

1. INTRODUCTION

Heterogeneous azeotropic distillation is used for separating non-ideal mixtures. The technique uses minimum-boiling azeotropes and liquid-liquid immiscibilities in combination to break the azeotropes or tangent pinches in the mixture that would prevent the desired separation. However, other configurations are possible. Azeotropic distillation processes are developed using residue curve maps to explain the behavior of entire systems of heterogeneous azeotropic distillation columns as well as the individual columns that make up the system (Pham and Doherty 1990a, 1990b, 1990c). This conceptual design is a starting point to most rigorous design. Nevertheless, to generate a good conceptual design it is necessary to have a non-ideal solution model capable of predicting vapor-liquid equilibrium, liquid-liquid equilibrium, vapor-liquid-liquid equilibrium, homogeneous and heterogeneous azeotropic points (Cairns and Furzer, 1990). Recently, a surprising feature of azeotropic distillation columns, multiple steady states, was discovered. It refers to output multiplicities, that is, that a column of a given design exhibits different column profiles at steady state for the set of inputs and the same values of the operating parameters. This aspect, multiple steady states (MSS), should be studied with azeotropic distillation simulation.

In this paper we discuss a recommendation to correlate heterogeneous azeotropic ternary systems. The reliability of the use of the recommended correlation is analyzed through heterogeneous azeotropic distillation.

2. METHODS AND MODELS

We have modeled the phase equilibria in heteroazeotropic systems in two steps: first we estimated binary parameters using all information we had at our disposal, and second we designed a distillation column to see if the parameters were adequate. Our calculations were done with commercial software: DISTIL and HYSYS.

2.1 Estimation of Parameters

All phase equilibria were described using activity coefficient models. The vapor phase was assumed to be ideal because equilibrium pressure was low and compounds in the systems under study did not associate. The numbers that are presented in this work for the seven ternary systems shown in Table 1 and Table 2 were obtained with UNIQUAC. The procedure used to estimate the binary parameters was: for the homogeneous binary systems we had chosen the DISTIL-HYSYS database binary parameters and in the case that these parameters were missing we used binary vapor-liquid equilibrium data. For the heterogeneous binary we have calculated two parameters (a and b : $a + b T$) for each binary parameter. The criterion for this election was to adjust the best possible the binary

phase equilibrium of each system. The objective function used was minimization of the separation factor (Minimize $f = \sum (S^{\text{cal}} - S^{\text{exp}})$) and was done with a local method. Different initial guesses were tried and a unique set parameters was found.

2.2 Distillation Column Design

The method we used for the design of distillation columns is based on the boundary-value design method as described by Julka and Doherty (1990) and implemented in DISTIL. For a one-feed, two-product distillation column, we define the feed, specify completely distillate and bottoms (using component and overall mass balances) and select the internal flow of the column (by specifying reflux or reboil ratio and using an energy balance). The composition profiles are then calculated using a combination of flashes and mass balances starting from both ends. If the composition profiles for rectifying and stripping sections of the column cross in the composition space, the column is feasible and the number of stages in each section of the column can be counted. For the most common heterogeneous systems the distillation column requires a top decanter. Then, for a ternary distillation column with one feed, two products and a top decanter the boundary-value design method algorithm can be summarized as follows:

1. Specify feed composition and thermodynamic state.
2. Specify column pressure.
3. Specify bottoms composition.
4. Select top vapor composition in the liquid region close to the ternary azeotrope.
5. Calculate the remaining mole fraction of the product using mass balances.
6. Guess a value for the reflux ratio.
7. Calculate reboil ratio using energy balance.
8. Compute the composition profiles for the rectifying and stripping sections of the column starting from distillate and bottoms compositions.
9. Repeat steps 5 to 7 until composition profiles intersect in the composition space.
10. Repeat steps 2 to 7 to optimize reflux ratio and pressure.
11. Count the number of stages in each section of the column.

In addition we did a rigorous column simulation with HYSYS. It is important to note that the number of specifications in DISTIL and in HYSYS are the same, what it is different is which variable is selected as specification. In HYSYS the specifications that normally are set include: feed compositions, number of stages, feed plate composition, reflux rate and distillate or bottom flow rate. Product compositions, heat duties are the results of the simulation. In DISTIL product compositions are specified, while number of plates and feed plate location are calculated. Both programs, HYSYS and DISTIL, are capable of dealing with the presence of two liquid phases.

