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Re-evaluating 2-heptanol as solvent for the extraction of 2,3-butanediol from water

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ABSTRACT

The performance of an extraction-distillation process for separating 2,3-butanediol from H_2O was evaluated in a recent study, finding high efficeincy when using 2-heptanol as solvent for extraction. Since the study was based on liquid-liquid equilibrium (LLE) data mainly derived from molecular simulations, the aim of this communication was to consolidate the database by providing experimental phase equilibrium data and to re-evaluate 2-heptanol as solvent. Based on LLE experiments, a solvent-to-feed ratio (S/F) of 3.175 was required to recover 95 % of 2,3-BDO in a counter-current extraction column. This S/F is 21.9 times higher than the estimation derived from the data based on molecular simulations. The high S/F results in a strong dilution of 2,3-BDO in the extract. Experimental investigation of the boiling point data of the 2,3-BDO – 2-heptanol system for subsequent distillation revealed the presence of a temperature minimum azeotrope at low 2,3-BDO concentrations, which limits the feasibility of the overall process. Since the use of 2-heptanol as solvent is oftentimes referred to in the community of diol separation, the results presented in the work at hand are relevant to a broad readership.

1. Introduction

2,3-butanediol is a precursor for numerous products, such as pharmaceuticals, cosmetics, flavoring agents or biofuels [1]. While its production is still mainly petrochemically based, the market share of bio-based 2,3-BDO is expected to rise in the upcoming years [2]. Besides the fermentative production and the corresponding feedstock costs, the product separation from fermentation broth is the main cost driver [3]. Currently, product separation is conducted via filtration and distillation in industrial scale at GS Caltex [2], which is highly energy intensive [4]. Several alternative process concepts have been proposed in academia [5], whereby solvent extraction is the most promising technology to be used in industrial scale. To this end, the separation of 2,3-BDO from aqueous solution via solvent extraction was studied extensively in literature, thereby focusing on the identification of a suitable solvent [6–8]. Experimental liquid-liquid equilibrium (LLE) data for various solvents were provided by multiple groups, mainly focusing on long chain alcohols [9–20]. Among the tested systems, C4 alcohols such as 1-butanol and isobutanol exhibited the highest distribution coefficients (0.68–0.88), which decreased with increasing carbon chain length (e.g. decanol with distribution coefficients in a range from 0.16 to 0.26) [9,10]. Several branched alcohols were also investigated, showing slightly enhanced selectivity due to branching, however, the chain length was found to be the more decisive factor. Consequently, oleyl alcohol (C18) was identified as the most selective solvent within this group, although its practical applicability is limited by its high viscosity and boiling point [21]. Furthermore, particularly high distribution coefficients were reported for phenolic solvents such as thymol, carvacrol, and nonylphenol, yet their industrial use is constrained by low density gradients between the phases, which complicate phase separation [17,19]. For selected solvents (1-butanol, isobutanol, oleyl alcohol, 2-heptanol, and carvacrol) process concepts have been published, claiming progressively improved performance of the extraction-distillation processes [19–23].

The most efficient process concept so far used 2-heptanol as a solvent for the separation of 2,3-BDO and is based on liquid-liquid equilibrium data derived from molecular simulations which were only partially verified by experiments. There are several studies emphasizing the importance of accurate phase equilibria in process design [24–26] and especially highlight the sensitivity of LLE data therein [27–30]. Hence, the need for consolidation of the LLE data of the ternary system (2,3-BDO – H_2O – 2-heptanol) for the scientific community is raised, especially since multiple reviews and techno-economic analysis refer to 2-heptanol as promising solvent and rely on the published results [3,31,

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32].

