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Standardization of *Sodium Acetate Trihydrate* for Potential Heat Therapy

Viswanath Srinivasan[1], Apurva Srinivas[2], Subashini Rajakannu[3]

[1, 2, 3]Department of Biomedical Engineering, Sri Sivasubramaniya Nadar College of Engineering, Chennai, India

Abstract: ***The purpose of the current study is to standardize the sodium acetate quantity for efficient heat therapy by finding the optimal solute to solvent ratio of sodium acetate and water used in the reaction solution. solute to solvent (STS) ratio is a quantityof sodium acetate to water in the solution prepared. Though the crystallization of sodium acetate phase change is commonly known as Hot ice experiment, there is no standard work for using the heat in heat therapy applications, which often lie in the usable range for superficial heat treatments because of fewer data available and works carried out. The study concentrates on deriving the optimal STS ratio for efficient heat therapy. Sodium acetate crystallization produces enough heat from 50°C to 60°C which lies within the human bearable range. The standardization is possible with the novel concept of Value Assessment principle and the scale narrow down approach. These two methods reduce the computation needed for standardizing the STS ratio. Values obtained using different STS ratios are represented graphically and results are interpreted from the experiment performed. The results show STS of 5.46 produces 55°C of heat and can be used ideally for superficial heat therapy.***

Keywords: Exothermic Heat; Heat therapy; Phase transition; crystallization; material

1. Introduction

Heat therapy refers to the treatment which is offered for stiffness and pain related problems by employing heat as the prime factor. These are some health conditions which are more prevalent in today's economy.Heat enhances the treatment by increasing the tissue temperature. (Dehghan M et al., 2014; Brosseau L et al., 2013) (Malanga GA et al., 2006; French SD et al., 2006). Heat therapy thereby increases the metabolism and elasticity of tissues alongside the rise in temperature. There are various modalities for providing heat therapy such as hot packs, ultrasound etc.Conversion of other form of energy into heat (e.g., shortwave diathermy, microwave diathermy, ultrasound) is regarded as deep heat therapy (Malanga GA et al., 2006). With the application of heat to the injured region, there will occur an increase in the supply of oxygen and other nutrients to the region, thereby enabling faster healing (Malanga GA et al., 2006; Charkoudian N 2010). The efficiency of heat therapy can be recognized based on the changes induced in the visco-elastic properties of the injured tissue. (Malanga GA et al., 2006). Applying heat directly on the skin increases both deep tissue temperature and blood flow (Nadler SF et al., 2006). Conductive topical heat treatment employed on the knees of healthy subjects increased the popliteal artery blood flow with suitable temperature of heat applied. The deep tissue blood flow was found to increase considerably in the trapezius muscle of healthy volunteers with heating pad treatments, resulting in increase in the skin temperature (Charkoudian N 2010 ; Nadler SF et al., 2006). Water is employed as the major component in all the treatment modalities. Sodium acetate ,CH_3COONa, also abbreviated as NaOAc, is thesodiumsaltofacetic acid. With being widely used in several industries, including, food, textile, health and beauty, sodium acetate also feature as a prime component in medical industries for manufacturing various modalities of heat therapy. Sodium acetate trihydrate crystal melts at 58 °C on dissolving in their water of crystallization (French SD et al., 2006 ; J. William Myrer et al., 2011). When they are heated past the melting point and subsequently allowed to cool, the aqueous solution becomes saturated.

The solution is capable of cooling to room temperature without forming crystals. Once when a solid form of chemical is introduced into the supersaturated solution, the liquid crystallizes and liberates heat (French SD et al., 2006 , Conner WW 2012). The major outcome of this reaction will be ample amount of heat produced, which is being employed for the process of heat therapy.

