Caffeine Extraction from Spent Coffee Grounds by Solid-liquid and Ultrasound-assisted Extraction: Kinetic and Thermodynamic Study

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Abstract

Coffee is the most essential drink today, aside from water, the high consumption of coffee and the byproducts of its soluble industries such as spent coffee grounds can have a negative effect on the environment as a source of toxic organic compounds. Therefore, caffeine removal from the spent coffee ground can be applied as a method to limit the effect of its production on the environment. The aim of this study is to determine the kinetics and thermodynamics parameters and develop models for both processes based on the process parameters by using traditional solid-liquid extraction and Ultrasound-assisted extraction methods. The processes were performed at a temperature range of 25 to 55 °C for traditional and ultrasound baths, and experimental time ranged from 5- 60 min. The results demonstrated that under the above conditions, the extraction process applies to the pseudo-first-order reaction, where the rate constant K value increases with temperature. The transition state parameters were also discussed where these parameters indicated that the system of the process exhibited an activated complex formation state resulting in a thermodynamically unfavorable process, and the thermodynamic parameters at the equilibrium state were also evaluated in terms of the obtained yield percentage. The results also showed that the ultrasound-assisted bath process showed a spontaneous behavior at temperatures of 45 °C and 55 °C with Δ°G of -1192.9703 and - 2725.25 J/mole. On the other hand, for the traditional method, the extraction process was approaching a spontaneous behavior with the temperature increasing where at 25 °C the Δ°G value was 10379.944 J and at a temperature of 55 °C it reached 8004.26 J/mole.

1- Introduction

Coffee consumption as a beverage started a long time ago and until the present day, coffee consumption culture is growing, where it's consumed by millions of people on a daily basis [1]. The main ingredient to produce coffee drinks is green coffee beans, where these beans are harvested and treated in a long treatment path up to the point where they can be utilized for the making of coffee beverages [2], The long path of treatment for green coffee beans, and the process of preparing coffee beverages in houses and cafes, produces and wide range of by-products such as husks pulp sliver skin, and spent coffee ground [3].

Spent coffee grounds are the most valuable by-product of the coffee production process, its produced in cafes, restaurants, and houses from soluble industries of coffee preparation. The importance of spent coffee grounds comes from its high production rate, where 650 kg of spent coffee ground is produced per one ton of green coffee beans [4]. Spent coffee grounds' value comes from its high content in a wide range of organic compounds such as polyphenols and caffeine, which have an important value commercially and can be used in a wide range of applications [5, 6].

However, these organic compounds give spent coffee grounds a toxic nature, whereas when untreated spent coffee grounds are disposed of in the environment, their decomposing can produce greenhouse gases such as carbon dioxide and methane contributing to global warming. Furthermore, its disposal can alter the acidity of the landfill and the surrounding area's soils, which can affect the environment negatively [7].

Caffeine is an alkaloid that is contained in spent coffee grounds, where 9 mg of caffeine is contained per 1 g of spent coffee grounds [8]. Due to the high rate of coffee consumption, which resulted in high amounts of spent coffee ground production from soluble coffee industries, high amounts of caffeine accumulated in the environment. This high accumulation led caffeine to be considered an emerging pollutant, which is a material that might affect the environment negatively in the near future. Through changing its water and soil nature, affects the living

organisms at macro and micro levels including humans [9].

On the above bases, Caffeine removal from spent coffee grounds can limit its effect on the environment. Furthermore, Caffeine is an important compound with a wide range of industrial and pharmaceutical applications, therefore its recovery can be of economic industrial benefit [10, 11].

The recovery of caffeine can be performed by solid-liquid extraction which is a process that depends on the concentration gradient between the solid matter and the solvent and includes the transformation of the solute through the pores of the solid matter from the bulk of the solid matter to the bulk of the immiscible solvent [12]. This process can be performed into methods, the traditional method, which is a well-established method for caffeine extraction, where circular mixing occurs to enhance the mass transfer rate of the solute through the solvent [13-15]. Alternative green nontraditional methods such as ultrasound methods, can also be used for caffeine recovery.

In these methods, ultrasounds are assisted to enhance the penetration of solute through the solid matrix [16-18]. Also microwave extraction method is another nontraditional technology that can be used for the purpose of caffeine extraction, where the microwaves are assisted to enhance the extraction process [19].

