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# Synthesis of Caffeine from Tea Leaves Using Different Extraction Techniques and Its applications

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UV spectroscopy

**ABSTRACT:**
Caffeine is a central nervous system (CNS) stimulant of the methylxanthine class drug discovered by German chemist Friedrich Ferdinand Runge. The pure state of Caffeine is a bitter, white crystalline, which is mostly used in pharmaceutical industry as caffeine sodium benzoate. Caffeine is the most widely used substance on the planet and is also one of the most researched in regards of how it affects the human body. In the present study Camellia sinensis assameca tea leaves are collected for the extraction of caffeine and then it will be isolated directly from tea leaves. The extraction of caffeine was carried out in two stages, namely solid liquid extraction (SLE) and liquid extraction (LLE). In the SLE operation, distilled water is used. The solubility of caffeine in water varies based on temperature. The LLE process is carried by various solvents which include di-chloro methane (DCM), Chloroform, Methyl acetate and many others which have less solubility towards the aqueous phase. Based on the percentage content of the caffeine in the tae sample, end user application of caffeine and federal government regulations, the selection of the solvent was carried.

The Experimental study was carried in a batch operation using two solvents dichloride methane and chloroform. 3- levels of extraction periods 30min, 45min and 60 minutes, 3- levels of temperatures 40, 50 and 60°C and 3-levels of mole ratios, i.e; water- tea leave weight ratio (Brew Ratio)(WTR) 10,15,20 are considered in the study. The procedure adopted for the analysis of caffeine uses the UV spectroscopy, which is calibrated in this section. Temperature is the parameter, which plays a crucial role in the extraction of caffeine as the solubility of the compound varies (increases) drastically at temperatures of 40°C and 60°C, the solubility of caffeine is 2.2 and 66.7 (% wt/wt) respectively. For lower WTR moles of '15, the yield is lesser order and at temperatures beyond to 50°C, there is drastic improvement of yield and is independent of extraction period. With higher water moles of 20, the caffeine yield is independent of extraction period for lower temperatures and is decreasing with time for higher temperatures of 60°C. A maximum of 2.42g of caffeine can be formed for 100g of tea leaves for the case. For the DCM solvent, the better range of the parameters observed are WTR= 20 and temperature of 60°C. In the selection of solvent for the extraction, various factors are to be accounted along with the yield, distribution coefficient other factors such as labour, health and environmental aspects.

**1.1: Introduction:** Caffeine (1,3,7 – trimethyl Xanthin-2,6-dihydroxy purine) is a psychoactive CNS stimulant drug. It is a bitter, white crystalline and is mostly used in pharmaceutical industry as caffeine sodium benzoate, caffeine citrate and in combination with painkillers such as aspirin and acetaminophen. Caffeine is present in the compounds like coffee, cocoa beans, kola nuts, tea leaves and a variety of exotic berries in a substantial amount.

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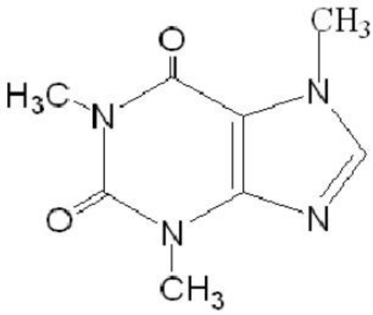
caffeine is widely consumed in the form of a beverage all over the world; it is a cardinal stimulant of the central nervous system with specific action on blood vessels. Caffeine is classified as a stimulant as it increases the activity of cardiovascular, digestive and sympathetic nervous system and produces the sense of alertness in the brain. It can have a lethal effect ( acute intoxication) when ingested at amounts of 1-5 g, with plasma concentrations higher than 80mg/ml and the first intoxication signs appear at about 250mg. Due to the various applications of the compound, different extraction techniques are developed to produce the compound on commercial scale.




**Figiure 1.1: The structural formuale of Caffeine**

**Table.1.1. Physical properties of Caffeine**

| | |
|---|---|
| Formula | $C_8H_{10}N_4O_2$ |
| Molar mass | 194.19 g/mol |
| IUPAC ID | 1,3,7-Trimethylpurine-2,6-dione |
| Melting point | 238 °C |
| Boiling point | 178 °C |
| Density | 1.23 g/cm³ |

**1.2. Various Extraction Processes of caffiene:**

The extraction of caffeine, also called, decaffeination, used to be carried out by treating the green coffee beans with a small amount of hot water and then exposing to a solvent (trichloroethylene) until 97% of the caffeine was removed. Residual solvent was removed after extraction by steam distillation. The process also removes wax from the beans, which are then roasted in the usual way. In these solvent based methods, the coffee beans are extracted as many as 10 times, maybe for as long as 10h until the required level of decaffeination has been reached. Caffeine can be extracted from cocoa by various methods, such as water extraction, supercritical carbon dioxide extraction and organic solvent extraction. The heat reflux extraction is one of the common methods used to extract caffeine from cocoa seed on a laboratory scale.

