Isobaric Vapor-Liquid Equilibrium Data for the Isopropanol-Water System

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Abstract

This work presents experimental isobaric vapor-liquid equilibrium data for the isopropanol-water system collected at 1.5 bar, 2 bar, 2.5 bar and 3 bar at Process Thermodynamics laboratory (PT lab) of Politecnico di Milano. The system is strongly non-ideal, with the presence of a minimum boiling azeotrope which has been found at all the analyzed pressures. Data at the considered pressures for the system are not available in the literature, though being of interest for the thermodynamic modeling based on the use of models for the description of strongly non-ideal mixtures which employ thermodynamic parameters regressed on the basis of experimental points, as the NRTL method. The reliability of the operation of the experimental unit and of the measurements has been checked by determining the vapor pressure curve of the single components and by comparing it with the ones calculated using the Antoine equation, for which parameters are consolidated for these components, and by comparing the collected data for the binary system with those available in the literature at atmospheric pressure. In addition, the test on thermodynamic consistency has been performed for all the collected data.

Keywords

Isopropanol-water, VLE data, isobaric curve, PT lab.

1. Introduction

The increasing greenhouse gas emissions and the resulting global climate change, joined with a growing world population, are key challenges that are leading to an increased interest in processes able to produce fuels and chemicals from alternative, renewable resources. In this respect, the production of bioethanol can be mentioned, which can be used as raw material for ethylene production by its dehydration (Rossetti et al., 2017) or hydrogen production by steam reforming (Rossetti et al., 2015). Also butanol is an important commodity chemical and an attractive biofuel, which can be produced through the Acetone-Butanol-Ethanol (ABE) fermentation by clostridia that is characterized by high process costs, due to the large volumes required and the downstream product recovery from dilute broths, usually performed by distillation (Lodi et al., 2018). These processes involve mixtures containing alcohols and water, which make the downstream processing a potentially difficult separation challenge due to the formation of azeotropes. Another system of this type is the one involving isopropanol and water.

Nowadays, isopropanol (2-propanol, also known as Iso Propyl Alcohol – IPA), is a solvent and an intermediate for chemicals production. For example, it is used for the production of mono-isopropylamine and isopropyl acetate both as a solvent and as an intermediate (Rodriguez and Kroon, 2015). IPA is commonly used as a solvent also in pharmaceutical and electronic industries. It is proposed as a substitute for hexane in vegetable oil extraction (Capellini et al., 2021) because of the advantages regarding safety and it can be partially recovered from the extract only by cooling due to its partial miscibility with oil.

Isopropanol can be found in a mixture with water in several processes in which it is involved and in its production by indirect hydrogenation or by fermentation of cellulosic materials. To obtain pure IPA, the raw product stream needs to be dehydrated. Since the mixture IPA + water forms an azeotrope (at 1 atm at about 87.5 wt.%), the system is strongly non-ideal and the separation into almost pure components is complex and energy-intensive. The isopropanol-water separation started to raise interest early in the last century and has been then studied in recent years to develop efficient methods to obtain pure isopropanol. Several processes have been suggested, as the azeotropic distillation (Pienaar et al., 2013), the pressure swing distillation (Knapp and Doherty, 1992), a single unit of pervaporation membrane as well as multi-stage arrangements for dehydration of isopropanol under adiabatic and ideal isothermal conditions (Vatankhah et al., 2021), the liquid-liquid extraction (Shekaari et al., 2010), the reactive distillation (Wang and Wong, 2006), the adsorption (Mujiburohman et al., 2006), the adoption of ionic liquids for breaking the azeotrope (Boli et al., 2018) and the extractive distillation through deep eutectic solvents, also known as low transition temperature mixtures (LTTMs) (Haider et al., 2021).

The properties of the isopropanol-water mixture were studied in the XIX century as reported by Young in 1902 (Young, 1902), which determined some boiling points at atmospheric pressure. In 1921 Lebo (Lebo, 1921) investigated the specific gravity and proposed data of vapor-liquid equilibrium for the distillation, reporting that *"the boiling point and composition of the vapor from any liquid mixture depend upon the composition of the liquid"*, therefore confirming the importance of vapor-liquid equilibrium data.

1.1. Isobaric data available in the literature

To the authors' knowledge, the works that propose vapor-liquid equilibrium (VLE) data in the last century mainly investigate the atmospheric conditions, with only a few works focusing on pressures different from 1 atm. In 1952 Wilson and Simons (Wilson and Simons, 1952) investigated the azeotropic mixture at the pressure of 4.12 bar. Barr-David and Dodge in 1959 (Barr-David and Dodge, 1959) published a study in which the pressure was investigated in the range of about 5.2-123.5 bar, though considering only isothermal vapor-liquid equilibrium curves. Table 1 and Table 2 reports the isobaric data found in the literature for the considered system. No isobaric VLE data in the pressure range from 1.5 bar to less than 4 bar, which are the object of the study presented in this work, were found.

Table 1. Experimental vapor-liquid equilibrium data for the isopropanol-water system at atmospheric pressure.

