Supporting Information

Measurement and correlational study of phase equilibria in aqueous solutions of N,N-Dimethylacetamide with 1-pentanol and 1-hexanol at 298.15 and 308.15K

Nassima Lami[a], Abdelkrim Merzougui[b], Hasan USLU[c]
[1]*Department of Chemical Engineering, University of El-ouad, Algeria*
[2]*Department of Chemical Engineering, University of Biskra, Algeria*
[c] *Nigde Omer Halisdemir University, Faculty of Engineering, Food Engineering Department, Nigde, 51240, Turkey*

*E-mail: merzouguikarim@yahoo.com
*Phone: +213 553751938, +213 33525325

Elephant herding optimization (EHO) parameters adjustment

As the key parameters (α scale factor, β factor and n_{Clan}) used in EHO are believed to play a key role in the performance of the optimization solver, many paper have made contribution to the research of parameter setting strategy (i.e. experimental, empirical, dynamical,...). In this work we used the experimental strategy for the parameter setting of EHO. It has to be noted that for the statistical analysis, 30 independent runs over each ternary mixture have been performed. The benchmarking mixture involves the predictions of LLE for (water + DMAC + 1-pentanol) ternary system at 298.15K. All experiments are implemented on Sony Vaio- Intel Core i3-3227U GHz- 4 GB RAM.

Experiment results and analysis

Effects of α scale factor, β factor and n_{Clan} on the performance of EHO

The RMSD values obtained using different α and β values are reported in Tables S1-S2 and Figures S1, respectively (The best results are highlighted in bold face).

As can be seen from Table S1 and Figures S1, the results of a sensitivity analysis of α scale factor has an effect on the results obtained by the proposed optimization solver. When α is 0.5, optimization precision and stability of the proposed solver are the most excellent for both thermodynamic models.

The results of a sensitivity analysis of β factor on binary parameter identification of the NRTL and UNIQUAC activity coefficient equations as shown in Table S2 and Figures S1. As the β value is decreased, the performance of the EHO is improved. As can be seen from Table S2 and Figures S1, a relatively small value (β = 0.1) produces the optimal solution (the value of RMSD are low) for both activity coefficient models.

Moreover, the convergent process of the EHO with closure equations with variation in α and β, during LLE data fitting of (water + DMAC + 1-pentanol) ternary system at 298.15K are reported in Figures S2-S3 for both thermodynamic models, respectively. In particular, Figures S2 shows that the EHO solver converges faster as the β value decreases. Therefore, it is generally better to use a small value for the β to enhance the performance of the optimization solver. A high β value causes deterioration in the performance of the solver.

As can be seen from Figure S3, that the EHO solver may reach a high precision in the solution obtained for LLE parameter identification as the: $0.3 \leq \alpha \leq 0.7$. When α is 0.5, the EHO solver has faster convergence speed and achieves better results on all the considered ternary systems.

On the other hand, the effect of the number of clan $\boldsymbol{n_{Clan}}$ on absolute objective function value is shown in Figure S4. It is observed that $\boldsymbol{n_{Clan}} = 5$ is able to find the best solution for both activity coefficient models.