**1.3. Industrial and health applications of caffeine:**

To list the industrial applications of the compound include;

The caffeine can be converted into items that we use in our everyday lives - sodas, cosmetics & pharmaceutical products. Diet pills and cosmetic companies are the largest consumers of caffeine.

It is used in manufacturing body wash, soap, lip-balm, facial scrub and several other products such as caffeine lipstick. Caffeine increases memory, a 200 mg caffeine pill helped boost memory consolidation. The compound mixed with carbs replenishes muscle glycogen concentrations faster after exercise. Caffeine detoxes the liver and cleanses the colon when taken as a caffeine enema, relieves post-workout muscle pain by up to 48%., relieves pain associated with sleep loss better than analgesics. Caffeine may protect against Parkinson's disease. It prevented skin cancer in hairless mice and the showed that caffeinated coffee drinkers have less risk of developing melanoma.

**Deleterious effects of excessive caffeine consumption**

Under low to moderate consumption caffeine is healthier, but beyond to the limits it causes many physical and psychological disorders. Some of the more deleterious effects of excessive caffeine consumption can include the following.

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Men who drank more than four cups of coffee per day had a 21% increased risk of all-cause mortality compared with non-coffee drinkers. They also found that men and women who consumed excessive amounts of coffee were more likely to smoke and be in poor physical condition and Women who consume a lot of caffeine are 70% more likely to develop incontinence.

**2.1: Materials and Methods:** Various chemicals are used to carry out the extraction operation and to be listed they are, $Na_2CO_3$, Dichloromethane, Chloroform, Anhydrous $Na_2SO_4$, Black Tea (Leaves). **3.1: Calculation of Caffeine Yield:** In the process of extraction of caffeine, the reaction progress is defined in terms of yield, where ,

%Yield = (Weight of Caffeine/Weight of Sample)*100

**3.2 Distribution coefficient ($K_D$):** The distribution coefficient is defined as the ratio of the concentration of the solute in one phase to the concentration of the solute in the other phase under equilibrium conditions. It is the better a measure of the distribution of a solute among two in soluble phases usually aqueous and organic phases.

**4.0: Experimental Studies:** Caffeine is the compound which has high commercial value and can be extracted from various natural compounds such as coffee beads, fruits and tea leaves etc.The process of extraction of caffeine attracting many researchers, due to the commercial importance of the compound.

Extraction of caffeine involves the boiling of the source material in water to a specific higher temperature over a period of time and Sodium carbonate was added to the contents. The contents are further filtered to collect the aqueous layer and cooled to room temperature. The contents are transferred to a separating funnel and known amounts of Dichloride methane, DCM, were added and allowed to mix by gentle vibration such that no emulsion was formed. The contents are allowed to settle for separation of two layers. The bottom organic layer, which contains the desired compound, caffeine, is collected into a beaker and sodium sulphate was added. The contents are mixed well so that the associated water amounts are being entrapped by the salt.
The contents are further filtered and clear organic layer of caffeine was collected. The organic layer was allowed to heat to higher temperatures at which the DCM was completely evaporated and caffeine was formed. For the detailed analysis of the extraction of caffeine from tea leaves, types of organic solvents used and various parameters considered are presented in the following.

**Table.4.1: various parameters and their range considered in the study**

| Parameters | Range |
|---|---|
| Type of Tea leaves | Black Tea |
| Water- to- Tea ratio, (weight terms) | 10,15,20 |
| Organic Extractants used | Dichloromethane and Chloroform |
| Extraction Temperature | 40, 50 and 60 $^{o}$C |
| Period of Extraction | 30,45,60 min |
| Pressure | 1 atmosphere |

**4.2. Experimental:**
The extraction of caffeine from tea leaves experiment was carried in a batch operation. In a typical reaction, 10 grams of tea leaves and 10grams of sodium carbonate are weighed and transferred to 400ml beaker. 100ml of distilled water was added to the contents, mixed thoroughly with glass rod. The contents are placed in an oil bath and the temperature was increased to 40$^{o}$C and the extraction process was carried for 30minutes. After the specified time of heating, the contents all filtered using a filter paper.

Figure 4.1: (a) weighting of tea leaves

(b) Boiling of tea leaves with water and $Na_2CO_3$

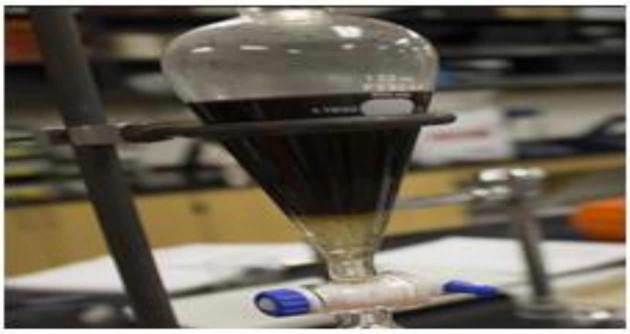

Figure4.2: Addition of first lot of DCM solvent ( 5ml) to the filtare and settling process