3. RESULTS AND DISCUSSIONS

Seven ternary systems have been studied. The systems are presented in Table 1. Four of the systems share a common residue curve map: two minimum boiling binary homogeneous azeotropes, one minimum boiling binary heterogeneous azeotrope and a minimum boiling ternary heterogeneous azeotrope. The others three systems hold small differences with that common residue curve map: one system has a minimum boiling ternary homogeneous azeotrope (ethylacetate-ethanol-water); a second system has two minimum boiling binary heterogeneous azeotropes (cyclohexane-isobutanol-water); and in the last system a minimum boiling binary homogeneous azeotrope is missing (acetone-chloroform-water).

3.1 Estimation of Parameters

Tables 1 and 2 report the results of data reduction following the estimation procedure recommended and using UNIQUAC as the non ideal solution model. UNIQUAC parameters and vapor pressure parameters are listed in Appendix A. Table 1 presents a comparison between experimental and predicted azeotropic points. Table 2 shows deviation between measured and predicted vapor-liquid equilibrium and liquid-liquid equilibrium.

Azeotropic points are predicted quite well, most of the calculated points are inside the range of experimental values. When the calculated azeotropic are outside the range of the experiments, differences are small. Figure 1 displays the difference between experimental and calculated azeotropic points for 2-isopropoxypropane-2-propanol-water. In this case the calculated 2-propanol-2-isopropoxypropane azeotrope is not in the range of the data. The same situation happens with the heterogeneous azeotrope between 2-isopropoxypropane-water. On the contrary for the minimum boiling binary homogeneous azeotrope 2-propanol-water, and the minimum boiling ternary heterogeneous azeotrope the agreement is excellent. To compare the performance of UNIQUAC with other model in Appendix B, Table B1 presents azeotropic point calculation with UNIFAC.

Vapor-liquid equilibrium is predicted with reasonable precision as presented in Table 2 and displayed in Figure 1 for the 2-propanol-2-isopropoxypropane-water. Liquid-liquid equilibrium is well predicted for most of the systems as it is shown in Table 2 for the boiling temperature at atmospheric pressure. The system cyclohexane-2-propanol-water is the worst case calculated, phase envelope is larger and calculated tie lines have opposite directions than the experimental ones. The graphs in Table 2 show in a qualitative way that liquid-liquid description is good. The graphs are drawn to see area and tie-lines deviations. Differences between prediction and experiment at a lower temperature, 25 °C e.g., a feasible decanter temperature, are less extreme. The difference between the behavior of the model when ethanol is added to cyclohexane - water (good agreement) against when

Table 1. Experimental and calculated azeotropic points.