The aim of this work is to provide the first comprehensive experimental validation of the ternary LLE (2,3-BDO – H_2O – 2-heptanol) and binary boiling point data (2,3-BDO – 2-heptanol), thereby closing the data gap left by previous simulation-based studies. The novel experimental LLE data and binary boiling point data are accompanied by an uncertainty analysis based on Gaussian error propagation. These results enable a more reliable process design and offer a critical benchmark for evaluating the accuracy of predictive models such as those proposed by Lee *et al.* [20]. The LLE and boiling point data are correlated using the non-random two-liquid (NRTL) model, and it is assessed whether key parameters such as the distribution coefficient and selectivity are accurately represented by the correlation. The minimal solvent-to-feed ratio (S/F) resulting from the NRTL parameters documented by Lee *et al.* [20] is compared with the values obtained from this work. Furthermore, the feasibility of the overall process concept is discussed with regard to the required S/F ratio and subsequent solvent regeneration via distillation, based on the new experimental boiling point data.

2. Materials and methods

Within the following section, an overview on the chemicals used (Section 2.1), the experimental procedures for the determination of LLE data (Section 2.2) as well as boiling point data (Section 2.3), the used simulation methods for data correlation (Section 2.4) and the determination of solvent demand (Section 2.5) is given.

2.1. Chemicals

All experiments are conducted using the chemicals listed in Table 1.

2.2. Experimental determination of liquid-liquid equilibrium data

The LLE experiments are conducted in 20 mL screw-cap glass vials in an HLC Heating-ThermoMixer MHR 23 from DITABIS. The vials are filled with compositions of distilled water and 2-heptanol, maintaining a mass ratio of 1:1 (distilled water to 2-heptanol). For ternary LLE data 2,3-BDO is added. The vials are shaken for at least 16 h at 298.15 K at 500 rpm to assure equilibrium is reached (see Fig. S1 in the SI), as conducted in [19]. In Before sampling, the vials are held at temperature with no shaking to allow for settling. All measurements are conducted as triplicates.

In Fig. 1, a schematic representation of the used methods to experimentally derive mass fractions of the ternary system H_2O, 2,3-BDO, and 2-heptanol is given. To determine the mass fraction of 2,3-BDO in the aqueous and organic phase, high performance liquid chromatography (HPLC) is used. The mass fractions of 2,3-BDO in the aqueous and organic phase were determined with an Agilent 1200 HPLC equipped with a Nucleodur C18ec column. Therefore, HPLC samples are diluted with methanol in volumetric ratio of 1:1. For detection of 2,3-BDO, a Refractive Index Detector (RID) is used. Two eluents are used to create a gradient throughout the measurement and eluent A is a mixture of 945 mL water, 50 mL methanol, and 5 mL trifluoracetic acid. Eluent B is pure methanol. At a constant flow of 0.5 mL/min eluent A is applied for 4 min. A gradient to a composition 25 % A and 75 % B is applied for 1 min. The ratio of 25A/75B is held for 7.5 min and is then changed back to pure solvent A. To achieve optimal results, the RID is purged for 4 min before every injection.

Table 1
Component, CAS registry number, supplier, purity.

Component	CAS Reg No.	Supplier	Purity
2,3-butanediol	513–85–9	VWR Chemicals	≥ 98 %
2-heptanol	543–49–7	VWR Chemicals	≥ 99 %
Ethanol	64–17–5	VWR Chemicals	≥ 99.8 %
Methanol	67–56–1	VWR Chemicals	≥ 99.8 %
Trifluoracetic acid	76–05–1	Carl Roth GmbH	≥ 99.9 %
Acetonitrile	75–05–8	VWR Chemicals	≥ 99.9 %

To determine the water content in the organic phase, it was analyzed via Karl-Fischer Titration (KF). The KF samples are prepared by diluting 1 g of the organic phase with 1 g of acetonitrile.

To determine the mass fraction of 2-heptanol in the aqueous phase, gas chromatography (GC) is used. For GC analysis an Agilent 7890 GC is used with a column obtained from CS-Chromatography of the type FS-CW 20 M-CB-1 (PEG 20,000, i.d. 530 µm; 25 m x 1 µm). The oven is heated in a gradient (80 °C hold 3.5 min, to 180 °C with 50 °C/min, hold 2.5 min, to 200 °C with 50 °C/min, hold 3 min). A sample volume of 2 µL, a flow rate of 8 mL/min helium and a split ratio of 5:1 is applied. GC samples are prepared by taking 100 µl from the aqueous phase and adding them to 900 µl ethanol for dilution. The remaining mass fractions (water in aqueous phase and 2-heptanol in organic phase) are calculated via closing condition. In Table 2 a summary of the used analytical techniques for the determnation of each compound in the ternary LLE is given.