The determination of the kinetic and thermodynamic properties on the solid-liquid extraction process provides a better understanding of the nature of the reaction, in terms of whether it's spontaneous or not, and how the chosen parameters affect the extraction of the chosen material [20, 21], therefore, the kinetic and thermodynamic parameters for the extraction of bioactive compounds were covered in a number of studies such as, Hamadamin, 2022 which performed caffeine extraction from tea leaves while studying the effect of *Citrus aurantifolia* on the process, the results obtained by this study showed that the process of caffeine applies to the pseudo first order model, and extraction exhibited a spontaneous reaction behavior at a temperature range of 30 to 100 °C with activation energy values up to Ea = 9.89 kJ/mol [22], and another study which used the Peleg's model to describe the extraction process of bioactive compounds from a number of plants dandelion, marigold and yarrow, the results obtained by this study showed that the chosen model was the best to describe the extraction process, and the best achieved recovery of bioactive compounds and polyphenols was at a temperature of 80 °C, however, regardless of the high recovery the process remained thermodynamically unfavorable and nonspontaneous [23].

The current study focused on studying the effect of temperature and time on the rate constant values. Furthermore, the study included the kinetic study, thermodynamic study, and finding the order of the reaction and the best model that describes the results obtained from the experimental work, also our study involved the determination of the yield percent of caffeine, and the calculations of the equilibrium rate

constant and thermodynamic parameters at the equilibrium state

2- Experimental Work

2.1. Plant materials

Spent coffee grounds were collected from (House of Dough, Baghdad Al-Jadriya), which is a local bakery. The percolation method was used to prepare coffee beverages using a high-pressure professional coffee-preparing machine. Samples were collected each week for a number of months, and the obtained samples showed that the spent coffee grounds are produced on an average of 0.5-1 kg each week. Obtained samples were dried at 110 °C for 4 hours, and were stored in a closed serialized container at room temperature.

2.2. Sample preparation and extraction processes

Five grams of spent coffee grounds were weighed and suspended in 100 ml of distilled water, the sample was prepared in a 200 ml Duran, and the total caffeine spent coffee grounds content was determined by a microwave oven (model: AO-08895-14) where the sample was placed in a microwave oven and samples were obtained after 25 sec for the first sample and every 5 min for the remaining samples. An incubator shaker (model: G-24 M1036-0000G) was used to perform the traditional process under the condition of (mixing speed= 250rpm, pH = 6) the sonication process was performed in a sonication bath (model: AO-08895-14), temperature effect was studied in the range of (25-55 °C) for a time period of (5- 60 min) for each method, the first sample was obtained after 5 min and the remaining samples were taken every 15 min, all the above samples were obtained using a 5ml syringe and the samples were filtered using a syringe filter of 0.22 μm filter and were placed in a sample tube for further analysis. For the determination of the total caffeine content in the sample the same weight of 5g of spent coffee ground was suspended in 100 ml of water and microwave-assistant extraction was performed to determine the saturation concentration.

2.3. High-performance liquid chromatography (HPLC) analysis

The analysis was performed using an HPLC device with the following specifications: (model 1514 Shimadzu Corporation) Zorbax Eclipse Plus 18 C Column, pore size 5μ, internal diameter 4.6nm and length 150 mm, Reverse phase – ODS and Flow rate of 1 ml/min (constant). The column temperature was at 40 °C and the UV detector was set at 275 nm. The mobile phase was water: methanol (60:40) where both are HPLC grade. The injection sample volume was 10 μ.

2.4. Kinetic and thermodynamic analyses equations

The equations below were used to fit the obtained concentration data to the pseudo-first-order model, where

values of K the rate constant were determined at each temperature, using the values of the obtained caffeine concentrations:

$$\frac{dC_t}{dt} = k(C_s - C_t) \tag{1}$$

Where: K ($Lmg-1\ min-1$): is the rate constant for the 1st order model. Cs (mg/L): is the concentration of caffeine at saturation (extraction capacity). Ct (mg/L): is the concentration of extracted caffeine at any time t (min). Eq .2 is generated by combining variables:

$$\frac{dC_t}{(C_s - C_t)} = k\ dt \tag{2}$$

With the boundary conditions being: $t = 0, C_t = 0$.
Eq .3 was obtained by the integration of the rate equation for a 1st order model and further, the linearization Equation may be rearranged to this formula:

$$ln(Cs - Ct) = kt + lnCs \tag{3}$$

Cs which is the extraction capacity, and the k rate constant of pseudo first order 1st extraction, can be calculated experimentally and by the linear Eq.2plotting, where t vs ln (Cs-Ct) whereby k is determined from the slope of the linear plot, and Cs from the intercept respectively.