Source	**Number of experimental points**	**T_{min} [K]**	**T_{max} [K]**
(Marzal et al., 1996)	27	352.65	372.78
(Sevgili and Senol, 2006)	17	353.16	373.15
(Wilson and Simons, 1952)	26	353.11	373.00
(Brunjes and Bogart, 1943)	27	353.03	371.87
(Khalfaoui et al., 1997)	12	352.25	373.13
(Udovenko and Mazanko, 1967)	18	353.53	369.66
(Lin and Tu, 2014)	17	353.22	373.15
(Lebo, 1921)	42	353.65	373.15
(Dobroserdov, 1959)	14	353.31	366.32

Table 2. Isobaric experimental vapor-liquid equilibrium data for the isopropanol-water system at pressures different from 1 atm.

Source	Pressure [bar]	Number of experimental points	T_{min} [K]	T_{max} [K]
(Marzal et al., 1996)	0.3	25	325.33	342.33
(Marzal et al., 1996)	0.6	26	340.52	359.14
(Wilson and Simons, 1952)	0.1266	24	308.78	323.71
(Wilson and Simons, 1952)	0.3866	24	322.23	338.29
(Wilson and Simons, 1952)	0.5066	25	336.9	354.68
(Wilson and Simons, 1952)	4.11566	16	393.4	477.61

1.2. Aim of the work

This work aims at collecting isobaric vapor-liquid equilibrium data for the isopropanol-water system at pressures intermediate between 1 atm and 4 bar, for which no data can be found in the literature, in particular at 1.5 bar, 2 bar, 2.5 bar and 3 bar. These data are fundamental for choosing the correct thermodynamic model to be used for the simulation of the processes where isopropanol and water are present, both in chemical and in energy processes. Indeed, separation operations play a central role in the practice of chemical engineering and engineering design of processes requires equipment that takes into account the thermodynamic and hydrodynamic characteristics of the system to be treated.

2. Experimental set-up

2.1. Chemicals

Demineralized water (ISO 3696 Q3, ASTM D 1193 TYPE 4) was used and isopropanol (CAS 67-63-0) was supplied by Sigma Aldrich, with a purity of at least 99.8%, molecular weight of 60.10 g/mol and specific gravity < 0.7840. Nitrogen (>99.99%, mole) coming from a tank storing N_2 in the liquid phase is used for pressurizing the VLLE unit (Fisher Labodest VLLE 602) up to the desired pressure and as a carrier for the gas-chromatograph.

2.2. Apparatus

The Process Thermodynamics laboratory (PT lab) of Politecnico di Milano is located at Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta” and has been created within the “Ingegneria Chimica – Energia (ICE)” collaboration with the aim of collecting experimental data of phase equilibria of mixtures of interest for which no points can be found in the literature or in other existing databases.

The laboratory, which has been recently improved with a thermostatic bath for the study of Liquid-Liquid Equilibria (LLE) at different temperatures, is composed of a unit for Vapor-Liquid Equilibria Fisher Labodest VLLE 602 (Figure 1) and a gas-chromatograph Agilent 7820A, with a TCD detector.

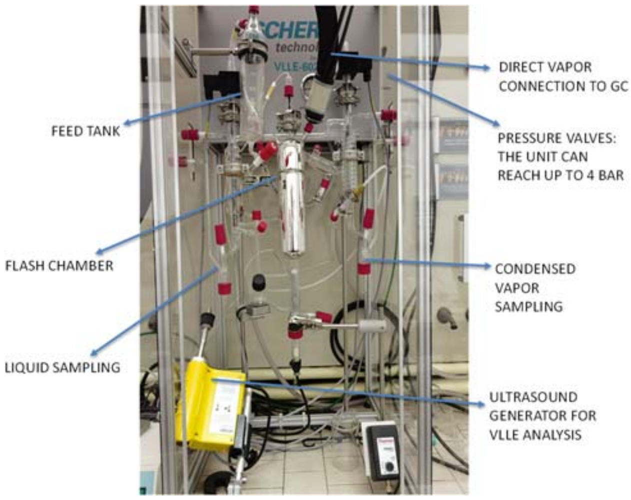


Figure 1. Unit for the study of VLE at the PT lab.

The VLLE unit is an all-glass recirculating still that ensures that both liquid and vapor phases are in intimate contact during boiling and in contact with the temperature probe. The system can be used at atmospheric pressure, vacuum and overpressure conditions up to 4 bar. The equilibrium temperature is measured with a digital temperature logging module and a Pt 100 resistance thermometer. The accuracy is ±0.1°C, as indicated by the supplier. A precision pressure transmitter is used to measure and control the pressure in the equilibrium cell, with a pressure accuracy of ±1 mbar as indicated by the supplier. This apparatus allows reaching pressures higher than atmospheric pressure (up to 4 bar) by injection of high purity nitrogen, under pressure control of two manual valves and under automatic control.

3. Experimental procedure and validation

3.1. Experimental procedure

The experimental procedure employed for the work presented in this paper is basically divided into four steps:

1. preparation and feeding;

2. setting the operating conditions and reaching equilibrium;
3. sampling;
4. emptying the unit.

Preparation and feeding. A check that the ventilation valves, the PTFE valves for pressure balance in the side branches and the sampling valves are open is made, then the mixture to be fed is prepared under the hood in the beaker (100 ml) and it is fed to the feed tank of the VLLE unit. The heater is then filled in, so that the electric heating element is completely submerged.