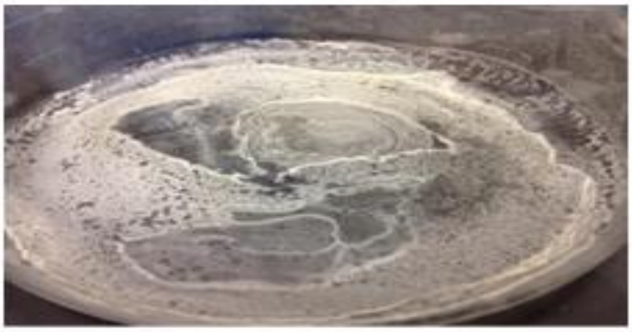

Figure 4.3: Caffeine extract observed after the drying of the DCM layer

The filtrate was allowed to cool to room temperature, transferred to a separating funnel and 20 ml of organic solvent (DCM) was added , in four equal lots (4x5 =20ml) , mixed the contents gently for 2 minutes and allowed to settle for 5 minutes. The bottom layer was collected into a conical flask. All the FOUR lots of the solvent layers are added together and 5g of $Na_2SO_4$ was added and mixed well to absorb the water content that present in the extract. The contents are further filtered to get the DCM layer which consists of caffeine, the desired compound. The DCM layer was heated gently to 30$^{o}$C at which the entire DCM solvent was evaporated and remains the Caffeine crystals.

**4.3. Analytical Procedure for Caffeine:**

**Preparing the calibration standards:** using a pipette add 25ml, 12.5ml, 10ml, 7.5ml, 5ml and 2.5ml to each of 6x 50ml volumetric flasks. Make the standards up to the 50ml volume using purified water. These amounts will create 100ppm, 50ppm, 40ppm, 30ppm, 20ppm and 10ppm calibration standards respectively (ppm = mg/L)

**Preparing the samples: A**dd 3.2g of dried tea leaves to a 250ml beaker and add 200ml boiling purified water. Stir at 500 rpm on a magnetic stirrer for 30 seconds, then leave to cool to room temperature without further stirring.

**Extract of caffeine from the samples:** take 50ml of the calibration standard or sample and it to a separating funnel. Use the measuring cylinder to add 25ml of dichloromethane. Invert the separating funnel 3 times and then vent to avoid pressure build-up. Put the funnel in a stand and allow the layers to separate, before removing the dichloromethane layer to a labelled conical flask. Return the calibration standard or sample to the separating funnel and repeat twice more, until 3x 25ml dichloromethane layers have been combined in the conical flask.

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**Measuring the calibration curve;** use a dropper pipette to add the calibration standards to the quartz cuvette for measurement. First measure purified water only as a blank, and then measures each of the calibration standards in increasing order of concentration. Tabulate the results of caffeine concentration in ppm vs. absorbance at 260nm.

**Calculation of the calibration curve;** use a spread sheet to create a line graph of the calibration curve results. Find the linear regression equation of the calibration curve, y = mx +c, where y is absorbance and x is concentration.

**Measuring the samples:** use a dropper pipette to add your first sample to the (cleaned and dried) cuvette. Take a measurement and record the absorbance at 260nm. Repeat for each sample, taking care to clean and dry the cuvette carefully between samples.

**Calculating the results;** using the calibration graph, concentrations of samples are calculated. Substitute y for the absorbance value recorded for that sample, keeping 'm and 'c constant, and rearrange to solve for x. For some models of spectrophotometer, a concentration mode is available which allows the instrument to do this calculation based on y = mx + c equation, so the readout on the spectrophotometer will be in ppm directly.

### 4.4. Observations & Calculations:

Initial Weight of Tea leaves = 10g , Water added = 100ml (STP conditions), i.e 1: 10 weight ratio of tea leave and water content, Extraction temperature =60°C, Extraction time = 60min, Total volume of filtrate (aqueous layer) = 88ml

Volume of the DCM added for extraction process = 4lots x5 =20ml

Concentration of DCM layer (From GC-MS analysis) = 0.0104 g/ml

Concentration of aqueous layer after four lots of extraction (from GC-MS analysis) = 0.000806 g/ml.