The distribution coefficient D_i of component i and selectivity S are used to describe the thermodynamic equilibrium. The distribution coefficient is defined as

$$D_i = \frac{w_{i,E}}{w_{i,R}} \tag{1}$$

where $w_{i,E}$ denotes the mass fraction of the solute in the extract and $w_{i,R}$ the mass fraction of the solute in the raffinate. The selectivity is derived from the quotient of the distribution coefficients of the solute (i) and water (j):

$$S = \frac{D_i}{D_j} \tag{2}$$

For uncertainty determination Gaussian error propagation is applied to the measured mass fractions. The uncertainty of the measuring device, the slope of calibration, and the error resulting from replicates are included. The documented uncertainties and details on the procedure can be found in the supplementary information in Section 1 and Section 2

2.3. Experimental determination of boiling point data

Differential scanning calorimetry (DSC) was employed to determine the boiling points of the binary system 2,3-BDO – 2-heptanol. Calibration was performed using indium as a standard (melting point 429.75 K). Measurements were carried out on a DSC3 STARe System (Mettler Toledo). For each experiment, 40 µL of pure compounds or mixtures at different molar ratios were placed in aluminum crucibles (100 µL capacity) that were hermetically sealed; the pinhole was applied automatically by the DSC. A nitrogen flow of 50 mL min^{-1} was applied to prevent condensation in the furnace. All measurements were conducted in triplicate. The samples were equilibrated at 298.15 K for 2 min, then heated to 523.15 K at 25 K min^{-1}. The resulting DSC thermograms were analyzed using STARe Software (V19.0). The peak of the second derivative of the thermogram was used to determine the isobaric boiling point line at atmospheric pressure, following the procedure reported in the literature [33,34,19].

2.4. Thermodynamic modeling of phase equilibrium data

The well-known NRTL activity coefficient model is used to correlate experimental LLE data [35]. The following model equations are used to express the activity coefficient γ_i:

$$\ln\gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{kj}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right) \tag{3}$$

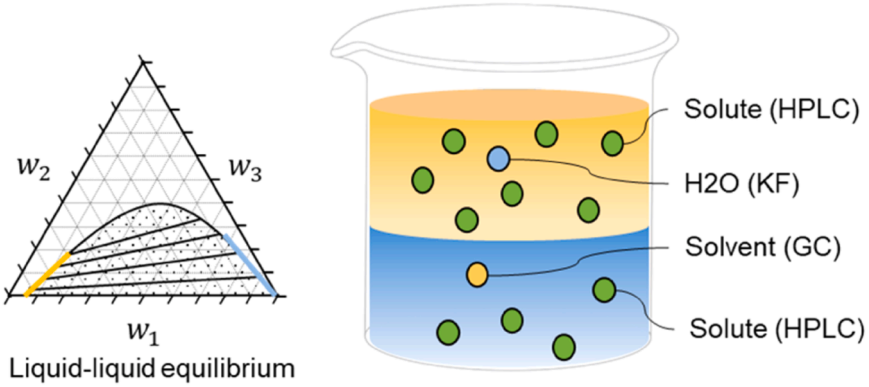

Fig. 1. Schematic representation of the used methods to experimentally derive mass fractions of the ternary system H_2O, 2,3-BDO, and 2-heptanol.

