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Study on Particle Swarm Optimization Variant and Simulated Annealing in Vapor Liquid Equilibrium Calculation

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Abstract

Phase equilibrium calculation plays a major rule in optimization of separation process in chemical processing. Phase equilibrium calculation is still very challenging due to highly nonlinear and non-convex of mathematical models. Recently, stochastic optimization method has been widely used to solve those problems. One of the promising stochastic methods is Particle Swarm Optimization (PSO) due to its simplicity and robustness. This study presents the capability of particle swarm optimization for correlating isothermal vapor liquid equilibrium data of water with methanol and ethanol system by optimizing Wilson, Non-Random Two Liquids (NRTL), and Universal Quasi Chemical (UNIQUAC) activity coefficient model and also presents the comparison with bare-bones PSO (BBPSO) and simulated annealing (SA). Those three optimization methods were successfully tested and validated to model vapor liquid equilibrium calculation and were successfully applied to correlate vapor liquid equilibrium data for those types of systems with deviation less than 2%. In addition, BBPSO shows a consistency result and faster convergence among those three optimization methods.

Keywords: *Phase equilibrium, stochastic method, particle swarm optimization, simulated annealing and activity coefficient model*

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INTRODUCTION

Optimization is one of important aspects that are encountered in chemical engineering especially in chemical process includes heat and mass exchange network synthesis (Lin and Miller, 2004), distillation column design, process design and control, and phase equilibrium calculation (Petriciolet and Hernández, 2010; Moodley, *et al.*, 2015; Hernández, *et al.*, 2015; Zhang, *et al.*, 2015; Zhou, *et al.*, 2017). Phase equilibrium calculation plays a major role in

optimization of separation process in chemical processing. Mathematical models or objective function used for parameter estimation in phase equilibrium calculation are usually highly non-linear and non-convex (Petriciolet, *et al.*, 2010) and often present several possible solutions. Therefore it is difficult for one to evaluate the first derivatives and to achieve the global optima solution with a reasonable amount of computation. The utilization of traditional search method for optimization in phase equilibrium calculation may fail to converge when initial estimates are not suitable (Petriciolet and Hernández, 2010) and may trap in local optima when the search space is multimodal (Rahman, *et al.*, 2009).

Because of those problems that are always encountered in traditional methods for parameter estimation in phase equilibrium calculation, several non-gradient based optimization methods have emerged. One of those promising non-gradient based optimization methods is Particle Swarm Optimization (PSO) due to its simplicity, robustness, and well-balanced mechanism to enhance global and local exploration abilities (Petriciolet, *et al.*, 2010).

There have been widely studies in the application of PSO in phase equilibrium calculation, mostly for vapor-liquid equilibria (Ahmadi, *et al*., 2014; Khalil, *et al*., 2016; Lazzús, 2014) and liquid-liquid equilibria calculation (Khansary and Sani, 2014; Ferrari, *et al*., 2009; Li, *et al*., 2015; Zhang, *et al*., 2011) applied bare bones of PSO in parameter estimation of vapor liquid equilibrium data. Lazzus (2016) made some research about the application of PSO in phase equilibrium calculation comprise optimization of activity coefficient in vapor liquid equilibrium for alcohol + water system. Ferrari *et. al*. (2009) also applied PSO in parameter estimation in the liquid-liquid phase equilibrium modeling. Li *et al*. (2015) performed succesfully The Non-Random Two Liquids (NRTL) activity coefficient model parameter regression for liquid-liquid equilibrium modeling using PSO method.

The aim of this study is to extend the application of PSO and implement bare-bones PSO (BBPSO) and Simulated Annealing (SA) in parameter estimation for vapor liquid equilibrium of mixture containing water and alcohols. Since the application of BBPSO in parameter estimation modelling in those systems is still scarce and very few, this study pioneers in evaluating the capability and robustness of the proposed PSO algorithm for parameter estimation in phase equilibrium calculation.

