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Interaction parameter estimation in liquid–liquid phase equilibrium modeling using stochastic and hybrid algorithms

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ABSTRACT

Metaheuristic methods Simulated annealing (SA) and Genetic algorithm (GA) combined with hybrid functions were investigated to estimate interactions parameters in liquid–liquid phase equilibrium systems. The Rastrigin and Rosenbrock functions with high number of variables were used as test functions to compare the performance of each algorithm. The experimental ternary LLE data for extraction of alcohol with dichloromethane (and diethyl ether) were considered in the NRTL and UNIQUAC activity coefficient model. The interaction parameters were carried out taking into account the closure equation. As a main conclusion, Hybrid algorithms have showed the best performance to estimate the interaction parameters comparatively to stochastic and deterministic algorithms.

1. Introduction

In the fluid phase equilibria [1–4], the estimation of physical properties and the equilibrium prediction of chemical systems require accurate methods of optimisation dealing with parameter estimation [4–8]. Both deterministic and stochastic optimisations are alternatives to estimate parameters in this field.

In literature stochastic algorithms were used as optimisation methods in phase equilibrium parameter estimations [1,5,6,9,10]. These methods may be based on genetic algorithms [5,11,12], simulated annealing [6,11,13], or particle swarm optimisation [14]. The advantage of such methods is principally the no-need of continuity or derivative function contrary to the deterministic method which can present instabilities or divergence near local minima [5]. Also the stochastic methods do not require an initial vector to start iteration contrary to classical and deterministic methods. Other methods like pattern search optimisation [15–18] and reactive search optimisation [19–21] may be used. Each method can present a particular advantage which is welcomed in parameter estimation calculations.

In the present paper, we have considered a few methods already used in literature but in different forms, based on the use of hybrid algorithms for estimating interaction parameters in LLE systems. The benefits of such methods are the ability to solve complex problems taking the advantage from each algorithm of the hybrid method. These methods are not affected by instabilities near local minima [5]. As a hybrid function, Nelder–Mead Simplex method has been used in this work owing to its ability to improve the results obtained by GA or SA methods. The hybrid strategy enables the stochastic algorithms such as GA or SA method, when the calculations stop in local minimum, to reach the global minimum. The main objective of this work is to compare the efficiency of several algorithms (SA, GA, SA-Hybrid and GA-Hybrid algorithms) and at last to find the best algorithm which gives the high performance. The main features of hybrid algorithms are the exploitation of the best characteristics belonging to two different methods (in this work: the stochastic and the deterministic method) to solve complex optimisation problems (high level of variables and non linear problems).

2. Genetic and simulated annealing algorithms

Genetic algorithm (GA) [5,8,9,22] and simulated annealing method (SA) [11,13,23,24] are classified in the category of the stochastic process and can be applied in estimating parameters such as interaction parameters.

Genetic algorithms tend to reproduce the biological process of natural selection so as to find the global optimum of an objective function. Because of the stochastic nature of GA method, convergence to exact optimum is not always guaranteed, but it is sufficiently strong to find values around the exact solutions. Each possible result in the solution space is identified as individual and

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Table 1
The parameters of GA-Hybrid algorithms used.

Parameter of GA-H algorithm	Value
Population size (GA)	200
Number of generation (GA)	100
Population type (GA)	Double vector
Selection mechanism (GA)	*Uniform*
Crossover probability (GA)	0.70
Mutation probability (GA)	0.01
Tolerance (GA)	1.E−6
Classical algorithm used	Nelder–Mead Simplex method
Maximum perturbation	1E−1
Minimum perturbation	1E−8
Maximum iteration	400
Maximum function evaluations	400
Tolerance of Simplex method	1E−4

classified according to its fitness function. Each individual, or chromosome, is characterized by a sequence of genes from a reliable alphabet. This later might be binary, floating point or integer numbers. The genetic algorithm is an iterative method which attempts to ameliorate the fitness of the population at each iterations step.

According to natural genetic, several operations intervene in the reproduction phase when two chromosomes are combined to give another one. Reproduction is just the process of transcribing an individual from one generation into the next.

The genetic method is able to solve optimisation problems which may present constraints. The GA algorithm is initially based on a natural selection process but also can be artificial because of the possible human intervention. Such a process leads to the biological evolution of species. The GA algorithm is based on three principle operators to create the next generation of the population, among which we can cite: Mutation, Selection and Crossover. The simulation with GA requires specifications of some options. In this work such options are summarized in Table 1.

In the other hand the simulated annealing method is inspired from metallurgy process which consists to reduce crystal defects. As in the metallurgic procedure, the basic steps of the simulated annealing algorithm consist to replace the obtained solution by a random one close to the exact solution. The parameter setting is a basic step in SA technique, so if the temperature (the global parameter T) is too low the algorithm may stop on local minimum and if the temperature is too high the optimum will be passed several times [23,24]. This parameter decreased gradually during the process. The annealing function should be specified (see Table 2). This function is used to perform next iteration. The option fast annealing is chosen as an annealing function in this work. Fast annealing is based on random steps proportional in size to temperature. Boltzmann annealing function [6] steps are proportional to the square root of the temperature. The temperature update function can be exponential, logarithmic or linear.

Table 2
The parameters of SA-Hybrid algorithms used.

