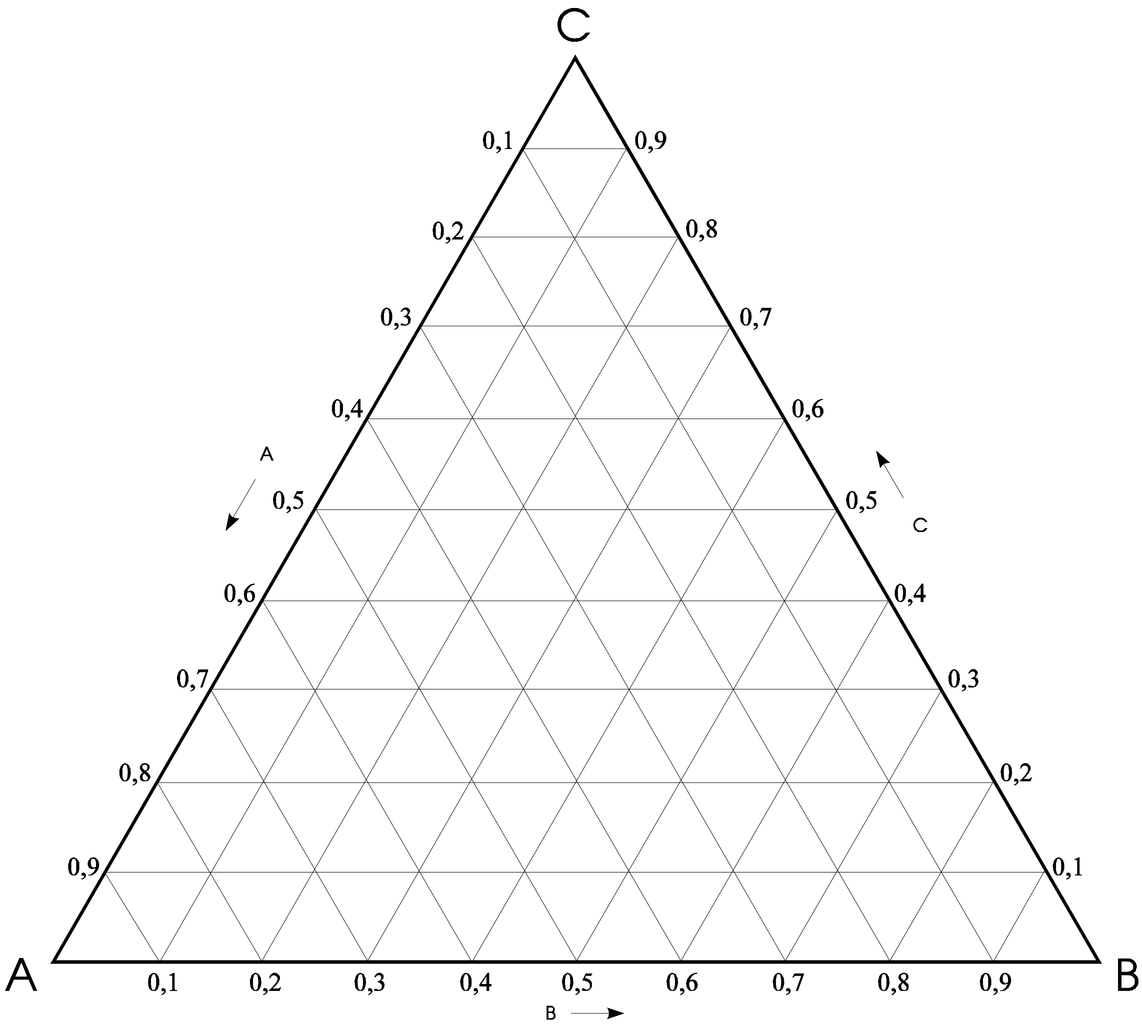
Example 1: Ternary Systems, Triangle Diagram

Two mixtures *R* and *E*, which contain both the three compounds *A*, *B*, and *C*, have to mixed in the ratio 1:2. This ternary system has no miscibility gap so that all compounds are completely soluble each other. The mixture *R* has a composition of $x_{A,R} = 0{,}7$ and $x_{B,R} = 0{,}2$; the mixture *E* exists of $x_{A,E} = 0{,}1$ and $x_{B,E} = 0{,}5$.