MATERIALS AND METHODS

Particle Swarm Optimization

Particle Swarm Optimization was first proposed by Kennedy and Ebehart (1995). It mimics the movement behavior of creatures that implement the underlying rules that enable large numbers of organisms (birds, fishes, herds) to move synchronously, often changing direction suddenly, scattering and regrouping. This method is population based and represented by particle. Each particle iteratively moves across the search space presented by velocity attracted to the position (location) of the best fitness (evaluation of the objective function) historically achieved by the particle itself (local best; pBest) and by the best among the neighbors of the particle (global best; gBest).

In essence, each particle continuously focuses and refocuses the effort of its search according to both local and global best. The basic flow of PSO algorithm is firstly initializing population of particle in the search space, and then secondly evaluating each particle to the fitness function. If the fitness is better than the particle's best experience (pBest), this algorithm will save the location vector for the particle as pBest. If the fitness is better than the best in the entire population (gBest), this algorithm will save the location vector for the particle as gBest. And finally update the particle's velocity and location based on pBest and gBest which are represented by Eq. (1) and (3) for velocity update and position update respectively.

$$\vec{v}_i(t+1) = w \times \vec{v}_i(t) + r_1 c_1(\vec{x}_{pBest} - \vec{x}_i(t)) + r_2 c_2(\vec{x}_{gBest} - \vec{x}_i(t)) \quad (1)$$

where t is the current iteration, w is the inertia weight, c_1 and c_2 are the acceleration constant, and r_1 and r_2 are random number in the range (0,1). The inertia weight responsible for balancing between local and global searches, hence it requires less iteration for the algorithm to converge. Larger value results in smoother, more gradually changes in direction (exploration), while smaller value allows particle to settle into the optima (exploitation). In this study, inertia value is set up to vary linearly from 1 to 0 during the optimization process based on Eq. (2)

$$w(t) = w_{\max} - \frac{t}{T}(w_{\max} - w_{\min}) \quad (2)$$

where t is the current iteration and T is the maximum iteration.

$$\vec{x}_i(t+1) = \vec{x}_i(t) + \vec{v}_i(t+1) \quad (3)$$

where x and v denote a particle position and velocity respectively. The PSO algorithm is described in detail in algorithm below.

Particle Swarm Optimization Algorithm

- Initializing swarm of number of particles with random location.
- Computing the fitness value of each particle (OF in the vapour liquid equilibrium calculation)
- Defining the pBest. For first iteration the pBest is the fitness value itself.
- Finding gBest from this iteration.

- Entering the loop:
  - Calculating the new velocity based on inertia weight using Eq. 1
  - Calculating the new location using Eq. 3
  - Computing the new fitness based on new location.
  - Finding the pBest of each particle by comparing it's pBest with new fitness. If the fitness is higher than the pBest, update the pBest. Set the pBest equals to fitness and the pBestLoc equals to new location.
- Doing the loop function until the loop limit reached.

For selected parameters in this algorithm are indicated in Table 1

Table 1. Parameter used in the PSO algorithm

PSO Parameter	Value
Number of particles	
Number of Iterations	250
Cognitive component (c_1)	500
Social component (c_2)	2.0
Minimum inertia weight (w_{min})	2.0
Maximum inertia weight (w_{max})	0
	1