The thermodynamics parameters were calculated using the following equations:
Firstly, the activation energy Ea in joule and Arrhenius constant in min-1 were evaluated from the Arrhenius model in its linearized formula:

$$lnk = \frac{-E_a}{R} * \frac{1}{T} + lnA \tag{4}$$

Where: K ($Lmg^{-1}\ min^{-1}$) = is the rate constant for the 1st-order model. Ea (J) = activation energy. R (J.K/mole) = gas constant. T (K) = experiments temperatures. A (min^{-1}) = Arrhenius constant.

After evaluating the activation energy value and the Arrhenius constant value the values of enthalpy ΔH entropy ΔS and Gibes energy ΔG energy of the process were calculated, respectively using the following transition state equations:

$$\Delta H^{\neq} = E_a - RT \tag{5}$$

$$A = \frac{RT}{Nh} e^{\frac{\Delta S^{\neq}}{R}} \tag{6}$$

$$\Delta G^{\neq} = \Delta H^{\neq} - T\Delta S^{\neq} \tag{7}$$

Where: ΔH$^{\neq}$ (J/mole) = enthalpy of the process. ΔS$^{\neq}$ (J.K/mole) = entropy of the process. ΔG$^{\neq}$ (J/mole) = Gibbs energy of the process. N (mol^{-1}) = avogadro's number. h (J.sec) = Planck constant

For the calculation of thermodynamics parameters at equilibrium the rate constant at equilibrium was calculated by the determination of the equilibrium yield,

the maximum yield, and the extracted yield at each temperature using the following equations:

$$yield = \frac{mass\ of\ the\ extract}{mass\ of\ the\ sample} * 100\% \tag{8}$$

$$Ye = \frac{maximum\ mass\ of\ caffiene\ extraction}{mass\ of\ sample} * 100\% \tag{9}$$

$$Yt = \frac{mass\ of\ maximum\ yield\ with\ temperature}{mass\ of\ the\ sample} * 100\% \tag{10}$$

$$Yu = Ye - Yt \tag{11}$$

$$Keq = \frac{Yt}{Yu} \tag{12}$$

$$\Delta G = -RTlnKeq \tag{13}$$

$$lnKeq = -\frac{\Delta H}{R}\frac{1}{T} + \frac{\Delta S}{R} \tag{14}$$

Where: Ye: is the yield of extraction percent at equilibrium. Yt: the maximum yield percent at each temperature. Yu: the extracted yield percent at each temperature. K= constant rate at equilibrium. T (k) = temperature of the experiment. R (J.K/mole) = gas constant. Δ°G (J/mole) = Gibbs free energy at equilibrium. Δ°H (J/mole) = Enthalpy at equilibrium. Δ°S (J/K mole) = Entropy at equilibrium

The values of enthalpy and entropy at equilibrium will be determined by the plot of lnK vs 1/T as shown in the linear Eq . 14, from the slope and the intercept of the line respectively.

3- Result and Discussion

3.1. Kinetic model

The kinetic model section includes a full decision of the extraction process kinetics representation for traditional shaker extraction and sonication extraction techniques of caffeine. The results attempted to assess the data shown in Table 1 obtained by using Eq. 1 and Eq. 2. and the linearity demonstrated in Fig. 1. to Fig. 8. to prove that the pseudo-first-order kinetic model applies to our study results.
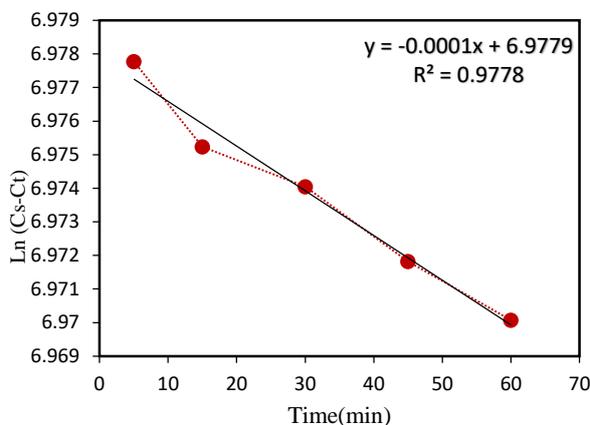
In general, the process of solid-liquid extraction of Caffeine consists of three stages firstly, solvent permeation through the matrix then, solute solubilization in the solvent and the diffusion of the solute through the solvent which is governed by Fick's law [24], all three stages were represented in the 1st order pseudo model, the first stage of the extraction is where water permeates through the walls of the spent coffee grounds particles reaching the insides of the particles, after the contact between the particles and the solvent the solute (caffeine) starts to dissolve in water, every technique assists the contact between the water and caffeine by different mechanisms, for the incubator shaker the circular mixing motion increase the surface area for the contact and the caffeine diffusion, for the ultrasound the power the ultrasound waves causes the destruction to the particle wall causing for contact enhancement, and a higher

