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Study of interaction parameters in liquid-liquid equilibrium of ternary systems with evolutionary algorithms

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Abstract

The study of phase equilibrium is very important for the optimization of separation processes. The interaction parameters are calculated based on the thermodynamic models UNIQUAC (Universal Quasi Chemical model) and NRTL (Non-Random Two Liquids model) from the liquid-liquid equilibrium data of the system Benzene, pyridine, water at 333.15 K and 288.15 K, and the system Heptane, Benzene, Methanol at 305.8 K and 279.8 K. Optimal results were obtained by optimization methods such as Genetic Algorithm GA, Threshold Acceptance Algorithm TA, and simulated annealing NMS Nelder-Mead-simplex method) using a MATLAB Code.

Keywords: Liquid-Liquid Equilibrium, Optimization, Genetic Algorithm GA, Threshold Acceptance Algorithm TA, simulated annealing NMS

Full length article **Corresponding Author*, e-mail: ngherraf@yahoo.com

1. Introduction

The thermodynamics of liquid-liquid equilibrium allow understanding the molecular interactions between the different species and the different phases. The most common processes are distillation, solvent extraction, absorption and leaching [1]. In industrial applications, there is often a problem of balance between pure-body and multi-component systems. The modeling of such systems is necessary to have a continuous data representation at equilibrium and to better understand the involved phenomena. Furthermore, modeling enables to reduce the amount of experimental data needed to design industrial processes. However, in order to obtain a satisfactory model, it is necessary to use fairly rigorous and strong thermodynamic tools. The presence of molecular interactions within a system marks a deviation from ideality depending upon the magnitude of these interactions. Most often, this deviation must be considered with respect to the complexity of the systems in question. In this case, the use of activity models is almost unavoidable. UNIQUAC and NRTL as phase balance activity prediction models are widely used because they have the advantage to provide a good representation of the liquid-liquid equilibrium by adjusting the necessary parameters. This adjustment is performed by an adequate method of minimizing the difference between experimental and calculated values. The accuracy of the calculation, therefore, depends on the chosen optimization method, if it leads to a local minimum instead of the global minimum, the calculation will be less precise, which will affect the calculation of the process involving the equilibrium predicts [2]. The solvent extraction processes is the best choice for separating organic compounds such as aromas, alcohols, etc., owing to their solubility in a series of organic or ionic solvents, and above all, their high performance, the efficiency and the relative cost of the equipment used leading to a high degrees of separation [3,4]. Because of the importance of liquid-liquid extraction, new programs are constantly developed, affecting both experimental and predictive aspects. The work in hand aims mainly to use experimental liquid-liquid equilibrium data from ternary systems containing liquids as solvents to determine new interaction parameters of the NRTL and UNIQUAC thermodynamic models.

The optimal values of the parameters obtained by a MATLAB calculation program based on the evolutionary optimization methods of the Genetic algorithm GA, the Threshold Acceptance TA method, and the deterministic and exact Nelder Mead Simplex NMS method will be used to calculate liquid-liquid equilibrium data.

2. Optimization algorithms

Different approaches such as Genetic algorithm GA, Threshold Acceptance algorithm TA and simulated annealing NMS which are classified in the category of the stochastic and evolutionary processes are considered in the

calculations of fluid phase equilibrium parameters. In order to estimate the parameters of interaction in UNIQUAC and NRTL models, a computer program in MATLAB using intrinsic function optimization based on genetic algorithm, threshold acceptance algorithm with a hybrid function based on the method of Nelder Mead Simplex was developed.

