Fluid Phase Equilibria 356 (2013) 11–17

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.elsevier.com/locate/fluid

Prediction of gas solubility in polymers by back propagation artificial neural network based on self-adaptive particle swarm optimization algorithm and chaos theory

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ARTICLE INFO

Article history:
Received 20 April 2013
Received in revised form 5 July 2013
Accepted 8 July 2013
Available online 18 July 2013

Keywords:
Solubility prediction
Gas in polymers
Artificial neural network
Chaos
Particle swarm optimization

ABSTRACT

A novel prediction method based on chaos theory, self-adaptive particle swarm optimization (PSO) algorithm, and back propagation artificial neural network (BP ANN) is proposed to predict gas solubility in polymers, hereafter called CSPSO BP ANN. The premature convergence problem of CSPSO BP ANN is overcome by modifying the conventional PSO algorithm using chaos theory and self-adaptive inertia weight factor. Modified PSO algorithm is used to optimize the BP ANN connection weights. Then, the proposed CSPSO BP ANN (two input nodes consisting of temperature and pressure; one output node consisting of gas solubility in polymers) is used to investigate solubility of CO_2 in polystyrene, N_2 in polystyrene, and CO_2 in polypropylene, respectively. Results indicate that CSPSO BP ANN is an effective prediction method for gas solubility in polymers. Moreover, compared with conventional BP ANN and PSO ANN, CSPSO BP ANN shows better performance. The values of average relative deviation (ARD), squared correlation coefficient (R^2) and standard deviation (SD) are 0.1275, 0.9963, and 0.0116, respectively. Statistical data demonstrate that CSPSO BP ANN has excellent prediction capability and high accuracy, and the correlation between predicted and experimental data is good.

1. Introduction

The development of polymer materials over the past several decades has caused polymers to become an important part of daily life. Solubility is one of the most important physicochemical properties of polymers compounds because it determines the compatibility of components of a blending system. Researchers are focusing their attention on gas solubility in polymers [1–4]. Solubility data provide useful criteria to determine requisite processing conditions that are mostly collected experimentally and by prediction [5–7]. Experimental studies mainly include phase-separation [4,8], pressure-decay [9], gravimetric [10], volumetric [11], and chromatographic [5,12] methods. Traditional prediction methods mainly consist of perturbed-hard chain theory, lattice-fluid theories, empirical models, and cubic equation of states [5,13–15]. Unfortunately, solubility data of gases in polymers within a wide range of pressure and temperature are limited [16–19] because some experimental studies are difficult to implement under many restricted conditions (i.e., time and material consuming). In addition, most traditional prediction methods have the shortcoming of being highly inaccurate [20–23].

Gas solubility in polymers is affected by temperature, pressure, and interactions among macromolecular chains. Given the nonlinear relationship among these factors, traditional methods of predicting gas solubility in polymers are insufficient to meet application requirements. Therefore, an effective and accurate prediction method for gas solubility in polymers must be developed. Methods involving artificial neural networks (ANN) are effective tools for calculating the phase equilibrium and thermodynamic properties of polymers blending systems and have thus been used in different areas of research and engineering practice [14,15,24]. Considering the nonlinear nature of gas solubility in polymers, ANN method can be considered as an alternative method for solubility prediction [14,25,26]. Thus far, numerous ANN models for predicting physicochemical properties have been proposed. Bakhbakhi [13] compared ANN with equation of states for predicting the solubility of 2-naphthol in ternary systems. They demonstrated

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http://dx.doi.org/10.1016/j.fluid.2013.07.017

Nomenclature

ANN	Artificial neural network
BP	Back propagation
PSO	Particle swarm optimization
CSPSO	Chaotic self-adaptive particle swarm optimization
PS	Polystyrene
PP	Polypropylene
ARD	Average relative deviation
R^2	Squared correlation coefficient
SD	Standard deviation
ANFIS	Adaptive neuro-fuzzy inference system
RBF	Radial basis function

that the ANN method is a powerful approach with better accuracy.

Back propagation (BP) algorithm is the most frequently algorithm used for ANN training. However, ANNs trained by BP algorithm suffer from converging too slowly and being easily trapped into a local optimum [13,27]. Researchers have recently discovered that the determination of ANN structure, parameters, and bias is crucial because the training process of ANN can be considered as a classical optimization problem [28,29]. With the development of the interdiscipline of information science and engineering technology, many intelligent algorithms such as genetic algorithm [30–32], simulated annealing algorithm [33,34] and particle swarm optimization (PSO) algorithm [35,36] can be used for this determination. PSO algorithm is a global and advanced algorithm with a strong ability to search global optimum. Compared with genetic algorithm and simulated annealing, the most important advantages of PSO are the few parameters needed to adjust and the easy implementation [37]. Lazzus [38] proposed PSO for modeling the phase equilibrium of complex mixtures. Zhang [39,40] introduced PSO algorithm for phase equilibrium calculations and for modeling vapor–liquid equilibrium data. Bonilla-Petriciolet [41] proposed a comparative study of PSO and several of its variants for solving phase stability and equilibrium problems. In addition, many ANN models based on PSO algorithm have been proposed. Lazzus [42] introduced a hybrid model based on ANN and PSO for estimation of solid vapor pressures of pure compounds at different temperatures. The studies have demonstrated that PSO is a powerful approach to ANN training [36,43]. Although PSO ANN shows high performance, it is easily trapped into a local minimum. Obviously, traditional PSO algorithm cannot be successfully used in some higher dimensional complex optimization problems.