surface area for the mass transfer, all the results were fitted and applied to the equation of the model with R2 ≥ 0.9, see Table 1.
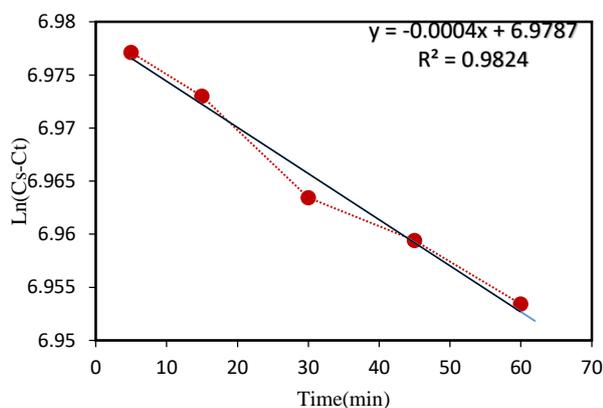
The modeling results showed that changing the temperature caused in increasing the reaction rate constant in a noticeable way, the rate constant remained increasing from 0.00013 at the temperature of 25 °C to 0.015976 at a temperature of 55 °C sonication bath process. For the shaker process, the reaction extraction constant increased from 0.000133 at a temperature of 25 °C to 0.001355 at 55 °C. The higher value of the rate constant in the sonication bath compared to the values in shaker extraction can be explained by the ultrasound waves enhancing the extraction process and increasing the extraction rate.

The values of the rate reaction constant are close to the values obtained in the literature, where according to Hamadamin, 2022 [22], the rate constant to extract caffeine at a temperature of 30 °C was around 0.0062 and when increasing the temperature to 60 °C the rate constant increased to 0.00155 when extraction caffeine from fresh tea by using an aqueous organic mixture at different temperatures of (30, 60, 80 and 100 °C) for a total stirring time of 40 min.

Table 1. Parameters of Pseudo 1st First Order Kinetic of Extraction Techniques

Extraction method	Temperature T °C	Rate constant K	Correction factor R²
Solid-liquid Extraction	25	0.000133	0.97
	35	0.000434	0.98
	45	0.001068	0.97
	55	0.001356	0.9
Sonication Bath Extraction	25	0.001024	0.98
	35	0.004114	0.96
	45	0.013579	0.93
	55	0.015976	0.98

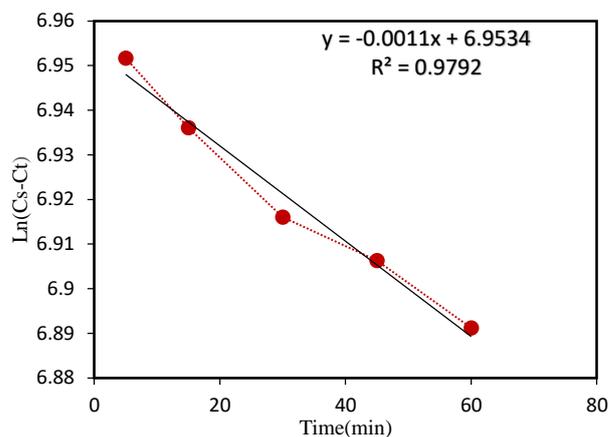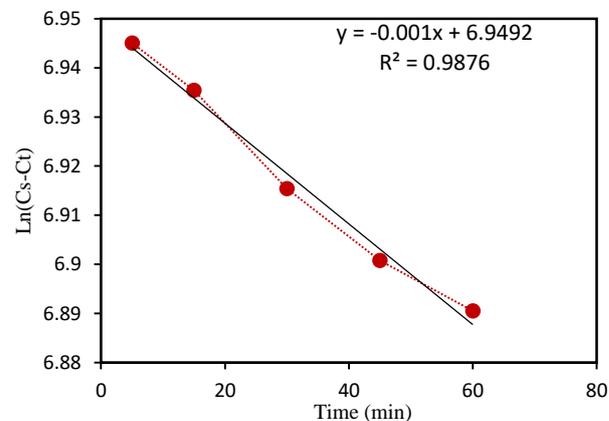**Fig. 3.** First Order Extraction Kinetics Via Incubator Shaker @ T= 45 ° C