2.1. Genetic algorithm

This approach is used to determine both constrained and unconstrained problems established on natural selection processes that imitates the biological evolution of species so as to find the global optimum of an objective function. In this method, convergence to exact optimum is not always assured, but it is sufficiently strong to find values around the exact solutions. In each gait, Genetic algorithm uses three operators in order to produce the next generation of the population; selection, crossover, and mutation. Moreover, it is more flexible in this space therefore, it is able to reach all points of the working area [5-13]. The functioning of a genetic algorithm described by Melanie (1996) is structured as follows:

1) Choose: the temperature, the number of constituents Nc, the number of Tie-lines k as well as the experimental data for each component and for each Tie-line.
2) Randomly generate a population of P chromosomes.
3) Evaluate the objective function of each chromosome.
4) Create a new population by repeating the following steps until the new population is completed:
   - ❖ Select two parent chromosomes based on their fitness.
   - ❖ Cross both parents to form two new chromosomes (children) with a probability of crossing. If both parents are not crossed, the children are an exact replica of the parents.
   - ❖ Mutating new children with a probability of mutation,
   - ❖ Place the two new children in the population.
5) Use the new population for the next run of the algorithm.
6) If the stop condition is satisfied, then stop the search and select the best solution; if not, continue.
7) Return to Step 2.

2.2. Threshold acceptance algorithm

Threshold acceptance method was stated by Dueck and Scheuer (1990), and was used in a number of fields (Economics, Management, etc.). It is a form of the Monte Carlo method similar to that of Simulated Annealing SA which uses a local search, in which a subset of solutions is explored by moving from one solution to a neighboring solution. Threshold acceptance method (TA) overcomes the stopping problem in local minima by also allowing upward movements, and also accepts new solutions leading to the higher values of the objective function. This method begins with a random feasible solution. Given any threshold order, length, and rounds, we can see that TA always accepts a solution that improves the objective function, but the deteriorations are only accepted if they are not worse than a particular threshold. Over time, the threshold decreases to zero, so TA is transformed into conventional local search.

The algorithm of this method is similar to Simulated Annealing SA, and is structured as follows:

- ❖ Choose the number of constituent Nc, the number of Tie-line k as well as the experimental data for each constituent and for each Tie-line.
- ❖ Choose an initial temperature (Threshold temperature $T = T_0$)
- ❖ Choose an initial solution $x = x_0$
- ❖ Generate a random solution in the vicinity of the current solution.
- ❖ Compare the two solutions according to the Metropolis criterion:

$$\Delta E = f(x^{new}) - f(x^0)$$

- ❖ Repeat 4 and 5 until statistical equilibrium is reached.
- ❖ Decrease the temperature and repeat until the system reaches the minimum.

2.3. Nelder mead simplex algorithm

This method is an extension of the Simplex method. It is a very intuitive and geometric approach that is classified in the category of 'Direct Search' algorithms (or direct search) because it only uses the evaluations of the objective function. It was proposed in 1965 by J. A. Nelder and R. Mead to minimize a function [14].

For a system with n variables the method starts with (n + 1) points thus defining an initial simplex. The first point (P_0) is estimated and the others are calculated by the following relation:

$$P_i = P_0 + \lambda \cdot E_i \qquad (1)$$

λ is a constant and E_i a vector.

The method consists of the following essential steps:

- Step 1: Reflection
- Step 2: Expansion
- Step 3: Contraction

Simulated annealing is the iterative practice of the Metropolis algorithm, to produce a sequence of configurations that tend toward thermodynamic equilibrium. The algorithm of this method is structured as follows:

- ❖ Choose the temperature, the number of constituents Nc and the number of Tie-lines k.
- ❖ Enter the experimental data for each constituent and for each Tie-line
- ❖ Evaluate an initial state for the NRTL or UNIQUAC model parameters.

- ❖ Optimize these parameters by minimizing the objective function using the Simplex-Nelder Mead minimization method NMS.
- ❖ Resume the calculations (iterations) until the stopping criterion.

3. Liquid-Liquid equilibrium systems and thermodynamic model

The calculation of the liquid-liquid equilibriums is based on the estimation of the activity coefficients which can be predicted using thermodynamic models such as NRTL, UNIQUAC that normally, should allow the calculation of biphasic or triphasic equilibrium with the same sets of parameters.