System	Components	Experimental azeotropes		Calculated azeotropes	
		Range T (°C) (type ^a)	Range y _i	T (°C) (type ^a)	y _i
Ethylacetate (1) Ethanol (2) Water (3)	(1) - (2)	70.90-72.14 (hom.)	0.5190-0.5750 (y ₁)	72.18 (hom.)	0.5337
	(1) - (3)	70.38-72.25 (het.)	0.6849-0.7150 (y ₁)	71.33 (het.)	0.6776
	(2) - (3)	78.00-78.20 (hom.)	0.8900-0.9050 (y ₂)	78.05 (hom.)	0.9074
	(1) - (2) - (3)	70.20-70.35 (hom.)	0.5950-0.6005 (y ₁) 0.1150-0.1242 (y ₂)	70.73 (het.)	0.5639 0.1350
Acetone (1) Chloroform (2) Water (3)	(1) - (2)	64.09-64.70 (hom.)	0.3300-0.3670 (y ₁)	63.81 (hom.)	0.3869
	(1) - (3)	-	-	-	-
	(2) - (3)	56.10-56.20 (het.)	0.8397-0.8548 (y ₂)	55.84 (het.)	0.8392
	(1) - (2) - (3)	60.40 (het.)	0.4643-0.4841 (y ₁) 0.3297-0.3533 (y ₂)	59.85 (hom.)	0.5764 0.2505
2-Isopropoxy propane (1) 2-Propanol (2) Water (3)	(1) - (2)	66.10-66.20 (hom.)	0.7820-0.8000 (y ₁)	66.74 (hom.)	0.7658
	(1) - (3)	62.20-63.00 (het.)	0.7800-0.7900 (y ₁)	62.82 (het.)	0.7766
	(2) - (3)	79.70-80.72 (hom.)	0.6645-0.7041 (y ₂)	80.09 (hom.)	0.6786
	(1) - (2) - (3)	61.60-61.90 (het.)	0.6926-0.7310 (y ₁) 0.0977-0.0610 (y ₂)	62.63 (het.)	0.7139 0.0680
Cyclohexane (1) 2-Propanol (2) Water (3)	(1) - (2)	68.80-69.60 (hom.)	0.5920-0.6300 (y ₁)	69.00 (hom.)	0.6052
	(1) - (3)	69.40 (het.)	0.7010 (y ₁)	69.33 (het.)	0.7010
	(2) - (3)	79.70-80.72 (hom.)	0.6645-0.7041 (y ₂)	80.09 (hom.)	0.6786
	(1) - (2) - (3)	64.30 (het.)	0.5484-0.5660 (y ₁) 0.1920-0.2220 (y ₂)	63.74 (het.)	0.5356 0.2467
Ethanol (1) Isooctane (2) Water (3)	(1) - (2)	< 72.40 (hom.)	<0.7366 (y ₁)	71.43 (het.)	0.6500
	(1) - (3)	78.00-78.20 (hom.)	0.8900-0.9050 (y ₁)	78.05 (hom.)	0.9074
	(2) - (3)	78.80 (het.)	0.5580 (y ₂)	79.92 (het.)	0.5338
	(1) - (2) - (3)	68.15-68.17 (het.)	0.4180 (y ₁) 0.3540 (y ₂)	69.51 (het.)	0.4640 0.3412
Ethanol (1) Cyclohexane (2) Water (3)	(1) - (2)	64.70-64.85 (hom.)	0.4300-0.4600 (y ₁)	65.41 (hom.)	0.4591
	(1) - (3)	78.00-78.20 (hom.)	0.8900-0.9050 (y ₁)	78.05 (hom.)	0.9074
	(2) - (3)	69.40 (het.)	0.7010 (y ₂)	69.33 (het.)	0.7010
	(1) - (2) - (3)	62.10-62.60 (het.)	0.2222-0.3121 (y ₁) 0.5220-0.5638 (y ₂)	62.85 (het.)	0.3121 0.5219
Cyclohexane (1) Isobutanol (2) Water (3)	(1) - (2)	78.10-79.80 (hom.)	0.8440-0.8675 (y ₁)	78.67 (hom.)	0.8538
	(1) - (3)	69.40 (het.)	0.7010 (y ₁)	69.33 (het.)	0.7010
	(2) - (3)	89.50-90.20 (het.)	0.3285-0.3350 (y ₂)	89.50 (het.)	0.3350
	(1) - (2) - (3)	69.50 (het.)	-	68.67 (het.)	0.6392 (y ₁) 0.0730 (y ₂)

a) hom.= homogeneous azeotrope; het.= heterogeneous azeotrope

Table 2. Deviation between measured and predicted phase equilibrium^{a)}.

System	Deviation in ternary LV equilibrium		Deviation in ternary LL equilibrium
	ΔT	ΔT_{\max}	
Ethylacetate (1) Ethanol (2) Water (3)	0.1528 (Soares et al., 1982) 0.2808 (Griswold et al., 1949)	-0.3593 1.295	<p>Ethanol (Beech and Glasstone, 1938)</p> <p>Water Ethylacetate</p>
Acetone (1) Chloroform (2) Water (3)	1.223 (Reinders and De Minjer, 1947)	-4.303	<p>Acetone (Reinders and Minjer, 1947)</p> <p>Water Chloroform</p>
2-Isopropoxypropane (1) 2-Propanol (2) Water (3)	0.2295 (Verhoeve, 1970)	-0.7570	<p>2-Propanol (Verhoeve, 1970)</p> <p>Water 2 Isopropoxypropane</p>
Cyclohexane (1) 2-Propanol (2) Water (3)	0.5418 (Verhoeve, 1968)	-1.045	<p>2-Propanol (Verhoeve, 1968)</p> <p>Water Cyclohexane</p>
Ethanol (1) Isooctane (2) Water (3)	0.2324 (Ruiz et al., 2002)	0.9812	<p>Ethanol (Ruiz et al., 2002)</p> <p>Water Isooctane</p>
Ethanol (1) Cyclohexane (2) Water (3)	5.781 (Cui et al., 2004) 0.4470 (Antosik et al., 2004) 0.1453 (Connemann et al., 1990)	12.84 -2.781 0.3911	<p>Ethanol (Connemann et al., 1990)</p> <p>Water Cyclohexane</p>
Cyclohexane (1) Isobutanol (2) Water (3)	6.829 (Cui et al., 2004)	13.16	<p>Isobutanol</p> <p>Water Cyclohexane</p>