Figures

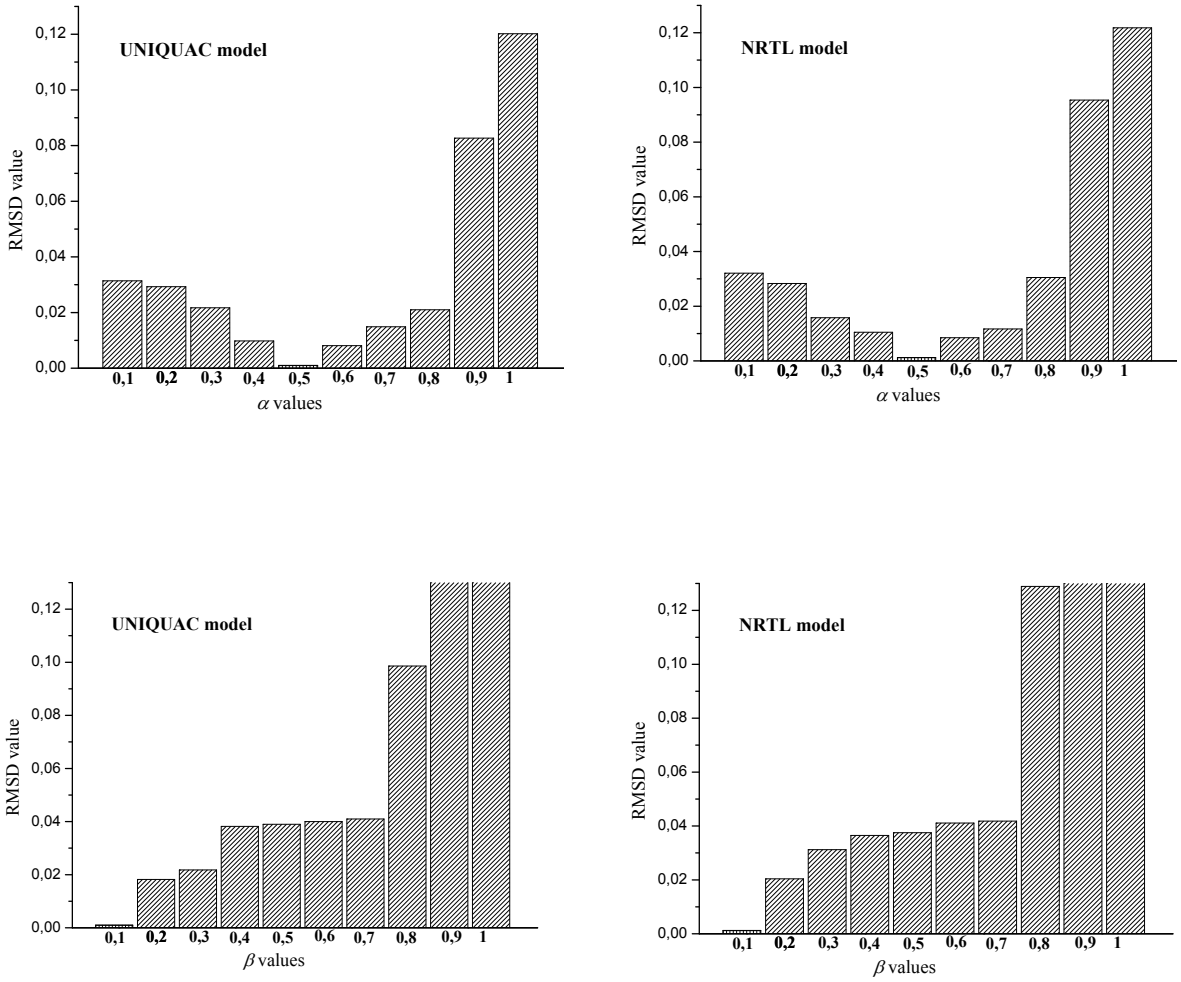
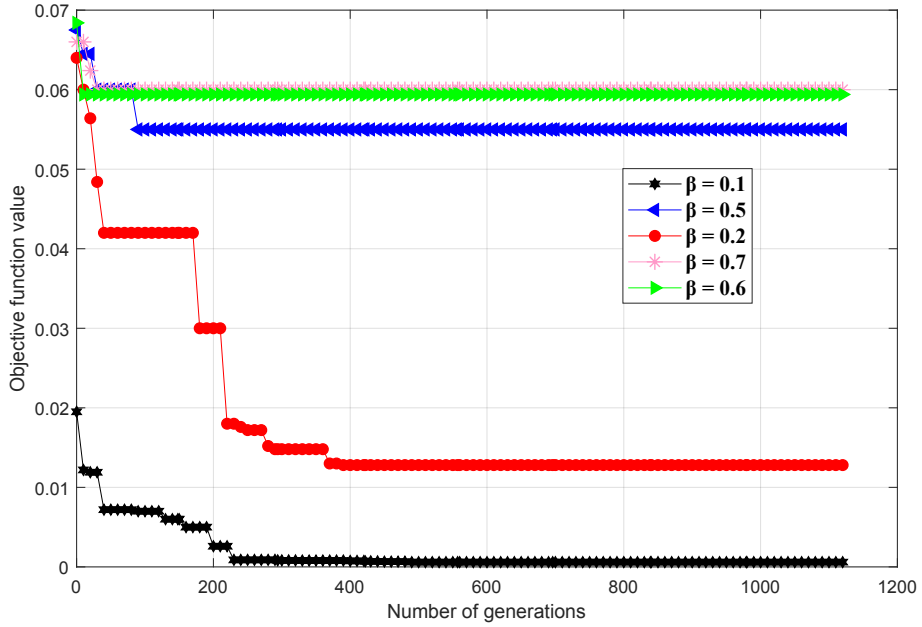


