

Supporting Information

Synthesis and characterization of diethyl citrate and phase equilibria in mixtures with ethanol and water

Claudia Berdugo, Andrea Suaza, Miguel A. Santaella, Orlando A. Sánchez, Gerardo

*Rodríguez, Alvaro Orjuela **

Department of Chemical and Environmental Engineering, Grupo de Procesos Químicos y Bioquímicos, Universidad Nacional de Colombia, 111321 Bogotá D.C., Colombia.

*Corresponding author. Tel (+571) 3165000 x 14303. E-mail address: aorjuelal@unal.edu.co

Table S.1. Normal boiling temperatures (Tb) calculated by Gani Method and reported in available literature

Component	Tb (°C)	
	Gani Method	Literature ¹
CA	359.1	
1-MEC	344.2	
2-MEC	347.5	
1,2-DEC	328.2	
2,3-DEC	331.7	
TEC	314.6	294

Table S.2. Antoine coefficients. P in bar and T in °C in the form

$$\ln P = c_1 + \frac{c_2}{c_2+T} + c_4 * T + c_5 * \ln(T) + c_6 * T^{c_7}$$

Components	CA	MEC	DEC	TEC	ETOH	H2O	DEE
c₁	218.647	190.324	166.369	7605.741	61.791	62.136	125.387
c₂	-29279	-24953.730	-21369.762	-266065.82	-7122.3	-7258.2	-6954.3
c₃	0	0	0	0	0	0	0
c₄	0	0	0	1.57875338	0	0	0
c₅	-26.801	-23.358	-20.437	-1264.405	-7.142	-7.304	-19.254
c₆	3.87E-18	4.38E-18	4.99E-18	-4.47E-16	2.89E-06	4.17E-06	0.024508
c₇	6	6	6	6	2	2	1

Table S.3. UNIQUAC Binary interaction parameters (B_{ij} , B_{ji}) for the reactive system. Parameters in gray areas were regressed from experiments. All other were estimated by UNIFAC

Component i	Component j					
	CA	MEC	DEC	TEC	EtOH	H ₂ O
CA	0	-239.036	16.300	-753.282	116.262	-770.242
MEC	27.544	0	-239.310	-896.607	-146.110	-218.814
DEC	7.458	285.802	0	-646.946	422.450	-323.344
TEC	143.487	128.681	797.487	0	25.075	41.719
EtOH	-450.428	663.757	-318.359	-586.137	0	A: 6060.665 B: -16.67
H ₂ O	-446.262	372.278	823.542	-68.640	A: -6293.266 B: 20.73	0

Parameters estimated with UNIFAC were reported in literature ².

UNIQUAC equation in Aspen Plus calculates $\tau_{ij} = e^{-\frac{u_{ij}-u_{ii}}{RT}} = e^{-\frac{\Delta u_{ij}}{RT}}$ as

$$\ln(\tau_{ij}) = A_{ij} + \frac{B_{ij}}{T}$$

$$\Delta u_{ij} = -RTA_{ij} - RB_{ij}$$

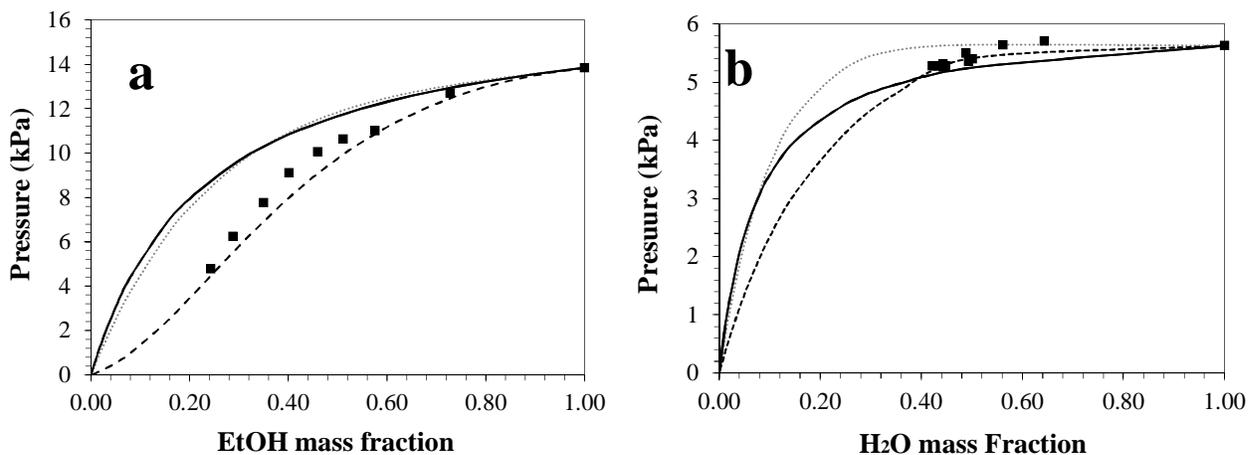


Figure S1. Mass basis binary P - x diagram for binary mixtures at 308 K. (a) DEC+EtOH. (b) DEC+H₂O. Solid curve – Ideal model. Dotted gray line – Kolah *et al* model². Dashed curve – Regressed UNIQUAC model.

References

- (1) Weast, R. Grasselli, J. **1989**. CRC Handbook of Data on Organic Compounds, 2nd Edition, Weast,R.C and Grasselli, J.G., ed(s)., CRC Press, Inc., Boca Raton, FL, 1989.
- (2) A.K. Kolah. N.S. Asthana. D.T. Vu. C.T. Lira. D.J. Miller. Reaction kinetics of the catalytic esterification of citric acid with ethanol. *Ind. Eng. Chem. Res.* **2007**. 46. 3180–3187.