The aforementioned works have achieved a high level of solubility prediction accuracy in some cases. However, improving the performance of the prediction model is still the first-line goal of academic and industrial used by the aforementioned works to conduct this study, which focuses on using BP ANN based on a modified PSO algorithm and chaos theory to investigate gas solubility in polymers. To develop an effective and accurate prediction method, we propose a BP ANN trained by hybrid algorithm based on self-adaptive PSO and chaos theory, hereafter called CSPSO BP ANN. In the proposed CSPSO BP ANN, the traditional PSO is modified by chaos theory and self-adaptive inertia weight factor to overcome its premature convergence problem and accelerate the converging speed. Then, the modified PSO algorithm [also called chaotic self-adaptive PSO (CSPSO)] is used to tune and optimize the connection weights of BP ANN. Using CSPSO BP ANN, gas solubility in polymers is investigated within a wide range of temperature and pressure. A comparison among different neural networks is carried out in detail to reveal that our proposed CSPSO BP ANN outperforms BP ANN and PSO ANN.

2. Theory

In this work, BP ANN tuned by hybrid algorithm is developed to investigate its capability in predicting gas solubility in polymers. We propose a hybrid algorithm based on self-adaptive PSO and chaos theory, hereafter called CSPSO algorithm. In the proposed CSPSO algorithm, the global best fitness, average local best fitness, and acceleration coefficients generated by chaotic sequence are proposed to avoid prematurity and accelerate the converging speed.

2.1. PSO algorithm

PSO algorithm is an evolutionary computation algorithm inspired by the social and collective behaviors of bird flocking or fish schooling [28,35]. By randomly initializing the PSO algorithm with candidate solutions, PSO successfully leads to a global optimum. Compared with the genetic algorithm and simulated annealing algorithm, PSO algorithm has the advantages of easy implementation and high performance and is thus widely used [28,32,44]. In PSO algorithm, we assume that in an n-dimensional search space, the total number of particles is m, the swarm is denoted as: $x = (x_1, x_2, \ldots, x_m)^T$, the position of the ith particle is $x_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,n})^T$, the velocity of the ith particle be expressed as the vector $v_i = (v_{i,1}, v_{i,2}, \ldots, v_{i,n})^T$, the best position of the ith particle $p_i = (p_{i,1}, p_{i,2}, \ldots, p_{i,n})^T$, and the best position of the neighboring particles $p_g = (p_{g,1}, p_{g,2}, \ldots, p_{g,n})^T$.

PSO algorithm performs searching based on orientation by keeping track of two variables; one is called "*Plbest*" (the best position a particle has traversed so far), and the other is called "*Pgbest*" (the best position that any neighbor particle has traversed so far). When a particle takes the whole population as its neighborhood, "*Pgbest*" becomes the global best called "*Gbest*." In the standard PSO algorithm, the position and velocity are updated as follows:

$$v_{i,d}^{k+1} = \omega v_{i,d}^{k} + c_1(p_{i,d}^{k} - x_{i,d}^{k}) + c_2(p_{g,d}^{k} - x_{i,d}^{k}) \quad (1)$$

$$x_{i,d}^{k+1} = x_{i,d}^{k} + v_{i,d}^{k+1} \quad (2)$$

where $i = 1,\ldots,m$; $x_{i,d}^{k}$ and $v_{i,d}^{k}$ denote the position and velocity of the ith particle at d-dimension and the kth iteration, respectively; ω denotes the inertia weight; c_1 and c_2 are acceleration coefficients; $p_{i,d}^{k}$ represents the best position of the ith particle in d-dimension, and $p_{g,d}^{k}$ denotes the global best position.

2.2. Chaotic self-adaptive PSO algorithm

PSO is a metaheuristic as it makes few or no assumptions about the problem being optimized and can search very large spaces of candidate solutions. However, PSO do not guarantee an optimal solution is ever found. More specifically, the conventional PSO is easily trapped into a local minimum. To avoid premature convergence and accelerate the converging speed, an improved PSO algorithm called CSPSO algorithm is proposed in this work. The difference between standard PSO and CSPSO algorithms lies in two points: one is a self-adaptive inertia weight factor proposed for the balance between exploration and exploitation, and the other is chaos theory used to generate chaotic sequences for adapting acceleration coefficients (c_1 and c_2). In formula (1), the inertia weight ω greatly affects the algorithm performance. A larger inertia weight facilitates global exploration, and a smaller one facilitates local exploitation. To balance between exploration and exploitation, a self-adaptive inertia weight factor was defined as follows:

$$\omega = \omega_{\max} - Pgbest(k)/Plbest_{\text{ave}} - (\omega_{\max} - \omega_{\min}) \times k/k_{\max} \quad (3)$$