

The recovery of Gallic acid with Triphenylphosphine Oxide and modelling with Artificial Intelligence

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Abstract

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Abstract

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Key words: Reactive extraction, gallic acid, organophosphorus extractant, triphenylphosphine oxide.

Introduction

Fossil fuel sources are finite and the consumption of them is directly associated with environmental pollution and climate change. During the last years, a global effort has been made to replace fossil fuels with renewable energy sources. Biomass is one of the promising renewable energy sources and can be converted into valuable products [1]. Great progresses have been made in science and technology for bio-based carboxylic acid production. Carboxylic acids are the best known type of organic acids that have at least one carboxylic group in the structure [2]. They are broadly used in the chemical, pharmaceutical, food and fuel industries. They are versatile building blocks for the synthesis of chemicals, pharmaceuticals, cosmetics, bioplastics, biopolymers and biofuels [3]. There are several publications addressing carboxylic acid production from biomass. Various carboxylic acids were produced via fermentation of biomass (carbohydrates, glucose, sucrose, cellulose, lignin etc.) by using engineered cultures [2, 4–6].

Gallic acid (3,4,5 trihydroxybenzoic acid) is a carboxylic acid of great interest. It has antimicrobial, antioxidative, anticancer, and antidiabetic properties [7]. Gallic acid is broadly used in chemical and pharmaceutical industries [8]. The production of gallic acid (HGA) is possible by microbial fermentation [9–13]. The separation of HGA from the fermentation broth and aqueous solutions has been the subject of several publications. HGA was adsorbed onto Na-montmorillonite [14], and a coal-based activated carbon [15]. HGA was extracted by molecular imprinted polymers [16], ethanol [17], tributyl phosphate [18, 19], trioctyl amine and aliquat 336 [20, 21]. All of these separation methods have their advantages and disadvantages in terms of selectivity, simplicity, performance, and cost [22, 23].

The recovery of carboxylic acids from the fermentation broth is cost intensive and time consuming [6]. Separation is the major cost driver in the total cost for the downstream process [22, 23]. The most common acid recovery techniques are liquid-liquid extraction, adsorption, distillation, reverse osmosis, electro dialysis, and reactive extraction. Purity, high extent of recovery, low energy consumption, little waste generation, and modest investment cost are the critics of the separation process selection [5]. Reactive extraction process meets all these requirements. In the reactive extraction process, reactive extractants are used with the solvents to recover the acid. Since the reactive extractants are viscous, solvents are used to regulate their physical properties (viscosity, surface tension, and density). Alcohols, ketones, esters etc. are the conventional solvents used with the reactive extractants to recover acids. In the reactive extraction process, acid reacts with the extractant molecule, and so an acid-extractant complex forms. Further, the formed complex solubilizes in the solvent. Organophosphorus extractants and aliphatic amines are the most efficient type of reactive extractants [24–26]. When compared to the other techniques, reactive extraction presents several advantages. Extractants are selective towards acids. In-situ acid removal is possible without damaging the microorganisms. The nature of the reaction is reversible so extractants can be back-extracted to the system.

To the best of our knowledge, there has been no paper reported so far dealing with the separation of HGA by triphenylphosphine oxide (Ph_3PO), which belongs to the family of organophosphorus compounds. The current study addressed this gap in the literature. For the solvent screen, five solvents were chosen from different categories. Reactive extraction results were evaluated regarding the distribution coefficient (K_D) of the acid, extraction efficiency ($E\%$), and loading factor (Z). The acid-extractant complexations were predicted by Mass Action Law Model. A temperature study was executed to determine the thermodynamic parameters. This study provides useful guidelines for the separation of HGA by reactive extractant of Ph_3PO .

