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Construction of Ternary Phase Diagram for Three Component System [Oil-Water-Surfactant]



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ABSTRACT

A ternary graph, triangle plot is a barycentric plot on three variables which sum to a constant. It graphically depicts the ratios of the three variables as positions in an equilateral triangle. It is used in physical chemistry and other physical sciences to show the compositions of systems composed of three species. In a ternary plot, the proportions of the three variables a , b , and c must sum to some constant, K . Usually, this constant is represented as 100%. Because $a + b + c = K$ for all substances being graphed, any one variable is not independent of the others, so only two variables must be known to find a sample's point on the graph, for instance, c must be equal to $K - a - b$. Because the three proportions cannot vary independently - there are only two degrees of freedom - it is possible to graph the intersection of all three variables in only two dimensions. It is sometimes necessary to know the mutual solubilities of liquids in a two-phase system. For example, you may need to know how much water is dissolved in oil with which it is in contact, and also the amount of the oil that is in the aqueous phase. In this experiment, you will consider a three-component mixture (oil-water-surfactant at 37 °C) and construct the corresponding ternary phase diagram. In this experiment, we investigate the behavior of a system of three liquids oil-water-surfactant. Surfactant is miscible with both oil and water, but oil and water are quite insoluble in each other. Every point on a ternary plot represents a different composition of the three components. According to the phase rule, a single phase in a three-component system may possess four degrees of freedom. $F = C - P + 2$ $F \equiv$ degree of freedom; $C \equiv$ component; $P \equiv$ phase. These are temperature, pressure and the compositions of two of the three components. Because of the difficulty in graphically so many variables, temperature and pressure are generally held constant. This is the same special form of the phase rule that applies to two component systems of constant pressure only.

INTRODUCTION

The advantage of using a ternary plot for depicting compositions is that three variables can be conveniently plotted in a two-dimensional graph. Ternary plots can also be used to create phase diagrams by outlining the composition regions on the plot where different phases exist. Every point on a ternary plot represents a different composition of the three components. There are three common methods used to determine the ratios of the three species in the composition. The first method is an estimation based upon the phase diagram grid. The concentration of each species is 100% (pure phase) in each corner of the triangle and 0% at the line opposite it. The percentage of a specific species decreases linearly with increasing distance from this corner, as seen. By drawing parallel lines at regular intervals between the zero line and the corner fine divisions can be established for easy estimation of the content of a species. For a given point, the fraction of each of the three materials in the composition can be determined by the first. For phase diagrams that do not possess grid lines, the easiest way to determine the composition is to set the altitude of the triangle to 100% and determine the shortest distances from the point of interest to each of the three sides. The distances (the ratios of the distances to the total height of 100%) give the content of each of the species

Phase diagrams for ternary systems are usually represented using a triangle. This graph accounts for the fact that only two variables are required. Along the phase boundary, only one variable is required. Regions, where one or two phases appear, have also been indicated in Fig. 1. Note that the line drawn is hypothetical, the real curve will be determined in this experiment. When the solution is stirred, the transition from one region to another can be observed by appearance (or disappearance) of cloudiness or turbidity in the solution. The turbidity results from scattering of light by the large number of very small “oily” droplets of the second phase that are produced when the system is stirred. Sometimes it is easier to see this when stopping the stirring briefly. If the three components are mixed to give an overall system composition that falls in the 2-phase region, the system will separate into two phases: a phase rich in water and another rich in 1-butanol. The compositions of the phases that form are given by the intersections of a tie line with the phase boundary. The tie line must also contain the point describing the overall system composition. A graphical demonstration and an interpretation of a tie line are given in Fig. 1. Note that in the case of Fig. 1 only the mass fraction of 1-butanol must be given when the system

remains on the phase boundary line. This determines the mass fractions of water and acetic acid. Hence the phase rule holds with $f = 5 - p = 3$ (i.e., mass fraction for 1-butanol, temperature and pressure). If the system was initially in the two-phase region, the tie line uniquely connects the points along the phase separating line. Given the point 'A' in Fig. 1 (depending on the 1-butanol mass fraction in phase 1), the points 'B' and 'C' are uniquely determined. Thus only the 1-butanol mass fraction in phase 1, temperature and pressure are required for complete description of the system, which had separated into two phases. This is again in accordance with the phase rule [3, 5, 7].