The distribution coefficient $K_D$ is defined as

$$K_D = \frac{Concentration\_of\_Caffeine\_in\_Organic\_Phase}{Concentration\_of\_Caffeine\_in\_Aqueos\_Phase}$$

= (0.0104 g/ml) / (0.000806 g/ml) = 12.9

Weight of caffeine extracted upon drying operation = 0.192g

Yield = (0.199/10) *100 = 1.92 g/100g of tea leaves taken

Calculations are carried for the both organic layer and aqueous layer and further the distribution coefficient is reported

**Table 4.1 Sample calculation for distribution coefficient for the extraction operation carried using DCM solvent (on Organic Layer Side)**

| | Calculation for Organic Layer | | | | |
|---|---|---|---|---|---|
| Extraction Period (min) | Temperature (oC) | Organic layer volume (ml) | Concentration of organic layer (g/ml) | Caffeine collected (g) | %Yield |
| 30 | 40 | 19.1 | 0.0053 | 0.1013 | 1.013 |
| | 50 | 18.4 | 0.0066 | 0.1217 | 1.217 |
| | 60 | 18.3 | 0.0080 | 0.1466 | 1.466 |

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**Table 4.2: Sample calculation for distribution coefficient for the extraction operation carried using DCM solvent (on Aqueous Layer Side)**

| Calculation for Aqueous Layer | | | | |
|---|---|---|---|---|
| Extraction Period (min) | Temperature (°C) | Aqueous Layer volume (ml) | Concentration of Aqueous Layer (g/ml) | Distribution Coefficient KD |
| 30 | 40 | 95.5 | 0.0006 | 8.4146 |
| | 50 | 92.1 | 0.0007 | 9.1861 |
| | 60 | 89.6 | 0.0008 | 10.139 |
| | | | $K_{D\,avg}$ | 9.24 |

**5.0: Results and Discussion:**

Detailed experimental study for extraction of caffeine from the tea leaves was presented and various parameters are considered for the analysis of the process. Effect of the all the parameters on the yield of caffeine were studied, using the two organic solvents dichloro methane, DCM and chloroform and were presented in the following.

**5.1 Extraction studies using the DCM solvent:**

Dichloromethane (or methylene chloride), DCM is a non-polar organic compound with the formula $CH_2Cl_2$. DCM's volatility and ability to dissolve a wide range of organic compounds made it a useful solvent for many chemical processes. In the present section, the effect of various parameters on the extraction of caffeine using the DCM solvent was presented.

**5.1.1. Effect of Water- Tea leaves weight ratio (Brew Ratio), WTR:**

Weight ratio of water to tea leaves plays an important role in the extraction of caffeine. As the solubility of caffeine is limited in water and is depending on the temperature, an optimum range of the WTR will be useful for the economic operation of the process. Figures 5.1 through 5.2 presents the effect of the Water-Tea leaves weight ratio on the yield of the caffeine.

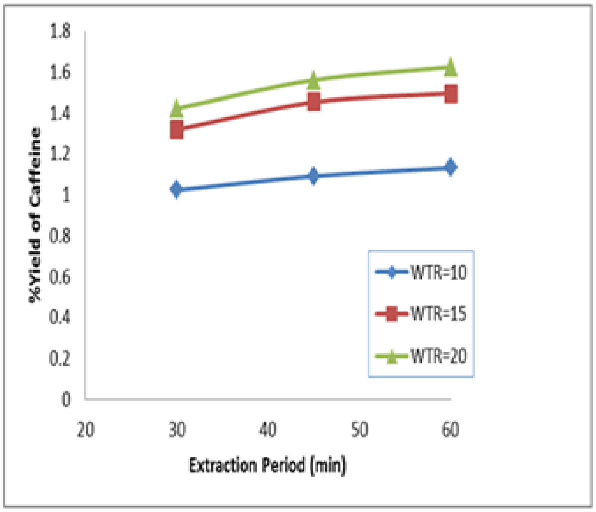


**Figure 5.1: Effect of WTR ratio on the Percentage Yield of Caffeine at 40°C using DCM solvent**

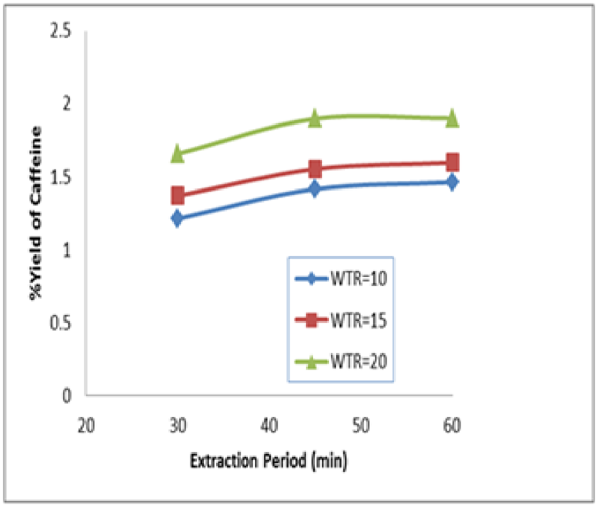


**Figure 5.2: Effect of WTR ratio on the Percentage Yield of Caffeine at 50°C**

From the figures, it was observed that, with increasing the water moles the yield is also increases gradually at the fixed parameters. At lower water moles, there is maximum yield that attained at the extraction time of

30minutes. Beyond to this, there is no much considerable increment.