Method and Materials

All chemicals used in the experiments are listed in Table 1. The chemicals were of reagent grade and they were used without further purification. The mother stock HGA solution was prepared by distilled water. The initial concentration of HGA was $0.06 \text{ mole kg}^{-1}$. It was prepared based on its concentration in the fermentation broth. pH of initial HGA solution was read on a pH meter (Mettler Toledo, SevenMulti). For the reactive extraction experiments, 5 mL aqueous phase ($0.06 \text{ mole kg}^{-1}$) was mixed with 5 mL organic phase in a conical flask. Ph_3PO concentration was varied in the solvents from 12 to 44 % by volume to see its effect on the extraction efficiency. The mixture was shaken in a temperature-controlled shaker (Nüve, ST30) at 120 rpm for 2 hours. Based on the preliminary experiments, 2 hours shaking was found to be sufficient. Phase separation was done by centrifugation (Nüve, ST200) at 4000 rpm for 10 minutes. After phase separation, aqueous

phase was taken by a syringe. The residual acid concentration was analyzed by a UV-vis spectrometer at the maximum adsorption wavelength of 260 nm. Since Ph_3PO has a low affinity to water, the water co-extraction to the organic phase was found to be negligible. The extracted HGA concentration was calculated by mass balance. The physical extraction experiments were performed with pure solvents alone. The thermodynamic study was conducted from 298.2 K to 318.2 K to estimate the thermodynamic parameters. All the experiments were repeated in triplicate in order to ensure the consistency. The distribution coefficient and the extraction efficiency were calculated to evaluate the extraction performance.

$$K_D = \frac{[\text{HGA}]_{\text{org}}}{[\text{HGA}]_{\text{aq}}} \quad (1)$$

$$E \% = \frac{K_D}{1 + K_D} \cdot 100 \quad (2)$$

where $[\text{HGA}]_{\text{org}}$ is the HGA concentration in the organic (extract) phase, $[\text{HGA}]_{\text{aq}}$ is the HGA concentration in the aqueous (raffinate) phase.

Table 1

Physicochemical properties of the chemicals.

Chemical	IUPAC name	Molecular weight (kg kmole ⁻¹)	Density (kg m ⁻³)	Supplier	Purity (% w)
Gallic acid	3,4,5 Trihydroxybenzoic acid	170.12	1700	Sigma-Aldrich	[?]98%
Triphenylphosphine oxide	Triphenyl-λ ⁵ -phosphanone	278.28	1212	Sigma-Aldrich	[?]98%
Oleyl alcohol	(Z)-Octadec-9-en-1-ol	268.48	849	Sigma-Aldrich	[?]99%
Isobutanol	2-methylpropan-1-ol	74.122	802	Sigma-Aldrich	[?]99%
Dimethyl adipate	Dimethyl hexanedioate	174.19	1060	Sigma-Aldrich	[?]99%
Isopropyl methyl ketone	3-Methylbutan-2-one	86.13	803	Sigma-Aldrich	[?]99%
Methyl ethyl ketone	Butan-2-one	72.11	805	Sigma-Aldrich	[?]99%

1.

2. Results and Discussion

3. Physical Extraction Results

Physical extraction studies were executed by using pure solvents alone. Oleyl alcohol and isobutanol were the types of alcohol, isopropyl methyl ketone and methyl ethyl ketone were the types of ketone, and dimethyl adipate was the type of ester used in the physical extraction experiments. The initial acid concentration was varied from 0.04 to 0.06 mole kg⁻¹ and the results were expressed in terms of K_D and E % (see Table 2). As seen from the E % values, ketones appeared to be the most effective solvents for HGA extraction, followed by alcohols. About 54 % extraction efficiency was achieved by isopropyl methyl ketone, and about 48 % extraction efficiency was achieved by methyl ethyl ketone. Ketones here seemed to be more successful at forming hydrogen bonds and dipole-dipole interactions with the acid molecule. For the ketones, the weakness

of the bonds between water and acid molecules provided easy accessibility to the acid molecules. Dimethyl adipate gave the lowest extraction efficiency of 21 %, which could be due to the higher affinity of HGA towards water than dimethyl adipate.

The initial pH of HGA was measured to be less than pK_a of HGA ($pK_a = 4.48$), showing that the maximum number of acid molecules was present in the undissociated form and could be distributed to the organic phase [27–29]. The physical extraction success is dependent on two main parameters; namely the distribution of undissociated acid molecule into the aqueous and organic phases and the dimerization of undissociated acid molecule in the organic phase [30, 31]. The distribution coefficient of acid was presented by Kertes and King [32]:

$$K_D = P + 2P^2D[HA]_{aq} \quad (3)$$

where P and D represent the partition coefficient and dimerization constant of acid, respectively. P is obtained from the slope and D is obtained from the intercept when K_D is plotted versus $[HA]_{aq}$ [29]. Dimer formation between the acid molecules occurs when acid-acid interactions dominate over the acid-solvent interactions. Thus, lower dimerization constant is expected for higher extraction efficiency. As seen in Table 2, P and D values have already an inverse relationship, which supports the assumption mentioned above. The solvents showing higher extraction efficiency are more successful at breaking the dimer formation between acid molecules and forming hydrogen bonds with acid molecules. As seen from the extraction efficiency and distribution coefficient results in Table 2, solvents alone were not capable to efficiently extract HGA. Therefore, for further experiments, Ph_3PO as a reaction-enhancing reagent was used together with the solvents to achieve higher extraction efficiencies and distribution coefficient values.

Table 2

Physical extraction results.

Diluent	[HGA] _{in} (kg mole ⁻¹)	[HGA] _{aq} (kg mole ⁻¹)	[HGA] _{org} (kg mole ⁻¹)	K_D	E %	P	D	R^2
Oleyl alcohol	0.06	0.046	0.014	0.304	23	0.78	19.59	0.99
	0.05	0.042	0.008	0.194	16			
	0.04	0.037	0.003	0.090	8			
Dimethyl adipate	0.06	0.047	0.013	0.276	21	0.32	62.64	0.99
	0.05	0.041	0.008	0.194	16			
	0.04	0.035	0.004	0.122	10			
Isobutanol	0.06	0.033	0.026	0.805	44	0.09	1308.34	0.99
	0.05	0.029	0.020	0.704	41			
	0.04	0.024	0.015	0.613	38			
Methyl iso- propyl ketone	0.06	0.027	0.032	1.213	54	0.41	20.34	0.99
	0.05	0.024	0.025	1.058	51			
	0.04	0.021	0.018	0.850	45			
Methyl ethyl ketone	0.06	0.030	0.029	0.942	48	0.27	152.60	0.99
	0.05	0.026	0.023	0.858	46			
	0.04	0.022	0.017	0.764	43			

Reactive Extraction Results

The complex formation between acid and extractant molecules is the chief difference between the reactive and solvent extractions. Trioctylphosphine oxide, tributyl phosphate, and Cyanex 23 are the types of organophosphorus extractants that have been broadly used to recover carboxylic acids [5, 28, 33–36]. Organophosphorus extractants have good chemical stability, they are effective in acid recovery and their recycle is possible. Besides, they co-extract water in negligible amounts. The phosphoryl group present in the organophosphorus extractant and the carboxylic group of the carboxylic acid react with each other, and so an acid-extractant complex forms.

Reactive extraction results are presented in terms of K_D and $E\%$ in Table 3. Fig. 1a-b shows the change in K_D and $E\%$ values versus the change in Ph_3PO concentration. The results in the presence of reactive extractant were better compared to the conventional solvents alone. The physical extraction efficiencies were 23, 21, 44, 54, and 48 % with oleyl alcohol, dimethyl adipate, isobutanol, methyl isopropyl ketone, and methyl ethyl ketone, respectively. Methyl isopropyl ketone and methyl ethyl ketone showed the best performance in terms of extraction efficiency, followed by isobutanol, dimethyl adipate, and oleyl alcohol. As seen, inadequate extraction efficiencies were obtained in the case of physical extraction. For the reactive extraction experiments, Ph_3PO was varied from 12 % to 44 % by volume in the solvents to see its effect on the efficiency. Remarkably, in the presence of Ph_3PO , the efficiencies increased up to 61, 76, 86, 67, and 84 %, respectively. All the reactive extraction efficiencies, even at the lowest TPPO amount, are quite higher than those obtained in the physical extractions. These great differences emphasize the importance of the reactive extractant. As seen from Fig. 1 and Table 3 that K_D values followed identical sequences with $E\%$ values. It is clear from the reactive extraction results that the acid-extractant complex was poorly solved by oleyl alcohol and dimethyl adipate, and thus the use of them with Ph_3PO would not be suggested. Whereas, acid-extractant complex was efficiently solved by the ketones and isobutanol, and therefore the use of isobutanol, methyl isopropyl ketone, and methyl ethyl ketone with Ph_3PO would be suggested. Acid recovery is highly dependent on the extractant concentration. However, the extractants are expensive. For the sake of the economy, the extractant amount should be optimized. Irrespective of cost, a further increase in the Ph_3PO amount can cause a third phase formation if solvent amount would not be enough to solve the complex.