Fig. 1. First Order Extraction Kinetics Via Incubator Shaker @ T= 25 °C
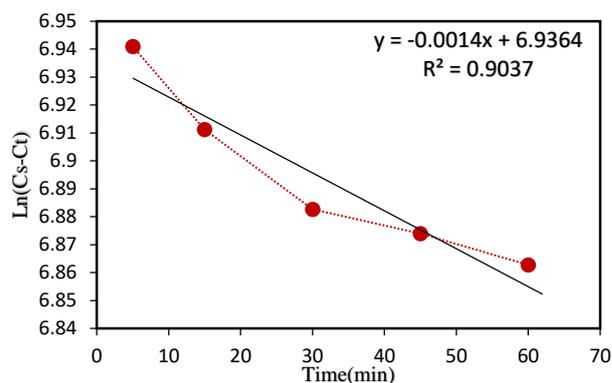
Fig. 4. First Order Extraction Kinetics Via Incubator Shaker @ T= 55 °C
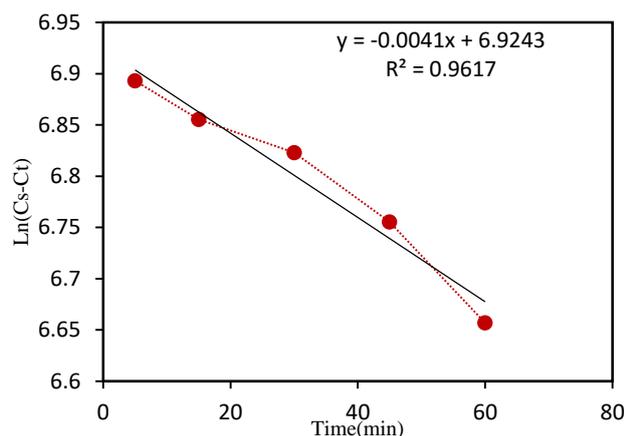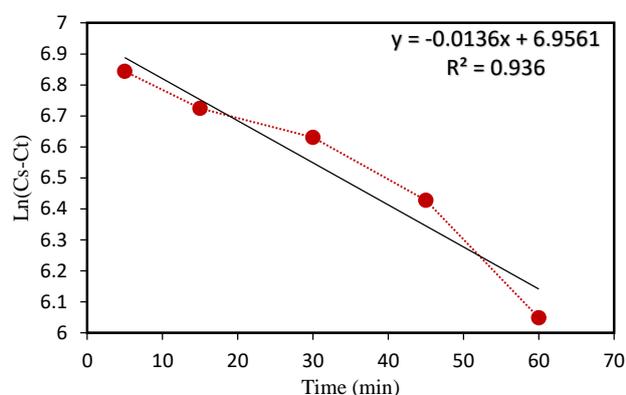

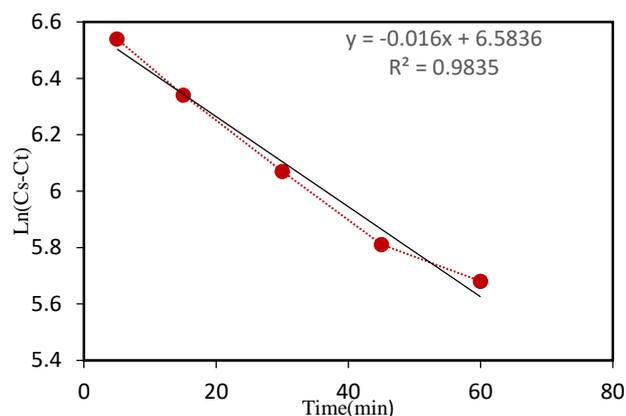**Fig. 2.** First Order Extraction Kinetics Via Incubator Shaker @ T= 35 °C