3.1 Universal quasi chemical UNIQUAC model

The UNIQUAC model for a solution with n components is as follows [13]:

$$\ln \gamma_1 = \ln\frac{\emptyset_i}{x_i} + \frac{z}{2} q_i \ln\frac{\theta_i}{\emptyset_i} + l_i - \frac{\emptyset_i}{x_i}\sum_{j=1}^{n} x_j l_j + q_i \left[1 - \ln\left(\sum_{j=1}^{n} \theta_j \tau_{ji}\right) - \sum_{j=1}^{n} \frac{\theta_j \tau_{ij}}{\sum_{k=1}^{n} \theta_k \tau_{kj}}\right] \quad (2)$$

where:

$$\theta_i = \frac{q_i x_i}{q_T}, \qquad q_T = \sum_{k=1}^{n} q_k x_{k,} \qquad \emptyset_i = \frac{r_i x_i}{r_T}, \qquad r_T = \sum_{k=1}^{n} r_k x_k \quad (3)$$

$$l_i = \frac{z}{2}(r_k - q_k) + 1 - r_k, \quad \tau_{ij} = \exp\left(-\frac{A_{ij}}{T}\right) \quad (4)$$

$$z = 10 \text{ (Coordination number)} \quad (5)$$

3.2 The non-random two-liquid NRTL model

The NRTL model for a solution with n components is as follows:

$$ln\gamma_i = \frac{\sum_{j=1}^{n} \tau_{ji} G_{ji} x_j}{\sum_{k=1}^{n} G_{ki} x_k} + \sum_{j=1}^{n} \frac{x_j G_{ij}}{\sum_{k=1}^{n} G_{kj} x_k}\left(\tau_{ij} - \frac{\sum_{l=1}^{n} x_l \tau_{lj} G_{lj}}{\sum_{k=1}^{n} G_{kj} x_k}\right) \quad (6)$$

where:

$$\tau_{ji} = \frac{g_{ji} - g_{ii}}{RT} = \frac{A_{ji}}{T}, \qquad G_{ji} = \exp\left(-\alpha_{ji}\tau_{ji}\right), \quad \alpha_{ji} = \alpha_{ij} \quad (7)$$

For ternary equilibrium, the fugacities in both phases are equal, and as follows:

$$f_1^{aq} = f_1^{org} \quad (8)$$

$$f_2^{aq} = f_2^{org} \quad (9)$$

$$f_3^{aq} = f_3^{org} \quad (10)$$

And the normalization of molar fraction for ternary systems is as follows:

$$x_1^{aq} + x_2^{aq} + x_3^{aq} = 1 \quad (11)$$

$$x_1^{org} + x_2^{org} + x_3^{org} = 1 \quad (12)$$

4. Results and discussions

The interaction parameters are frequently obtained from experimental liquid-liquid equilibrium data (figures 1-14), by minimizing objective function for all studied systems of the UNIQUAC and NRTL models, as well as the results concerning the prediction of liquid-liquid equilibrium by these models. The objective function is given as follows [4]:

$$\min f = -\sum_{k=1}^{m}\sum_{j=1}^{2}\sum_{i=1}^{n} W_{ijk}\left(x_{ki}^{cal} - x_{ki}^{Exp}\right)^2 \quad (13)$$

In the present work, results between the observed and calculated mass fractions were obtained in terms of the root mean square deviation RMSD defined as [4]:

$$RMSD = \left(\frac{-f}{2mn}\right)^{0.5} \quad (14)$$

m and **n** are the total number of tie lines and components respectively. The tie lines are estimated by liquid-liquid separation using an iterative method.

RMSD is used to measure the quality of the correlation. Several algorithms were used to calculate interaction parameters using Genetic algorithm GA, Threshold Acceptance Algorithm TA, and simulated annealing NMS using a MATLAB Code.