Setting of operating conditions and reaching equilibrium. The desired pressure value is set, the ventilation valves are closed and the opening of the lateral throttle valves (the one on the right to increase and the one on the left to lower the pressure) is set until the set point pressure is reached. The magnetic stirrer is activated and the thermal power to be supplied to heat up the mixture is provided, then time is waited for the mixture to boil. When the temperature of the liquid and of the vapor phases are very similar and remain almost constant for 5-10 minutes (depending on the stability of the system) and the formation of 1-2 drops of condensate per second is observed, equilibrium is considered to be reached.

Sampling. The gas chromatograph is prepared and the analysis of the composition of the liquid phase and of the vapor phase is performed. The VLLE unit at PT lab is in-line with the gas-chromatograph, so that the vapor phase can be analyzed directly in line (in case the carrier is not present as component of the mixture to be analyzed) or, as done in this work, in its condensate phase. The gas and the liquid analyses are repeated at least three times making sure that the temperature at which the equilibrium is evaluated is always the same, to guarantee the repeatability of the experiment.

Emptying the unit. At the end of the experimental procedure the unit is emptied.

3.2. Validation of the experimental procedure

To validate the unit at PT lab, data of water vapor pressures and VLE data for the IPA-water binary mixture at a pressure of about 1 atm have been collected and compared with the results obtained with the Antoine equation (Dortmund Data Bank, 2021) for vapor pressure estimation (Figure 2) and with the available experimental data at 1 atm for the binary mixture VLE (Figure 3). Because of the high number of sources available in the literature at 1 atm, in Figure 3b) a selection has been made to make the plot understandable to the reader.

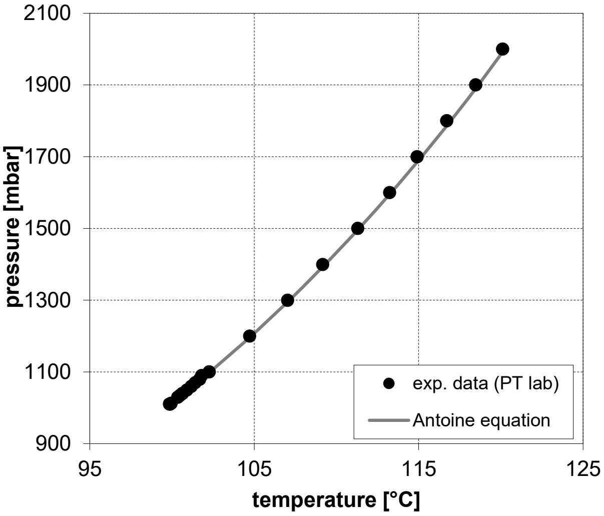
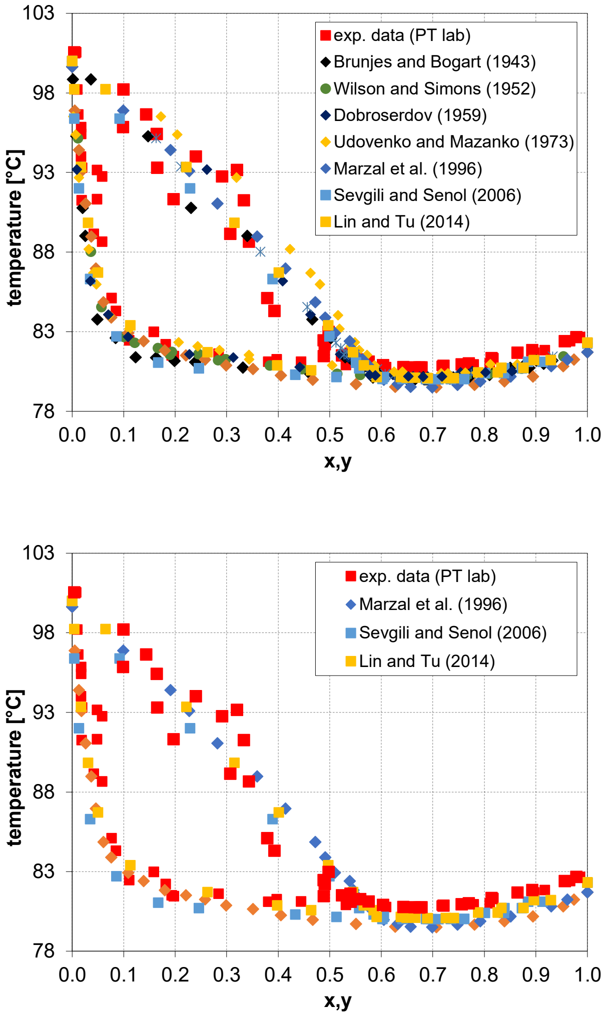


Figure 2. Vapor pressures of water obtained experimentally at PT lab and with the Antoine equation.



a)

b)

Figure 3. Experimental VLE data collected at PT lab and from literature sources for the system isopropanol-water at about 1 atm considering a) most of all the literature sources and b) a selection of the most recent available literature sources.

Both for the water vapor pressure and for the VLE of the binary mixture at about 1 atm a good agreement is obtained, confirming that the experimental procedure and the collection of points at different temperatures and compositions can be considered suitable.