Parameter of SA-H algorithm	Value
Annealing function (SA)	Fast annealing
Reannealing interval (SA)	100
Temperature update (SA)	Exponential
Initial temperature (SA)	100
Tolerance (SA)	1E−6
Classical algorithm used	Simplex (Nelder–Mead)
Stall iterations	1000
Tolerance of Simplex method	1E−4

2.1. The Genetic algorithm

The GA-Hybrid algorithm considered in this work is a combination between a stochastic method (GA) and the deterministic NM-Simplex method. The basic steps of the algorithm can be summarised as follows [5,12]

1. Fitness function definition
2. Setting the parameters
   a. Population size
   b. Generation
   c. Selection
   d. Crossover
   e. Mutation
3. Initialization of population of individuals
4. Evaluation of the fitness function of each individual in that population
5. Continue repeatedly on this generation until convergence achieved
6. Choose the best-fit individuals for reproduction
7. Mate individuals using crossover and mutation operations to give birth to new individuals
8. Evaluation the fitness function of new individuals
9. Save least-fit population with new individuals as a vector of solution
10. Use the obtained vector by GA as initial vector to be used by Hybrid function
11. Calculating new vector by Hybrid function (Nelder–Mead Simplex method)
12. Checking the objective function
13. Repeat calculation until convergence

2.2. The Simulated Annealing algorithm

For the SA-Hybrid algorithm we choose the same hybrid function as with GA-Hybrid method, so we can sum up the algorithm in the following general steps:

1. Running the SA algorithm [6,11]
2. Checking the convergence
3. Choose a hybrid function (Nelder–Mead Simplex method)
4. Repeat calculation until convergence

3. Liquid–liquid equilibrium systems

In liquid–liquid equilibrium calculations, UNIQUAC and NRTL models can be used to predict interaction parameters where recent applications can be found in Refs. [1–3,25].

The experimental protocol has been previously discussed in Ref. [9]. The experimental results for the extraction of alcohol (methanol, ethanol and 1-propanol) from water by diethyl ether and Dichloromethane at 293.15 K were adopted. The interaction parameters using universal quasi chemical UNIQUAC and non two-liquid NRTL models have been considered in this work.

3.1. The Universal quasi chemical UNIQUAC model

$$\ln\,\gamma_i = \ln\frac{\phi_i}{x_i} + \frac{z}{2}q_i\,\ln\frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i}\sum_{j=1}^{n}x_j l_j + q_i\left[1 - \ln\left(\sum_{j=1}^{n}\theta_j\tau_{ji}\right) - \sum_{j=1}^{n}\frac{\theta_j\tau_{ij}}{\sum_{k=1}^{n}\theta_k\tau_{kj}}\right] \quad (1)$$

where:

$$\theta_i = \frac{q_i x_i}{q_T}, \quad q_T = \sum_{k=1}^{n} q_k x_k, \quad \phi_i = \frac{r_i x_i}{r_T}, \quad r_T = \sum_{k=1}^{n} r_k x_k \tag{2}$$

$$l_i = \frac{z}{2}(r_k - q_k) + 1 - r_k, \tau_{ij} = \exp\left(-\frac{A_{ij}}{T}\right) z$$
$$= 10\,(\text{coordination number}) \tag{3}$$

3.2. The non random two-liquid NRTL model

The NRTL model for a solution with n components is in the following form:

$$\ln\ \gamma_i = \frac{\sum_{j=1}^{n} \tau_{ji} G_{ji} x_j}{\sum_{k=1}^{n} G_{ki} x_k} + \sum_{j=1}^{n} \frac{x_j G_{ij}}{\sum_{k=1}^{n} G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_{i=1}^{n} x_i \tau_{ij} G_{ij}}{\sum_{k=1}^{n} G_{kj} x_k}\right) \tag{4}$$

where:

$$\tau_{ji} = \frac{g_{ji} - g_{ii}}{RT} = \frac{A_{ji}}{T}, \quad G_{ji} = \exp(-\alpha_{ji}\tau_{ji}), \quad \alpha_{ji} = \alpha_{ij} \tag{5}$$

4. Closure equation

The closure equation for ternary system can be written (see Refs. [7,8]), as follows:

$$A_{12} - A_{21} + A_{23} - A_{32} + A_{31} - A_{13} = 0 \tag{6}$$

Better results have been reported with the use of closure equation than without it (Refs. [7,8]) when calculating the root mean square deviation (RMSD). The authors showed that the binary interaction parameters are related together through Eq. (6) (the six parameters are dependent) for ternary system using non-random NRTL model. So, in this work we choose to consider the closure equation in our calculation of binary interaction parameters of the quasi chemical UNIQUAC and NRTL models. The structural parameters for pure component and supplementary data considered in this work may be found in Ref. [9].