Fig. 5. First Order Extraction Kinetics Via Incubator Shaker @ T= 25 °C

Fig. 6. First Oder Extraction Kinetics Via Sonication @ T= 35 °C

Fig. 7. First Order Extraction Kinetics Via Sonication @ T= 45 °C

Fig. 8. First Oder Extraction Kinetics Via Sonication @ T= 55 °C

3.2. Thermodynamic analysis

This section includes a discussion of the thermodynamic parameters of caffeine extraction in both traditional solid-liquid extraction and sonication extraction. The thermodynamic parameters were calculated in transition and equilibrium state using the equations from Eq. 5 to Eq. 14, all the obtained data is demonstrated in Fig. 9. and Fig. 10, and Table 2 to Table 5. The values of thermodynamic parameters at the transition state showed

that the process of extraction is endothermic and energy is needed to enhance the rate of the reaction. Furthermore, negative values for the entropy obtained at the transition state can be explained as a loss in degrees of freedom due to the reacting species joining themselves to form a state transition during the extraction process known as activated complex formation, as a result, unfavorable thermodynamic conditions will occur, see Table 2, Table 4 [24-26].

However, regardless of the transition state showing a nonspontaneous process. The results showed in Table 3. and Table 5. of the evaluated Gibbs free energy at equilibrium depending on the equilibrium rate constant and yield percent, demonstrated that the extraction process is an endothermic process, and increasing the temperature will increase the value of spontaneous Gibbs energy by increasing the entropy of the system, which was achieved by the ultrasound effect which enhanced the penetration of solvent in the solute particles reaching a spontaneous state of -1192.975703-and -2725.25806 at temperatures of 45 and 55 °C, respectively. These results fall in line with the results obtained by Hamadamin, 2022 [22], when boiling tea with lime as an extraction catalyst, where the extraction process reached a spontaneous state at a temperature of 30 °C. For the shaker extraction process, the values of Gibbs free energy remained positive, this indicates that the energy consumption for the disorganization of the solid particles in the solvent medium $\Delta°H$ is greater than the energy consumed for the solid particles reorganization $(T\Delta°S)$, resulting a thermodynamically unfavorable process [22, 27]. These positive values were found to be decreasing with temperature increasing, where at a temperature of 25 °C $\Delta°G = 10.377$ Kj/mole and it decreased to $\Delta°G = 8.004$ Kj/mole at a temperature of 55 °C, which indicates that increasing the temperature leads to a more spontaneous process.

Table 2. The Values of the Transition State Via the Shaker Method

T(K)	S*(J/mole.K)	H*(J/mole)	G*(J/mole)
298.15	-135.64	5266.442	45707.82
308.15	-135.91	5183.30	47065.61
318.15	-136.18	5100.16	48426.10
328.15	-136.43	5017.02	49789.20
E(J)= 7745.261898			
LnA(1/Sec)= 13.14282035			

Table 3. The Values of Equilibrium Yield (Ye), Total Yield at Each Temperature (Yt), Un Extracted Yield (Yu), Rate Constant at Equilibrium (Keq), Gibes Free Energy at Equilibrium ($\Delta°G$), Entropy at Equilibrium ($\Delta°S$), and Enthalpy at Equilibrium ($\Delta°H$) for Shaker

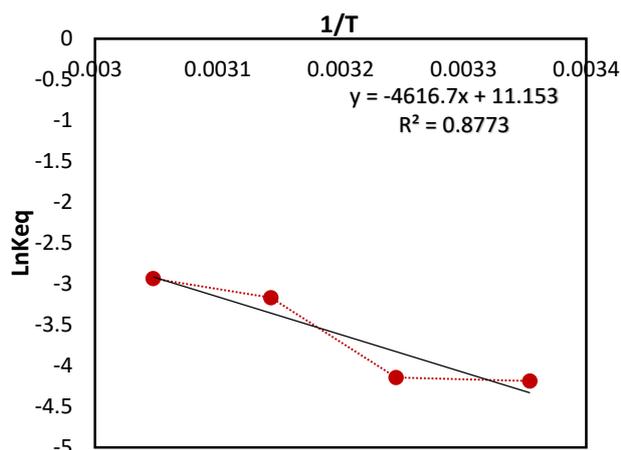| Ye	Yt	Yu	Keq	lnkeq	$\Delta°G$ J/mole
2.178	0.0490	2.1289	0.0152	-4.1875	10379.94
2.178	0.0842	2.0938	0.0159	-4.1441	10616.93
2.178	0.2104	1.9676	0.0420	-3.1699	8384.84
2.178	0.2655	1.9125	0.0532	-2.9339	8004.26
$\Delta°H$(J/mole)=38382.97702					
$\Delta°S$(J/K.mole)=92.72330141					