2. Materials and Methods

2.1 Principle

Exothermic reaction

Sodium acetate trihydrate is prepared from baking soda ($NaHCO_3$) with vinegar (CH_3COOH). It consist of sodium cations, Na (+), and acetate ions, $C_2H_3O_2$(-), which makes up sodium acetate, CH3COONa.

$$\mathbf{CH_3COOH + NaHCO_3 \rightarrow CH_3COONa + CO_2 + H_2O \text{ - (1)}}$$

As it exhibits more solubility in water, large quantity of Sodium acetate trihydrate is dissolved into water and heated at a temperature large enough to dissolve the salt to obtain the liquid form (Alberto gianinetti 2013 ; Wada T et al., 2010).When this liquid solution is allowed to reach the room temperature they still remain to occur in liquid phase and when this solution is exposed with a solid crystals of Sodium acetate trihydrate solid phase [$CH_3COONa.3H_2O(s)$] (Wada T et al., 2010).Then the entire liquid and solid form gets converted into solid phase Sodium acetate trihydrate

[$CH_3COONa.3H_2O(s)$] (Myrer JW et al., 2013).We all know that energy can neither be created nor be destroyed but it can be converted from one form to another. (Wada T et al., 2010). Thus, the **phase transition energy** is converted into **heat energ**y. Any chemical reaction which liberates heat is termed as **Exothermic energy.** Thus, the mentioned reaction is an exothermic reaction.

$$\mathbf{CH_3COONa.3H_2O(l) + CH_3COONa\ .3H_20(s) \rightarrow CH_3COONa.3H_20(s) - (2)}$$

The above equation explains the reaction that has taken place between various phases of sodium acetate trihydrate.

Phase transition and Entropy:

Entropy can be regarded as the measure of randomness or disorderliness of a system. The second law of thermodynamics states that the entropy of an isolated system never decreases spontaneously. Such systems turn towards the equilibrium state with maximum entropy. Non-isolated systems suffer a loss in their entropy if the environmental entropy increases by more or less the same amount. Since entropy is a function ofstate of the system, a change in entropy of a system is determined by its initial and final states. This applies to all the systems regardless of their reversibility condition . The combined entropy of both the system and environment gets increased in case of irreversible process. The change in entropy (ΔS) of a reversible system was defined by Rudolf Clausiusas:

$$\Delta S = \delta Q_{rev} / T - (3)$$

where T is the absolute temperature of the system, dividing an incremental reversible transfer of heat into that system (δQ_{rev}). (If heat is transferred out, the sign would be reversed thereby giving a decrease in entropy of the system.) The above definition is sometimes called the macroscopic definition of entropy because it can be used without regards to any microscopic description of the contents of a system (J. William Myrer et al., 2011). Thus, we can infer that solution having high entropy indicates high degree of randomness and vice versa and also the change in entropy is directly proportional to the heat transfer into the system and inversely proportional to the absolute temperature.

From the equation (2) we can clearly see a phase change has happened between the molecules of sodium acetate trihydrate in solid and liquid phase. The solid phase at room temperature indicates lesser degree of freedom and randomness due to closely packed structure of molecules and thus lesser entropy (Alberto gianinetti 2013). In liquid phase at room temperature indicating more degree of freedom and randomness due to freely packed structure of molecules thus greater entropy. So, during the phase transition between solid and liquid phase there is clearly an entropy change that has happened. This change will follow equation (3) since it is a macroscopic and reversible system. From equation (3), we have three parameters which has a dependent relationship on each other. First the entire reaction is carried out in a constant room temperature. Thus, absolute temperature of the system becomes a constant, T = constant. Since T is constant ,the entropy change ΔS of a system is directly proportional to the transfer of heat into that system , $\delta Q_{rev.}$ This δQ_{rev} is the heat that is liberated as a result of exothermic reaction explained in the previous sub-section. (Alberto gianinetti 2013) Thus the phase change between the molecules (entropy change) has brought the heat liberation required for heat therapy, which will be measured for various samples using value assessment and scale narrow down approach.