The solvent properties like dielectric constant, boiling point, density, molecular weight, Dimroth-Reichardt E_T parameter, and dipole moment (μ) have been attempted to correlate with K_D [37]. E_T parameter gives information about the ionization power of the solvent. However, there was no significant correlation found between K_D and them.

$$Z = \frac{[HGA]_{org}}{[Ph_3PO]} \quad (4)$$

The loading factor (Z) is the ratio of organic phase acid concentration to the organic phase extractant concentration. Basically, it is the fraction that shows how many acid molecules are loaded on an extractant molecule. The loading factors were calculated and written in Table 3. As seen, the higher extractant concentrations were used in the solvents, the less were the loading factor values, which can be expressed by the definition of Z [37]. The loading factor values were calculated to be less than 0.5, showing that there was no overload on the extractant molecule. In other words, one extractant molecule reacted with one acid molecule, showing 1:1 acid-extractant complex formation. The reaction between carboxylic group and phosphoryl group is shown in Fig. 2. The complexation constant K_E gives information about the type of the formed complex and estimated from the loading factors. If loading factors are less than 0.5, complexation constant values are calculated as in the below Eq. (5) [37, 38]:

$$\frac{Z}{1-Z} = K_E [HGA]_{aq} \quad (5)$$

where K_E is the experimental complexation constant of 1:1 acid-extractant complex formation, and it is found from the slope when $\frac{Z}{1-Z}$ is plotted versus $[HGA]_{aq}$ [39].

Mass Action Law Model explains the nature and type of the formed complex. First, acid and extractant

molecules interact with each other at the interphase, then complexation occurs, and afterwards the formed complex is solubilized in the solvent. Dipole-dipole interactions and hydrogen bonding enable dissolution of the complex in the solvent. Although according to the Mass Action Law model, activities of species are proportional to the concentrations of species, a non-ideal behavior can be observed for the equilibrium constant. The following equation gives the relationship of distribution coefficient with Mass Action Law model's equilibrium constant [27, 37]:

$$\text{Log } K_D = \text{Log } K_{E,\text{MAL}} + s \text{ Log } [\text{Ph}_3\text{PO}]_{\text{org}} \quad (6)$$

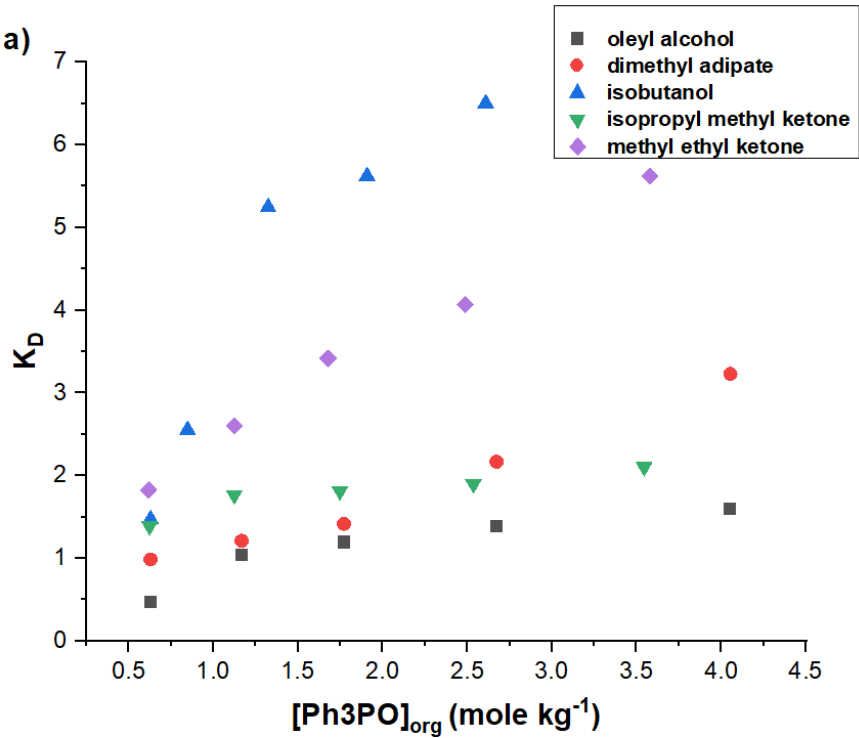
where $K_{E,\text{MAL}}$ is the equilibrium constant of the Mass Action Law model, s is the solvation number. $[\text{Ph}_3\text{PO}]_{\text{org}}$ is the organic phase Ph_3PO concentration. $K_{E,\text{MAL}}$ might be obtained from the intercept, when $\text{Log } K_D$ is plotted against $\text{Log } [\text{Ph}_3\text{PO}]_{\text{org}}$. Higher $K_{E,\text{MAL}}$ value means higher complexation. In this circumstance, solvent would have strong ability to solve the complex and the extractant would display high complexation potential with the acid [27]. $K_{E,\text{MAL}}$ values were found to be dissimilar to K_E values.