Please determine:

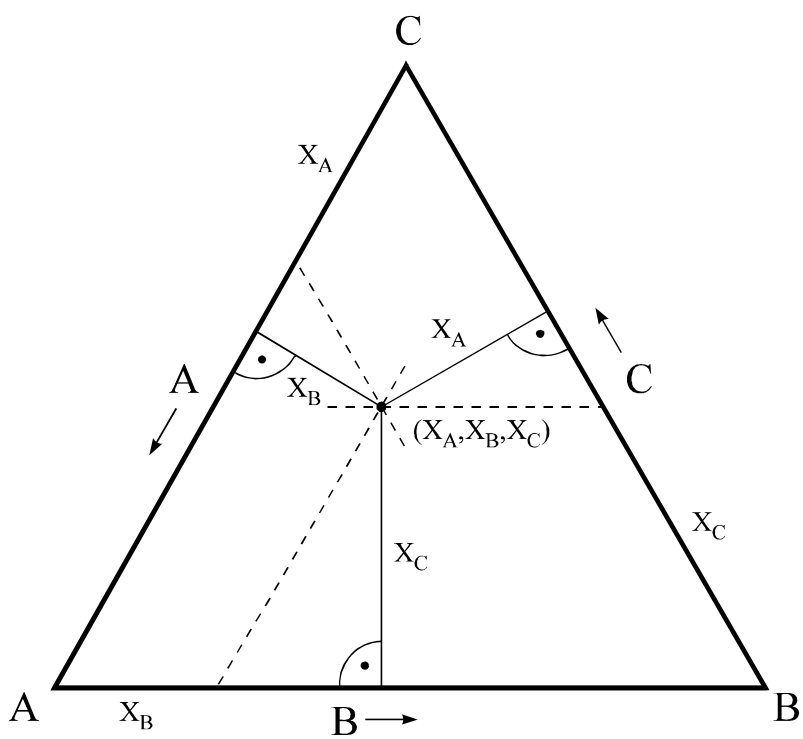
a) The points *R* and *E* in the triangle diagram and the concentration of the active agent *C* and

b) the mixing point (calculation and graphical determination).



a.) Mixtures in the triangle diagram

For a partial solubility of substances *A* and *B*, which is essential for extraction, all three compounds have to be taken into account for drawing of the phase equilibrium. For this reason triangle co-ordinates are used, where each of the vertexes represents the pure compounds. Points at the triangle side represent the composition of the binary system and points inside the triangle the composition of the ternary system.
The representation of a ternary point is based on the fact that the sum of the normal distances in a equal sided triangle is corresponding to the height of the triangle. If the height of the triangle is set 100% so result the concentrations of the single compounds from the normal distances (see figure).



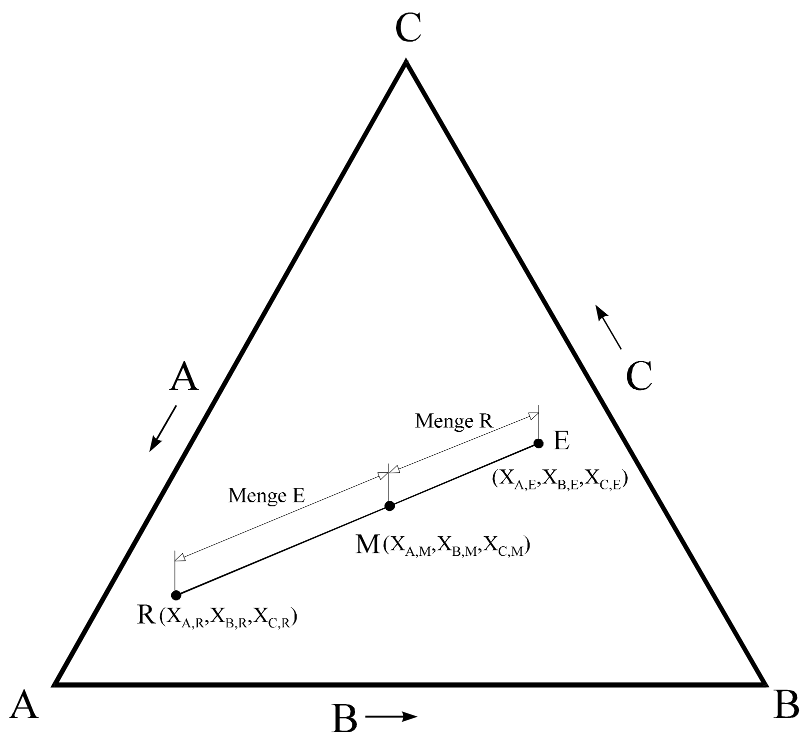
The given points *R* and *E* can therefore be drawn in the diagram.
From these points the concentration of C can be determined.