Value assessment principle:

Value assessment principle will be the key to find the sodium acetate quantity required for thermo (or) heat therapy. This will be based upon two parameters which will produce the necessary output. The key outcome of this method is the solute-to-solvent ratio which will be obtained. The solute to solvent ratio is the ratio of quantity of solute dissolved in the particular amount of solvent. Thus, the two terms involved in this principle will be solute and solvent quantity Let us assume the solute quantity to be X; and the solvent quantity to be Y. The ratio will be the heat produced and this can be represented as,

$$\textbf{STS ratio} = \mathbf{X/Y} - (4)$$

The ratio ought to be in the range of 55°C to 60°C which is regarded as the clinical usable range of temperature. In order to find this value, which is the quantity of salt used, we need to keep Y as a constant throughout the experiment. It can be taken as any value, but the shorter value is preferred because it requires a smaller quantity of salt to make up the same value of STS ratio (i.e.) smaller the value of solvent, smaller will be the value of solute. e.g. To produce a ratio of 1, let us consider the below two cases.

Case 1: If we assume 20ml as solvent concentration, then Y becomes 20ml. Thereby the ratio becomes,

$$X/20 = 1$$
$$X = 20g$$

Thus, 20g of solute must be dissolved in 20ml of solvent to make the ratio 1.

Case 2: If we assume 40ml as solvent concentration, then Y becomes 40ml. Thereby the ratio becomes,

$$X/40 = 1$$
$$X = 40g$$

Thus, 40g of solute must be dissolved in 40ml of solvent to make the ratio 1.

On comparing the results of case 1 and case 2, one can infer that taking smaller quantity of Y will demand smaller quantity of X, thereby reducing the quantity of salt to make up the same ratio. Now, throughout the experiment which is going to be carried on in the upcoming section, Y value will be fixed as 30ml. The solute-to-solvent ratio will be

$$\textbf{STS ratio} = \mathbf{X/30}$$

Where X will be selected based on the scale narrow down approach which will be described later to yield the appropriate clinical heat range of 55°C to 60°C.

Scale narrow down approach

Scale narrow down approach will be a useful tool to reduce the computation needed and the number of trial s needed to reach the desirable output, say 55°C. Using this method, we can find the value of X which was described in the VA principle where we fixed Y as a constant. This approach involves assuming certain initial value of X say z. Fix their scaling factor to an arbitrary value *say s*.
Begin the trial 1 with X value as (s+z).
Hence, X = s + z

Where X is the quantity of absolute which is to be dissolved in the pre-determined value of Y. The scaling factor for the next trial is selected based on the results obtained during the trial 1. Based on the results, we can either increment or decrement the scaling factor. By repeating this method, the difference between the actual values obtained and the desirable value decreases, which will finally yield the value of temperature produced. To understand this process, go through the following example. e.g. Now let us assume the desirable value of temperature to be 100°C; the initial value of z to be 0g; the scaling factor to be 20. Therefore, X becomes 20g (0+20). This value is used to obtain the STS ratio which is described in the VA principle and having the value of Y to be 30ml. Hence STS = 20/30 is taken as the first trial and the temperature obtained is about 50°C.

Temperature difference (Ɵ) = Observed temperature (O1) ± Desirable temperature (D) = 50°C- 100°C = -50°C

Hence, the difference is 50°C. For trial 2, the scaling factor be decrement from 20 to 10. Now the value of X becomes,

X = 20 + 10
X = 30g & Y = 20ml

Therefore, the STS Ratio is X/Y = 30/30

In this trial, the temperature reached is 90°C. Therefore, O2 becomes 90°C temperature difference Ɵ = O2 ± D = 90 ± 100 = -10°C

The above steps are again repeated until the temperature difference Ɵ becomes 0. We could see a gradual reduction in the temperature difference as we move further. Why to use this method? If this method is not used to calculate the quantity of solute, then the no. of trials taken to reach the desirable value will go very long and the process will become quite tedious. For example, to obtain the STS ratio as 1, have X = 50g and Y = 50ml for producing 100°C. Nearly 50 trials are to be performed from 0 to 50g. Whereas using scale narrow down approach, the desired value can be obtained within 10 trials, thereby reducing the manual work to a greater extent.

3. Procedure

Before beginning the experiment, one must have a clear understanding of the VA principle and scale narrow down approach.