Table 2
Analytical techniques for determination of ternary LLE data.

	w_{H2O}	$w_{2,3-BDO}$	$w_{2-heptanol}$
Aqueous phase	$\sum_i w_i = 1$	HPLC – RID	GC – FID
Organic phase	KF	HPLC – RID	$\sum_i w_i = 1$

$$G_{ij} = \exp\left(-\alpha_{ij}\tau_{ij}\right) \tag{4}$$

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T} \tag{5}$$

$$\tau_{ii} = 0 \tag{6}$$

$$\alpha_{ij} = \alpha_{ji} = 0.3 \tag{7}$$

$$\alpha_{ii} = 1 \tag{8}$$

To model the LLE data, the binary interaction parameters of water and 2-heptanol are regressed by adjusting b_{ij} using an objective function (OF) based on molar fractions of the binary LLE while a_{ij} is fixed to zero, since only isothermal LLE data is correlated. The remaining binary pairs are regressed to the ternary LLE by only adjusting b_{ij}. In all cases, the non randomness parameter α_{ij} is fixed to 0.3 as typical value [36,37].

$$OF_{LLE}(x) = RMSD(x)_{aq} + RMSD(x)_{org} \tag{9}$$

$$RMSD(x)_{aq/org} = \sqrt{\frac{1}{I \cdot N}\sum_{i=1}^{I}\sum_{j=1}^{N}\left(\frac{x_{i,n}^{exp} - x_{i,n}^{NRTL}}{u_{i,n}(x)}\right)^2} \tag{10}$$

To correlate boiling temperatures for pTx vapor-liquid equilibrium (VLE) data, an individual set of NRTL parameters was regressed.

$$OF_{VLE}(T) = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(\frac{T_n^{exp} - T_n^{NRTL}}{u_n(T)}\right)^2} \tag{11}$$

2.5. Calculation of minimal solvent to feed ratio

Aspen Plus V11 is used to evaluate the minimal S/F for the separation of 2,3-BDO from water using 2-heptanol as solvent. The NRTL model is chosen to cover non-idealities in the liquid phase. The feed stream consists of an aqueous stream with 10 wt % of 2,3-BDO at 298.15 K. The extraction process is modeled using the multistage counter-current extraction column model with 10 theoretical separation stages in isothermal operation mode at 25 °C and atmospheric pressure. The recovery of 2,3-BDO is specified to be 95 % to be comparable to the published processes assessment. The S/F is minimized via sensitivity analysis while maintaining the recovery of 2,3-BDO.

3. Results and discussion

To re-evaluate the extraction process using 2-heptanol, LLE data was collected within this work. Binary (water – 2-heptanol) and ternary LLE systems consisting of water, 2,3-BDO, and 2-heptanol were measured experimentally at 298.15 K. The mass fractions of 2,3-BDO are in the relevant concentration range for feed streams from fermentation (below 15 wt % 2,3-BDO in the feed [38]). The mass fractions were determined as described in Section 2.2. The experimentally derived mass fractions in organic (org) and aqueous (aq) phase and uncertainties are given in Table 3.

The obtained LLE data was correlated as described in Section 2.4 using the NRTL model. The corresponding NRTL parameters used for process design can be found in Table 4.

In Fig. 2, the experimental tie-lines (black) and the correlated tie-lines (grey) are shown. The correlation of the experimental tie-lines using the NRTL model results in a RMSD (as defined in Section 2.4) of 79.3. The measured cross-solubility ($x_{H_2O}^{org}$= 0.27) is in good agreement with the published one from Stephenson *et al.* ($x_{H_2O}^{org}$= 0.25) [39].

The distribution coefficient and selectivity are depicted in Fig. 3. In the supplementary information in Section 3, the numerical values of distribution coefficients and selectivities as well as the uncertainty, following Gaussian error propagation in a 95 % confidence interval, are tabulated.

The experimentally measured distribution coefficients of 2,3-BDO in 2-heptanol and water are slightly dependent on the content of 2,3-BDO and within the range of 0.29 and 0.34. Further, all calculated distribution coefficients and selectivities using the NRTL model are within the range of uncertainty of the experimentally measured data points.