The observations of the extraction process at the higher temperatures are quite different as shown in Figure 5.2. By increasing the water moles, there is drop in the yield of caffeine with extraction time of the order of 4.1%. Higher loss of the solvent water at the higher WTR ratios will be reason for the phenomena. This study concludes that, though the percentage yield is increased with the WTR ratios, the operation is to be conducted in the time periods of 45min and with WTR ratio 20, which yields an amount of 2.426% of caffeine.

### 5.1.2. Effect of Extraction Temperature:

Temperature is the parameter, which plays a crucial role in the extraction of caffeine as the solubility of the compound varies (increases) drastically with temperature. At the temperatures of 25ºC and 100ºC, the solubility of caffeine is 2.2 and 66.7 (% wt/wt) respectively.

The detailed study of the temperature effect will determine the optimum range of the temperature for maximization of the caffeine yield in an energy efficient way. Based on the literature, three levels of extraction temperatures are accounted for the operation, i.e. 40, 50 and 60 ºC and the effect of temperature was studied by varying the other governing parameters.

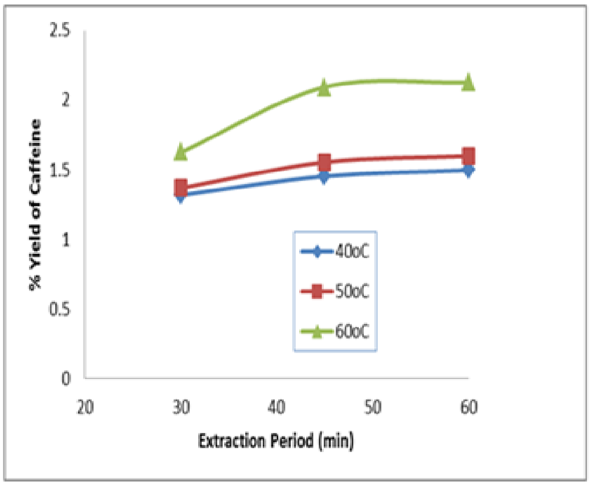


**Figure 5.3: Effect of temperature on the Percentage Yield of Caffeine for WTR ratio 15.**

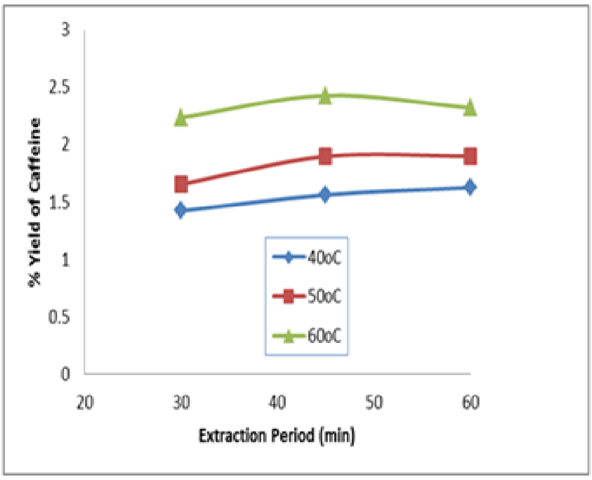


**Figure 5.4: Effect of temperature on the Percentage Yield of Caffeine for WTR ratio 20.**

From the figures 5.3 and 5.4, it was observed that yield of caffeine is depending directly on temperature. For lower WTR moles of '15, the yield is lesser order and at temperatures beyond to 50ºC, there is drastic improvement of yield and is independent of extraction period. With higher water moles of 20, the caffeine yield is independent of extraction period for lower temperatures and is decreasing with time for higher temperatures of 60ºC. A maximum of 2.42g of caffeine can be formed for 100g of tea leaves for the case.

### 5.1.3. Effect of Extraction period:

It is important to determine the duration of the extraction process (extraction period) to extract most of the desired compound. Typically, this would be the time at which equilibrium of solvent concentration between the inner and outer cells of tea leaves established. Using this information, suitable duration can be selected and operating cost for the process can be reduced. For the DCM solvent, the better range of the parameters observed are WTR= 20 and temperature of 60ºC. The effect of the time parameter under the specified operating parameters is presented in Figure 5.5.

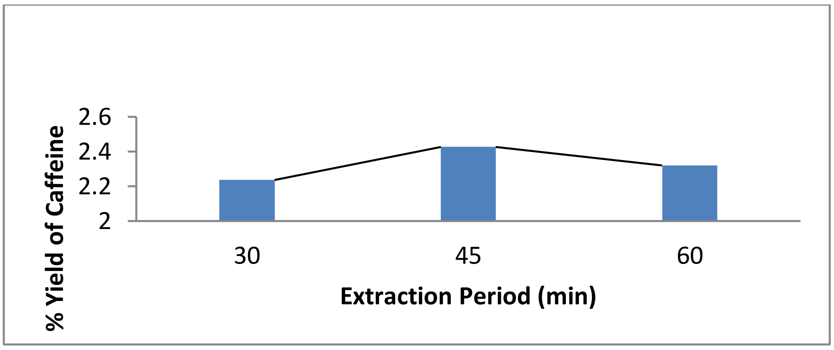


**Figure 5.5: Effect of extraction period on the percentage yield of caffeine for the water moles of (WTR) '20 and temperature of 60°C**

At the extraction period of 45minutes, maximum yield of caffeine can be attained in comparison to 60 minutes. As the extraction time (period) is prolong, leads to the evaporation the aqueous phase, resulting the deviation from the equilibrium and further causes decrement in the yield. A detailed doctorial research will establish the insight of the phenomenon.