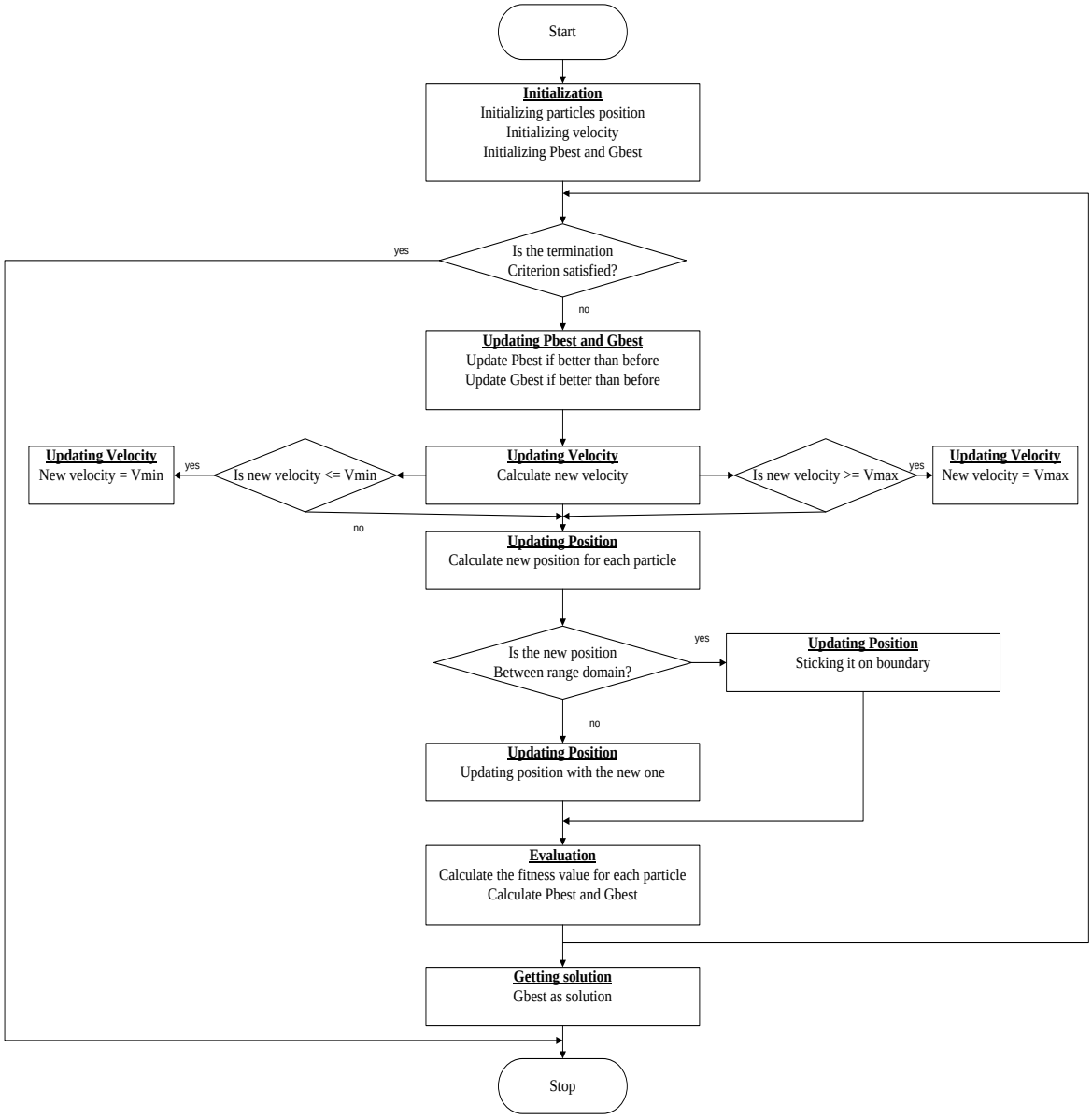

Figure 1. Flowchart of PSO method

Bare-Bones PSO (BBPSO)

This algorithm was first developed by Kennedy (2003). Basically, BBPSO is similar with original PSO, however in this algorithm the next position will be updated by directly sampling from a Gaussian distribution of mean and standard deviation:

mean = (pBest + gBest)/2 (4)

std_dev = | pBest-gBest | (5)

$$\vec{x}_i(t+1) = N\left[\frac{\vec{x}_{pBest} + \vec{x}_{gBest}}{2}, \left|\vec{x}_{pBest} - \vec{x}_{gBest}\right|\right] \quad (6)$$

If the current particle's pbest happens to be the same as that of gbest, it means that the value of standard deviation in Eq. (5) is zero. As standard deviation is zero, Gaussian normal distribution becomes zero, particle whose value of gbest will not be updated.

In this study a possible approach to fix this problem is assign a small fix value (such as 0.001) for standard deviation when the value is zero. In BBPSO we don't need to specify the parameter value such as inertia weight and acceleration constant. The flowchart for this optimization method is presented in Fig. 1.