The calculated minimal S/F using a multistage counter-current extraction column as described in Section 2.5 is presented in Fig. 4a. When comparing the S/F resulting from this work (3.175) and the S/F from Lee *et al.* [20] (0.145), it becomes evident that the parametrization resulting from predictive LLE data underestimated the S/F by orders of magnitude (a factor of 21.9).

In Fig. 4b, a representation of the ternary equilibrium data measured and calculated by Lee *et al.* [20] and data from this work is given. It can be observed that the calculated tie-lines reported by Lee *et al.* [20] are considerably steeper than those obtained experimentally by Lee *et al.* [20] and than those obtained within this work. This indicates that within the calculations of Lee *et al.* [20] the distribution coefficients are overestimated and therefore the S/F is underestimated, leading to a reduced energy demand in solvent regeneration. Additionally, a non-existent miscibility gap between water and 2,3-BDO is modeled, further indicating that the NRTL correlation is insufficient. The slopes of the experimental tie-lines are in the same range for both studies, while the cross-solubility of water in the organic phase is different. The cross-solubility of 2-heptanol and water was already published by

Table 3
The experimental ternary LLE data for the ternary systems consisting of water, 2,3-BDO, and 2-heptanol at 298.15 K at atmospheric pressure.

$w^{org}_{H_2O}$	$u^{org}_{w,\ H_2O}$	$w^{org}_{2,3-BDO}$	$u^{org}_{w,\ 2,3-BDO}$	w^{org}_{2-hept}	$u^{org}_{w,\ 2-hept}$	$w^{aq}_{H_2O}$	$u^{aq}_{w,\ H_2O}$	$w^{aq}_{2,3-BDO}$	$u^{aq}_{w,\ 2,3-BDO}$	w^{aq}_{2-hept}	$u^{aq}_{w,\ 2-hept}$
0.0537	0.0007	0.0000	0.0000	0.9463	0.0007	0.9968	0.0002	0.0000	0.0000	0.0032	0.0002
0.0558	0.0006	0.0128	0.0003	0.9314	0.0007	0.9529	0.0008	0.0439	0.0011	0.0032	0.0001
0.0581	0.0006	0.0229	0.0003	0.9190	0.0007	0.9187	0.0006	0.0780	0.0015	0.0033	0.0001
0.0604	0.0006	0.0349	0.0004	0.9049	0.0007	0.8819	0.0010	0.1146	0.0023	0.0035	0.0001
0.0629	0.0007	0.0474	0.0009	0.8897	0.0011	0.8476	0.0006	0.1487	0.0027	0.0037	0.0001
0.0668	0.0006	0.0620	0.0007	0.8712	0.0009	0.8148	0.0004	0.1811	0.0032	0.0041	0.0001

Table 4
NRTL parameters for correlation of ternary LLE data.

Component *i*	Component *j*	a_{ij} / -	a_{ji} / -	b_{ij} / K	b_{ji} / K	α_{ij} / -
H_2O	2,3-BDO	0	0	−2220.7187	370.9282	0.3
H_2O	2-heptanol	0	0	2476.4177	479.1804	0.3
2,3-BDO	2-heptanol	0	0	156.5994	−2148.3727	0.3

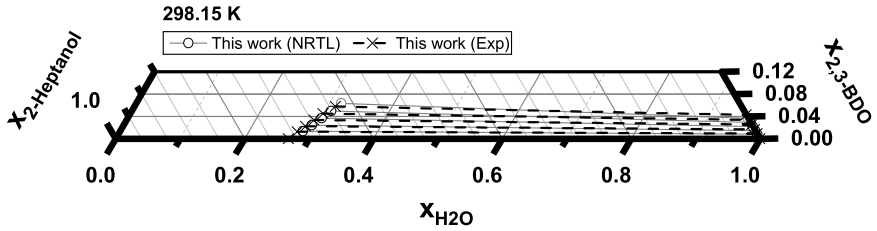

Fig. 2. Representation of the mole fractions of the ternary system water, 2,3-BDO, and 2-heptanol at 298.15 K. Black crosses indicate experimental tie-line data and open circles represent the corresponding correlation using the NRTL model.