In order to calculate the optimal interaction parameters with the UNIQUAC and NRTL models, we have developed programs based on the minimization methods, Genetic Algorithm GA, Threshold Acceptance Algorithm TA, and simulated annealing NMS using a MATLAB Code.

The interaction parameters of the UNIQUAC and NRTL models for all studied systems as shown in tables 1-12 are optimized by minimizing the objective function defined previously using all the chosen experimental results. The results will be analysed and compared to the experimental.

Table 1: Interaction parameter results with GA algorithm using UNIQUAC and NRTL models for the system Benzene, Pyridine, Water at 333.15.

	UNIQUAC			**NRTL**		
	RMSD=0.2065	**fob**=1.8240		**RMSD**=0.3344	**fob**=4.6958	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-6.543	15.553	0.000	-4.171	14.578
(2)	1.742	0.000	7.689	8.054	0.000	-9.849
(3)	17.531	9.060	0.000	19.544	5.546	0.000

Table 2: Interaction parameter results with TA algorithm using UNIQUAC and NRTL models for the system Benzene , Pyridine, Water at 333.15.

	UNIQUAC			**NRTL**		
	RMSD=0.030815	**fob**=0.0398821		**RMSD**=0.08807911	**fob**=0.3311220	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	433.929	-188.008	0.000	-297.899	947.835
(2)	705.569	0.000	928.632	103.628	0.000	-280.501
(3)	1.575	826.496	0.000	817.044	865.933	0.000

Table 3: Interaction parameter results with NMS algorithm using UNIQUAC and NRTL models for the system Benzene, Pyridine, Water at 333.15.

	UNIQUAC			**NRTL**		
	RMSD=0.00302	**fob**= 0.00038		**RMSD**= 0.00259	**fob**=0.000283	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-413.756	-160.583	0.000	-387.148	3.144
(2)	865.269	0.000	6.426	41.913	0.000	6.833
(3)	1.616	1.186	0.000	5.684	5.931	0.000

Table 4: Interaction parameter results with GA algorithm using UNIQUAC and NRTL models for the system Benzene , Pyridine, Water at 288..15K

	UNIQUAC			**NRTL**		
	RMSD=0.2669	**fob**=2.9937		**RMSD**=0.3537	**fob**=5.2563	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.0000	-5.8878	20.1294	0.0000	3.7547	17.4088
(2)	1.1145	0.0000	-2.6371	-1.7274	0.0000	945.1501
(3)	19.9407	12.7861	0.0000	17.8646	-6.7759	0.0000

Table 5: Interaction parameter results with TA algorithm using UNIQUAC and NRTL models for the system Benzene, Pyridine, Water at 288..15K

	UNIQUAC			**NRTL**		
	RMSD=0.0533	**fob**=0.1192		**RMSD**=0.0599	**fob**=0.1511	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-214.105	187.357	0.000	196.225	600.454
(2)	368.783	0.000	186.434	325.719	0.000	-473.686
(3)	986.305	501.054	0.000	1.514	1804.218	0.0000

Table 6: Interaction parameter results with NMS algorithm using UNIQUAC and NRTL models for the system Benzene, Pyridine, Water at 288.15K

	UNIQUAC			**NRTL**		
	RMSD=0.0022		**fob**=0.00021	**RMSD**=1.8169		**fob**=0.000138
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-226.546	9.351	0.000	1.036	1.977
(2)	7.889	0.000	4.498	-21.865	0.000	1.766
(3)	419.809	627.512	0.000	9.089	3.553	0.000

Table 7: Interaction parameter results with GA algorithm using UNIQUAC and NRTL models for the system Heptane, Benzene, Methanol 279.8K

	UNIQUAC			**NRTL**		
	RMSD=0.2669	**fob**=2.9937		**RMSD**=0.3537667	**fob**=5.2563	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-1.410	20.646	0.000	5.726	21.279
(2)	-1.662	0.000	2.885	1.656	0.000	4.009
(3)	18.545	-2.103	0.000	17.895	-1.452	0.000