Table 3

The reactive extraction results.

Solvents	$[\text{Ph}_3\text{PO}]_{\text{org}}$ (mole kg^{-1})	$[\text{HGA}]_{\text{aq}}$ (mole kg^{-1})	$[\text{HGA}]_{\text{org}}$ (mole kg^{-1})	K_D	E %	Z	K_E	$K_{E,\text{MAL}}$
Oleyl alcohol	0.628	0.040	0.019	0.469	31	0.030	1.20	4.16
	1.166	0.029	0.030	1.033	50	0.026		
	1.771	0.027	0.032	1.193	54	0.018		
	2.672	0.025	0.034	1.386	58	0.013		
Dimethyl adipate	4.054	0.023	0.036	1.595	61	0.009		
	0.628	0.030	0.029	0.986	49	0.047	1.91	6.30
	0.847	0.027	0.032	1.211	54	0.038		
	1.323	0.024	0.035	1.416	58	0.026		
Isobutanol	1.908	0.018	0.041	2.166	68	0.021		
	2.609	0.014	0.045	3.229	76	0.017		
	0.623	0.024	0.035	1.472	59	0.057	2.55	7.76
	1.122	0.016	0.043	2.551	71	0.038		
Methyl iso-propyl ketone	1.746	0.009	0.050	5.245	83	0.028		
	2.536	0.009	0.050	5.623	84	0.020		
	3.545	0.007	0.052	6.501	86	0.014		
	0.616	0.025	0.034	1.388	58	0.056	8.81	1.62
Methyl ethyl ketone	1.122	0.021	0.038	1.764	63	0.034		
	1.676	0.021	0.038	1.813	64	0.023		
	2.487	0.020	0.039	1.899	65	0.015		
	3.577	0.019	0.040	2.104	67	0.011		
Methyl ethyl ketone	0.673	0.021	0.038	1.826	64	0.057	3.97	4.36
	1.130	0.016	0.043	2.606	72	0.038		
	1.740	0.013	0.046	3.417	77	0.026		
	2.577	0.011	0.048	4.070	80	0.018		

Solvents	$[\text{Ph}_3\text{PO}]_{\text{org}}$ (mole kg^{-1})	$[\text{HGA}]_{\text{aq}}$ (mole kg^{-1})	$[\text{HGA}]_{\text{org}}$ (mole kg^{-1})	K_D	E %	Z	K_E	$K_{E,MA}$
	3.609	0.009	0.050	5.623	84	0.014		