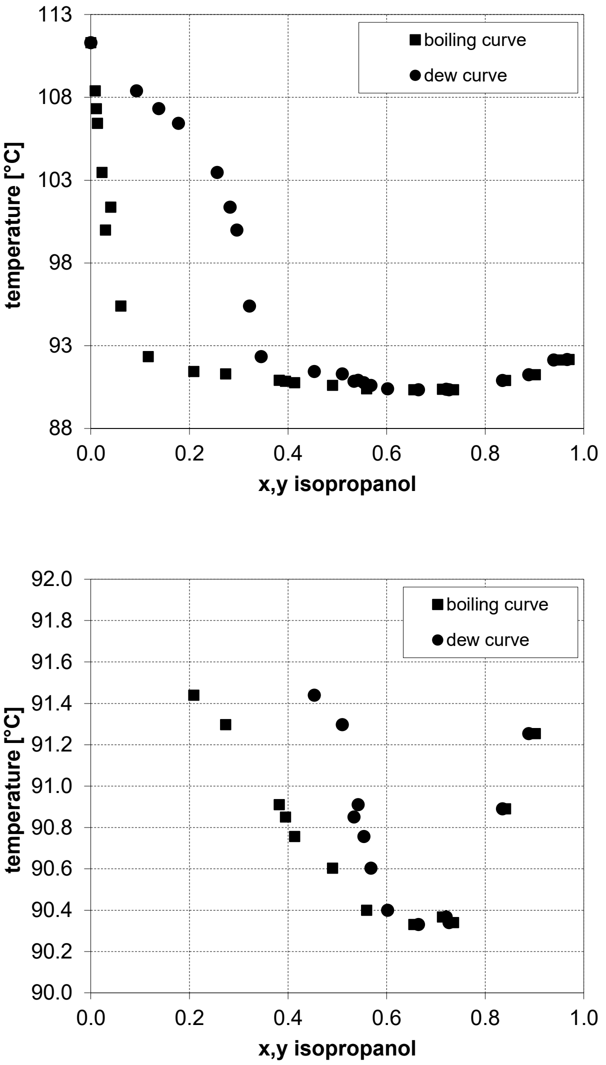
In addition, the test on the thermodynamic consistency based on the methodology proposed by Redlich and Kister (Wisniak et al., 2017) has been performed for all the obtained experimental results.

4. Results

Results for the different isobaric vapor-liquid equilibrium curves are reported in Figure 4 at 1.5 bar, in Figure 5 at 2 bar, in Figure 6 at 2.5 bar and in Figure 7 at 3 bar. The resulting experimental points are also reported in Table 3 to Table 6 in the Appendix, together with the estimated uncertainties for temperature, pressure and composition of the vapor and of the liquid phases.

As for the uncertainty for the composition of phases a coverage factor equal to 2 has been considered, which gives an appropriate 95% level of confidence for the interval.

The method adopted in this work for evaluating and expressing the uncertainty of measurement results follows the policy instituted at NIST (National Institute of Standards and Technology) in 1992. This policy is based on the approach recommended by the CIPM (International Committee for Weights and Measures) in 1981 (Taylor and Kuyatt, 1994).



a)

b)

Figure 4. Experimental VLE data collected at PT lab for the isopropanol-water system at 1.5 bar a) for a mole fraction of isopropanol ranging from 0 and 1 and b) detail for the composition range close to the azeotropic point.

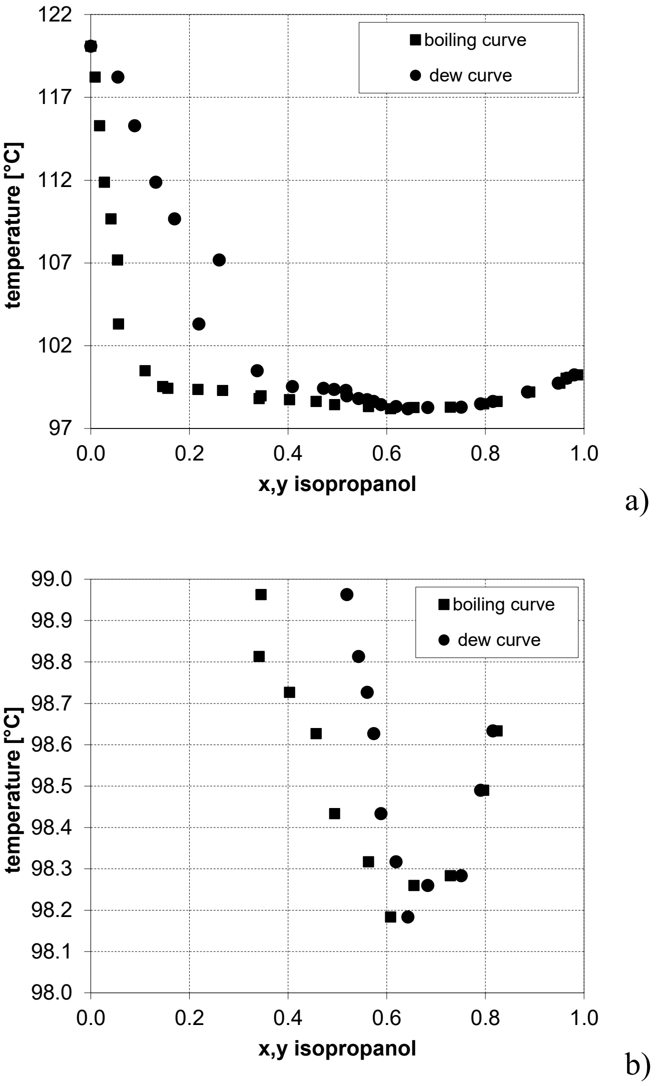


Figure 5. Experimental VLE data collected at PT lab for the isopropanol-water system at 2 bar a) for a mole fraction of isopropanol ranging from 0 and 1 and b) detail for the composition range close to the azeotropic point.