**5.2.1. Effect of Water- Tea leaves weight ratio, WTR:**

Weight ratio of water to tea leaves plays an important role in the extraction of caffeine. Three levels of WTR ratios are considered by varying the other governing parameters and the observation arte presented in Figures 5.6 through 5.8.

From the figures, it was observed that, the caffeine yield was increases gradually with the amount of the water moles introduced. For all the three temperature levels considered, at higher water moles of the order 20 moles, there is slight drop in the yield. At the lower temperature level of 40°C, this observation is very specific, which suggests the high temperature operation for the process. The caffeine yield with WTR ratio 15 is just closes that for the ratio 20, suggesting the better operational water moles as 15. Lower water moles also minimize the labour and economics of downstream processes. An amount of 2.451g of Caffeine can be extracted under such operations, which is in line with the reported literature.

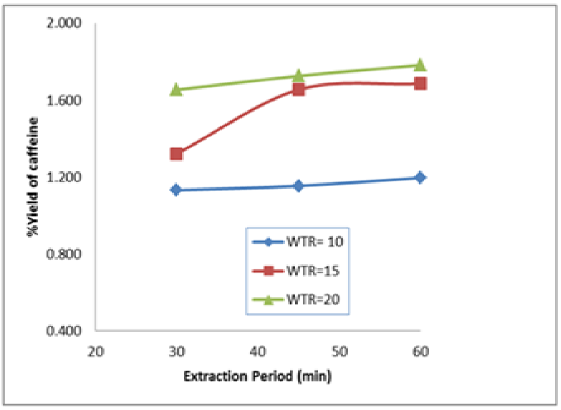


**Figure 5.6: Effect of WTR ratio on the Percentage Yield of Caffeine at 40°C using Chloroform solvent**

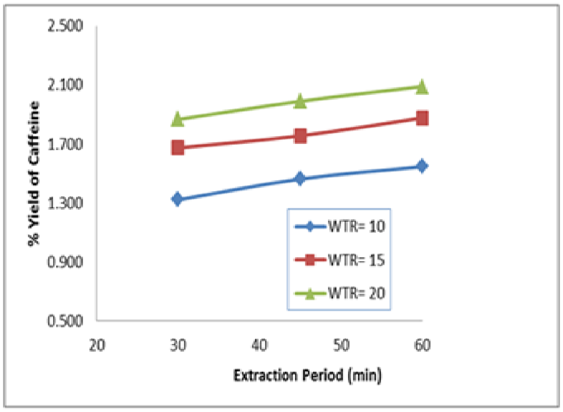


**Figure 5.7: Effect of WTR ratio on the Percentage Yield of Caffeine at 50°C using Chloroform solvent**

**5.2.2. Effect of Extraction temperature:**

Studying the effect of temperature of a extraction process is an important aspect which deals with the operational cost. For most of the components, the solubility is increase with temperature. As the temperature of a solution is increased, the average kinetic energy of the molecules that make up the solution also increases. This increase in kinetic energy allows the solvent molecules to more effectively break apart the solute molecules that are held together by intermolecular attractions. The average kinetic energy of the solute molecules also increases with temperature, and it destabilizes the solid state. The increased vibration (kinetic energy) of the solute molecules causes them to be less able to hold together, and thus they dissolve more readily.

The detailed study of the temperature effect will determine the optimum range of the temperature for maximization of the caffeine yield in an energy efficient way. Based on the literature, three levels of extraction temperatures are accounted for the operation, i.e. 40, 50 and 60°C and the effect of temperature was studied for WTR ratios of 10 and 15 and the study was presented in figures 5.10 and 5.11.

