Application of adaptive neuro-fuzzy inference system for solubility prediction of carbon dioxide in polymers

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ABSTRACT

Solubility of carbon dioxide in poly(vinyl acetate) (PVAc), poly(2,6-dimethyl-1,4-phenylene ether) (PPO), polypropylene (PP), and high-density polyethylene (HDPE), poly(butylene succinate) (PBS), poly(butylene succinate-co-adipate) (PBSA) and polystyrene (PS) are modeled by adaptive neuro-fuzzy inference system (ANFIS) in wide range of pressure and temperature. The results obtained in this work indicate that ANFIS is effective method for prediction of solubility of carbon dioxide in polymers and have better accuracy and simplicity compared with the classical methods.

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1. Introduction

Solubility of gases in polymers has been a subject of interest for chemical engineers for several decades. Data of the solubility are important to design the polymerization processes made to withdraw unreacted monomers and solvent from products in polymer industry. To describe gas solubility in polymer, the statistical mechanics-based models are often used. For example, the perturbed-hard chain theory (Doghieri, De Angelis, Giacinti Baschetti, & Sarti, 2006; Feng, Wen, Xu, & Wang, 2001; Lee, Rangaiah, & Chiew, 2001), the lattice-fluid theories of Sanchez and Lacombe (Enders, Kahl, & Winkelmann, 2005; Li, Li, Turng, Gong, & Zhang, 2006) and cubic equation of states (EOSs) Louli & Tassios, 2000; Zhong & Masuoka, 1998 have been extended to describe phase behavior of polymer solution.

Much attention has been paid to solubility of CO2 in polymers, because polymer processing with CO2 is an important application of green chemistry (Nalawade, Picchioni, & Janssen, 2006). Also, carbon dioxide (CO2) is the favorite matter because it has a relatively low critical temperature and pressure and because it is inexpensive, non-flammable, non-toxic and readily available. Therefore, numerous studies have been carried out to measure and predict CO2 solubility in various polymers (Aubert, 1998; Bos, Puent, Wessling, & Straathoff, 1999; Sato et al., 1999; Sato, Takikawa, Yamane, Takishima, & Masuoka, 2002).

Use of conventional methods is cumbersome, for example, vapor–liquid or solubility calculation based on EOS required adjustable parameters such as the binary interaction parameters and the mixing rules. As alternative approaches, ANN and ANFIS extract the desired information directly from experimental data, and need not take into account the detailed information of structures and interactions in the systems and improve the prediction accuracy compared to the conventional thermodynamic models and they have been used widely (Mohanty, 2005; 2006).

Fuzzy logic reduces the possible difficulties in modeling and analysis of complex data and also, it is appropriate for incorporating the qualitative aspects of human experience within its mapping rules, which are to provide a way of catching information. Artificial neural networks (ANNs) have also been used to identify models of complex systems because of their high computational rates, robustness and ability to learn. For the same purpose Neuro-fuzzy systems are fuzzy systems which use ANNs theory in order to determine their properties (fuzzy sets and fuzzy rules) by processing data samples. A specific approach in neuro-fuzzy is the adaptive neuro-fuzzy inference system (ANFIS) that is one of the first integrated hybrid neuro-fuzzy models (Jang, 1993), but has shown significant results in modeling nonlinear functions and is faster in convergence when compared to the other neuro-fuzzy models (Akcayol, 2004).

In this work, in order to show the applicability of ANFIS for prediction of carbon dioxide solubility in polymers a hybrid grid partitioning ANFIS was used. Also one of the main objectives of this study is comparing the results of ANFIS by the ANN results in previous our work (Khajeh, Modarress, & Mohsen-Nia, 2007) and results obtained by using EOS are available in the literature.