$x_{C,R} = 0{,}1$ $x_{C,E} = 0{,}4$

(Control: The sum of the components *A*, *B* and *C* must be equal 1)
The triangle diagram can also be given in weight percent *wt%*.

b) Mixing point

If two mixtures with given composition in the triangle diagram are mixed then the resulting mixing point lays on the connection line between these two points. The position of the mixing point can be calculated by a mass balance or graphically by the use of the law of balance.



Calculating:

Total balance:

$$R + E = M$$

Mass balance for compound C:

$$R \cdot x_{C,R} + E \cdot x_{C,E} = M \cdot x_{C,M} \quad \rightarrow$$

$$x_{C,M} = \frac{R \cdot x_{C,R} + E \cdot x_{C,E}}{R + E}$$

with $\frac{R}{E} = \frac{1}{2}$ the mass *R* and *E* can be eliminated, which results in

$$x_{C,M} = \frac{0{,}5 \cdot x_{C,R} + x_{C,E}}{1{,}5}$$

or $x_{C,M} = \frac{0,5 \cdot 0,1 + 0,4}{1,5}$

$$\boxed{x_{C,M} = 0,3}$$

Analogous results therefore

$\boxed{x_{A,M} = 0,3}$ and $\boxed{x_{B,M} = 0,4}$

Graphically:

Law of balance:

$$\frac{\overline{RM}}{\overline{ME}} = \frac{E}{R}$$

with $\frac{R}{E} = \frac{1}{2}$ follows $\frac{\overline{ME}}{\overline{RM}} = \frac{1}{2}$

From the diagram the length of the distance $\overline{RE}$ can be determined with 77 mm.

$$\overline{RE} = \overline{RM} + \overline{ME} \quad \Rightarrow \quad 0,5 = \frac{77 - \overline{RM}}{\overline{RM}}$$