a) ΔT = Average $[(\text{abs}(T^{\text{cal}} - T^{\text{exp}}) / T^{\text{exp}}) * 100]$; ΔT_{\max} = Maximum $[(\text{abs}(T^{\text{cal}} - T^{\text{exp}}) / T^{\text{exp}}) * 100]$; - - - Experimental; — Predicted. In parenthesis data reference.

Table 3. Design of azeotropic column.

System	Total number of plates	Feed plate	Reflux ratio	Multiplicity
Ethylacetate (1) Ethanol (2) Water (3)	a)	a)	a)	a)
Acetone (1) Chloroform (2) Water (3)	29	12	22.30	b)
2-Isopropoxypropane (1) 2-Propanol (2) Water (3)	20	2	6.85	yes
Cyclohexane (1) 2-Propanol (2) Water (3)	11	2	1.21	yes
Ethanol (1) Isooctane (2) Water (3)	28	2	2.16	yes
Ethanol (1) Cyclohexane (2) Water (3)	24	2	2.43	yes
Cyclohexane (1) Isobutanol (2) Water (3)	27	4	0.19	yes

a) Ternary azeotrope too close to phase envelope does not allow to cross distillation regions.

b) Distillation column has not decanter.

2-propanol is added (bad agreement) is well documented in the literature (Plackov and Stern, 1992). Semi empirical models (UNIQUAC, NRTL) show good results on systems of cyclohexane-water with methanol, ethanol and butanols as the alcohol component. It seems that the domination of one group, OH or alkyl, in the alcohol components leads to “more predictable” behavior that when two groups have effects of about equal importance, as in the case of propanols, then complicated behavior results. Figure 2 displays comparison between experimental and calculated vapor-liquid-liquid equilibrium and between experimental and calculated residue curve lines, as shown predictions are fair. It is possible to see that calculated residue curves follow very closely the experimental ones. From Figure 2 it is possible to see that calculated ternary azeotropic point is homogeneous. On the contrary, experimental ternary azeotropic point is heterogeneous, as it is written down in Table 1. This situation, homogeneous or heterogeneous azeotrope differences between calculated and experimental points, also happen with the ethylacetate-ethanol-water system. In all the other cases there are azeotropic point agreement between experiment and calculation.