Figure S1. Variation of the RMSD value with change in α and β of the EHO-C solver for ternary system (water + DMAC + pentanol) at 298.15K.

a)



b)

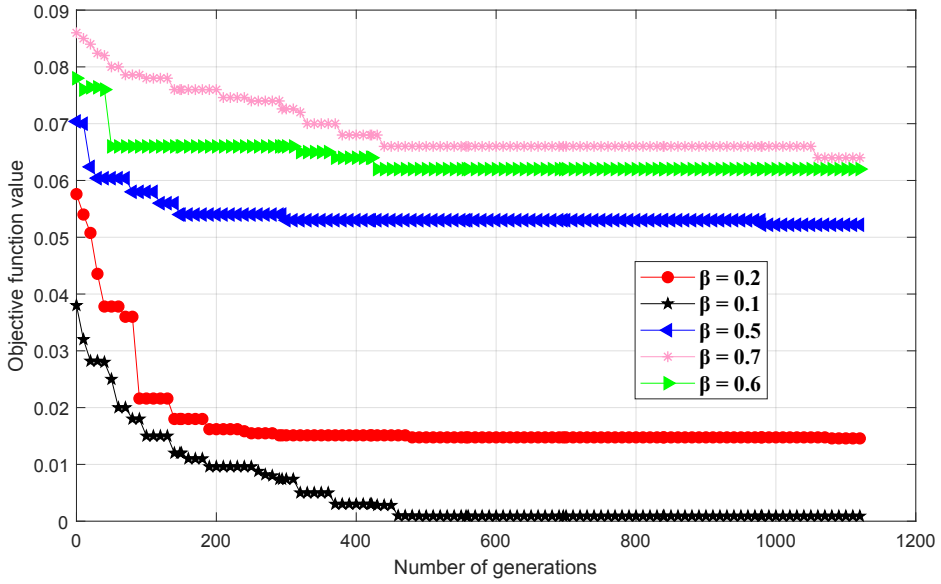
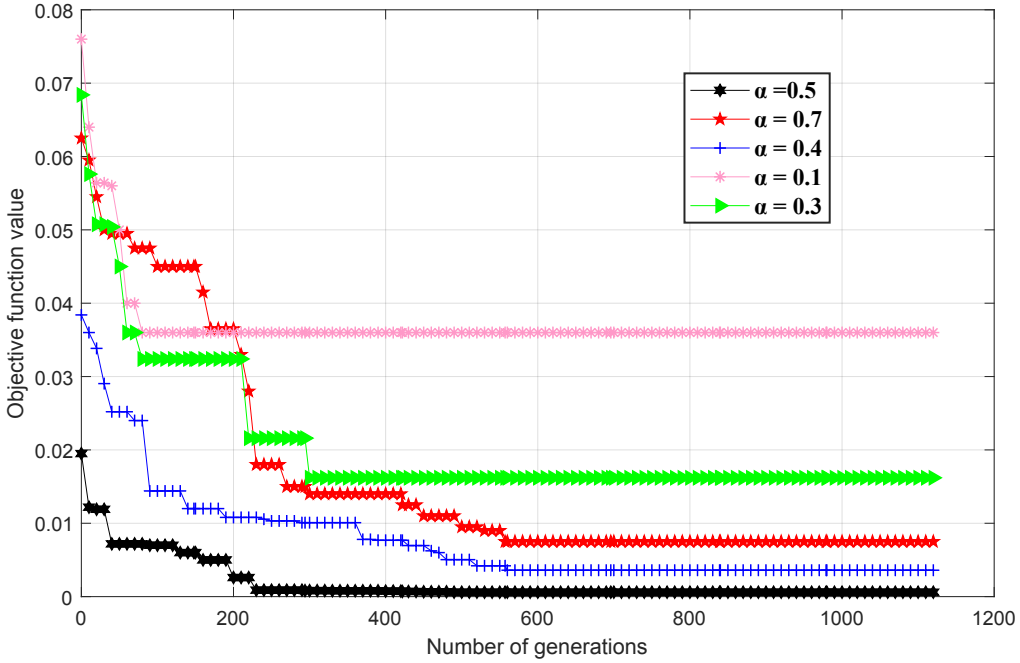