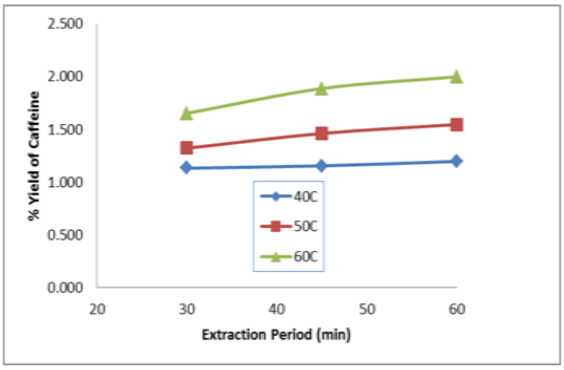


**Figure 5.10: Effect of temperature on the Percentage Yield of Caffeine for WTR ratio 10**

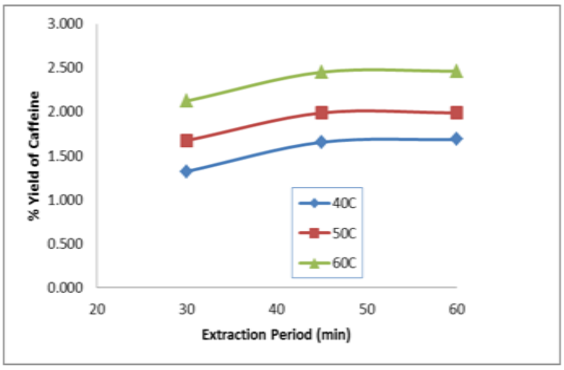


**Figure 5.11: Effect of temperature on the Percentage Yield of Caffeine for WTR ratio 15.**

From the figures, it was observed that with increasing the temperature from 40 to 60°C, the yield also increases gradually. At lower temperatures, the yield is independent of extraction period lower water moles of 10, whereas at higher temperatures it is increasing. The increase in solubility of caffeine with temperature might be the cause for the observed phenomena.

The effect of extraction period for the case of chloroform solvent studies was carried at the optimum range of the parameters, i.e, WTR= 15 and temperature of 60°C, which was presented in Figure 5.12. from the figure , it was observed that the maximum yield was attained with the extraction period of 45minutes and above to that, there is bit loss in the compound.

### 5.2.3. Effect of Extraction period:

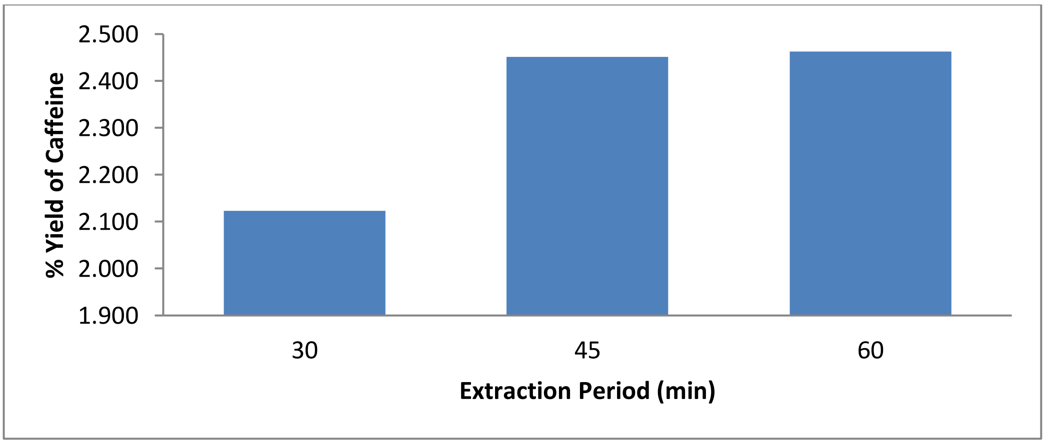


**Figure 5.12: Effect of extraction period on the percentage yield of caffeine for the water moles of (WTR) '15 and temperature of 60°C**

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**.3. Comparison of the performance of the two solvents DCM and chloroform:**

The previous two sections have presented the ability of the two solvents DCM and Chloroform towards the extraction of caffeine from tea leaves. The two solvents are believed to be performed well for the process of extraction.

The two parameters namely Percentage yield of caffeine formed (%Y) and Distribution coefficient $K_D$ are the aspects to be accounted in selection of the solvent. The detailed study of the yield terms are presented in the previous sections. In terms of yield of caffeine and WTR, chloroform is superior, which yields 2.451g of caffeine per 100g of tea leaves with the less water moles of 15. Calculation of Distribution coefficient $K_D$, for the two cases of extraction time 30 minutes and 60 minutes and for the two solvents DCM and chloroform respectively.

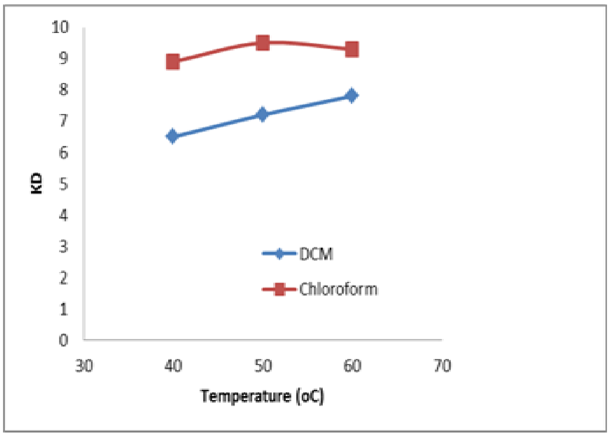


**Figure 5.12: Dependency of $K_D$ with temperature for the two solvents and for WTR =10 and extraction time of 60minutes.**