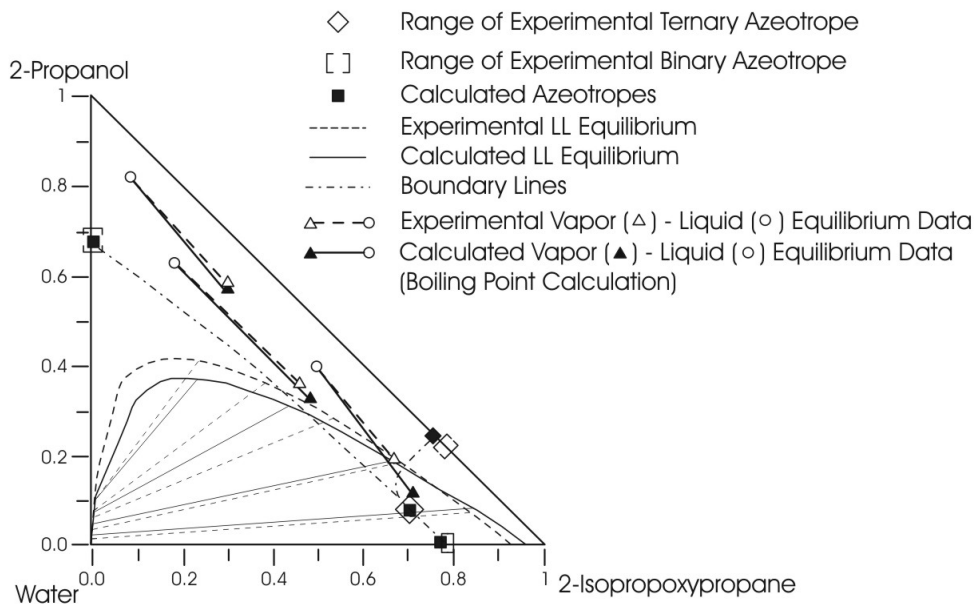


Figure 1. Phase diagram at 1 atm calculated with UNIQUAC.

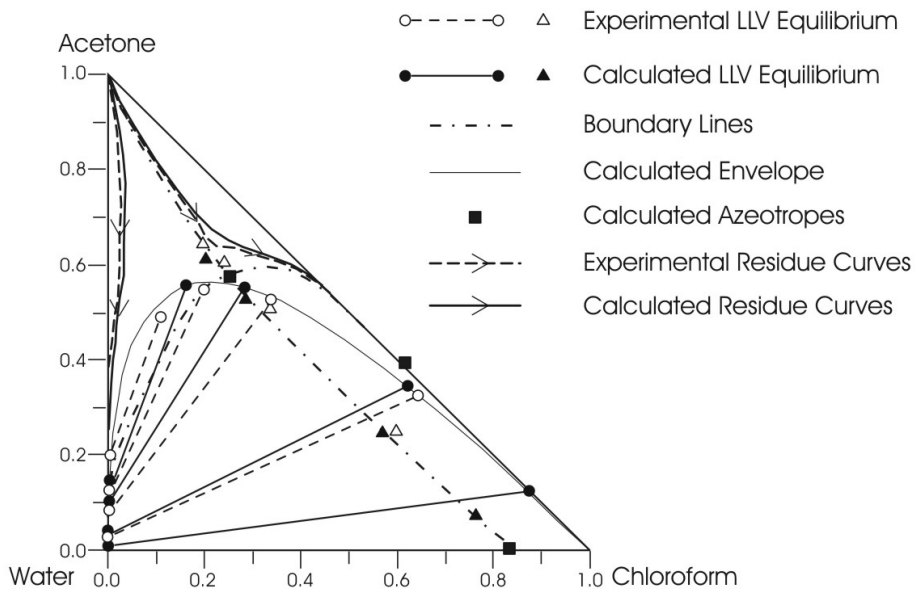


Figure 2. Phase diagram and residue curve map at 1 atm calculated with UNIQUAC.