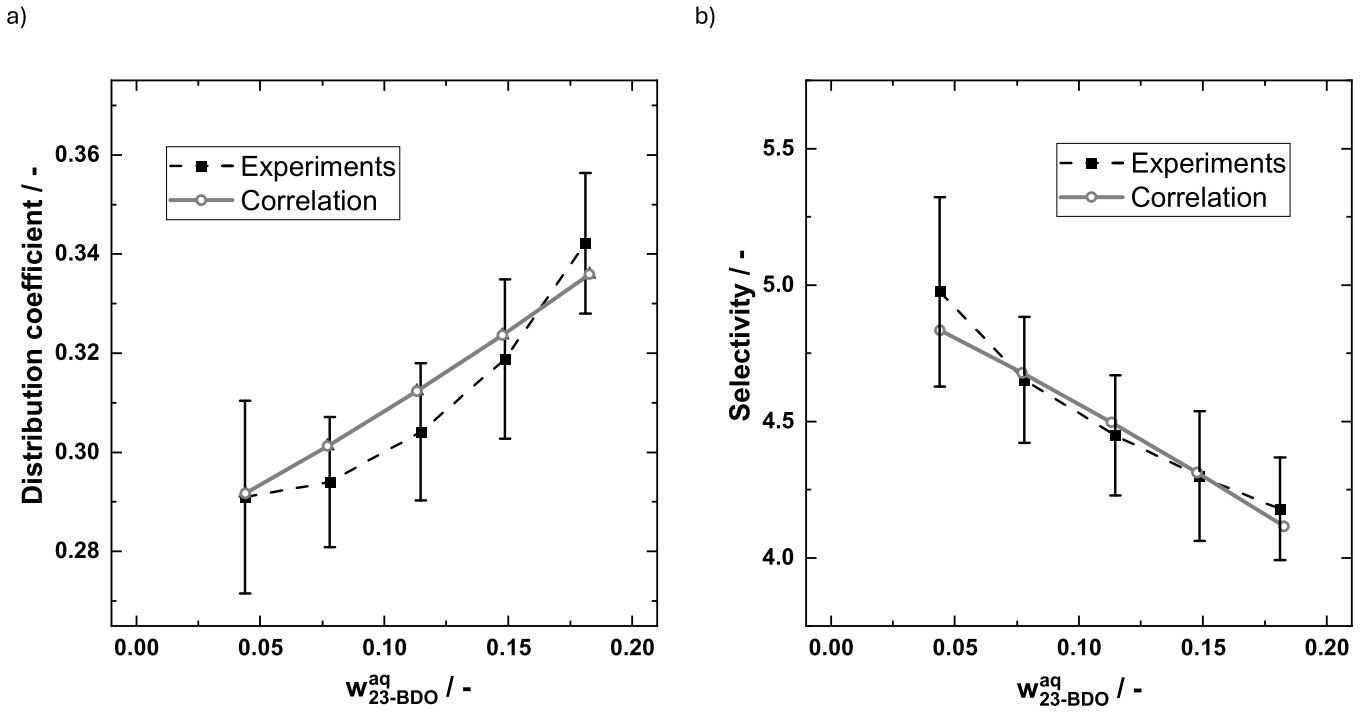

Fig. 3. Experimental distribution coefficients of 2,3-BDO (a) and selectivities for 2,3-BDO (b) in the ternary system water, 2,3-BDO, and 2-heptanol (black squares) as a function of the weight fraction of 2,3-BDO in the raffinate. The uncertainty of both, distribution coefficient and selectivity, follows Gaussian error propagation in a 95 % confidence interval. Further, distribution coefficient and selectivity calculated using the NRTL correlation derived in this work are shown (grey circles).

Stephenson *et al.* [39] ($x^{org}_{H_2O} = 0.25$) and is in good agreement with the cross-solubility measured within this work. Consequently, the resulting S/F values are lower compared to those derived within this study which facilitates solvent regeneration, due to highly concentrated solute (higher distribution coefficients) and a lower water content in the extract (lower cross-solubility).