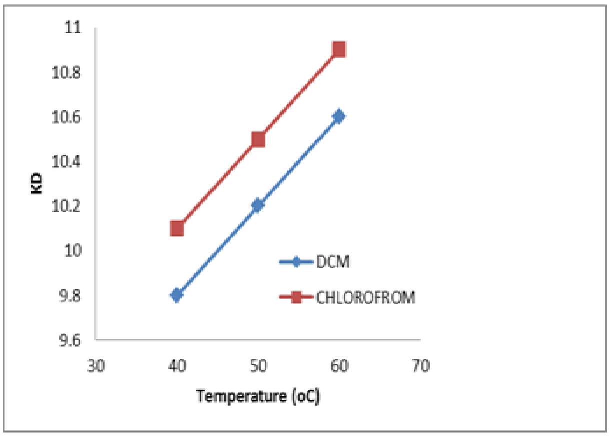


**Figure 5.13: Dependency of $K_D$ with temperature for the two solvents and for WTR =20 and extraction time of 60minutes.**

Figures 5.13 and 5.14 present the variation of $K_D$ with temperature for the two solvents. At the values of WTR=10 and 20 respectively. The plots indicate the chloroform is superior in terms of distribution of the solute, i.e, caffeine more in organic solvent.

In the selection of solvent for the extraction, various factors are to be accounted along with the yield, distribution coefficient other factors such as labour, health and environmental aspects. Regular exposure of mankind to the chloroform may causes many ill effects and associated hath hazards. So, based on the end use of the compound caffeine, level of purity the selection criterion depends. For high purity applications, caffeine derived from DCM extraction is suggestible than to chloroform.

## 6. Conclusions:

- The observations of the extraction process at the higher temperatures are quite different as shown in eth previous sections. By increasing the water moles, there is drop in the yield of caffeine with extraction time of the order of 4.1%. Higher loss of the solvent water at the higher WTR ratios will be reason for the phenomena. This study concludes that, though the percentage yield is increased with the WTR ratios, the operation is to be conducted in the time periods of 45min and with WTR ratio 20, which yields an amount of 2.426% of caffeine.
- From the extraction processes, increasing the water moles the yield is also increases gradually at the fixed parameters. At lower water moles, there is maximum yield that attained at the extraction time of 30minutes. Beyond to this, there is no much considerable increment.
- The yield of caffeine is depending directly on temperature. For lower WTR moles of '15, the yield is lesser order and at temperatures beyond to 50$^o$C, there is drastic improvement of yield and is independent of extraction period. With

higher water moles of 20, the caffeine yield is independent of extraction period for lower temperatures and is decreasing with time for higher temperatures of 60ºC. A maximum of 2.42g of caffeine can be formed for 100g of tea leaves for the case. At the extraction period of 45minutes, maximum yield of caffeine can be attained in comparison to 60 minutes. As the extraction time (period) is prolong, leads to the evaporation the aqueous phase, resulting the deviation from the equilibrium and further causes decrement in the yield.

- For all the three temperature levels considered, at higher water moles of the order 20 moles, there is slight drop in the yield. At the lower temperature level of 40ºC, this observation is very specific, which suggests the high temperature operation for the process. The caffeine yield with WTR ratio 15 is just closes that for the ratio 20, suggesting the better operational water moles as 15. Lower water moles also minimize the labour and economics of downstream processes. An amount of 2.451g of Caffeine can be extracted under such operations, which is in line with the reported literature.
- The caffeine yield was increases gradually with the amount of the water moles introduced. For all the three temperature levels considered, at higher water moles of the order 20 moles, there is slight drop in the yield. At the lower temperature level of 40ºC, this observation is very specific, which suggests the high temperature operation for the process. The caffeine yield with WTR ratio 15 is just closes that for the ratio 20, suggesting the better operational water moles as 15. Lower water moles also minimize the labour and economics of downstream processes. An amount of 2.451g of Caffeine can be extracted under such operations, which is in line with the reported literature.
- The two parameters namely Percentage yield of caffeine formed (%Y) and Distribution coefficient $K_D$ are the aspects to be accounted in selection of the solvent. The detailed study of the yield terms are presented in the previous sections. In terms of yield of caffeine and WTR, chloroform is superior, which yields 2.451g of caffeine per 100g of tea leaves with the less water moles of 15.The chloroform is superior in terms of distribution of the solute, i.e, caffeine more in organic solvent.
- In the selection of solvent for the extraction, various factors are to be accounted along with the yield, distribution coefficient other factors such as labour, health and environmental aspects. Regular exposure of mankind to the chloroform may causes many ill effects and associated hath hazards. So, based on the end use of the compound caffeine, level of purity the selection criterion depends. For high purity applications, caffeine derived from DCM extraction is suggestible than to chloroform.

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