$$\overline{RM} = 51,3\,\text{mm}$$

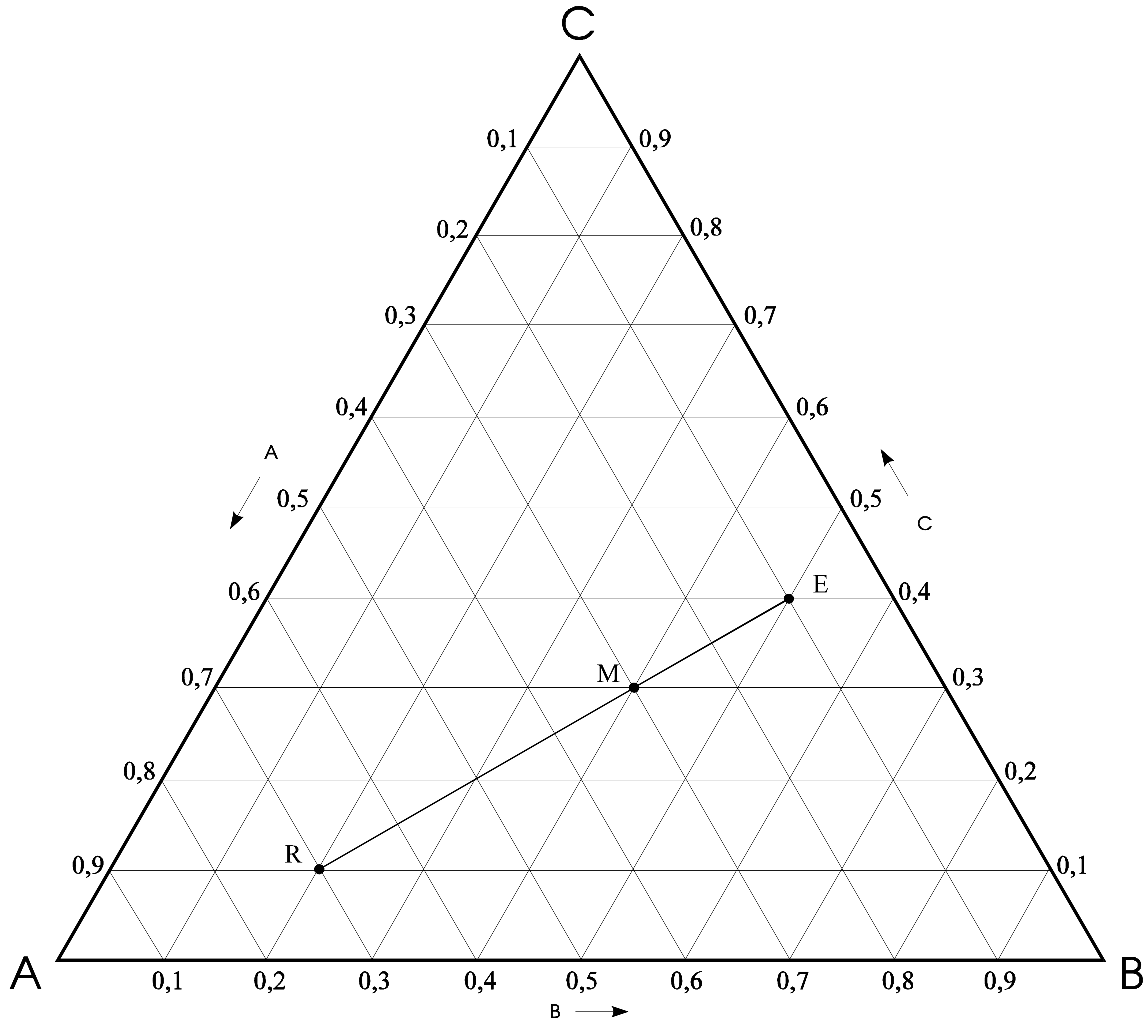
Drawing this length in the diagram results the mixing point *M* and the concentrations of the compounds can be determined.

$$\boxed{x_{A,M} = 0,3}$$

$$\boxed{x_{B,M} = 0,4}$$

$$\boxed{x_{C,M} = 0,3}$$

Triangle diagram



Example 2: Ternary system with mixing gap

A waste water from a process is loaded with acetone, which should be extracted with chlorobenzene.

The equilibrium data for the ternary system water / acetone / chlorobenzene are given.

composition of the coexisting phases in equilibrium in wt%					
water phase			organic phase		
water	acetone	chlorobenzene	water	acetone	chlorobenzene
99,89	0,00	0,11	0,18	0,00	99,82
89,79	10,00	0,21	0,49	10,79	88,72
79,69	20,00	0,31	0,79	22,23	76,98
69,42	30,00	0,58	1,72	37,48	60,80
58,64	40,00	1,36	3,05	49,44	47,51
46,28	50,00	3,72	7,24	59,19	33,57
27,41	60,00	12,59	22,85	61,07	15,08
25,66	60,58	13,76	25,66	60,58	13,76

You have to determine:

a.) the triangle diagram including the phase equilibrium line and connodes.

b.) The water and chlorobenzene content of the aqueous phase (raffinate) with an acetone concentration of 45 % and of the coexisting phase.

c.) Which amount of acetone has to be added to a mixture, existing of 110 g chlorobenzene and 90 g water? What is the composition of the mixing point?

d.) What is the water free composition of this mixing point?

a) Construction of the phase equilibrium in the triangle diagram

The given ternary system ha a mixing gap which separates the system in a homogeneous one phase region and a heterogeneous two phase region. The boundary is the binodal curve.