Simulated annealing

Simulated annealing was first developed by Kirkpatrick *et al.* (1983). This optimization method mimics the annealing process of metals. If solid material is heated past its melting point and then cooled back into a solid state, the structural property

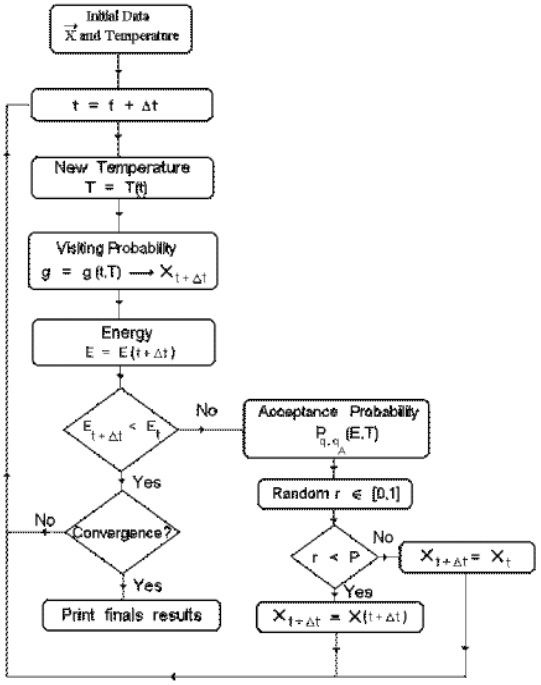

Figure 2. Flowchart of SA optimization method (Mundim and Ellis, 1999)

Table 2. Parameter used in the SA algorithm

SA Parameter	Value
Initial Temperature	600
Number of Iterations	100
Cooling step (k)	1
α	0.95

depends on the cooling rate. The idea of this optimization method is each step of the Simulated Annealing (SA) algorithm replaces the current solution by a random "nearby" solution, chosen with a probability that depends on the difference between the corresponding function values and on a global parameter T (temperature) that is gradually decreased during the process. In this study, geometrical cooling schedule as described in Eq. (7) was used with parameter shown in Table 2.

$$T(k) = T_0\alpha^k \quad (7)$$

The flowchart for this optimization method is presented in Fig. 2.

Algorithm for Vapour Liquid Equilibrium Calculation

The algorithm for isothermal vapour liquid equilibrium calculation is described in detail in the following algorithm. Isothermal Vapour Liquid Equilibrium Calculation:

1. Calculate Pisat for each component using Antoine equation given in Eq. (8).

$$\log(P_i^{sat}/kPa) = A - \frac{B}{[(T/K)+C]} \quad (8)$$

A, B, and C are Antoine constant which is obtained from published data.

2. Calculate γiexp for each component using Eq. (9)

$$\gamma_i^{\exp} = \frac{y_i\varphi_i P}{x_i P_i^{sat}} \quad (9)$$

3. Calculate γical using activity coefficient model Wilson, Non Random Two Liquids (NRTL), Universal Quasi-Chemical (UNIQUAC). In this calculation we set binary interaction parameter.
4. Minimizing objective function shown in Eq. (10) to obtain binary interaction from this optimization process and all optimization algorithms used in this study where n is number of component and N is number of data.

$$OF = \sum_{j=1}^{N}\sum_{i=1}^{n}\left(\frac{\gamma_i^{cal} - \gamma_i^{\exp}}{\gamma_i^{\exp}}\right)^2 \quad (10)$$

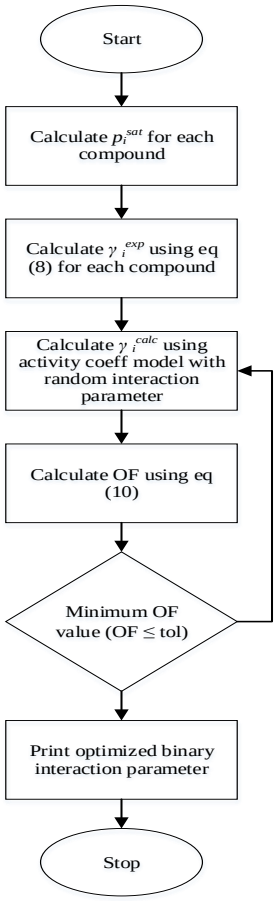

Figure 3. Flowchart of VLE calculation

This optimization method was performed by employing Matlab® Software. To evaluate the performance of optimization method used in this study, we compared experimental data and calculated data for pressure, and it was then expressed as deviation calculated in eq. (11).