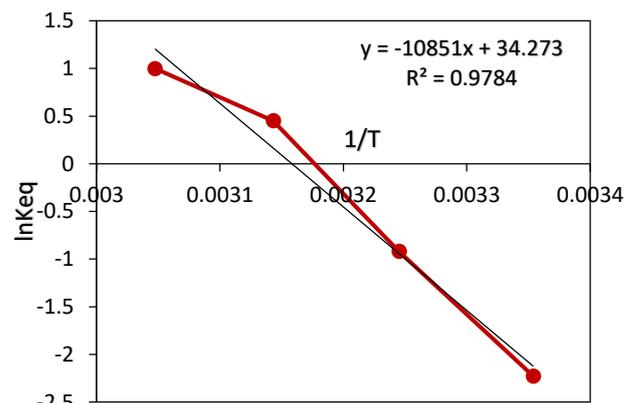**Fig. 9.** Thermodynamic Parameters at Equilibrium for Shaker

Fig. 10. Thermodynamic Parameters at Equilibrium for Sonication

Table 4. The Values of the Transition State via the Sonication Method

T(K)	S*(J/Kmole)	H*(J/mole)	G*(J/mole)
298.15	-74.92023333	-1359.93	20977.53449
308.15	-75.19451187	-1443.07	21728.11575
318.15	-75.4600302	-1526.21	22481.39553
328.15	-75.71733064	-1609.35	23237.28897
E(j)=1118.886019			
LnA(1/Ses)= 20.44626			

Table 5. The Values of Equilibrium Yield (Ye), Total Yield at Each Temperature (Yt), Un Extracted yield (Yu), Rate constant at Equilibrium (Keq), Gibes Free Energy at Equilibrium (Δ°G), Entropy at equilibrium (Δ°S), and Enthalpy at Equilibrium (Δ°H) for Sonication Extraction

Ye	Yt	Yu	Keq	lnkeq	Δ°G J/mole
2.178	0.2118	1.9658	0.107753387	-2.227910117	5522.58615
2.178	0.6212	1.5564	0.399117021	-0.91850062	2353.161021
2.178	1.3302	0.8473	1.569902654	0.451013613	-1192.975703
2.178	1.5915	0.5861	2.715313291	0.998907339	-2725.25806
Δ°H (j)= 90219.26					
Δ°S(j/K)=284.9442					

4- Conclusions

This research aimed to show spent coffee ground as a possible source for caffeine extraction, two methods were utilized for the caffeine extraction under the effect of temperature effect in the range of (25- 55 °C) and for a time range of (5-60 min), The results showed that the extraction of caffeine was more efficient via sonication method, where after 60 min caffeine recovery reached up to 795.7 mg/L ,whereas, for the shaker method its only reached 132 mg/L, the efficiency of sonication is due to the combined effect of ultrasound to provide a higher contact level between the solute and the solvent , with the effect of temperature which produced a higher caffeine recovery , furthermore, the kinetic analysis demonstrated that our data fits to the pseudo first order model, where the correction factor for every figure was $R^2 \geq 0.9$, and the rate constant increased with temperature increasing reaching its highest value at K=0.001356 for the shaker traditional extraction and K= 0.015976 for the ultrasound-assisted extraction both at a temperature of 55 °C, caffeine is a bioactive important compound there for its extraction hold a high importance and the above kinetics

data can help in the process of sizing a reactor/extractor , furthermore the obtained equilibrium data can help with determining the best operating conditions., The thermodynamic study at equilibrium showed that the extraction process system for the shaker approached a spontaneous behavior with the temperature increasing, where the value of Gibbs energy at equilibrium decreased from 10379.94 J at a temperature of 25 °C to 8004 J/mole at a temperature of 55 °C showing that the process is approaching a favorable spontaneous state with the temperature increasing, in addition, the ultrasound-assisted process reached a favorable spontaneous state at the temperatures of 45 and 55 °C, where Gibbs free energy at equilibrium reached up to -1192.975703 and -2725.25806 J/mole, both of the extraction systems approaching a spontaneous state and achieving a spontaneous state indicates that the spontaneous nature of the extraction process increases with increasing the temperature, lastly, the positive values of the processes enthalpies Δ°H of 38382.97702 J/mole and Δ°H of 90219.26 J/mole indicated that the extraction process is endothermic, and the positive values of entropies of Δ°S

of 92.72330141 and $\Delta^{\circ}S$ of 284.9442 J/K.mole indicated that the process of caffeine extraction is an irreversible process.