Solution preparation

Begin your trial 1 with an initial value of z and scaling factor s. Take a fixed volume of Y, say 30ml.Mix the X g in Y ml thoroughly and allow them to dissolve partially in the beaker. Now place the beaker containing X and Y to the Bunsen burner / hot plate or any other heat adjustable modality and start heating the beaker containing the sample. Stir until the complete salt gets dissolved in the Y ml of solvent. A clear solution is obtained at the end of dissolution. The clear solution is labelled as sample A and the heating process is stopped. Allow the solution to cool to room temperature by sufficiently placing it in the external environment.

Crystallization process

Once the solution A is brought back to room temperature, place the temperature measuring device, say thermometer onto the sample A.Initiate the crystallization process by adding a same pinch of sodium acetate crystal onto the sample A. The solution begins to change its phase from liquid to solid phase. Start your stop watch and note down the temperature changes in the tabulation for about 10 minutes at an interval of 30s.The solution will begin to liberate heat, due to exothermic principle discussed in the introduction section.

Calculation

The maximum temperature is obtained at an interval of time and the value of maximum temperature is noted as On, n = 1,2,3…. etc. On represents the observed temperature of the scale narrow down section. Now find the temperature difference, Ɵn by finding the difference in between the observed temperature On and the desirable temperature (D). This Ɵn will help us in selecting the further values of scaling factor s for the coming trials.

Time Vs Temperature graph

The readings of time and temperature which are obtained are graphically represented by plotting a graph with X and Y axis as temperature and time. Thus, the temperature vs time graph is obtained. In graph, obtain the line equation by interpolating the graph into various points. Once the above steps are completed, repeat them once again to obtain trial 2 of sample A. Now a new temperature vs time table is formed by taking.

The readings of time and temperature which are obtained are graphically represented by plotting a graph with X and Y axis as temperature and time. Thus, the temperature vs time graph is obtained. In graph, obtain the line equation by interpolating the graph into various points. Once the above process is completed, repeat them once again to obtain trial 2 of sample A. Now a new temperature vs time table is formed by taking the mean values of the new trials for every 30s .This equation will be of the form y = ± mx + c where +m for increasing slope and –m for decreasing slope. We are interested in finding a solution concentration which produces maximum heat and is able to withstand the temperature. Such a solution will be regarded as the ideal solution for this experiment. Once this is completed, use scale narrow down method and scaling factor is adjusted suitably to reduce the value of Ɵn, n = 1,2,3…etc. All the steps from 1–21 are repeated for two trials and a graph for time vs temperature is plotted and the line equation is obtained. These steps are repeated until the Θn value reaches 0. All the graphs are plotted in a single sheet from A, B….to n and the inference is obtained.

4. Graphical Interpretation

Sample A:
Initial value of X, z = 0
Scaling factor, s = 50
Solute quantity, X = 50g (s+z)
Solvent quantity, Y = 30ml

No crystallization has taken place in this reaction because the amount of solute quantity dissolved in the solvent quantity is not sufficient enough to make up the highly saturated solution because the 50g of sodium acetate salt gets easily dissolves in 30 ml of water under room temperature indicating that it is a normal solution not the highly saturated solution which produces the exothermic heat reaction under exposed with tiny particle of sodium acetate salt.

Sample B:
Initial value of X, z = 50
Scaling factor, s = 50
Solute quantity, X = 100g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = 12.85°C O_2 = 42.15°C [Fig 1A near here]

Sample C:
Initial value of X, z = 100
Scaling factor, s = 25
Solute quantity, X = 125g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = 9.9°C O_2 = 45.1°C [Fig 1B near here]

***Sample D*:**
Initial value of X, z = 125
Scaling factor, s = 25
Solute quantity, X = 150g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = 7.2°C O_2 = 47.8°C [Fig 1C near here]

Sample E :
Initial value of X, z = 155
Scaling factor, s = 5
Solute quantity, X = 155g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = 9.9°C O_2 = 45.1°C[Fig 1D near here]

***Sample F* :**
Initial value of X, z = 155
Scaling factor, s = 5
Solute quantity, X = 160g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = 4.6°C O_2 = 50.4°C [Fig 1E near here]

Sample G:
Initial value of X, z = 160
Scaling factor, s = 2
Solute quantity, X = 162g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = 4.4°C O_2 = 50.6°C [Fig 1F near here]

Sample H:
Initial value of X, z = 162
Scaling factor, s = 2
Solute quantity, X = 164g (s+z)
Solvent quantity, Y = 30ml
Θ_2 = -0.35°C O_2 = 55.35°C [Fig 1G near here]
= 0 (approx.)

