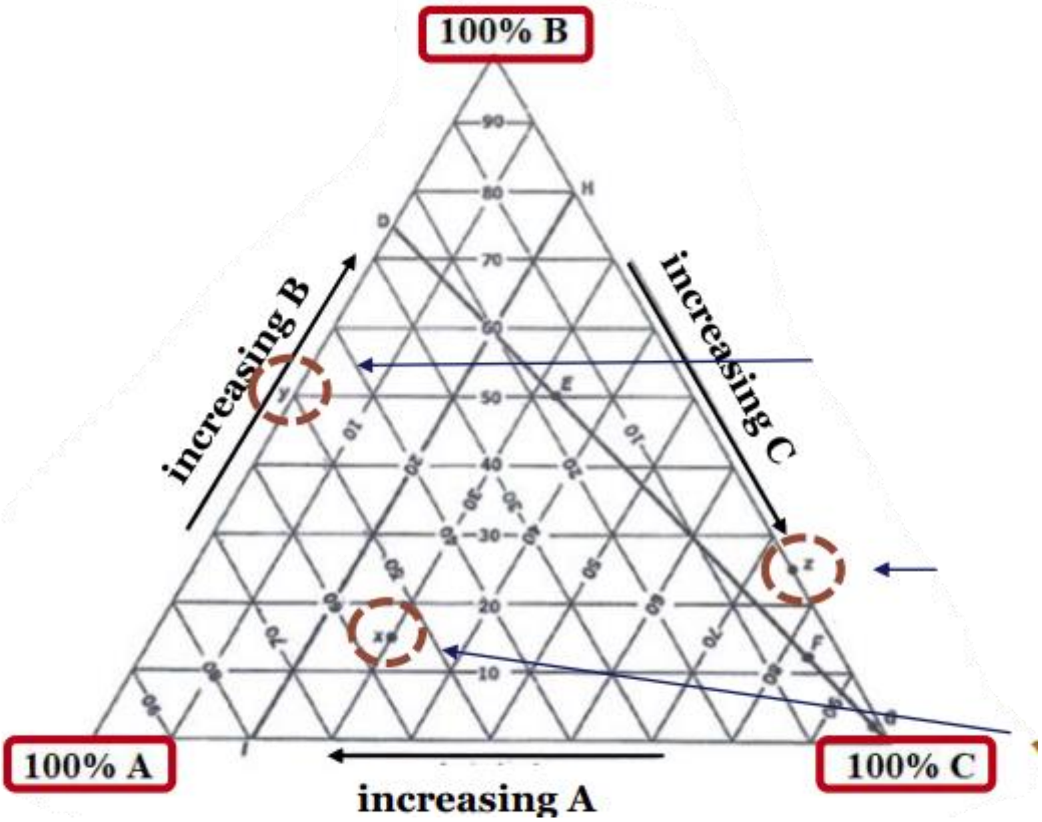
THREE-COMPONENT SYSTEMS. EXTRACTION.

A three-component diagram delimits the homogeneous and heterogeneous regions in a three-component system at constant temperature and pressure (usually atmospheric). When we want to observe changes in equilibrium composition at different temperatures, we have to use three-dimensional diagrams.

- In a non-condensed system containing three components but only one phase, F=3-1+2=4 (temperature, pressure, and the concentrations of two of the three components)
- Only two concentration terms are required because the sum of these subtracted from the total will give the concentration of the third component.
- If we regard the system as condensed and hold the temperature constant, F=2, thus we can use a planar diagram (generally triangular graphs are used) to illustrate the phase equilibria.
- Several areas of pharmaceutical processing such as Crystallization, Salt form selection, and Chromatographic analyses rely on the use of ternary systems for optimization

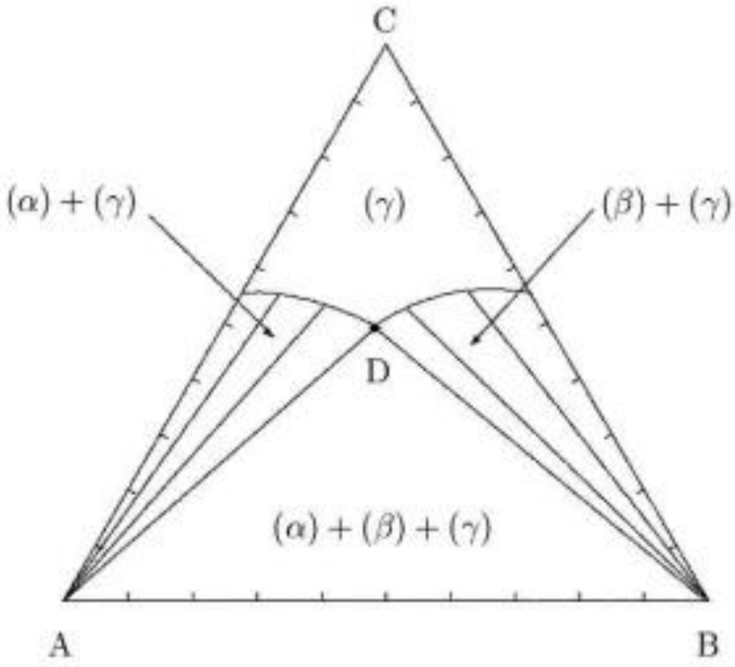
RULES RELATING TO TRIANGULAR DIAGRAMS



- The concentration in ternary systems are accordingly expressed on a weight basis. 100 % B 0 % A, 0 % C increasing A