Figure S2. Convergence behavior of the EHO-C solver on different β values for ternary system (water + DMAC + pentanol at 298.15K), a) UNIQAC, b) NRTL model.

a)



b)

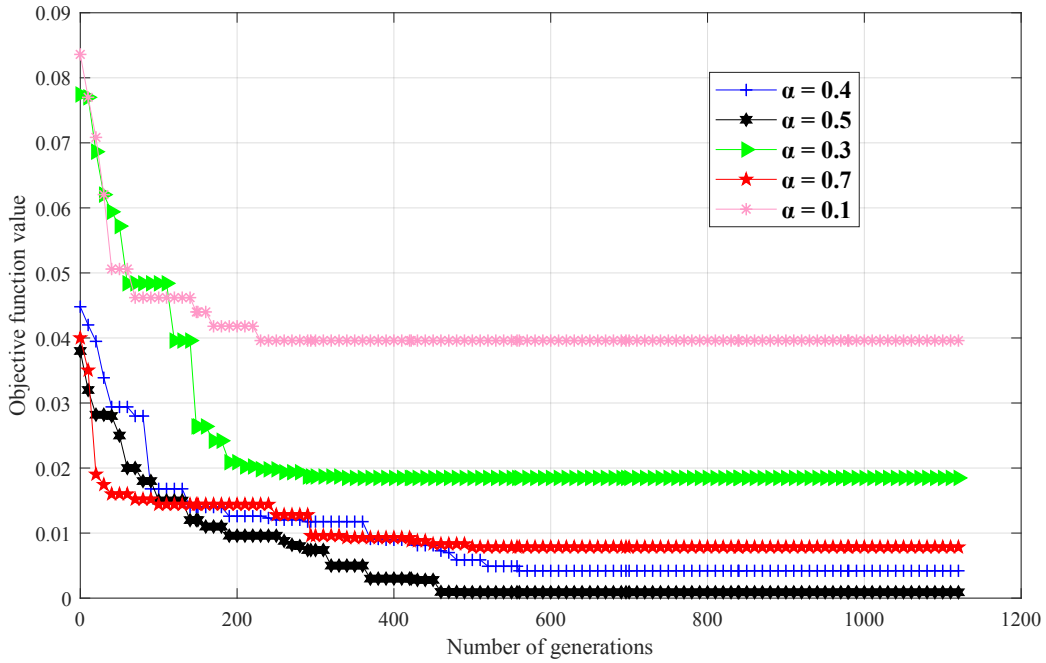


Figure S3. Convergence behavior of the EHO-C solver on different α values for ternary system (water + DMAC + pentanol at 298.15K), a) UNIQAC, b) NRTL model.