Table 8: Interaction parameter results with TA algorithm using UNIQUAC and NRTL models for the system Heptane, Benzene, Methanol 279.8K

	UNIQUAC			**NRTL**		
	RMSD=0.0620425	**fob**= 0.1616692		**RMSD**=0.0694473	**fob**=0.202563	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-297.727	773.557	0.000	-706.952	498.800
(2)	236.628	0.000	-642.940	295.949	0.000	-125.972
(3)	341.255	539.189	0.000	1623.700	774.051	0.000

Table 9: Interaction parameter results with NMS algorithm using UNIQUAC and NRTL models for the system Heptane, Benzene, Methanol 279.8K

	UNIQUAC			**NRTL**		
	RMSD=0.0058723 **fob**=0.00 14483			**RMSD**=0.004804	**fob**=0.0009693197	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-93.613	356.523	0.000	-261.304	929.883
(2)	0.141	0.000	-81.753	-1.615	0.000	-113.459
(3)	319.953	107.771	0.000	938.334	133.499	0.000

Table 10: Interaction parameter results with GA algorithm using UNIQUAC and NRTL models for the system Heptane, Benzene, Methanol 305.8K

	UNIQUAC			**NRTL**		
	RMSD=0.1457087	fob= 0.8917032		RMSD= 0.2669922	fob=2.994	
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-2.475	22.340	0.000	-1.431	18.924
(2)	4.519	0.000	-2.849	6.566	0.000	3.274
(3)	19.466	4.337	0.000	21.066	6.753	0.000

Table 11: Interaction parameter results with TA algorithm using UNIQUAC and NRTL models for the system Heptane, Benzene, Methanol 305.8K

	UNIQUAC			**NRTL**		
	RMSD= 0.0768468		**fob**= 0.2480279	**RMSD**= 0.0322863		**fob**=0.0437811
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	-329.130	-63.132	0.000	843.773	806.698
(2)	472.475	0.000	-82.226	518.607	0.000	-322.769
(3)	912.280	226.136	0.000	899.123	166.788	0.000

Table 12: Interaction parameter results with NMS algorithm using UNIQUAC and NRTL models for the system Heptane, Benzene, Methanol 305.8K

	UNIQUAC			**NRTL**		
	RMSD=0.0074906		**fob**= 0.0023566	**RMSD**=0.0070187		**fob**=0.0020690
i-j	(1)	(2)	(3)	(1)	(2)	(3)
(1)	0.000	2421.2	1237	0.000	866.185	179.608
(2)	-0.983	0.000	3637.9	0.201	0.000	647.962
(3)	-174.041	1535	0.000	2980.2	658.757	0.000

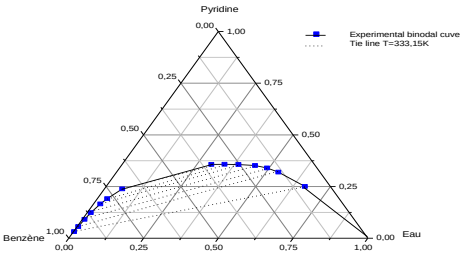

Fig.1. The miscibility curve for the system Benzene, Pyridine, Water at 333.15k

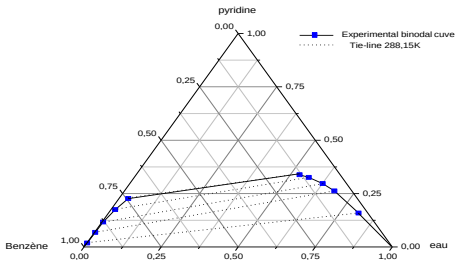

Fig.2. The miscibility curve for the system Benzene, Pyridine, Water at 288.15k

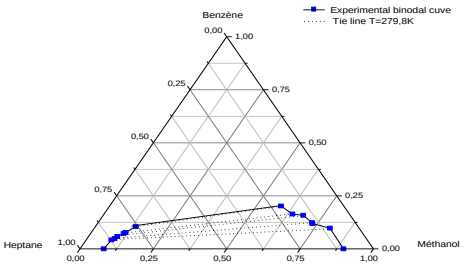

Fig.3. The miscibility curve for the system Heptane, Benzene, Methanol at 279.8k.