5. Discussion and conclusion

The interaction parameters for UNIQUAC and NRTL models were calculated with implementation of the closure equation (with respect to interaction parameters), just a single equation is needed for ternary systems (Eq. (6)), and the results are collected in Tables 3 and 4 respectively. RMSD formula of Ref. [9] is used to calculate the root mean square deviation to measure the quality of correlation. Several algorithms were used to estimate interaction parameters using GA (Genetic Algorithm), SA (Simulated Annealing), NMS (Nelder–Mead Simplex), SA-NMS (hybrid) and GA-NMS (hybrid). All the algorithms used in this work are suitable for LLE calculations but the hybrid algorithm GA-NMS show the best performance among the others, so it is selected to adjust values of tie lines of (water(X) + alcohols(Y) + dichloromethane(Z)). Looking to the values of the number of iteration (Niter) and the objective function values from Tables A.1 and A.2 (see Appendix A), the GA-NMS show better results than those given by GA, SA, NMS and SA-NMS algorithms used in this work. For high number of variables, the X and Y vector values are summarized in Table A.3 of Appendix A. Figs. 1–3 depict the ternary phase diagram of water–methanol–dichloromethane, water–ethanol–dichloromethane and water–1-propanol–dichloromethane respectively. The simulation results were adjusted to experimental data using Uniquac model for calculating

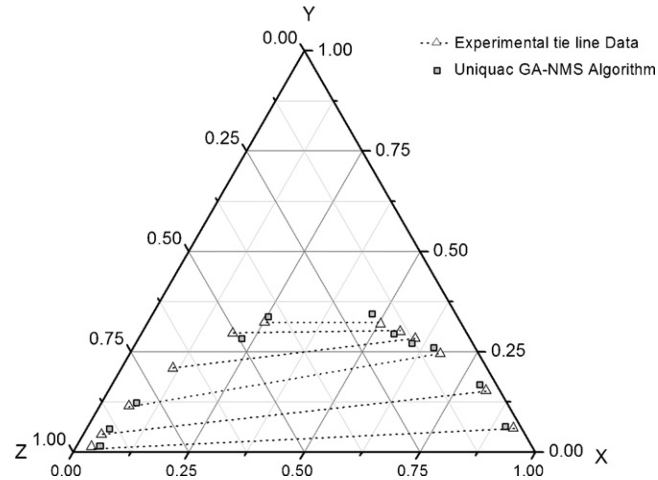

Fig. 1. Experimental and adjusted data LLE of (water(X) + methanol(Y) + dichloromethane(Z)) at 293.15 K using GA-NMS algorithm.

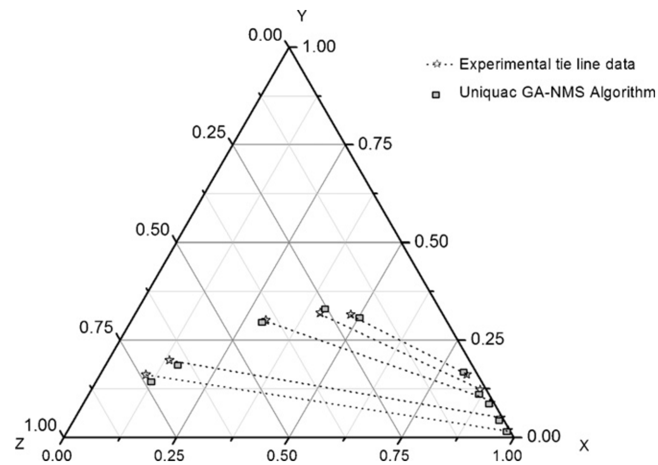

Fig. 2. Experimental and adjusted data LLE of (water(X) + ethanol(Y) + dichloromethane(Z)) at 293.15 K using GA-NMS algorithm.

interaction parameters. Figs. 4 and 5 present a comparison of the RMSD values when using GA-NMS instead of GA-LM hybrid genetic based algorithm of Ref. [9]. In Fig. 4 the values of RMSD for Uniquac model have approximately the same values as in Fig. 5 when NRTL model was used. In Tables 3 and 4 a comparison of RMSD values from Ref. [9] and this work reveal some discrepancies between

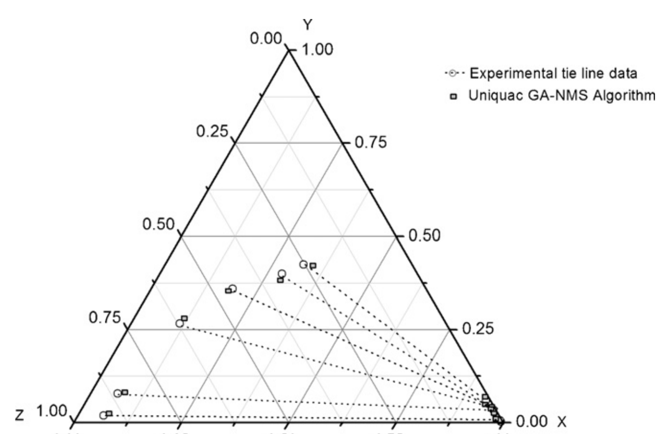

Fig. 3. Experimental and adjusted data LLE of (water(X) + 1-propanol(Y) + dichloromethane(Z)) at 293.15 K using GA-NMS algorithm.

Table 3
The UNIQUAC binary interaction parameters with closure equation and RMSD values using GA-NMS algorithm.