$$\Delta P = \frac{100}{N}\sum_{N}\left(\frac{\left|P_{\exp} - P_{cal}\right|}{P_{\exp}}\right) \qquad (11)$$

where N is number of data. Where $Pcal$ is defined as

$$P_{cal} = \sum_{i=1}^{k} x_i \gamma_i^{cal} P_i^{sat} \qquad (12)$$

The flowchart for VLE calculation is presented in Fig. 3.

RESULTS AND DISCUSSIONS

Validation of Algorithm

The system used for testing this algorithm is isothermal vapor liquid equilibrium data obtained by Kurihara *et al.* (1995) at 323.15 K. To evaluate the performance of both PSO and BBPSO algorithm, in this study we run the algorithm in three times and the comparison of convergence history is shown in Fig. 4 for methanol (1) – water (2) system.

From Fig. 4 we can see that convergence time resulted from BBPSO is faster than PSO. BBPSO shows a consistency result and faster convergence. In general way, the algorithms implemented in this study showed an interesting strategy for other phase equilibrium calculation. In this study, the comparison between PSO algorithm and SA algorithm was also be made in term of result consistency. From Table 3 we can see that in multiple running PSO is more consistent than SA since SA always gives different result in each run.

Optimization Results

The algorithms developed in this study were used to correlate vapour liquid equilibrium data and to obtain binary interaction parameter for three activity coefficient models (Wilson, NRTL, and UNIQUAC) for evaluating the capability of these algorithms were shown in Fig. 4-6.

From Figure 4-6 we can see that convergence time resulted from BBPSO is faster than PSO.The binary interaction parameters obtained from all algorithms were shown Table 4. Table 5 shows comparison between PSO algorithms, SA algorithm in terms of the deviation in pressure which is defined in eq. (11).

Table 3. Comparison between PSO and SA for methanol (1)-water (2) system

Parameter	methanol (1)-water (2)			
	Run 1		Run 2	
	PSO	SA	PSO	SA
Wilson				
Λ_{12}	0.6496	0.6490	0.6496	0.6496
Λ_{21}	0.8125	0.8131	0.8125	0.8123
NRTL				
(g_{12} - g_{22})	82.7167	83.1024	82.7167	81.6167
(g_{21} - g_{11})	315.6817	315.1349	315.6817	316.6361
UNIQUAC				
(u_{12} - u_{22})	460.1274	459.7533	460.1274	460.1476
(u_{21} - u_{11})	-227.5596	-227.4077	-227.5596	-227.5829

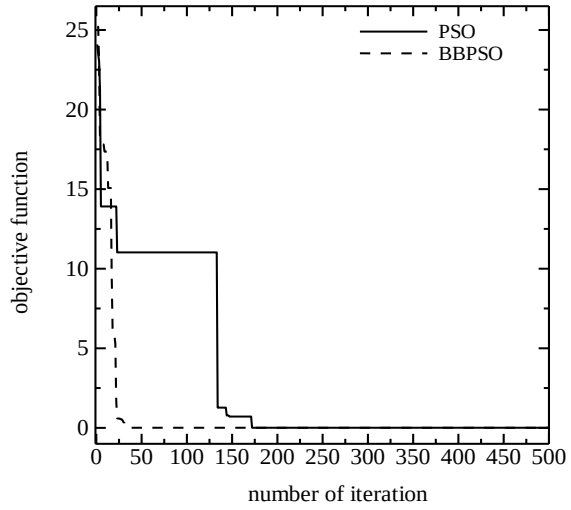

Figure 4. Comparison between PSO and BBPSO for methanol (1) – water (2) system using Wilson Model