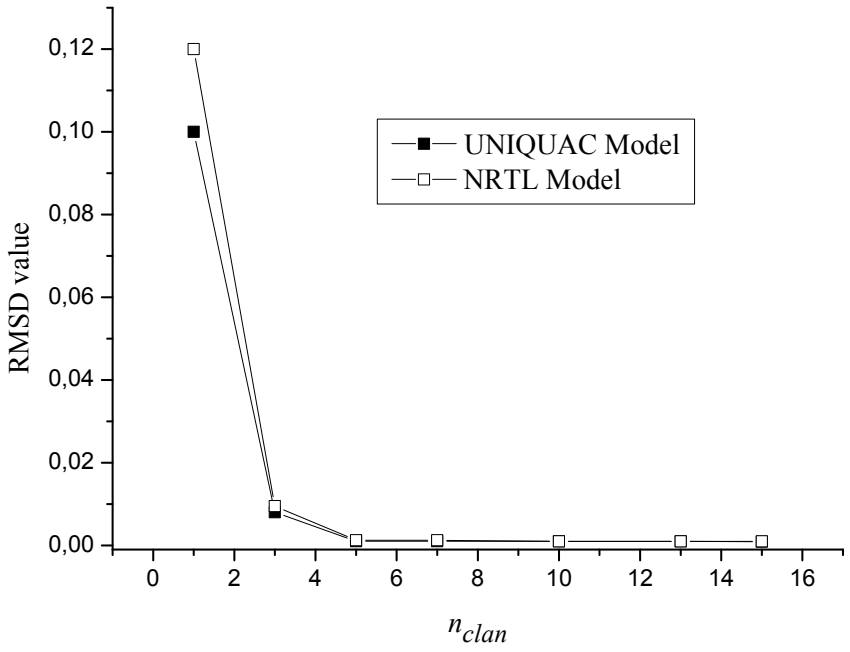


Figure S4. RMSD value *vs*. number of clan n_{Clan} with closure equations for LLE of ternary system (water + DMAC + pentanol) at 298.15 K

Tables

Table S1. Effects of α scale factor on the performance of EHO (β = 0.1 and n_{Clan} = 5)

	UNIQUAC		NRTL	
α	EHA	EHA-C	EHA	EHA-C
0.1	0.0334	0.0314	0.0328	0.0321
0.2	0.0315	0.0293	0.0327	0.0283
0.3	0.0221	0.0217	0.0198	0.0158
0.4	0.0106	0.0098	0.0045	0.0105
0.5	**0.0013**	**0.0010**	0.0015	**0.00125**
0.6	0.0085	0.0081	0.0088	0.0085
0.7	0.0152	0.0149	0.0175	0.0117
0.8	0.0253	0.0210	0.0325	0.0305
0.9	0.0882	0.08270	0.0965	0.0954
1	0.1214	0.1202	0.1258	0.1218

Table S2. Effects of β scale factor on the performance of EHO (α = 0.5 and n_{Clan} = 5)

	UNIQUAC		NRTL	
β	EHA	EHA-C	EHA	EHA-C
0.1	0.0013	**0.0010**	0.0015	**0.00125**
0.2	0.0193	0.0182	0.0250	0.0204
0.3	0.0235	0.0218	0.0361	0.0312
0.4	0.041	0.0382	0.0395	0.0365
0.5	0.0418	0.0390	0.0398	0.0375
0.6	0.0457	0.040	0.0418	0.0411

0.7	0.0460	0.041	0.0506	0.0418
0.8	0.1078	0.0986	0.1302	0.1289
0.9	0.1452	0.1415	0.1450	0.1452
1	0.1552	0.1421	0.1680	0.16052