System	UNIQUAC parameters (cal/mol)			RMSD [9]	RMSD
	i–j	A_{ij}	A_{ji}		
Water(1) + methanol(2) + dichloromethane(3)	1–2	−217.1951	46.5882		
	1–3	42.3663	1271.1305	0.0747	0.022
	2–3	−280.5650	684.4159		
Water(1) + ethanol(2) + dichloromethane(3)	1–2	−89.6319	2240.3147		
	1–3	−428.3353	1931.0817	0.0447	0.025
	2–3	−152.2494	−122.7789		
Water(1) + 1-propanol(2) + dichloromethane(3)	1–2	749.4678	87.9214		
	1–3	302.4683	558.1047	0.0068	0.0433
	2–3	−152.7824	764.4004		
Water(1) + methanol(2) + diethyl ether(3)	1–2	−425.2475	61.8336		
	1–3	−69.3835	266.9906	0.0695	0.0224
	2–3	−50.8059	−201.5128		
Water(1) + ethanol(2) + diethyl ether(3)	1–2	−376.3916	297.6616		
	1–3	404.5385	2223.6400	0.0719	0.0219
	2–3	−597.3111	547.7371		
Water(1) + 1-propanol(2) + diethyl ether(3)	1–2	505.6760	1466.0026		
	1–3	−509.9159	824.5981	0.0024	0.0376
	2–3	170.6516	544.8391		

Table 4
The NRTL binary interaction parameters with closure equation and RMSD values using GA-NMS algorithm.

System	NRTL parameters (cal/mol)			α_{ij}	RMSD [9]	RMSD
	i–j	A_{ij}	A_{ji}			
Water(1) + methanol(2) + dichloromethane(3)	1–2	406.1868	166.8307	0.2		
	1–3	−105.6348	654.9997	0.2	0.0114	0.021
	2–3	95.8629	1095.8535	0.2		
Water(1) + ethanol(2) + dichloromethane(3)	1–2	542.9969	−409.2277	0.2		
	1–3	1430.5448	1225.9778	0.2	0.0608	0.024
	2–3	−1766.2854	−1018.6278	0.2		
Water(1) + 1-propanol(2) + dichloromethane(3)	1–2	614.5465	912.7817	0.2		
	1–3	−53.7939	146.4881	0.2	0.0359	0.0432
	2–3	−726.1428	−824.0959	0.2		
Water(1) + methanol(2) + diethyl ether(3)	1–2	−430.4609	546.1301	0.2		
	1–3	760.1399	2303.2226	0.2	0.0168	0.0223
	2–3	−310.6009	255.8908	0.2		
Water(1) + ethanol(2) + diethyl ether(3)	1-2	−793.5203	364.4957	0.2		
	1–3	424.0051	901.9363	0.2	0.0514	0.022
	2–3	−174.9669	−855.0516	0.2		
Water(1) + 1-propanol(2) + diethyl ether(3)	1–2	2047.6507	−2261.7976	0.2		
	1–3	212.0005	907.9738	0.2	0.0033	0.038
	2–3	−4763.5568	241.8649	0.2		

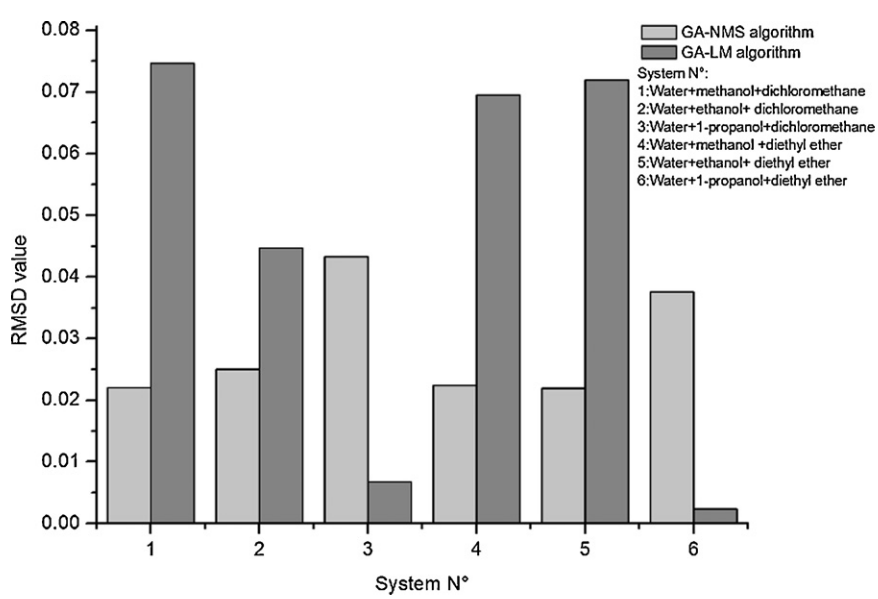

Fig. 4. Comparison of RMSD values for hybrid algorithm using Uniquac model.

