiently filter out the noise and provide better generalization performance over the conventional techniques.

Keywords: Neural network; Regularization network; Characterization; Optimization; Porous materials

1. Introduction

Several types of neural networks have been extensively used for empirical modeling of various chemical engineering processes (Himmelblau & Hoskins, 1988; Venkatasubramanian & Chen, 1989; Watanabe, Matsuura, Abe, Kubota, & Himmelblau, 1989; Nascimento, Oliveros, & Braun, 1994; Chan & Nascimento, 1994; Nascimento, Guardani, & Giulietti, 1997; Iliutaş & Lavric, 1999; Nascimento, Giudici, & Guardani, 2000; Guardani, Onimaru, & Crespo, 2001; Shaikh & Al-Dahhan, 2003; Lin, Chen, & Tsutsumi, 2003; Tarca, Grandjean, & Larachi, 2003). Although, characterization and optimization of solid porous materials have been considerably explored by many researchers (Szombathely, Brauer, & Jeroniec, 1992; Cascarini de Torre & Bottani, 1996; Lastoskie & Gubbins, 2001; Moussatov, Ayrault, & Castagnede, 2001), however, the application of neural network for such tasks is relatively new.

Real solids have complex micro-structure and majority...