To enable the modeling of the solvent regeneration process via distillation, binary boiling point data were determined experimentally as described in Section 2.3. In Fig. 5, the experimental boiling point data at atmospheric pressure (numerical values in supplementary information in Table 3) as well as the UNIFAC estimation that Lee *et al.* [20] used are presented.

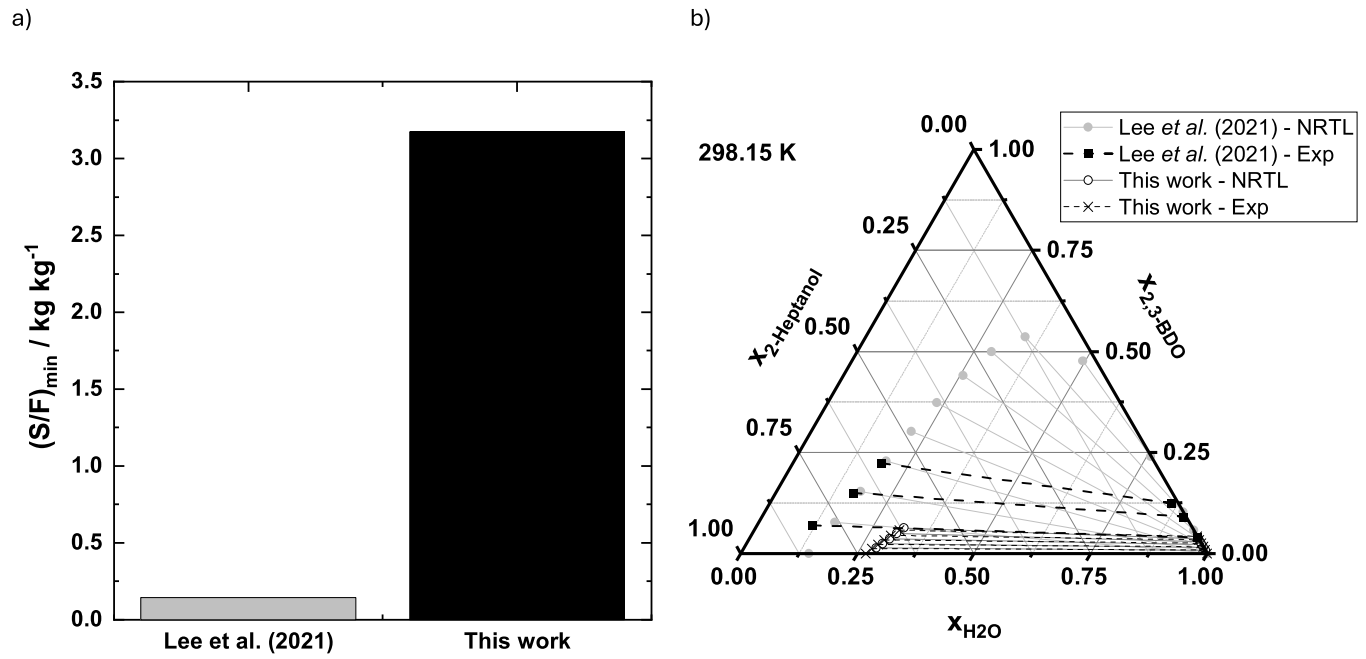

Fig. 4. Comparison of calculated minimal S/F using NRTL parameters from Lee et al. [20] and from this work (a). Representation of ternary equilibrium data: experimental data measured by Lee et al. [20] (black squares); calculated data by Lee et al. [20] (grey circles); experimental data from this work (black crosses); calculated data from this work (open circles) (b).

The boiling point data was used to correlate NRTL parameters as described in Section 2.4. To calculate the pure component vapor pressures, Antoine parameters taken from literature ([40]) are used (see Table 5 in the SI).