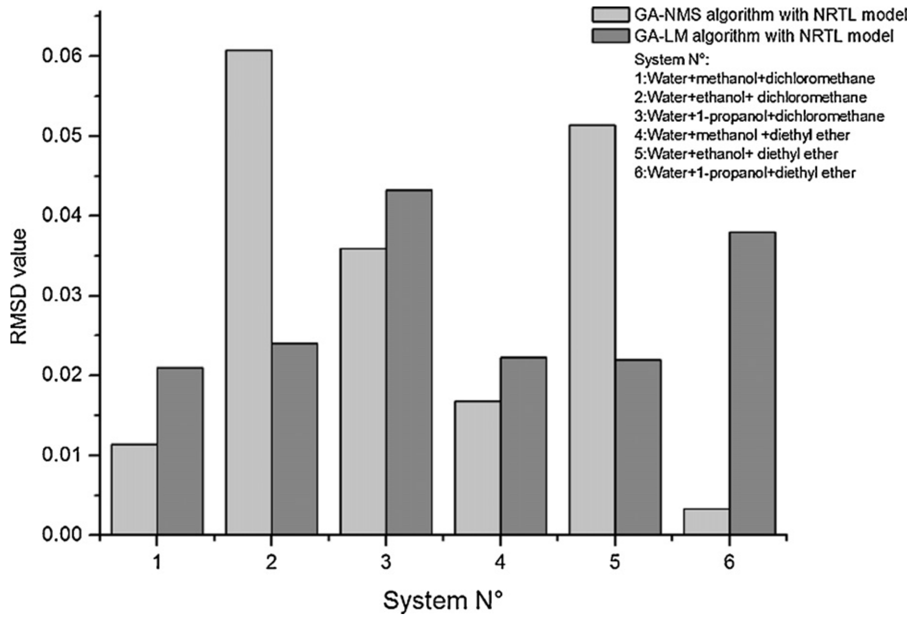

Fig. 5. Comparison of RMSD values for two hybrid algorithm using NRTL model.

Table 5
RMSD and Niter (number of iterations) values using GA, SA, NMS, GA-NMS, SA-NMS algorithms for UNIQUAC model.

System	Parameter	GA	SA	NMS	GA-NMS	SA-NMS
WMDC[a]	RMSD	0.026921	0.021967	0.021967	0.021966	0.021966
	Niter	51	9529	1236	51	5799
WEDC[a]	RMSD	0.030259	0.024950	0.024947	0.024947	0.024947
	Niter	51	5202	1221	51	6227
WPDC[a]	RMSD	0.055986	0.043284	0.043280	0.043280	0.043280
	Niter	51	7434	1213	51	5967
WMDE[a]	RMSD	0.027611	0.022391	0.022390	0.022390	0.022390
	Niter	51	5708	1241	51	6123
WEDE[a]	RMSD	0.026044	0.021939	0.21939	0.021940	0.021939
	Niter	51	4839	1218	51	6210
WPDE[a]	RMSD	0.047718	0.037655	0.037654	0.037655	0.037655
	Niter	51	7549	986	51	6701

[a] WMDC: water(1) + methanol(2) + dichloromethane(3); WEDC: water(1) + ethanol(2) + dichloromethane(3); WPDC: water(1) + 1-propanol(2) + dichloromethane(3); WMDE: water(1) + methanol(2) + diethyl ether(3); WEDE: water(1) + ethanol(2) + diethyl ether(3); WPDE: water(1) + 1-propanol(2) + diethyl ether(3).

the values which may be explained by the implementation of the closure equation in this work and the type of optimization method. The various RMSD and iteration number values of GA, SA, NMS, GA-NMS and SA-NMS are given in Tables 5 and 6 and depicted in Figs. 6–8. Fig. 6 present the performance of each algorithm used by giving the iteration number for six systems (WMDC, WEDC, WPDC, WMDE, WEDE, and WPDE), the order of algorithm considering minimum number of iteration may lead to the following classification:

1. GA-NMS (Genetic Algorithm-Nelder Mead Simplex method)
2. NMS (Nelder–Mead Simplex method)
3. SA-NMS (Simulated Annealing-Nelder Mead Simplex method)

Table 6
RMSD and Niter (number of iterations) values using GA, SA, NMS, GA-NMS, SA-NMS algorithms for NRTL model.

System	Parameter	GA	SA	NMS	GA-NMS	SA-NMS
WMDC[a]	RMSD	0.029881	0.021966	0.021966	0.021966	0.021966
	Niter	51	6665	1273	51	7446
WEDC[a]	RMSD	0.034160	0.024948	0.024947	0.024948	0.024947
	Niter	51	9478	1230	51	8252
WPDC[a]	RMSD	0.060286	0.043283	0.043280	0.043280	0.043280
	Niter	51	13381	1232	51	8667
WMDE[a]	RMSD	0.029741	0.022391	0.022390	0.022390	0.022390
	Niter	51	6098	1247	51	6827
WEDE[a]	RMSD	0.029713	0.021940	0.021939	0.021939	0.021939
	Niter	51	6652	1232	51	6407
WPDE[a]	RMSD	0.052205	0.037671	0.037654	0.037656	0.037654
	Niter	51	18828	1233	51	11640

[a] WMDC: water(1) + methanol(2) + dichloromethane(3); WEDC: water(1) + ethanol(2) + dichloromethane(3); WPDC: water(1) + 1-propanol(2) + dichloromethane(3); WMDE: water(1) + methanol(2) + diethyl ether(3); WEDE: water(1) + ethanol(2) + diethyl ether(3); WPDE: water(1) + 1-propanol(2) + diethyl ether(3).