Now lets us consider some more value of solute quantity (x) greater than 164g such as 165,180 and 190 and find their respective peak temperature and temperature difference

Sample I:
Solute quantity, X = 165 g
Solvent quantity, Y = 30 ml
$\Theta10$ = 4.4°C O_{10} = 50.6°C
The difference observed is 4.4°C higher than that obtained using the solute quantity of about 164g.

Sample J:
Solute quantity, X = 180 g
Solvent quantity, Y = 30 ml
$\Theta10$ = 10.4°C O_{10} = 44.6°C

The difference observed is 10.4°C higher than that obtained using the solute quantity of about 164g which is larger when compare to the 165g quantity. this indicates that there is a peak temperature drop with every increase in the solute quantity.

Sample K :
Solute quantity, X = 190 g
Solvent quantity, Y = 30 ml
$\Theta10$ = 10.9°C O_{10} = 44.1°C

The solute quantities 164g, 180g, 190g have their corresponding peak values of 50.6°C, 44.6°C, 44.1°C. This indicates a gradual decrease in the peak temperature compare to the 164g. Thus scale narrow down approach helps in calculating the least quantity of solute that provides the maximum amount of heat production than other method. Further this verification section proves that increasing the solute concentration beyond 164g will not result in increase in temperature conversely in results in decrease in reduction of peak temperature, thus reducing the efficiency of the process. [Fig 2 near here]

5. Results

We can infer from Table 1 as to how the value of solute quantity X increase with the corresponding changes in the z value and the scaling factor s. Z value is inversely proportional to the s value (i.e.) z value started from a value of 0g and reached a final value of 162g whereas the s value started with a value of about 50 and ended with a value of 2. since the solute quantity, X is summation of this quantity the vary directly proportional to z and inversely to s. temperature difference Θ_n in each case gradually decrease through the values of 12.85°C, 9.9°C, 7.2°C, 4.9°C, 4.6°C, 4.4°C, 0°C. This shows that the temperature difference between the ideal heat therapy 55°C temperature and the peak exothermic heat O_n coincide with each other at a particular point of solute quantity which is 164g [Table 1 near here]. The temperature produce will be used as Noninvasive and side effects free strategies which are commonly employed for stiffness related problems and others like sprains, spasms, joint related issues etc simply involves the application of heat which is termed as heat therapy. This method of employing heat for treatment purpose increases tissue metabolism, blood flow, connective tissue extensibility etc.

6. Discussion

The graphical representation of temperature vs time for different concentrations are shown Fig. 1A; Fig 1B; Fig 1C; Fig 1D; Fig 1E; Fig 1F; Fig 1G where the curve is interpolated to obtain the line equation which gives details about the duration of heat dissipation and point where the heat ceases to attain the room temperature. This is studied using the gradient factor, slope m of the equation. Since it is a decreasing curve the slope is often in negative value of m. Thus, the larger the slope value, larger will be the duration to reach the room temperature. The values of 50g, 100g, 125g, 150g, 155g, 160g, 162g, 164g are -0.3595, -0.5164, -0.6297, -0.3309, -0.3879, -0.1442, -0.1145 respectively out of which 0.1145 is the larger since the slope is in negation. Thus, 164g apart from being the peak temperature producer also acts as large duration heat producer.

Thus the solution having the quantity of solute **164g** and the quantity of solvent **30ml** making the STS ratio of **5.46** will be producing the clinical temperature required for treating the patient with heat therapy and the duration of heat production is calculated based on its corresponding line equation **$y = 0.6224x + 55.497$**, where **-0.6224** is the slope value shows the degradation of temperature with time. Based on the quantity of solution needed the values of solute or the solvents can be changed by fixing the other parameter as a constant for the STS ratio based on the Value assessment principle.