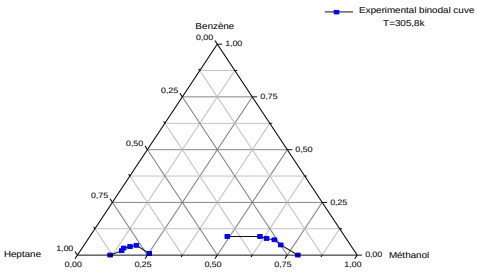

Fig.4. The miscibility curve for the system Heptane, Benzene, Methanol at 305.8k.

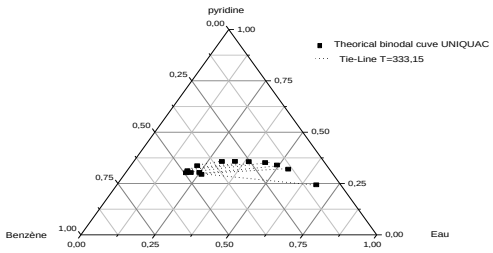

Fig.5. Binodal curve, experimental and theoretical tie-line GA algorithm using UNIQUAC model for the system Benzene, pyridine, water at 333.15K.

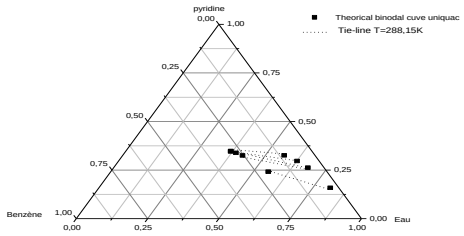

Fig.6. Binodal curve, experimental and theoretical tie-line GA algorithm using NRTL model for the system Benzene, pyridine, water at 288.15K.

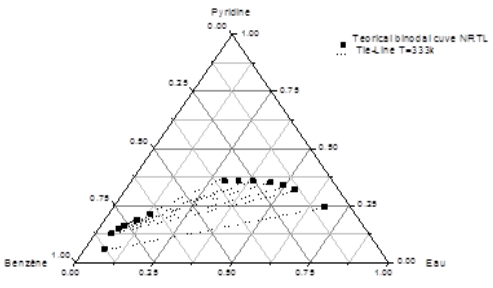

Fig.7. Binodal curve, experimental and theoretical tie-line TA algorithm using UNIQUAC model for the system Benzene, pyridine, water at 333.15K

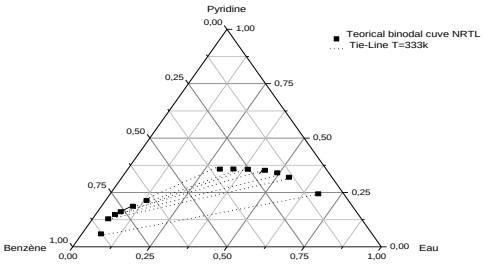

Fig.8. Binodal curve, experimental and theoretical tie-line TA algorithm using NRTL model for the

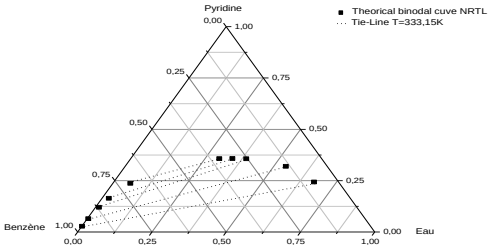

Fig.9. Binodal curve, experimental and theoretical tie-line NMS algorithm using NRTL model for the system Benzene, pyridine, water at 333.15K.