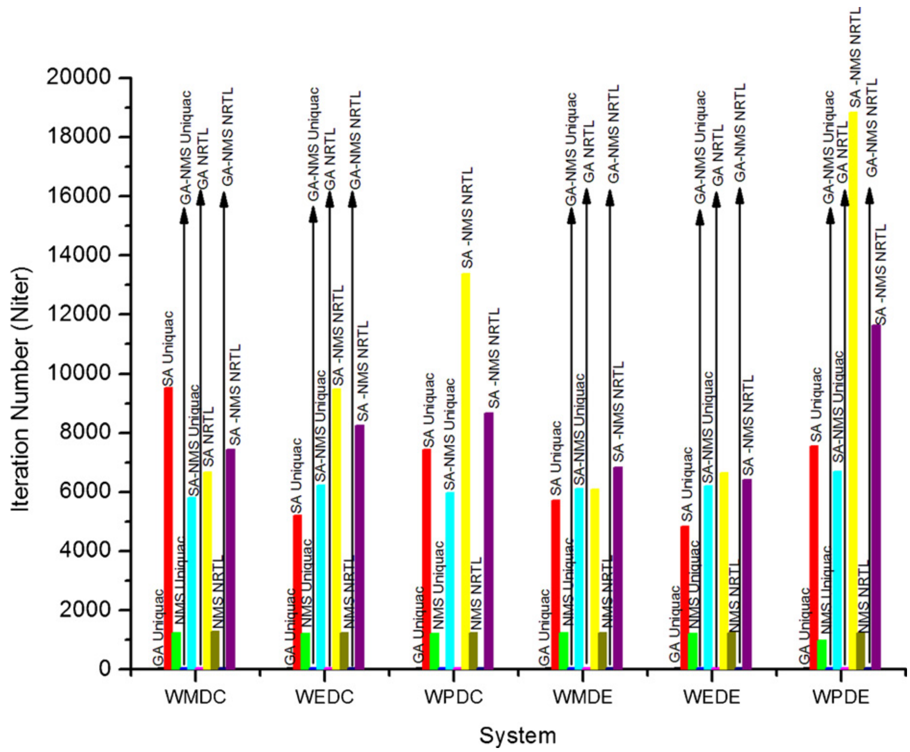

Fig. 6. Values of iteration number (Niter) using several algorithms for Uniquac and NRTL models.

4. SA (Simulated Annealing)
5. GA (Genetic Algorithm)

The SA-NMS and SA methods while the strong behavior of the algorithms in optimization comes in the last because of the huge number of iteration. The NMS algorithm requires more iterations than GA and GA-NMS but less than SA and SA-NMS algorithms. The genetic algorithm applied without hybrid function and according to the GA parameters summarized in Table 1 give a different value comparatively to those given by all the others algorithms.

If we exclude the GA algorithm which give different value of RMSD, all the others algorithms (SA, NMS, GA-NMS, SA-NMS) gives the same RMSD value for each system using UNIQUAC or NRTL model. As main conclusion the algorithm GA-NMS is recommended

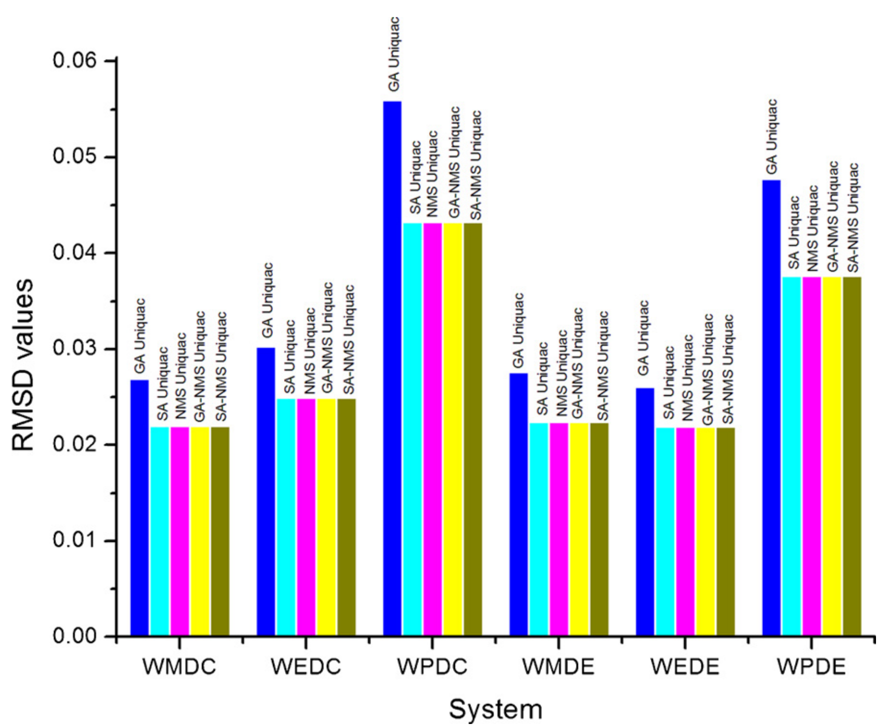

Fig. 7. Comparison of RMSD values for several algorithms using UNIQUAC model.