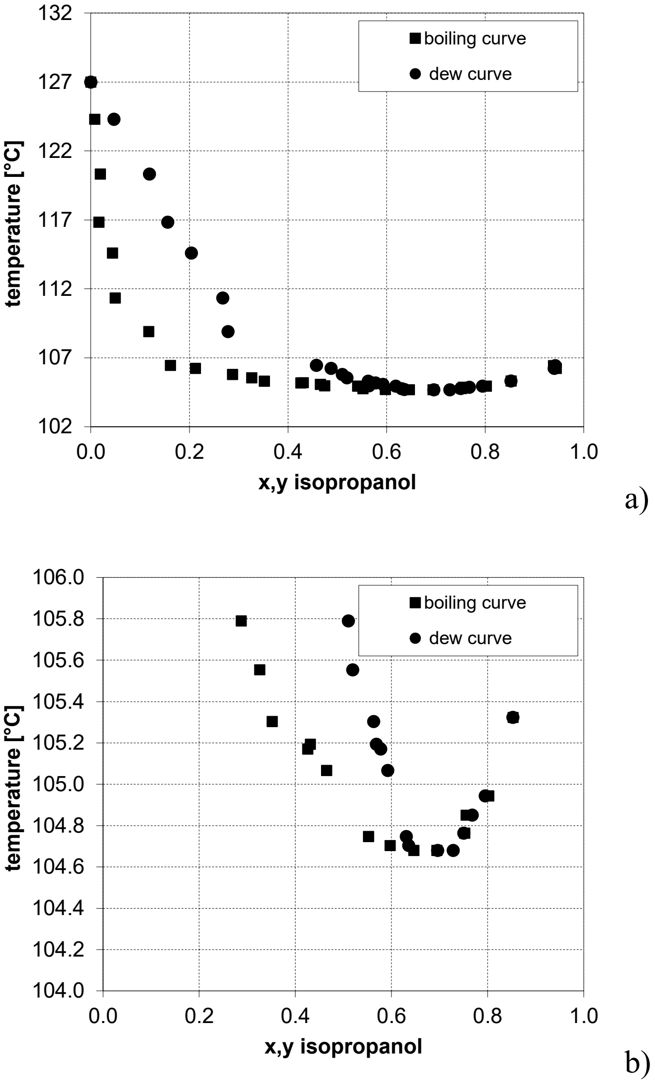


Figure 6. Experimental VLE data collected at PT lab for the isopropanol-water system at 2.5 bar a) for a mole fraction of isopropanol ranging from 0 and 1 and b) detail for the composition range close to the azeotropic point.

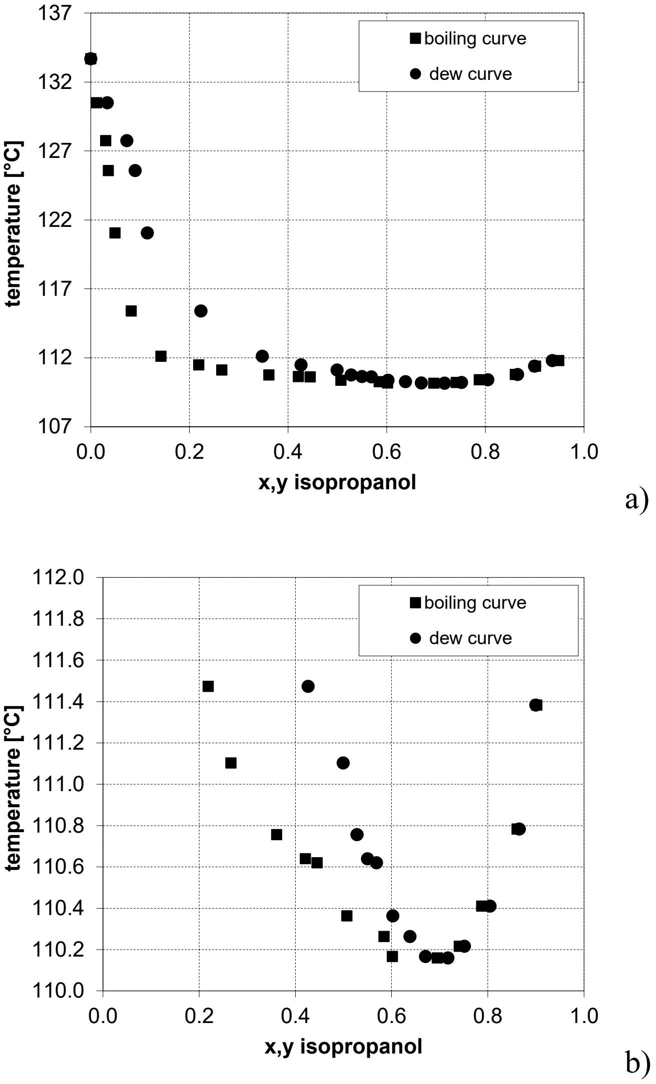


Figure 7. Experimental VLE data collected at PT lab for the isopropanol-water system at 3 bar a) for a mole fraction of isopropanol ranging from 0 and 1 and b) detail for the composition range close to the azeotropic point.