In the for the extraction interesting heterogeneous region a mixture splits in raffinate and extraction phase along a connode, which connects the two coexisting phases. The higher the amount of the active agent (extractable substance *C*) is the shorter the connodes become until they melt to one point, the critical point *K*. By this critical point *K* the binodal curve is split into two parts. Normally the part on the left side represents the raffinate phase *R*, which has a low content of solvent *B*, and the right side represents the solvent rich extract phase *E*.

According to the given table the coexisting phases (connodes) are given which can now be drawn in the triangle diagram. One line in the table corresponds to one connode.

1.connode point of the raffinate phase:

$w_{A,R} = 0{,}9989$ $w_{B,R} = 0{,}0011$ $w_{C,R} = 0{,}0$

1.connode point of the extract phase:

$w_{A,E} = 0{,}0018$ $w_{B,E} = 0{,}9982$ $w_{C,E} = 0{,}0$

Connecting these two points gives the first connode and analogous for the other given data. The last row corresponds to the critical point *K*. By connecting all raffinate and all extract points the result is the binodal curve.

b) Raffinate phase / Extract phase

Point in the raffinate phase

Drawing the acetone concentration of $w_{C,R} = 0{,}45$ on the right side of the triangle for the active agent *C* and crossing this with the binodal curve at the left side gives the point of the aqueous phase, so that the concentrations of water and chlorobenzene can be determined.

$w_{A,R} = 0{,}535$ $w_{B,R} = 0{,}015$

Point of the extract phase

The point of the extract phase has to be on a connode going through the already determined point on the raffinate side. But this connode is not given and has to be constructed.

Possibility 1:

By interpolation between the two connodes next to the point the connode through the given point can be constructed, but in a very inaccurate way.

Possibility 2:

With the help of the conjugation line the connode can be determined better and with higher accuracy. For this purpose the right and left triangle side has to be shifted parallel through the points of the connodes and the crossing of these two lines represents one point of the conjugation line. All these by this way constructed point and the critical point have to be connected to the conjugation line.

The searched coexisting phase can be constructed analogous: parallel shifting of the right triangle side through *R*, crossing with the conjugation line and crossing of the parallel shifted left triangle side through the point on the conjugation line with the right side of the binodal curve.

The by this way determined concentrations are:

$w_{A,E} = 0{,}04$ $w_{B,E} = 0{,}41$ $w_{C,E} = 0{,}55$

c) mixture near the phase boundary

First the binary mixture has to drawn at the basic side of the triangle diagram.

	mass [g]	weight-%
chlorobenzene	110	55
water	90	45
Σ	200	100

This point of the binary mixture has to be connected with the point *C*, pure acetone, and somewhere on this line the mixing point must be. The boundary between one and two phase region is the binodal curve. Therefore the searched mixing point *M* can be determined by crossing the line GC with the binodal curve. The necessary amount of acetone can be determine by the law of balance.

$$\overline{CM} = 40\,\text{mm} \qquad \overline{MG} = 69\,\text{mm} \qquad \overline{CG} = 109\,\text{mm}$$

$$\frac{G}{C} = \frac{\overline{CM}}{\overline{MG}} \rightarrow \frac{200}{C} = \frac{40}{69}$$

$$C = 345\,g$$

Composition of the mixing point M:

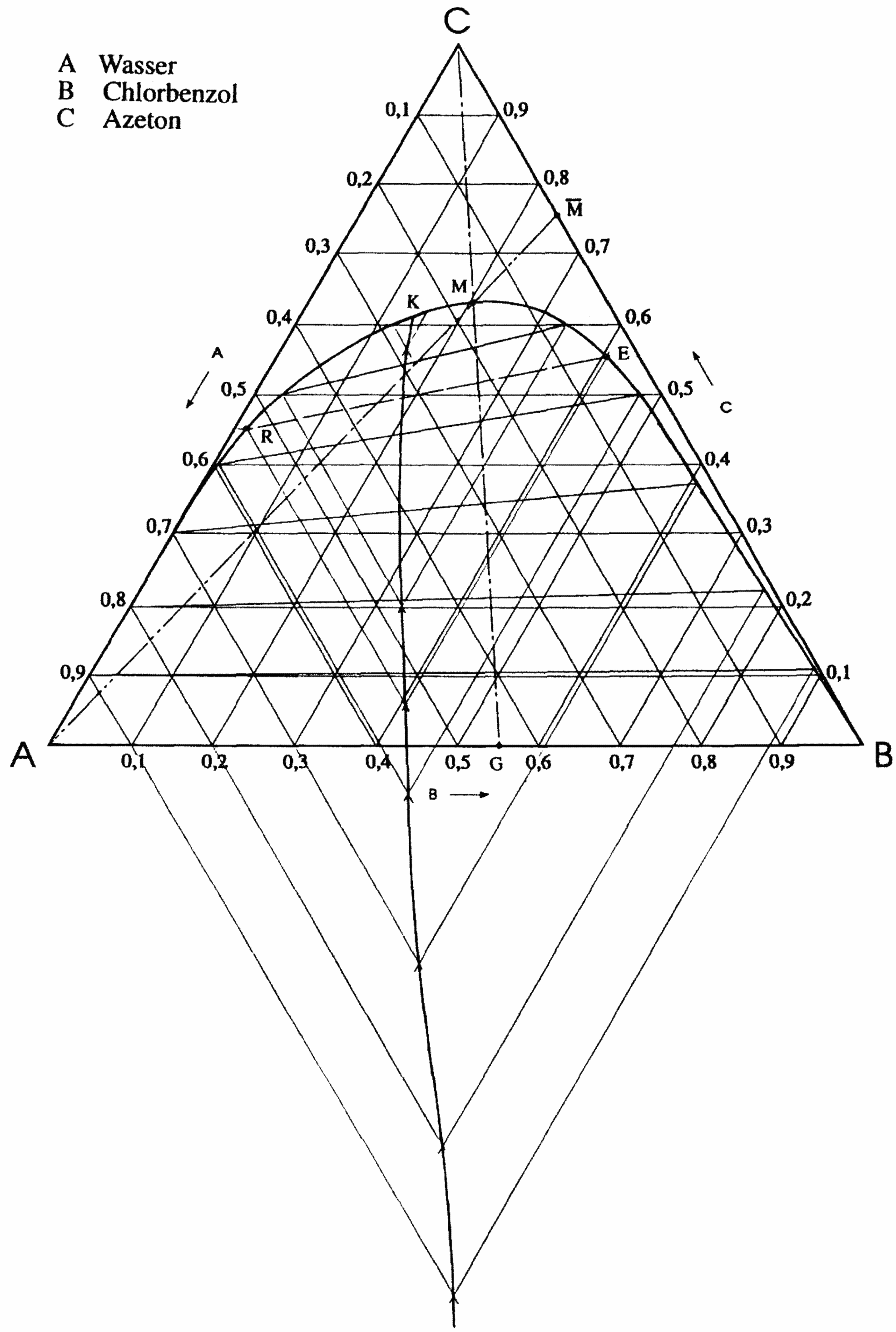
$$w_{A,M} = 0{,}16 \qquad w_{B,M} = 0{,}21 \qquad w_{C,M} = 0{,}63$$

d) water free mixing point:

To get the water free mixing point, the edge point A and the mixing point M hove to be connected and this line has to be prolonged to the right side of the triangle diagram, the water free side. The composition of the binary, water free mixture of acetone and chlorobenzene is:

$$\boxed{w_{B,\overline{M}} = 0{,}25} \qquad \boxed{w_{C,\overline{M}} = 0{,}75}$$

Triangle diagram



Example 3: Single Step Extraction

The basic mixture of 100 kg exists of 40 mole% acetone and 60 mole% water and has to be extracted with trichloroethane, which is preloaded with 15 mole% acetone. Your have to determine:

a) the phase diagram of the system acetone / water / trichloroethane in the triangle diagram.
b) the minimum and maximum amount of solvent,
c) the necessary amount of solvent, if the raffinate contains 4,82 mole% acetone,
d) the amount and composition of the produced raffinate and extract,
e) the extraction process in the triangle diagram