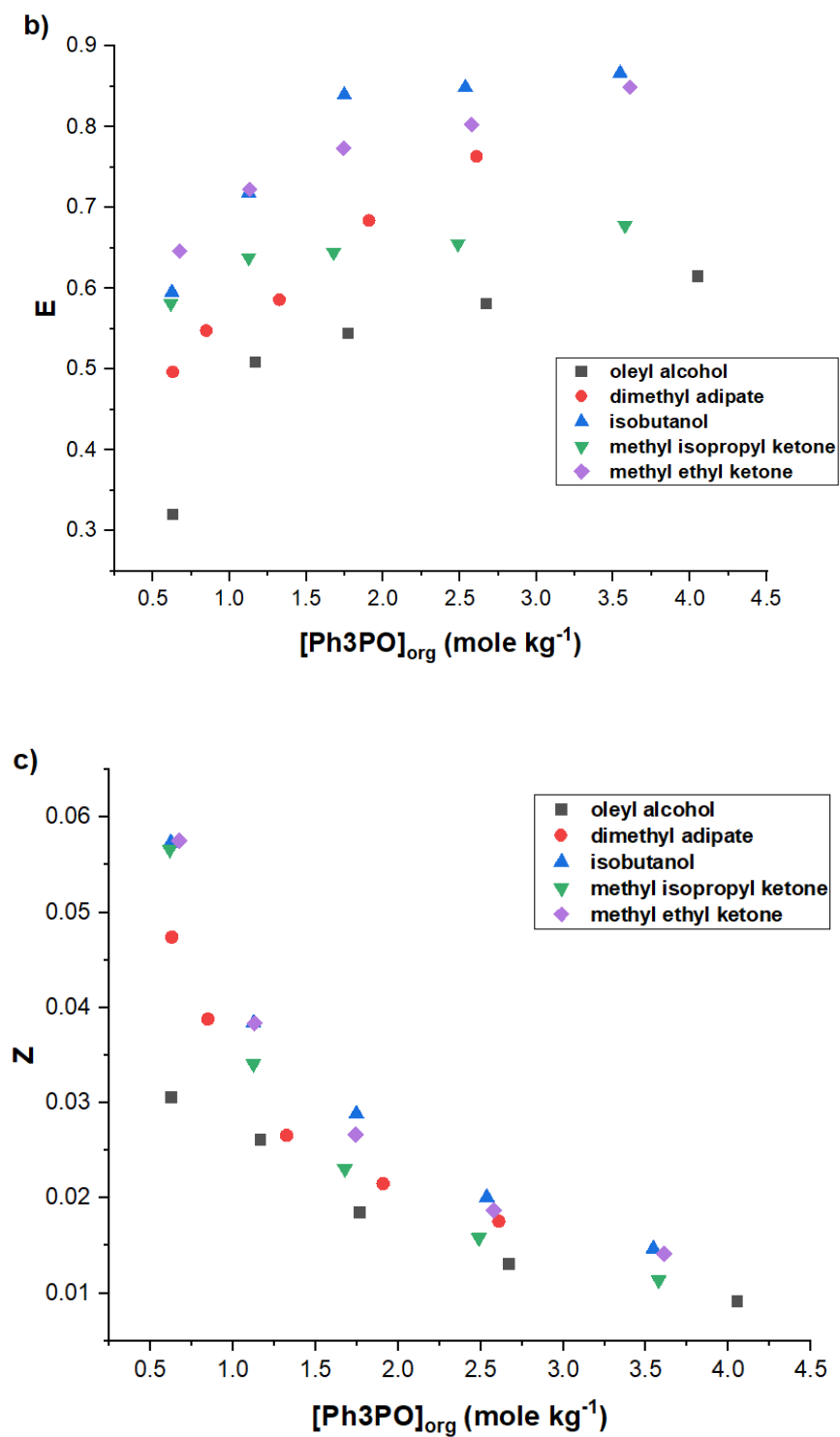


Fig. 1a-c. The change in concentration versus a) distribution coefficient, b) extraction efficiency, and c) loading factor.

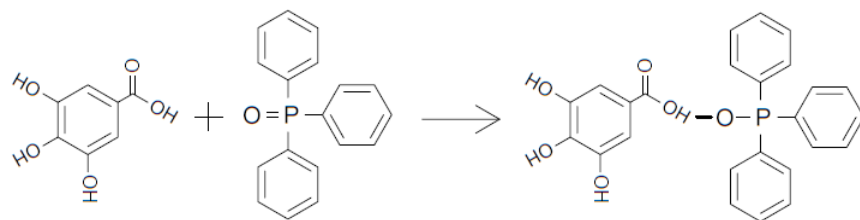


Fig. 2. The reactive extraction of HGA with Ph₃PO and the formation Ph₃PO-HGA complex.