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Figures

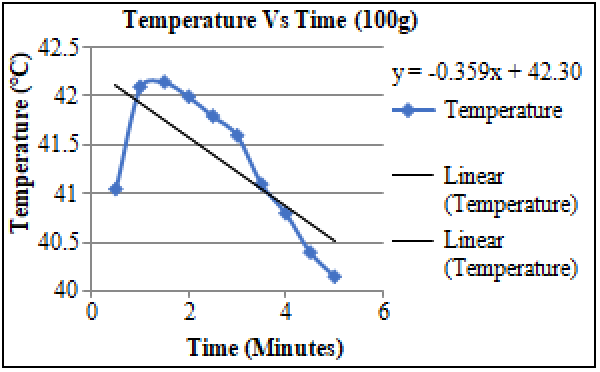

Figure 1 (A): Temperature vs Time graph for solute quantity 100g

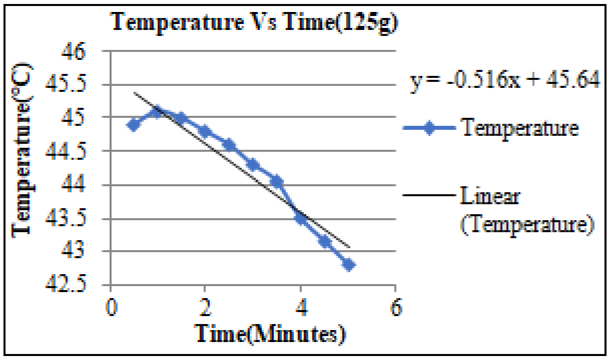

Figure 1 (B): Temperature vs Time graph for solute quantity 125g

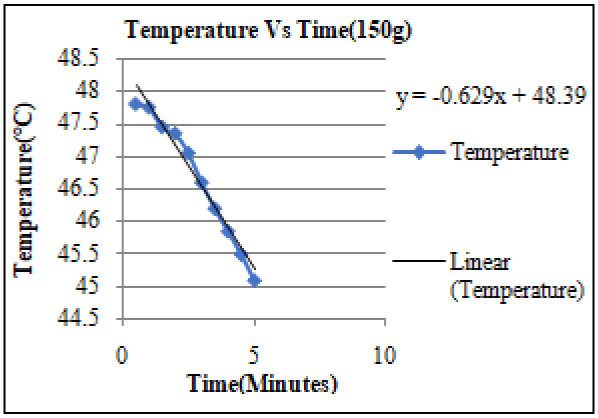

Figure 1 (C): Temperature vs Time graph for solute quantity 150g

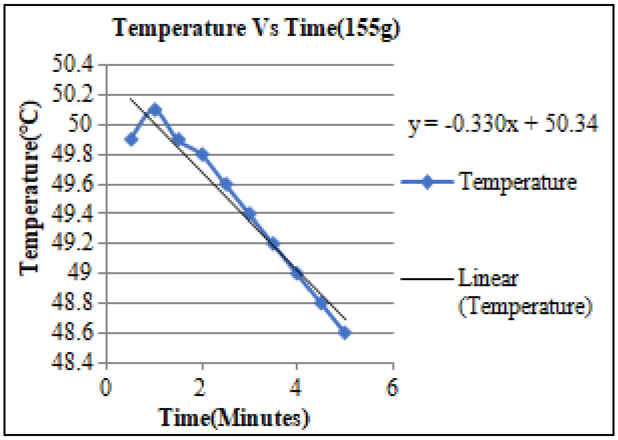

Figure 1 (D): Temperature vs Time graph for solute quantity 155g

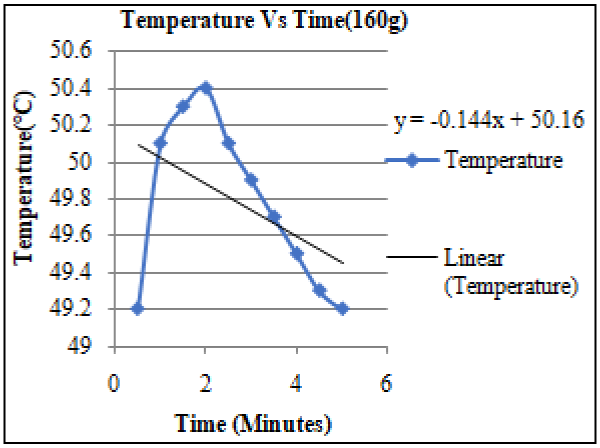

Figure 1 (E): Temperature vs Time graph for solute quantity 160g

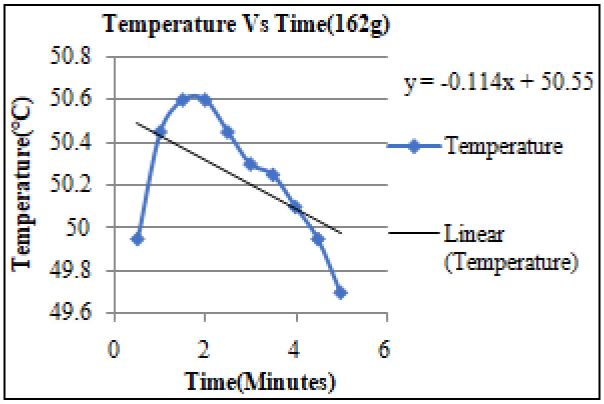

Figure 1 (F): Temperature vs Time graph for solute quantity 162g