Phase equilibria data for the system water / acetone / trichloroethane

phase equilibria data for the coexisting phases in mole%					
extract phase			raffinate phase		
trichloroethane	acetone	water	trichloroethane	acetone	water
80,18	17,7	2,	0,07	1,	97,9
59,01	35,9	5,	0,10	4,	95,0
49,17	44,0	6,	0,12	6,	93,0
35,99	53,7	10,	0,17	10,3	89,4
25,04	58,3	16,	0,29	14,9	84,7
14,56	56,9	28,4	0,78	21,9	77,2
9,94	52,4	37,	1,50	27,3	71,1

a) Phase equilibrium in the triangle diagram

Drawing of the single connode points analogous to example 2 and constructing the connodes and combining the single point to the binodal curve.
The critical point was not drawn because the composition is not given and therefore the exact position is not defined.

b) minimal / maximal amount of solvent

Drawing of feed and solvent

feed:

$$x_{C,F} = 0{,}4 \qquad x_{A,F} = 0{,}6$$

The point *F* is on the left triangle side (binary mixture).

solvent:

$$x_{C,L} = 0{,}15 \qquad x_{B,L} = 0{,}85$$

The point *L* is on the right triangle side (binary mixture).

The mixing point *M* has to be on the line between these two points *F* and *L* and *M* has to be in the two phase region, because for extraction the mixture has to separate in two phases. The minimal and maximal amount of solvent ($M_{\min}$ and $M_{\max}$) are the two crossings of the connection line $\overline{FL}$ with the binodal curve. By the length, which can be determined from the diagram, the searched amounts can be calculated.

Minimal amount of solvent:

$$\overline{FL} = 91{,}5\,\text{mm}$$

and

$$\overline{FM_{\min}} = 4\,\text{mm}$$

law of balance:

$$\frac{\overline{FM_{\min}}}{\overline{M_{\min}L}} = \frac{M_{\min}}{F} \rightarrow M_{\min} = F \cdot \frac{\overline{FM_{\min}}}{\overline{M_{\min}L}} = 100 \cdot \frac{4}{91{,}5 - 4}$$

$$\boxed{M_{\min} = 4{,}57\,\text{kg}}$$

Maximal amount of solvent:

$$\overline{M_{max}L} = 2\,\text{mm}$$

law of balance:

$$\frac{\overline{FM_{max}}}{\overline{M_{max}L}} = \frac{M_{max}}{F}$$

$$M_{max} = F \cdot \frac{\overline{FM_{max}}}{\overline{M_{max}L}} = 100 \cdot \frac{91{,}5 - 2}{2}$$

$$\boxed{M_{max} = 4.475\,\text{kg}}$$

c) effective amount of solvent

The acetone concentration of the produced raffinate *R*, which has to be on he binodal curve, must be 4,82 %. With the connode going through this point *R* the extract *E* is fixed.

The mixing point *M* of feed *F* and solvent *L* is the crossing of the connode *RE* with the connection line $\overline{FL}$. With the law of balance the necessary amount of solvent *L* can be calculated.

$$\overline{ML} = 45{,}5\,\text{mm}$$

law of balance:

$$\frac{\overline{FM}}{\overline{ML}} = \frac{L}{F}$$

$$L = F \cdot \frac{\overline{FM}}{\overline{ML}} = 100 \cdot \frac{91{,}5 - 45{,}5}{45{,}5}$$

$$\boxed{L = 101{,}1\,\text{kg}}$$

d) composition and amount of raffinate and extract

Raffinate R:

$$\boxed{x_{A,R} = 0{,}9508} \quad \boxed{x_{B,R} = 0{,}001} \quad \boxed{x_{C,R} = 0{,}0482}$$

Extract E:

$$\boxed{x_{A,E} = 0{,}0503} \quad \boxed{x_{B,E} = 0{,}5901} \quad \boxed{x_{C,E} = 0{,}3596}$$

amount of raffinate:

total balance: $E + R = F + L = 100 + 101{,}1 = 201{,}1\,\text{kg}$

law of balance: $$\frac{\overline{RM}}{\overline{ME}} = \frac{E}{R}$$

$\overline{RE} = 95\,\text{mm}$ $\overline{ME} = 26\,\text{mm}$

$$R = \frac{201{,}1}{\frac{95 - 26}{26} + 1}$$

$$\boxed{R = 55\,\text{kg}}$$

amount of extract:

$$E = F + L - R$$

$$\boxed{E = 146{,}1\,\text{kg}}$$

Triangle Diagram / Nernst Diagram