Column design

Solvent to feed ratio (S/F) and the number of theoretical units (NTU) are important parameters to design a liquid-liquid counter-current extraction column. Basically, the S/F and NTU are calculated to reveal the applicability of column design [37].

$$(S/F)_{\min} = \frac{X_{\text{in}} - X_{\text{out}}}{K_D X_{\text{in}} - Y_{\text{in}}} \quad (7)$$

$$E_X = K_D \frac{S}{F} \quad (8)$$

$$\text{NTU} = \frac{\ln \left[\left(\frac{X_{\text{in}} - Y_{\text{in}} / (K_D)}{X_{\text{out}} - Y_{\text{in}} / (K_D)} \right) (1 - 1/E_X) + \frac{1}{E_X} \right]}{\ln E_X} \quad (9)$$

where x_{in} and x_{out} are the HGA concentration in the feed and raffinate phases, Y_{in} is HGA concentration in the extract phase. As a known rule, $(S/F)_{\text{act}}$ is calculated by multiplying $(S/F)_{\min}$ by 1.5. The NTU are calculated from the Eq. (9) above by using a Modifier Kremser equation [30, 37]. Here, E_x is the separation factor. In this study, the column design parameters, $(S/F)_{\text{act}}$ and NTU, were calculated based on the maximum Ph₃PO concentrations used in the solvents, the results of which are given in Table 4. As seen, around 2 to 4 NTU are needed to meet the targeted extraction efficiencies.

Table 4

Column design parameters.

Solvent	X_{out} (mole kg ⁻¹)	K_D	$(S/F)_{\min}$	$(S/F)_{\text{act}}$	E_X	NTU
oleyl alcohol	0.023	1.59	0.38	0.58	0.92	1.79
dimethyl adipate	0.014	3.22	0.23	0.35	1.15	2.55
isobutanol	0.007	6.50	0.13	0.20	1.32	3.73
methyl isopropyl ketone	0.019	2.10	0.32	0.48	1.02	2.07
methyl ethyl ketone	0.009	5.62	0.15	0.22	1.27	3.28

Thermodynamic Study

The temperature effect on the extraction efficiency was studied in the thermodynamic study. The highest efficiency was obtained by Ph₃PO in isobutanol in the reactive extraction experiments, and therefore further thermodynamic study was executed with Ph₃PO in isobutanol. The thermodynamic study was carried out at 298.2 K, 308.2 K and 318.2 K. The thermodynamic parameters were calculated by Van't Hoff equation given below [38, 40]:

$$\ln K_E = \frac{-\Delta H^0}{RT} + \frac{\Delta \Sigma^0}{R}$$

englishR (10)

$$\Delta G^0 = -R T \ln K_E \quad (11)$$

where, K_E is the equilibrium complexation constant, R is the universal gas constant ($8.314 \text{ J mol}^{-1}\text{K}^{-1}$). ΔH^0 , ΔS^0 and ΔG^0 are the changes in enthalpy, entropy, and free Gibbs energy, respectively. ΔH^0 and ΔS^0 might be estimated from the slope and intercept when $\ln K_E$ is plotted versus $1/T$. Similarly, ΔG^0 might be estimated from the Eq. (11). The results of thermodynamic study are tabulated in Table 5. The results showed that increasing temperature from 298.2 K to 308.2 K and 318.2 K adversely affects the efficiency. Acid-extractant interactions seem to be reduced here with higher temperatures. However, the differences were not quite sharp. Likewise, Wasewar et. al. studied the reactive extraction of protocatechuic acid and found similar results [38]. The room temperature generally produces the best results for the recovery of carboxylic acids. From the thermodynamic parameters ΔH^0 , ΔS^0 and ΔG^0 were found to be negative. The negative ΔH^0 value revealed the exothermic nature of the complex formation. The negative ΔS value showed that the order of the system increased, which might be due to the complex formation. Lastly, the negative ΔG^0 value confirmed that the examined reactive extraction process is energetically favorable.

Table 5

Thermodynamic parameters.