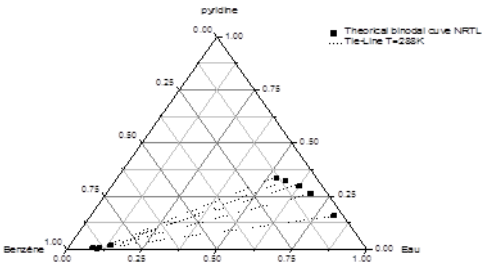

Fig.10. Binodal curve, experimental and theoretical tie-line TA algorithm using NRTL model for the system Benzene, pyridine, water at 288.15 K.

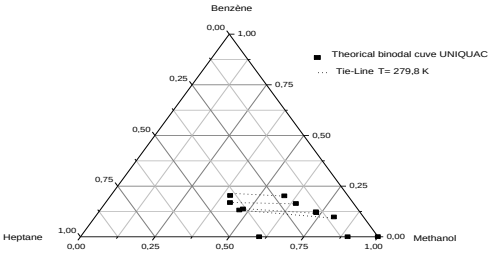

Fig.11. Binodal curve, experimental and theoretical tie-line GA algorithm using UNIQUAC model for the system Heptane, Benzene, methanol at 279.8 K.

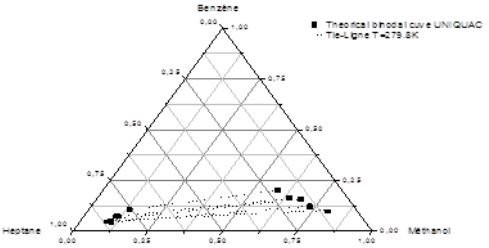

Fig.12. Binodal curve, experimental and theoretical tie-line NMS algorithm using UNIQUAC model for the system Heptane, Benzene, methanol at 279.8 K.

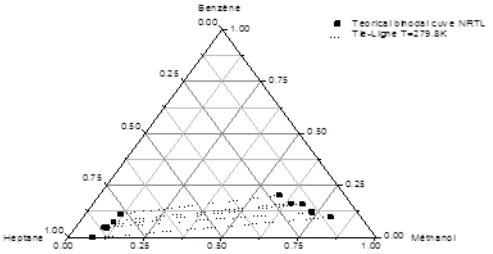

Fig.13. Binodal curve, experimental and theoretical tie-line NMS algorithm using NRTL model for the system Heptane, Benzene, methanol at 279.8 K.

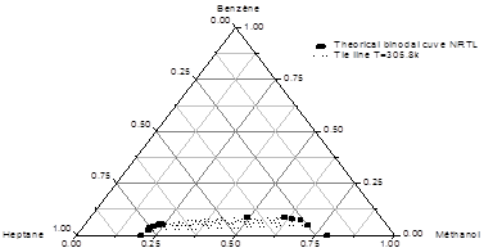

Fig.14. Binodal curve, experimental and theoretical tie-lineTA algorithm using NRTL model for the system Heptane, Benzene, methanol at 205.8 K.

Conclusions

In order to classify optimization methods, many criteria are considered such as the value of the RMSD and the objective function fob. For the deterministic method NMS, the results averred exact, but for stochastic methods GA and TA, results are random and never the same, and therefore, it is necessary to carry out several executions to retain the best results. The RMSD values obtained with GA, TA, and NMS methods are given previously in the tables 1-9 and they represent the performance of each method for the prediction of balances and the estimation of the interaction parameters of the models. It can be observed that the best performance is given by NMS algorithm comparatively to TA algorithm which is, in turn better than the GA algorithm. It can also be noted that the temperature and the thermodynamic models used have an importance on the calculation of the interaction parameters. Several future work prospects arise from this study: we propose to extend the study by experimental measurements of liquid-liquid equilibrium data, different ternary systems, as well as the application of other thermodynamic models and other methods (with hybridization) for the optimization of interaction parameters and the prediction of equilibrium.

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