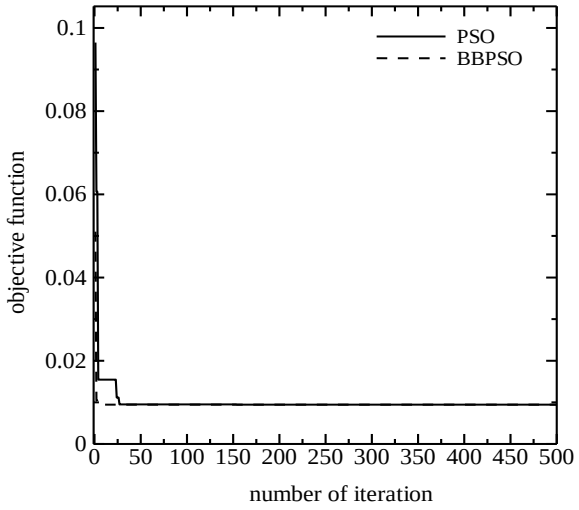

Figure 5. Comparison between PSO and BBPSO for methanol (1) – water (2) system using NRTL Model

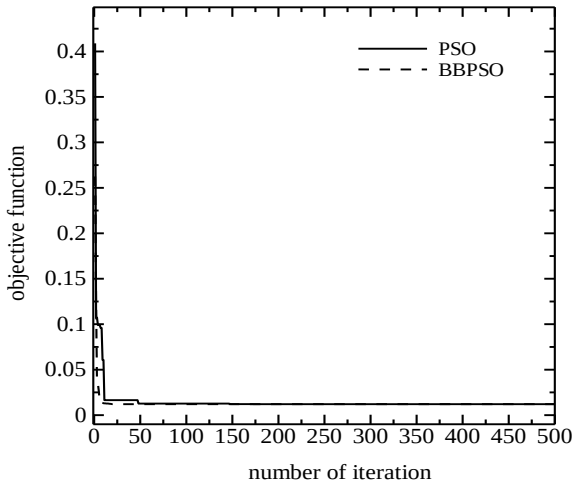

Figure 6. Comparison between PSO and BBPSO for methanol (1) – water (2) system using UNIQUAC Model

Table 4. Binary interaction parameters obtained from this correlation

Parameter	methanol(1)-water(2)	ethanol(1)-water(2)
Wilson		
Λ_{12}	0.6496	0.1723
Λ_{21}	0.8125	0.8532
NRTL		
$(g_{12} - g_{22})$	82.7167	-62.4882
$(g_{21} - g_{11})$	315.6817	1158.1634
α_{12}	0.30	0.30
UNIQUAC		
$(u_{12} - u_{22})$	460.1274	100.2397
$(u_{21} - u_{11})$	-227.5596	341.1725

Table 5. Comparison between deviations from PSO and SA algorithms

Activity Coefficient Model	ΔP (%)*			
	Methanol (1)-water (2)		Ethanol (1)-water (2)	
	PSO	SA	PSO	SA
Wilson	1.32	1.32	0.42	0.42
NRTL	1.29	1.29	0.13	0.14
UNIQUAC	1.34	1.35	0.15	0.15

* ΔP (%) obtained from Kurihara *et al*, 1995 was 1.49% and 0.17% for Methanol (1)-water (2) and Ethanol (1)-water (2), respectively using gradient method.

CONCLUSIONS

In this study, PSO, BBPSO and SA have been successfully applied to optimize three activity coefficient models (Wilson, NRTL, and UNIQUAC) and used to correlate isobaric vapor liquid equilibrium data of water in methanol and ethanol systems with deviation less than 2%. In summary, among those three algorithms, BBPSO shows a consistency result and faster convergence. In general way, the algorithms implemented in this study showed an interesting strategy for other phase equilibrium calculation.

The future study may be aimed to employ those three algorithms in different mixture system and different phase equilibrium such as liquid-liquid equilibrium and also calculation of phase equilibrium in high pressure since it is still challenging to provide better correlation and prediction of phase equilibrium experimental data. Hybridization of PSO and SA is interesting to be applied, where PSO can be used to explore in such large area of search space and SA can be used to exploit the near optimal area of the search space. or suggest applications and extensions.

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