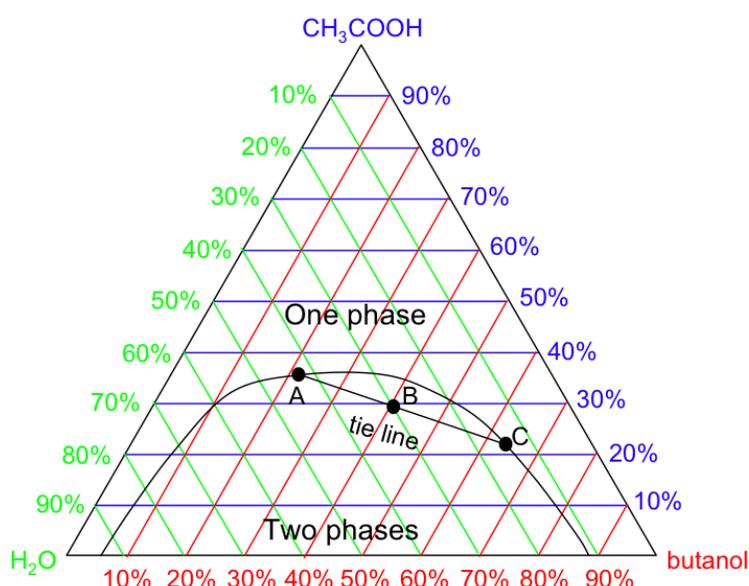


FIG. 1: Drawing of a tie line in a triangular phase diagram. The diagram may contain one or many tie lines. The point 'A' denotes the composition of phase 1, 'B' denotes the initial composition of the system, and 'C' the composition of phase 2.

In the above diagram, every corner of the triangle represents a pure component, which are 100% A, 100% B and 100% C. Each side represents one binary mixture and area in this triangular diagram represents ternary components. Rules relating to triangular diagrams are as below

Each of three corners or apexes of the triangle represent 100% by weight of one component (A, B, or C). As a result, that same apex will represent 0% of the other two components. The three lines joining the corner points represent two-component mixtures of the three possible combinations of A, B and C. Thus the lines AB, BC and CA are used for two-component

mixtures of A and B, B and C, and C and A, respectively The area within the triangle represents all the possible combinations of A, B, and C to give three-component systems addition of the third component into one pair of miscible liquids can change their solubility. If this third component is more soluble in either one from the two components, the solubility of both components will reduce. But if the third component is soluble in both components at the same time, the solubility increases. Thus, when ethanol is added to a mixture of benzene and water, the solubility of these two components will increase until a point is reached, where the mixture become homogenous. This application can be used in formulations of solutions.

MATERIALS AND METHODS

Table No-1

Sr. No.	Materials used	Supplier	Manufacturer
1.	Oil (Coconut Oil)	SD Fine Chemicals	SD Fine Chemicals
2.	Surfactant (SLS)	SD Fine Chemicals	SD Fine Chemicals
3.	Water	In House	In House

Method:-

1. In a Test Tube 1 ml each of water & oil was taken, two distinct layers can be seen which are indicative of two phase system.
2. Added Surfactant from burette to above mixture till homogenous single phase system is obtained.
3. Keeping the volume of oil constant added 1 ml water each time and titrated against surfactant so as to obtain homogenous phase.
4. From that calculated respective percentages of water, oil & surfactant for the construction of ternary phase diagram^[7, 8].