As a result of the thermodynamic consistency test, all data up to 2.5 bar fully satisfy the criteria; for the curve at 3 bar more experimental points for water-rich compositions could be added. However, it should be highlighted that also at 3 bar the obtained boiling curve and dew curve are in line with those obtained at about 4 bar (Figure 8) and at other pressures (Figure 9).

A minimum temperature azeotrope occurs for all the considered pressures, confirming the non-ideality of the mixture. On the right side of the azeotrope, for high mole fractions of isopropanol, the boiling curve becomes very close to the dew curve, differently from the trend at low isopropanol contents. These trends are confirmed also by comparison with the isobaric curve by Wilson and Simons (Wilson and Simons, 1952) at about 4 bar, in addition to the ones available at 1 atm from the literature.

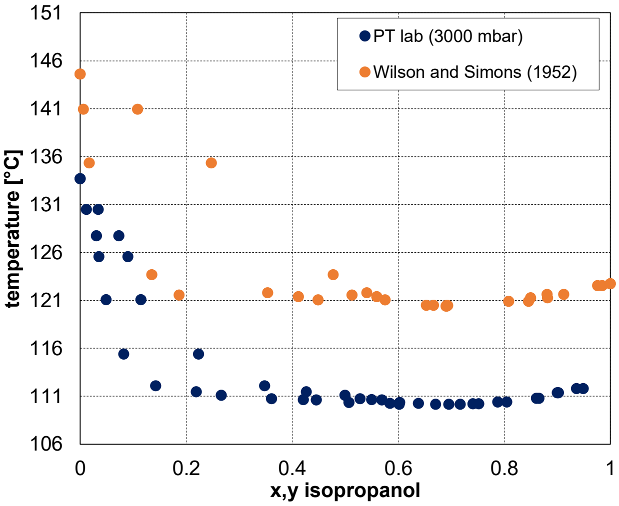


Figure 8. Comparison of the experimental VLE data collected at PT lab for the isopropanol-water system at 3 bar and the ones by Wilson and Simons (Wilson and Simons, 1952) at about 4 bar.

Figure 9 reports a comparison of the obtained curves at different pressures, which highlights the variation of temperature levels as expected with increasing pressure and of the azeotropic point, that slightly moves towards a higher mole fraction of isopropanol as the pressure increases.

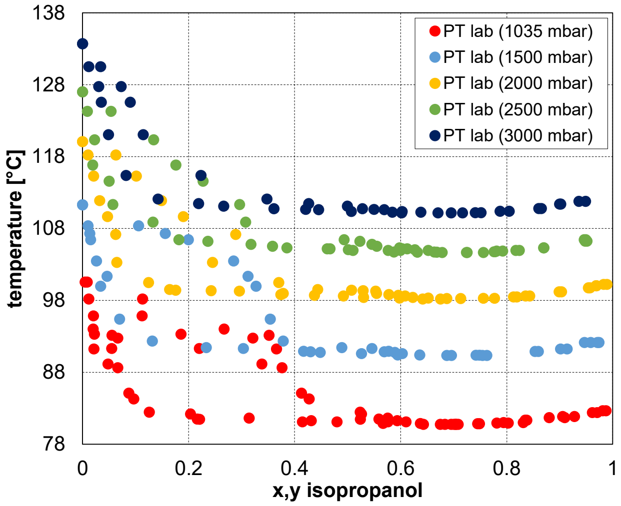


Figure 9. Comparison of the VLE experimental data collected at PT lab for the isopropanol-water system at different pressures.

5. Conclusions

This work presents isobaric experimental vapor-liquid equilibrium data for the system isopropanol-water at 1.5 bar, 2 bar, 2.5 bar and 3 bar to fill the gap existing in the literature. The equipment at the PT lab of Politecnico di Milano, consisting of an equilibrium unit and a gas-chromatograph, has been employed for this purpose, after validation with available experimental data from the literature at 1 atm. The collected experimental data were evaluated through the Redlich-Kister consistency test method. Future development of this work could focus on the collection of more experimental points at 3 bar and on the study of the vapor-liquid equilibrium curve at higher pressures up to 4 bar or under vacuum to extend the range of conditions for which experimental data for this system are available.

6. Appendix

Table 3. Data of temperature, pressure, composition in the liquid and in the vapor phases collected at PT lab at a pressure of 1.5 bar and related uncertainties (*x* is the mole fraction in the liquid phase and *y* is the mole fraction in the vapor phase of the most volatile component (isopropanol)).