Analogous to the VLE data estimated via the UNIFAC group contribution method, a close boiling region at low concentrations of 2,3-BDO can be observed for the experimental VLE data. In particular, a temperature minimum azeotrope appears to be located at approximately 4 mol % 2,3-BDO. When using a S/F of 3.175, the extract consists of only 3.5 mol % 2,3-BDO due to dilution in the high amount of solvent necessary for extraction. Hence, the efficiency of the distillation process is hindered due to the presence of an azeotropic point that displays a distillation boundary and the large amounts of solvent that would have to be evaporated resulting from the high S/F of 3.175.

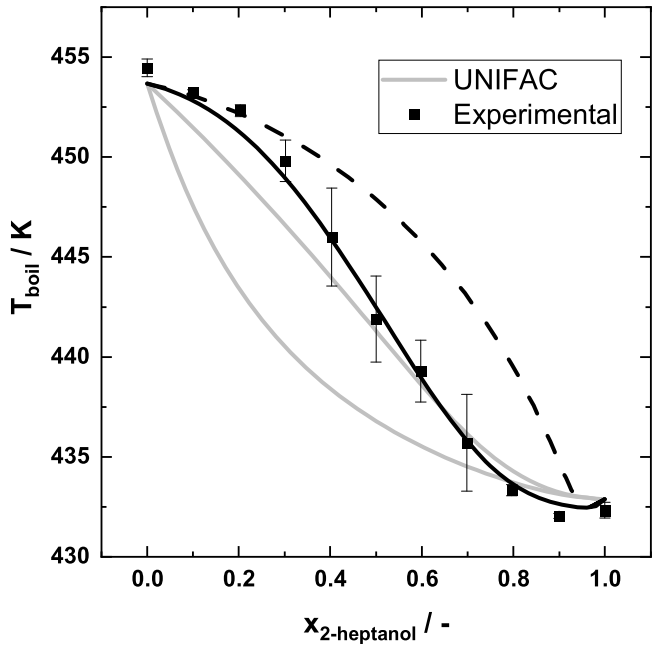

Fig. 5. Binary vapor-liquid equilibria data of 2,3-BDO – 2-heptanol based on experimental results (black squares) and UNIFAC estimation (grey line). The experimental boiling points are correlated using the NRTL model. The corresponding bubble point lines are presented as full lines and the calculated dew point lines are presented as dashed lines.

Table 5
NRTL parameters for correlation of binary boiling point data.

Component *i*	Component *j*	a_{ij} / -	a_{ji} / -	b_{ij} / K	b_{ji} / K	α_{ij} / -
2,3-BDO	2-heptanol	0	0	−736.438	1846.063	0.3

4. Conclusion

In this study, the use of 2-heptanol for separating 2,3-butanediol (2,3-BDO) from H_2O as a method of process intensification proposed by previous work that was mainly based on molecular simulations is re-evaluated. To this end, novel experimental LLE data of the ternary system as well as binary boiling point data is presented to provide additional experimental data for process analysis, including a comprehensive uncertainty analysis and data correlation using the NRTL model. Based on the experimental LLE data and correlation, a minimal S/F of 3.175 for the separation of 95 % of 2,3-BDO from aqueous solution was identified. The high S/F leads to a dilution of 2,3-BDO in the extract (3.5 mol % 2,3-BDO). The experimental investigation of the VLE of 2,3-BDO and 2-heptanol yielded the identification of a temperature minimum azeotrope at low concentration of 2,3-BDO, indicating potential limitations for the overall process feasibility. In conclusion, the re-evaluation of 2-heptanol as solvent for the separation of 2,3-BDO yielded that the extraction performance of 2-heptanol is only moderate and the subsequent solvent regeneration presents significant technical difficulties.

CRediT authorship contribution statement

William Graf von Westarp: Writing – review & editing, Writing – original draft, Methodology, Investigation, Formal analysis, Data

curation, Conceptualization. **Janik Hense:** Writing – review & editing, Methodology. **Moritz Haas:** Writing – review & editing, Methodology. **Andreas Jupke:** Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cep.2025.110591.

Data availability

Data will be made available on request.

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