Table No-2

Sr.No	Vol of Water (V ₁)	Vol of Oil (V ₂)	Vol of Surfactant (V ₃)	% of Water	% of Oil	% of Surfactant
1	1	1	1	36	30	33
2	2	1	1.5	47	19	32
3	3	1	2	53	14	32
4	4	1	2.5	56	11	31
5	5	1	3	58	09	31
6	6	1	3.6	59	08	32
7	7	1	3.1	66	07	25
8	8	1	2.5	72	07	20
9	9	1	2	77	07	15
10	10	1	1.6	81	06	11

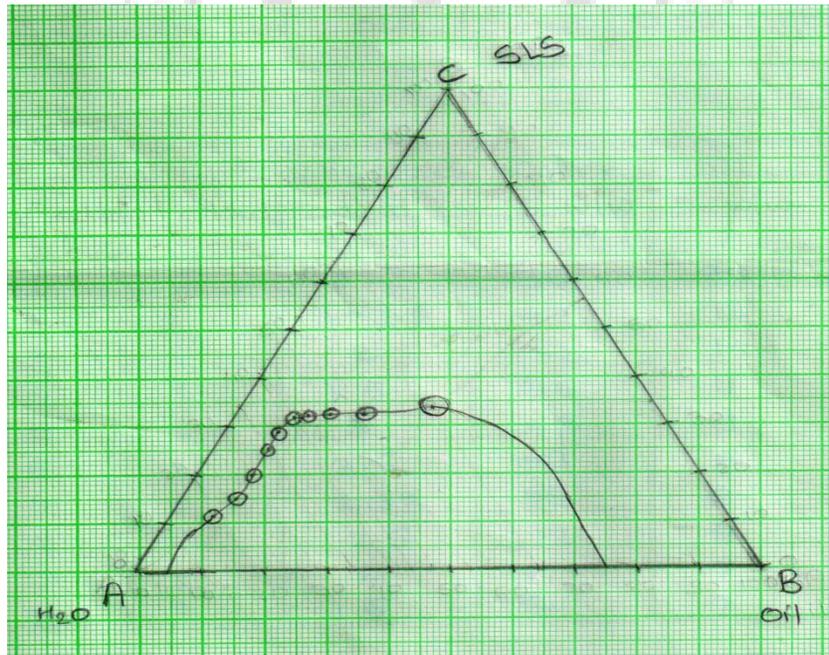


FIG.2: The curve represents the possible condition of water, oil, and surfactant. The Area above curve represents one phase (region of miscibility) while that below the curve represents two-phase (region of immiscibility) system.

Calculation for Determination of % Oil, Water & Surfactant^[8]

$$W_1 = V_1 \times \sigma_1$$

$$W_2 = V_2 \times \sigma_2$$

$$W_3 = V_3 \times \sigma_3$$

Where,

V_1, V_2, V_3 are the Volume of Water, Oil & Surfactant respectively.

$\sigma_1, \sigma_2, \sigma_3$ are the densities of Water, Oil & Surfactant respectively.

$$\% \text{ of Water} = \frac{W_1}{(W_1 + W_2 + W_3)} \times 100$$

$$\% \text{ of Oil} = \frac{W_2}{(W_1 + W_2 + W_3)} \times 100$$

$$\% \text{ of Surfactant} = \frac{W_3}{(W_1 + W_2 + W_3)} \times 100$$

RESULT AND DISCUSSION

The Ternary phase diagram for water, oil, and surfactant is shown in FIG.2 the curve represents possible condition of water, oil, and surfactant. The Area above curve represents one phase (region of miscibility) while that below the curve represents two-phase (region of immiscibility) system.

CONCLUSION

Oil, Water & Surfactant system is a ternary system with one pair of partially miscible liquid (Oil and water). The addition of sufficient amount of Surfactant to the Oil-water system would produce a single liquid phase in which all the three components are miscible and the mixture is homogenous.

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