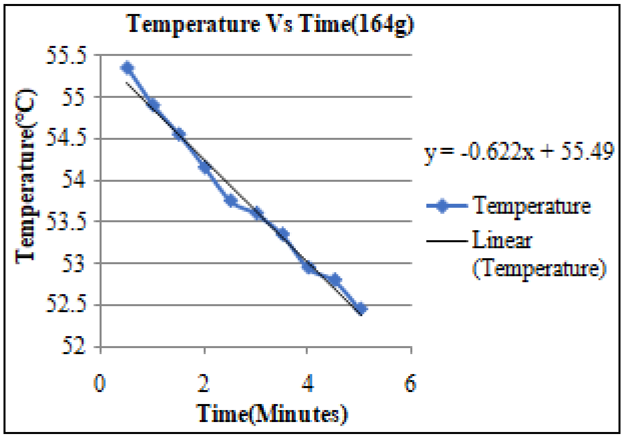

Figure 1 (G): Temperature vs Time graph for solute quantity 164g

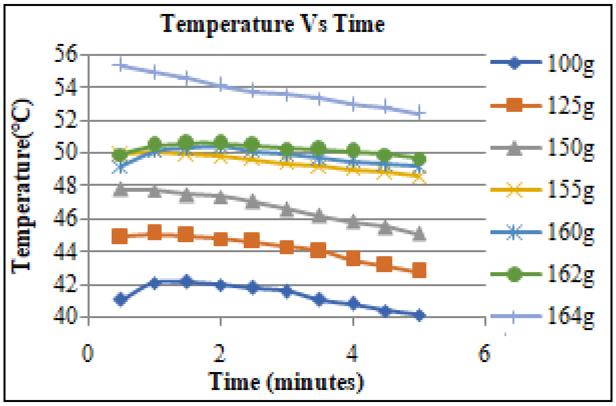

Figure 2: Temperature vs time graph of all experimented solute quantity

Table 1: Temperature difference, peak temperature and slope value for samples A to H with solvent quantity 30 ml

Sample	Initial X value z (g)	Scaling factor s(g)	Solute quantity X(g)	Temperature difference Θ_n (°C)	Peak temperature O_n (°C)	Slope m
A	0	50	50	-	-	-
B	50	50	100	12.85	42.15	-0.3595
C	100	25	125	9.9	45.1	-0.5164
D	125	25	150	7.2	47.8	-0.6297
E	150	5	155	4.9	50.1	-0.3309
F	155	5	160	4.6	50.4	-0.3879
G	160	2	162	4.4	50.6	-0.1442
H	162	2	164	0	55.35	-0.1145