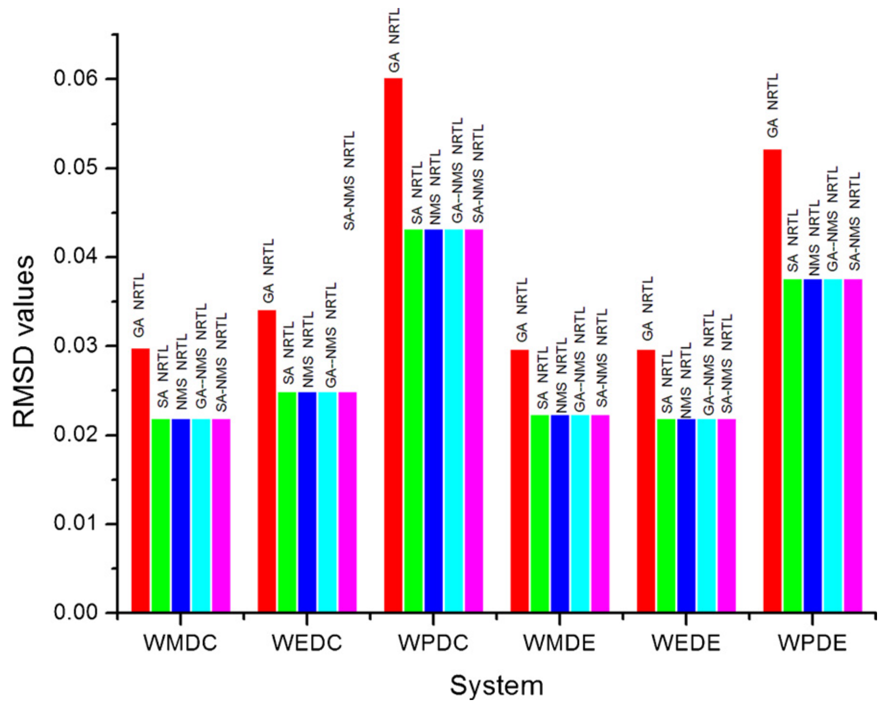

Fig. 8. Comparison of RMSD values for several algorithms using NRTL model.

in parameter interaction calculations in LLE systems, in general GA algorithm should be applied either with hybrid function [9] or testing other parameters such as selection [5], crossover and mutation operators.

Appendix A. Test functions

There are a number of test functions which can be used to evaluate the efficiency of algorithms namely Rosenbrock function, Levy function, Matyas function, Goldstein and price function, Zakharov function and Rastrigin function.

In this work Rosenbrock, Rastrigin functions were used in order to compare the performance of the algorithms discussed above:

A.1. Rosenbrock function

The Rosenbrock function [26], or Dejong's function (two variables), is quite often used as a test function in optimization problems because it converges slowly for most used methods. The Dejong's second function (two variables) can be written as:

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \quad (A.1)$$

The global minimum is given by : $f(x)$

$$= 0 \quad \text{for}(x) = (x_1, x_2) = (1, 1) \quad (A.2)$$

whereas the general Rosenbrock function is given by [26]:

$$f(x) = \sum_{j=1}^{n-1} (100(x_j^2 - x_{j+1})^2 + (x_j - 1)^2) \quad (A.3)$$

Several minima can be found when trying to optimise the Rosenbrock function considering the number of variables n.

$$\text{The search domain} : -5 \leq xj \leq 10 \quad \text{for}\, j = 1, 2 \ldots n \quad (A.4)$$

$$\text{The global minima}\, x = (1, 1 \ldots 1) \quad \text{for}\, f(x) = 0 \quad (A.5)$$

A.2. Rastrigin function

Containing several minima, the Rastrigin function [22] is generally used in genetic algorithm because the classical methods especially the gradient based present difficulties to find the global minimum. For two variables the Rastrigin function is given by the following function:

$$f(x) = 20 + x_1^2 + x_2^2 - 10(\cos(2\pi x_1) + \cos(2\pi x_2)) \quad (A.6)$$

The global minimum is given by : $f(x)$

$$= 0 \quad \text{for}(x) = (x_1, x_2) = (0, 0) \quad (A.7)$$

The general Rastrigin function is given by [22]:

$$f(x) = 10n \sum_{j=1}^{n} (x_j^2 - 10 \cos(2\pi \cdot x_j)) \quad (A.8)$$

$$\text{The search domain} : -5.12 \leq xj \leq 5.12 \quad \text{for } j = 1, 2 \ldots n \quad (A.9)$$

$$\text{The global minima } x = (0, 0 \ldots 0) \quad \text{for } f(x) = 0 \quad (A.10)$$

A.3. Levy function

The Levy function is a non-convex function used in optimization as a test function [6]. This function has 780 minima and only one global minimum if $a = 1$ and several global minima with several local minima if $a = 0$.

$$\text{The search domain} : -10 \leq xj \leq 10 \quad (A.11)$$

$$f(x) = \left(\sum_{j=1}^{5} (j \cos((j-1)x_1 + j)) \right) \left(\sum_{k=1}^{5} (k \cos((k+1)x_2 + k)) \right) + a((x_1 + 1.42513)^2 + (x_2 + 0.80032)^2) \quad (A.12)$$

See the following Tables A.1–A.3.

Table A.1
Comparison the performance of: GA, SA and NMS (Nelder–Mead Simplex) algorithms.