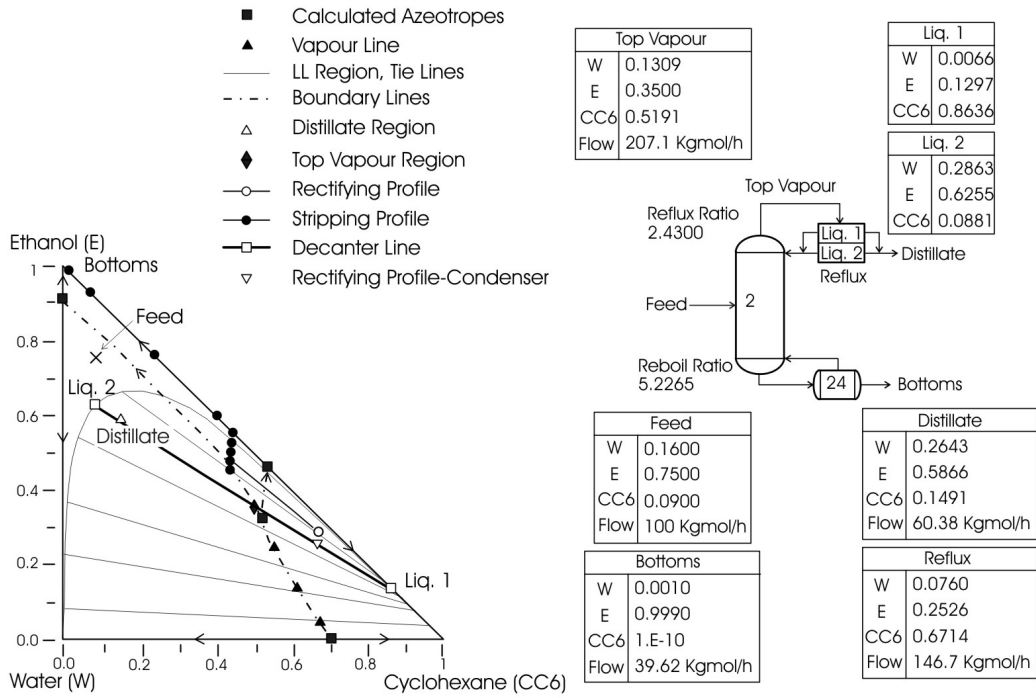


Figure 3. Column design for ethanol dehydration at 1 atm.

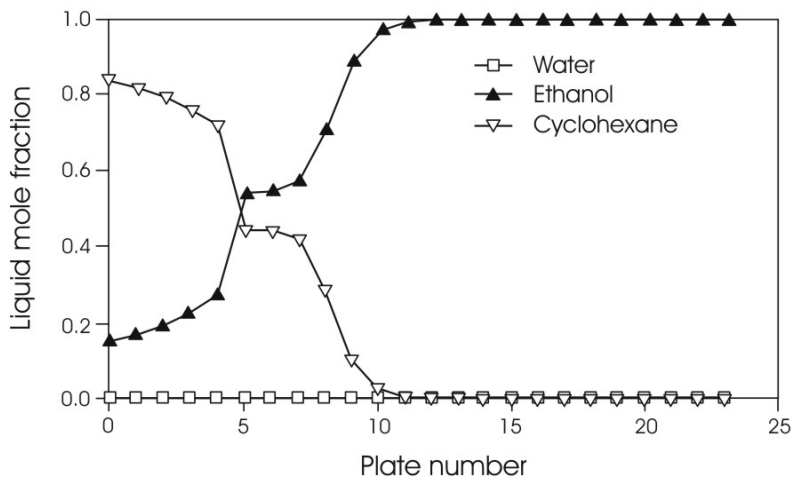


Figure 4. Liquid composition profile for heterogeneous distillation column.

3.2 Distillation Column Design

To see if the binary parameters were correct we designed the heterogeneous distillation columns of the sequences of distillation columns needed to separate the ternary mixture. One of the columns of the sequence has a decanter, it is the so called heterogeneous distillation column. For each ternary system a heterogeneous azeotropic distillation column was designed following the boundary-value design method algorithm as described in 2.2. Table 3 presents the main parameters of the heterogeneous azeotropic distillation column for each system of Table 1. Also, Table 3 displays if the topological structure of ternary diagram leads to MSS behavior (Hilmen et al., 2002). Figure 3 presents a feasible design for dehydration of ethanol. For the system ethanol - cyclohexane - water of Figure 3 the following parameters were specified: top vapor mole fraction of cyclohexane and water, and bottoms mole fraction of ethanol. Figure 3 presents a summary of the column inputs and calculated outputs. The figure displays rectifying profile, stripping profile, decanter tie line, mass balance, tray numbers and feed tray.

Although the design column is feasible it may not be optimal. Optimizing the column from a good conceptual design is easier than trying to simulate the column directly. Optimization of the column will take into account the effect of the reflux ratio and/or the effect of specification as well a more specific description of the phase equilibria in the column and in the decanter. A rigorous optimization of the columns was done with HYSYS. We did not explore the existence of MSS that the topological structure of the ternary mixture indicates. Figure 4 shows composition profiles for the heterogeneous distillation column of Figure 3. It is possible to see that the HYSYS profile is in agreement with the DISTIL profile (see stripping profile of Figure 3). Besides, the five top stages of HYSYS also display liquid-liquid equilibrium.

4. CONCLUSIONS

In this work we have modeled the thermodynamic behavior of seven ternary systems by picking up an activity coefficient model and by estimating its binary parameters. We show how well the model describes phase equilibrium experimental information. Furthermore, we present distillation column designs to show that with an adequate parameters election the activity coefficient model preserves all aspect that are essential for azeotropic distillation conceptual design.