- The lines AB, BC, and AC are used for two-component mixtures and can be divided into 100 equal units. Examples:
- Point y, on the line AB, represents a system containing 50% B and 50%A üPoint z, along BC, signifies a system containing 75%C.
- Point x, 15% of B 85% of A + C

ISOBARIC-ISOTHERMAL DIAGRAM OF A THREE-COMPONENT SYSTEM



The region (α) + (β) + (γ) is also heterogeneous. Here the system is formed by three phases: pure substance A, pure substance B, and a mixture of the composition given by point D

Three-component system containing two liquid phases

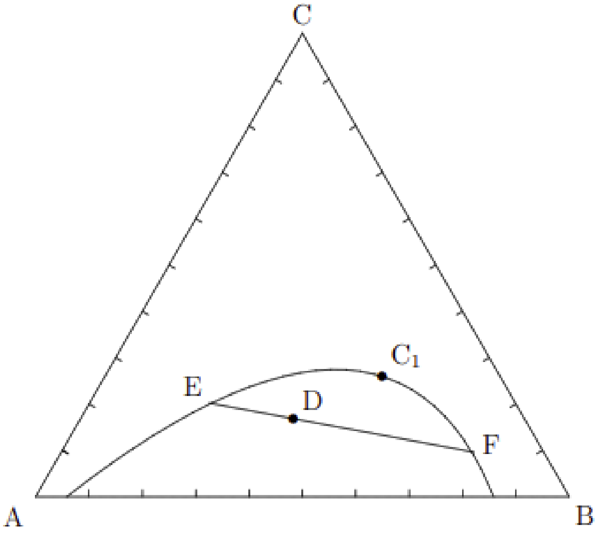


Figure shows a binodal line EC_1F and a tie line EDF. The system of a global composition given by point D split into two liquid phases whose composition is given by points E and F on the binodal line. The amount of substance ratio of both liquid phases is given by the lever rule. The compositions of both coexisting phases merge at point C_1 (the critical point).

The distribution coefficient is defined as the ratio of the molar fractions or concentrations of the *i* th component in one and the other liquid phase

$$K_{x,i} = \frac{x_i^{(\ell_2)}}{x_i^{(\ell_1)}} \qquad \text{or} \qquad K_{c,i} = \frac{c_i^{(\ell_2)}}{c_i^{(\ell_1)}}\,, \qquad i = 1, 2, 3\,.$$

The distribution coefficient generally depends on temperature, pressure and composition.

EXTRACTION

Extraction is a set of methods based on the use of differences in the extracted component solubility in two contacting immiscible phases (two liquid or liquid and solid).

Extraction is a process of distributing a substance between two immiscible liquid phases, as well as a method of extraction and separating substances, based on such a distribution.

In most cases, in analytics, a combination of two contacting immiscible liquid phases - organic the solvent and water solution of the partial (extract- able) substances is used.

Liquid extraction is based on using the capability of substances to be distributed between two immiscible contacting liquid phases, i.e., on their different solubility in these liquid phases. Liquid extraction can be used for both separation and concentration of substances.

- Let us consider the distribution of a substance A between the contacting immiscible liquid organic and aqueous phases at a constant temperature (T= const).

A(organic) = A(aqu.)

Equilibrium constant P, equal to

$$P = \frac{a(\text{organic})}{a(\text{aqu.})},$$

where ***a* (organic)** and ***a* (aqu.)** — are equilibrium activities of substance A in organic and aqueous phase respectively. The value P, in this case, is called the distribution constant (true thermodynamic), it is constant at a constant temperature for a given system.

DISTRIBUTION COEFFICIENT D

The distributed substance is often in present in the immiscible contacting liquid organic and aqueous phases in different chemical forms. For example, organic acids RCOOH, where R is an organic radical, in an aqueous solution undergo electrolytic dissociation:

$RCOOH + H_2O = RCOO^- + H_3O^+$

$2RCOOH = (RCOOH)_2$

$$D = \frac{\sum c_{\text{organic}}}{\sum c_{\text{aqu.}}},$$

where ∑C(ganic) - is the sum of the equilibrium concentrations in the organic phase of all forms of the distributed substance; ∑C(aqu.) - is the sum of the equilibrium concentrations in the aqueous phase of all forms of the distributed substance.

USE OF EXTRACTION

Extraction is one of the most effective methods of substances separation. Extraction methods are used for obtaining various components from herbal and mineral raw materials, for releasing gases from metals and alloys at high temperatures, for separation of solution components from each other, etc.