T (K)	[Ph ₃ PO] _{org} (mole kg ⁻¹)	[HGA] _{in} (mole kg ⁻¹)	[HGA] _{aq} (mole kg ⁻¹)	K _D	E %	Z	Ln K _E	$\Delta H^0 \text{ J mole}^{-1}$	$\Delta \Sigma^0 \text{ J mole}^{-1} \text{ K}^{-1}$
298.2	19.764	0.06	0.002	23.025	0.95	0.002	1.731	- 10697.15	-44.71
	12.936	0.05	0.004	11.549	0.92	0.004			
	8.384	0.04	0.008	6.225	0.86	0.006			
308.2	19.764	0.06	0.005	10.491	0.91	0.002	1.294		
	12.936	0.05	0.005	9.146	0.90	0.004			
	8.384	0.04	0.006	8.883	0.89	0.006			
318.2	19.764	0.06	0.006	8.171	0.89	0.002	0.593		
	12.936	0.05	0.007	6.818	0.87	0.004			
	8.3848	0.04	0.008	6.144	0.86	0.006			

3.2.3. Gradient Boosting

The Gradient Boosting algorithm is a machine learning technique for regression and classification problems, which produces a prediction model in the form of a set of weak prediction models, usually decision trees. It builds the model in steps like other reinforcement methods, and generalizes them by allowing the optimization of an arbitrary differentiable loss function [41, 42]. The algorithm's objective is to create a chain of weak models, where each one aims to minimize the error of the previous model through a loss function. The adjustments of each weak model are multiplied by a value called the learning rate. This value aims to determine the impact of each tree on the final model. The lower the value, the lower the contribution of each tree. Scikit-Learn has precisely and effectively implemented the Gradient Boosting algorithm for solving classification and regression problems. In this work, the Gradient Boosting algorithm is analyzed in a classification model. The data is provided by the library itself, which has a Dataset package. Table 6 shows the results of Gradient Boosting technique. The precision and accuracy of Gradient Boosting technique is tested by taken random data from Table 3. Table 6 analyzes the model's accuracy metrics in relation to the experimental data. The first row presented in Table 6 is the behavior of the explained variance. The explained variation measures the proportion for which a mathematical model is responsible for. Randomly taken values from Table 3 are written in Table 7 and calculated also by the model. The accordance between the model's and experimental values are approximately 92%, 95%, and 86% for K_D , E and Z values, respectively. In practice, these percentages show how accurate is the model. The second row presented in Table 6 is the

mean absolute error (MAE). In statistics, the MAE is a measure of errors between observation pairs that expresses the same phenomenon. A lower MAE value is desirable for an accurate model.

Table 6

Mean Absolute Error (MAE) results of Gradient Boosting algorithm.

Explained Variance	Explained Variance	Explained Variance
K_D	E %	Z
0.92894525	0.95382577	0.86591146
MAE	MAE	MAE
0.13146782	1.26640486	0.00679955

Explained Variance - If \hat{y} is the estimated target output, y the corresponding (correct) target output, and r^2 is Variance, the square of the standard deviation, then the explained variance is estimated. And If \hat{y} is the predicted value of the i -th sample, and y is the corresponding true value, then the mean absolute error (MAE) is estimated. (For detailed explanation see Supported Material.)

Table 7

The comparison between Experimental and Model Results.

		Experimental outcomes	Experimental outcomes	Experimental outcomes
	$\text{Ph}_3\text{PO}]_{\text{org}}$ (mole kg^{-1})	K_D	E %	Z
Methyl ethyl ketone	0.673	1.82	64	0.057
Dimethyl adipate	2.609	3.22	76	0.017
Isobutanol	0.623	1.47	59	0.057
Methyl isopropyl ketone	1.676	1.18	64	0.023

Conclusion

In this study, the reactive extraction of HGA by Ph_3PO was examined. The highest extraction efficiency of 86 % was achieved by Ph_3PO in the presence of isobutanol. Methyl ethyl ketone gave 84 % extraction efficiency. A remarkable improvement was achieved by oleyl alcohol and dimethyl adipate. The physical extraction efficiencies with oleyl alcohol and dimethyl adipate alone were 23 and 21 %, respectively. Whereas, their extraction efficiencies reached up to 61 and 76 % in the presence of 44 % Ph_3PO concentration by volume in the organic phase, respectively. The loading factor values were less than 0.5, proving the 1-1 acid-extractant complexation. The acid-extractant complex formations were also examined by equilibrium constant (K_E) values. The necessary number of theoretical units to design an extraction column was found to be between 2 and 4. From the thermodynamic study results, this examined reactive extraction process was revealed to be spontaneous, exothermic and feasible in nature. In this work, we presented the Gradient Boosting algorithm, which comprises a systematic strategy for building forecasting committees. The use of this algorithm in chemical engineering prediction problems is still quite recent, but the results presented in this work are encouraging.

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