Algorithm	Function test	Minimum point	Start point		F_{obj} value	Niter
GA	Rosenbrock (n = 30)	X_1[a]			191.69	52
GA	Rastrigin (n = 30)	X_2[a]			65.63	65
GA	Rosenbrock (n = 2)	X_3 = (0.965,0.934)			0.00174	51
GA	Rastrigin (n = 2)	X_4 = (0.000,0.019)			0.07	62
NMS	Rosenbrock (n = 30)	X_5[a]	0.0,. . .	. . .,0.0	28.07	5143
NMS	Rastrigin (n = 30)	X_6[a]	0.5,. . .	. . .,0.5	115.63	4989
NMS	Rosenbrock (n = 2)	X_7 = (1.0,1.0)	0.0	0.0	3.68e−10	79
NMS	Rastrigin (n = 2)	X_8 = (0.995,0.995)	0.5	0.5	1.99	38
SA	Rosenbrock (n = 30)	X_9[a]	0.0,. . .	. . .,0.0	22.31	82,230
SA	Rastrigin (n = 30)	X_{10}[a]	0.5,. . .	. . .,0.5	288.57	21,870
SA	Rosenbrock (n = 2)	X_{11} = (0.956,0.913)	0.0,. . .	. . .,0.0	0.002	4118
SA	Rastrigin (n = 2)	X_{12} = (0.000,0.995)	0.5	0.5	0.99	2148

[a] Values collected in Table A.3.

Table A.2
Comparison the performance of GA-H and SA-H algorithms (H = Nelder–Mead Simplex).

Algorithm	Function test	Minimum point	Start point		F_{obj} value	Niter
GA-H	Rosenbrock (n = 30)	Y_1[a]			24.71	177
GA-H	Rastrigin (n = 30)	Y_2[a]			0.246	158
GA-H	Rosenbrock (n = 2)	Y_3 = (1.0,1.0)			3.33e−10	51
GA-H	Rastrigin (n = 2)	Y_4 = (0.0,0.0)			6.10e−7	61
SA-H	Rosenbrock (n = 30)	Y_5[a]	0.0,. . .	. . .,0.0	23.02	84,702
SA-H	Rastrigin (n = 30)	Y_6[a]	0.5,. . .	. . .,0.5	297.5	43,256
SA-H	Rosenbrock (n = 2)	Y_7 = (1.0,1.0)	0.0	0.0	1.46e−10	1788
SA-H	Rastrigin (n = 2)	Y_8 = (0.0,0.0)	0.5	0.5	3.69e−10	2204

[a] Values collected in Table A.3.

Table A.3
The thirty $X_{i=2,5,6,9,10}$ and $Y_{j=1,2,5,6}$ vector values related to Tables A.1 and A.2 for Rosenbrock and Rastrigin functions using GA-H and SA-H algorithms (H = NMS, Nelder Mead Simplex).

X_2	X_5	X_6	X_9	X_{10}	Y_1	Y_2	Y_5	Y_6
1.112	0.433	2.187	0.988	−3.979	0.905	0.006	0.975	2.986
−3.979	0.905	0.006	0.975	2.986	0.843	−0.008	0.949	−0.995
2.986	0.843	−0.008	0.949	−0.995	0.718	−0.001	0.896	4.974
−0.995	0.718	−0.001	0.896	4.974	0.534	−0.006	0.806	0.994
4.974	0.534	−0.006	0.806	0.994	0.306	0.001	0.658	−0.993
0.994	0.306	0.001	0.658	−0.993	0.112	−0.004	0.44	2.983
−0.993	0.112	−0.004	0.44	2.983	0.008	−0.006	0.209	0.994
2.983	0.008	−0.006	0.209	0.994	0.008	−0.005	0.057	0.993
0.994	0.008	−0.005	0.057	0.993	0.022	0.004	0.017	2.984
0.993	0.022	0.004	0.017	2.984	0.019	0.009	0.011	0.991
2.984	0.019	0.009	0.011	0.991	0.002	−0.005	−0.008	2.986
0.991	0.002	−0.005	−0.008	2.986	0.011	0.002	0.015	1.986
2.986	0.011	0.002	0.015	1.986	0.004	0.002	0.016	1.992
1.986	0.004	0.002	0.016	1.992	0.006	−0.001	0.019	2.982
1.992	0.006	−0.001	0.019	2.982	0.024	0.008	0.029	−2.981
2.982	0.024	0.008	0.029	−2.981	0.019	0.018	0.006	0
−2.981	0.019	0.018	0.006	0	0.012	−0.012	−0.002	2.984
0	0.012	−0.012	−0.002	2.984	0.009	0	0.005	−1.991
2.984	0.009	0	0.005	−1.991	0.008	−0.002	0.023	8.954
−1.991	0.008	−0.002	0.023	8.954	0.013	0.002	0.025	−0.994
8.954	0.013	0.002	0.025	−0.994	0.01	−0.001	0.025	1.991
−0.994	0.01	−0.001	0.025	1.991	−0.007	0	0.005	−0.999
1.991	−0.007	0	0.005	−0.999	0.018	−0.001	0.01	−3.979
−0.999	0.018	−0.001	0.01	−3.979	−0.005	0.008	0.005	−1.99
−3.979	−0.005	0.008	0.005	−1.99	−0.004	−0.001	0.011	0.996
−1.99	−0.004	−0.001	0.011	0.996	−0.004	0.005	0.01	1.984
0.996	−0.004	0.005	0.01	1.984	0	0	0.002	1.989
1.984	0	0	0.002	1.989	0.017	0.01	0.01	4.9767
1.989	0.017	0.01	0.01	4.9767	0.004	0.001	0.007	5.967
4.9767	0.004	0.001	0.007	5.967	−0.002	0.006	−0.01	−3.98

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