Pressure [mbar]	Uncertainty in pressure [mbar]	Temperature [°C]	Uncertainty in temperature [±°C]	x [mol/mol]	Uncertainty in x [± mol/mol]	y [mol/mol]	Uncertainty in y [± mol/mol]
0.009287	0.006061	0.095277	0.034987	0.009287	0.006061	0.095277	0.034987
0.012044	0.004363	0.141372	0.227528	0.012044	0.004363	0.141372	0.227528
0.013664	0.007711	0.181677	0.019456	0.013664	0.007711	0.181677	0.019456
0.023292	0.010830	0.261701	0.067483	0.023292	0.010830	0.261701	0.067483
0.030588	0.014756	0.302090	0.019591	0.030588	0.014756	0.302090	0.019591
0.041495	0.017812	0.287799	0.034545	0.041495	0.017812	0.287799	0.034545
0.062549	0.031886	0.327961	0.034551	0.062549	0.031886	0.327961	0.034551
0.119259	0.071614	0.351590	0.017723	0.119259	0.071614	0.351590	0.017723
0.213430	0.036065	0.460195	0.018272	0.213430	0.036065	0.460195	0.018272
0.279047	0.014101	0.516686	0.016613	0.279047	0.014101	0.516686	0.016613
0.388827	0.022305	0.548865	0.013346	0.388827	0.022305	0.548865	0.013346
0.401720	0.025135	0.540328	0.015407	0.401720	0.025135	0.540328	0.015407
0.419883	0.013785	0.560613	0.013609	0.419883	0.013785	0.560613	0.013609
0.497237	0.015793	0.575035	0.011905	0.497237	0.015793	0.575035	0.011905
0.566203	0.012024	0.608418	0.011134	0.566203	0.012024	0.608418	0.011134
0.661428	0.013889	0.670526	0.010963	0.661428	0.013889	0.670526	0.010963
0.719062	0.022194	0.726312	0.020692	0.719062	0.022194	0.726312	0.020692
0.845077	0.010092	0.838549	0.011207	0.845077	0.010092	0.838549	0.011207
0.904021	0.004454	0.890974	0.007023	0.904021	0.004454	0.890974	0.007023
0.953419	0.013163	0.940617	0.017791	0.953419	0.013163	0.940617	0.017791
0.970853	0.004307	0.967450	0.004729	0.970853	0.004307	0.967450	0.004729

Table 4. Data of temperature, pressure, composition in the liquid and in the vapor phases collected at PT lab at a pressure of 2 bar and related uncertainties (*x* is the mole fraction in the liquid phase and *y* is the mole fraction in the vapor phase of the most volatile component (isopropanol)).

Pressure [mbar]	**Uncertainty in pressure [mbar]**	**Temperature [°C]**	**Uncertainty in temperature [±°C]**	**x [mol/mol]**	**Uncertainty in x [± mol/mol]**	**y [mol/mol]**	**Uncertainty in y [± mol/mol]**
2000	[1992;2000]	118.23	0.13778	0.009140	0.002856	0.056525	0.042610
2000	[1992;2000]	115.29	0.01951	0.018644	0.008450	0.091388	0.043635
2000	[1992;2000]	111.88	0.05321	0.028715	0.019834	0.134869	0.061798
2000	[1992;2000]	109.65	0.02083	0.042101	0.036840	0.173525	0.097727
2000	[1992;2000]	107.17	0.02778	0.055920	0.027808	0.265444	0.027060
2000	[1992;2000]	103.30	0.02333	0.057890	0.013611	0.224206	0.037181
2000	[1992;2000]	100.48	0.06028	0.112805	0.073794	0.343490	0.039407
2000	[1992;2000]	99.53	0.00214	0.149350	0.070187	0.415324	0.080367
2000	[1992;2000]	99.43	0.00964	0.159594	0.027474	0.478406	0.022025
2000	[1992;2000]	99.35	0.00124	0.221870	0.030028	0.500134	0.015955
2000	[1992;2000]	99.29	0.00981	0.272410	0.028942	0.523852	0.012147
2000	[1992;2000]	98.81	0.00481	0.347390	0.016765	0.549280	0.011882
2000	[1992;2000]	98.96	0.00381	0.351446	0.037963	0.525863	0.025289
2000	[1992;2000]	98.73	0.00301	0.409231	0.022257	0.567256	0.015650
2000	[1992;2000]	98.63	0.00021	0.463243	0.021406	0.580399	0.012468
2000	[1992;2000]	98.43	0.00008	0.501067	0.016706	0.594821	0.014417
2000	[1992;2000]	98.32	0.00004	0.569491	0.018021	0.625214	0.012541
2000	[1992;2000]	98.18	0.00028	0.614303	0.016570	0.649293	0.011875
2000	[1992;2000]	98.26	0.00003	0.661368	0.012008	0.688730	0.011047
2000	[1992;2000]	98.28	0.00001	0.733914	0.009398	0.756296	0.012660
2000	[1992;2000]	98.49	0.00010	0.800950	0.012197	0.794324	0.009055
2000	[1992;2000]	98.63	0.00008	0.827315	0.009731	0.819130	0.007270
2000	[1992;2000]	99.20	0.00074	0.892551	0.011097	0.888002	0.005781
2000	[1992;2000]	99.73	0.00023	0.952126	0.002126	0.948839	0.006525
2000	[1992;2000]	100.03	0.00001	0.964542	0.011918	0.965877	0.003613
2000	[1992;2000]	100.23	0.00003	0.987679	0.000642	0.980742	0.002576

Table 5. Data of temperature, pressure, composition in the liquid and in the vapor phases collected at PT lab at a pressure of 2.5 bar and related uncertainties (x is the mole fraction in the liquid phase and y is the mole fraction in the vapor phase of the most volatile component (isopropanol)).