5. APPENDIX A. Parameters for Phase Equilibrium Calculations.

Table A.1. Physical constants.

Component	Vapor pressure coefficient ^{a)}					Volume and area parameters	
	A	B	C	D	E	R	Q
Ethylacetate	88.3760	-7147.86	0	-10.9917	8.54613e-6	3.4786	3.1159
Ethanol	86.486	-7931.1	0	-10.2498	6.38949e-6	2.1054	1.9720
Water	65.9278	-7227.53	0	-7.17695	4.0313e-6	0.92	1.3997
Acetone	71.3031	-5952.0	0	-8.53128	7.82393e-6	2.5734	2.3359
Chloroform	73.7058	-6055.6	0	-8.9189	7.74407e-6	2.8698	2.41
2-Isopropoxypropane	86.6891	-6651.66	0	-10.9317	1.00417e-5	4.742	4.0879
2-Propanol	83.637	-8249.01	0	-9.54518	2.00272e-6	2.779	2.5078
Cyclohexane	70.9775	-6187.1	0	-8.46523	6.452e-6	4.0464	3.24
Isooctane	77.8121	-6805.06	0	-9.43901	6.75475e-6	5.8463	5.0079
Isobutanol	14.8561	-2874.72	-100.296	0	0	3.4535	3.048

a) $\ln P_{\text{vap}} = A + B/(C+T) + D \cdot \ln T + E \cdot T^F$, F=2 for all components, T(K), P_{vap} (kPa)

Table A.2. Binary parameters of the UNIQUAC model ^{a)}.

	a_{12}	a_{21}	b_{12}	b_{21}
Ethylacetate(1)/Ethanol(2)	363.9664	-62.7027	0	0
Ethylacetate(1)/Water(2)	2367.9928	-1008.1255	-5.269	3.932
Ethanol(1)/Water(2)	50.88	232.0099	0	0
Acetone(1)/Chloroform(2)	1566.005	-781.5877	0	0
Acetone(1)/Water(2)	601.6118	-52.3022	0	0
Chloroform(1)/Water(2)	32865.0	-1039.5792	0	4.0546
2-Isopropoxypropane(1)/2-Propanol(2)	413.7904	-89.3915	0	0
2-Isopropoxypropane(1)/Water(2)	1538.7338	70.2446	-1.145	0.3434
2-Propanol(1)/Water(2)	300.1896	109.5493	0	0
Cyclohexane(1)/2-Propanol(2)	807.0932	-171.298	0	0
Cyclohexane(1)/Water(2)	721.6136	-211.9998	5.8959	4.3143
Ethanol(1)/Isooctane(2)	-152.8457	1066.51	0	0
Isooctane(1)/Water(2)	7731.1379	-191.2775	-17.3278	3.9647
Ethanol(1)/Cyclohexane(2)	-112.4378	948.1325	0	0
Cyclohexane(1)/Isobutanol(2)	661.1688	-186.2545	0	0
Isobutanol(1)/Water(2)	303.7919	328.2438	0	0

a) $\tau_{ij} = \exp [(a_{ij} + b_{ij} T) / RT]$; $[a_{ij}] = \text{cal} / \text{gmol}$; $[b_{ij}] = \text{cal} / \text{gmol K}$.

6. APPENDIX B. Azeotropic point calculation with UNIFAC

Prediction of azeotropic points is as good as prediction with UNIQUAC (Table 1).

Table B1. Experimental and UNIFAC calculated azeotropic points.