Nomenclature

Symbols	Description	Units
Ea	Activation energy	J
A	Arrhenius constant	min^{-1}
N	Avogadro's number	mol^{-1}
C_o	Caffeine concentration in the control	mg/L
C_t	Caffeine concentration after degradation	mg/L
K	The constant rate at equilibrium	
R	Gas constant	J.K/mole
$\Delta^{\circ}G$	Gibbs free energy at equilibrium	J/mole
$\Delta G^{\neq}$	Gibbs free energy of the process	J/mole
$\Delta^{\circ}H$	Enthalpy at equilibrium	J/mole
$\Delta H^{\neq}$	Enthalpy of the process	J/mole
$\Delta^{\circ}S$	Entropy at equilibrium	J/K mole
$\Delta S^{\neq}$	Entropy of the process	J.K/mole
T	Experiments temperatures	K
h	Planck constant	J.sec
C_s	The concentration of caffeine at saturation (extraction capacity)	mg L
Ct	The concentration of extracted caffeine at any time t (min)	mg L
Yt	The maximum yield percent at each temperature	
Yu	The extracted yield percent at each temperature	
K	The rate constant for the 1st order model	L/mg.min
Ye	The yield of extraction percent at equilibrium	

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استخلاص الكافيين من القهوة المستهلكة عن طريق الاستخلاص السائل والسائل بمساعدة الموجات فوق الصوتية (دراسة حركية وديناميكية حرارية)

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الخلاصة

القهوة تعد المشروب الاكثر اهمية اليوم, باستثناء الماء, الاستهلاك العالي للقهوة والنواتج الجانبية من صناعات القهوة الذائبة مثل بقايا القهوة المستهلكة لها تأثير سلبي على البيئة,كمصدر للمواد العضوية السامة. لهذا السبب ازالة الكافيين من بقايا القهوة يمكن ان تطبق كطريقة للتقليل من اثر عملية انتاج القهوة على البيئة. الهدف من الدراسة الحالية هو تحديد موديل الديناميكا الحرارية وتطوير نماذج بناءً على معاملات العملية باستخدام طرق استخلاص السائل الصلب التقليدية و الاستخلاص بمساعدة الموجات فوق الصوتية. أجريت العمليات عند درجة حرارة تتراوح بين ٢٥ إلى ٥٥ م° للحمام التقليدي والموجات فوق الصوتية، وتراوح زمن التجربة من ٥ إلى ٦٠ دقيقة.

أظهرت النتائج أنه في ظل الظروف المذكورة أعلاه، ان عملية الاستخلاص تتطبق على تفاعل الدرجة الشبه اولية ، حيث تزداد قيمة المعدل K مع زيادة درجة الحرارة. تمت مناقشة معاملات الحالة الانتقالية أيضًا حيث أشارت هذه القيم إلى أن نظام العملية أظهر حالة تكوين لمعقد نشط مما أدى إلى عملية غير مفضلة من الناحية الديناميكية الحرارية، وتم أيضًا تقييم معاملات الديناميكية الحرارية في حالة التعادل من حيث نسبة الناتج التي تم الحصول عليها. أظهرت النتائج أن عملية الاستخلاص بمساعدة الموجات فوق الصوتية أظهرت سلوكاً تلقائياً عند درجات حرارة ٤٥ م° و٥٥ م° مع $\Delta G°$ من ١١٩٢,٩٧٠٣– و٢٧٢٥,٢٥– جول/مول. من ناحية أخرى، بالنسبة للطريقة التقليدية، كانت عملية الاستخلاص تقترب من السلوك التلقائي مع زيادة درجة الحرارة حيث كانت قيمة $\Delta G°$ عند ٢٥ م° هي ١٠٣٧٩,٩٤٤ جول وعند درجة حرارة ٥٥ م° وصلت إلى ٨٠٠٤,٢٦ جول/مول.

الكلمات الدالة: الكافيين، استخلاص السوائل الصلبة، الاستخلاص بمساعدة الموجات فوق الصوتية، دراسة الخواص الحركية، الديناميكا الحرارية.