Pressure [mbar]	**Uncertainty in pressure [mbar]**	**Temperature [°C]**	**Uncertainty in temperature [±°C]**	**x [mol/mol]**	**Uncertainty in x [± mol/mol]**	**y [mol/mol]**	**Uncertainty in y [± mol/mol]**
2500	[2490;2500]	124.30	0.10453	0.008162	0.004301	0.048137	0.018623
2500	[2490;2500]	116.83	0.00778	0.017095	0.010858	0.159829	0.015032
2500	[2490;2500]	120.33	0.03111	0.020164	0.011051	0.121862	0.098809
2500	[2490;2500]	114.59	0.01143	0.045315	0.062182	0.208416	0.119771
2500	[2490;2500]	111.33	0.03111	0.051058	0.007087	0.272929	0.065822
2500	[2490;2500]	108.90	0.44333	0.120363	0.072663	0.284064	0.110374
2500	[2490;2500]	106.45	0.04083	0.165215	0.031629	0.464422	0.019159
2500	[2490;2500]	106.23	0.05604	0.216685	0.107472	0.494187	0.014960
2500	[2490;2500]	105.79	0.02093	0.293206	0.011075	0.517045	0.011533
2500	[2490;2500]	105.55	0.05551	0.332295	0.039647	0.526230	0.021541
2500	[2490;2500]	105.30	0.00101	0.358317	0.018677	0.569768	0.021793
2500	[2490;2500]	105.19	0.00231	0.437863	0.011443	0.575040	0.011433
2500	[2490;2500]	105.07	0.02008	0.472193	0.018735	0.598953	0.011347
2500	[2490;2500]	104.97	0.00194	0.481042	0.011741	0.571177	0.025749
2500	[2490;2500]	104.95	0.00250	0.548052	0.035006	0.625162	0.017139
2500	[2490;2500]	104.75	0.00004	0.558968	0.012721	0.636851	0.010652
2500	[2490;2500]	104.70	0.00334	0.604007	0.011024	0.642010	0.014350
2500	[2490;2500]	104.68	0.00023	0.652484	0.010454	0.701609	0.012364
2500	[2490;2500]	104.68	0.00003	0.700123	0.009736	0.733809	0.013201
2500	[2490;2500]	104.76	0.00031	0.757297	0.010581	0.755443	0.014308
2500	[2490;2500]	104.85	0.00083	0.760231	0.025408	0.772709	0.012395
2500	[2490;2500]	104.94	0.00221	0.806487	0.015391	0.799106	0.011143
2500	[2490;2500]	105.32	0.00048	0.856325	0.011143	0.855781	0.006068
2500	[2490;2500]	106.43	0.00031	0.939994	0.028689	0.943494	0.019962
2500	[2490;2500]	106.23	0.00040	0.945562	0.007196	0.941811	0.005295

Table 6. Data of temperature, pressure, composition in the liquid and in the vapor phases collected at PT lab at a pressure of 3 bar and related uncertainties (*x* is the mole fraction in the liquid phase and *y* is the mole fraction in the vapor phase of the most volatile component (isopropanol)).

Pressure [mbar]	Uncertainty in pressure [mbar]	Temperature [°C]	Uncertainty in temperature [±°C]	x [mol/mol]	Uncertainty in x [± mol/mol]	y [mol/mol]	Uncertainty in y [± mol/mol]
3000	[2994;3000.5]	130.50	0.12368	0.012058	0.009583	0.034760	0.019129
3000	[2994;3000.5]	127.74	0.03768	0.031345	0.009485	0.074954	0.029797
3000	[2994;3000.5]	125.57	0.05204	0.036447	0.005717	0.091992	0.029686
3000	[2994;3000.5]	121.07	0.20111	0.050330	0.034665	0.117370	0.023071
3000	[2994;3000.5]	115.40	0.04333	0.084200	0.057570	0.227359	0.207754
3000	[2994;3000.5]	112.11	0.02404	0.145840	0.046008	0.353534	0.173920
3000	[2994;3000.5]	111.47	0.04748	0.223491	0.028501	0.432746	0.104394
3000	[2994;3000.5]	111.10	0.00874	0.271193	0.039519	0.506172	0.020115
3000	[2994;3000.5]	110.76	0.00521	0.367131	0.016672	0.534671	0.021883
3000	[2994;3000.5]	110.64	0.00610	0.427118	0.020811	0.556277	0.027682
3000	[2994;3000.5]	110.62	0.00640	0.451767	0.018618	0.575372	0.016294
3000	[2994;3000.5]	110.36	0.00334	0.513689	0.051124	0.608860	0.022220
3000	[2994;3000.5]	110.26	0.00474	0.590933	0.025036	0.644184	0.013999
3000	[2994;3000.5]	110.17	0.00124	0.607921	0.013526	0.676111	0.014965
3000	[2994;3000.5]	110.16	0.00010	0.700706	0.009687	0.722224	0.009244
3000	[2994;3000.5]	110.22	0.00001	0.745745	0.012445	0.756505	0.009423
3000	[2994;3000.5]	110.41	0.00070	0.791970	0.015515	0.808898	0.010383
3000	[2994;3000.5]	110.78	0.00214	0.863685	0.008390	0.868404	0.012737
3000	[2994;3000.5]	111.38	0.00724	0.904256	0.023686	0.902239	0.013321
3000	[2994;3000.5]	111.80	0.00141	0.950078	0.011903	0.937563	0.012210

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