System	Components	Experimental azeotropes		Calculated azeotropes	
		Range T (°C) (type ^a)	Range y _i	T (°C) (type ^a)	y _i
Ethylacetate (1) Ethanol (2) Water (3)	(1) - (2)	70.90-72.14 (hom.)	0.5190-0.5750 (y ₁)	71.05 (hom.)	0.5348
	(1) - (3)	70.38-72.25 (het.)	0.6849-0.7150 (y ₁)	70.78 (het.)	0.6865
	(2) - (3)	78.00-78.20 (hom.)	0.8900-0.9050 (y ₂)	77.93 (hom.)	0.8986
	(1) - (2) - (3)	70.20-70.35 (hom.)	0.5950-0.6005 (y ₁) 0.1150-0.1242 (y ₂)	-	-
Acetone (1) Chloroform (2) Water (3)	(1) - (2)	64.09-64.70 (hom.)	0.3300-0.3670 (y ₁)	64.37 (hom.)	0.3736
	(1) - (3)	-	-	-	-
	(2) - (3)	56.10-56.20 (het.)	0.8397-0.8548 (y ₂)	55.98 (het.)	0.8373
2-Isopropoxy propane (1) 2-Propanol (2) Water (3)	(1) - (2)	66.10-66.20 (hom.)	0.7820-0.8000 (y ₁)	64.61 (hom.)	0.7463
	(1) - (3)	62.20-63.00 (het.)	0.7800-0.7900 (y ₁)	63.25 (het.)	0.7718
	(2) - (3)	79.70-80.72 (hom.)	0.6645-0.7041 (y ₂)	80.20 (hom.)	0.6896
Cyclohexane (1) 2-Propanol (2) Water (3)	(1) - (2)	61.60-61.90 (het.)	0.6926-0.7310 (y ₁)	62.79 (het.)	0.7035
	(1) - (2) - (3)	61.60-61.90 (het.)	0.0977-0.0610 (y ₂)		0.0754
	(1) - (2)	68.80-69.60 (hom.)	0.5920-0.6300 (y ₁)	68.63 (hom.)	0.6209
Ethanol (1) Isooctane (2) Water (3)	(1) - (3)	69.40 (het.)	0.7010 (y ₁)	69.34 (het.)	0.7009
	(2) - (3)	79.70-80.72 (hom.)	0.6645-0.7041 (y ₂)	80.20 (hom.)	0.6896
	(1) - (2) - (3)	64.30 (het.)	0.5484-0.5660 (y ₁) 0.1920-0.2220 (y ₂)	63.74 (het.)	0.5573 0.2173
Ethanol (1) Isooctane (2) Water (3)	(1) - (2)	< 72.40 (hom.)	<0.7366 (y ₁)	71.11 (hom.)	0.6407
	(1) - (3)	78.00-78.20 (hom.)	0.8900-0.9050 (y ₁)	77.93 (hom.)	0.8986
	(2) - (3)	78.80 (het.)	0.5580 (y ₂)	79.75 (het.)	0.5370
	(1) - (2) - (3)	68.15-68.17 (het.)	0.4180 (y ₁) 0.3540 (y ₂)	69.32 (het.)	0.4683 0.3523
Ethanol (1) Cyclohexane (2) Water (3)	(1) - (2)	64.70-64.85 (hom.)	0.4300-0.4600 (y ₁)	64.60 (het.)	0.4391
	(1) - (3)	78.00-78.20 (hom.)	0.8900-0.9050 (y ₁)	77.93 (hom.)	0.8986
	(2) - (3)	69.40 (het.)	0.7010 (y ₂)	69.35 (het.)	0.7009
	(1) - (2) - (3)	62.10-62.60 (het.)	0.2222-0.3121 (y ₁) 0.5220-0.5638 (y ₂)	62.66 (het.)	0.3060 0.5393
Cyclohexane (1) Isobutanol (2) Water (3)	(1) - (2)	78.10-79.80 (hom.)	0.8440-0.8675 (y ₁)	77.87 (hom.)	0.8537
	(1) - (3)	69.40 (het.)	0.7010 (y ₁)	69.35 (het.)	0.7009
	(2) - (3)	89.50-90.20 (het.)	0.3285-0.3350 (y ₂)	90.28 (het.)	0.3151
	(1) - (2) - (3)	69.50 (het.)	-	68.22 (het.)	0.6402 (y ₁) 0.0782 (y ₂)

a) hom.= homogeneous azeotrope; het.= heterogeneous azeotrope

7. NOMENCLATURE

f	= objective function
LL	= liquid-liquid equilibrium
LLV	= liquid-liquid-vapor equilibrium
LV	= liquid-vapor equilibrium
S	= separation factor (x_L/x_H)
T	= temperature [°C]
x	= liquid mole fraction
y	= vapor mole fraction

Subscripts

H	= heavy phase
i	= component
L	= light phase
max	= maximum

Superscripts

cal	= calculated
exp	= experimental

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