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THE MULTIVARIATE CALCULATION OF MATERIAL BALANCES OF FLOWSHEETS FOR SEPARATING TERNARY MIXTURES OF DIFFERENT PHYSICAL-CHEMICAL NATURE*

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An approach to the determination of free variables required for calculating the material balance of the flowsheet of ternary mixtures separation is presented. Phase diagrams of the considered ternary systems are characterized by the presence of a two-phase splitting area and by the presence of different amounts of azeotropes (classes 3.1.0, 3.1.1, 3.2.1 and 3.3.1). For all the systems flowsheets containing three rectification columns and a florentine vessel for separation were suggested. The multivariance of the solution of the balance problem was shown. The approach was illustrated by the example of real ternary systems characterized by different phase diagrams (methanol – chloroform – water, butyl alcohol – water – toluene, nitromethane – hexane – water). The parameters of the rectification columns were presented.

Keywords: *rectification, separation flowsheet, splitting, material balance.*

Introduction

The concept of the number of degrees of freedom is widely used in various fields of knowledge: mathematics, mechanics, chemistry, chemical thermodynamics, chemical technology, etc. Generally, it is equal to the difference between the number of variables and the number of independent equations connecting them. One of forms of expressing the number of degrees of freedom is Gibbs' phase rule [1]. This concept is also the cornerstone of determining the number of independent variables characterizing a single device [2–4] or a flow diagram including several devices [5, 6]. The concept of the number of degrees of freedom is considered in detail in [7].

When developing process flow diagrams of separation focused on extreme conditions (infinite efficiency of a column and infinite reflux-to-product ratio [8]), calculation of rectification is preceded by calculation of the general and component-by-component mass balances. For separating complexes it is convenient to carry out the calculation with the use of the balance simplexes method [9], which coordinates the structure of the phase equilibrium diagram, the complex structure and the preset separation and allows determining the minimum possible volumes of recycle flows. In the presence of several (or even one) recycles and thermodynamic restrictions imposed by the phase equilibriums on the compositions of flows the balance task becomes rather nontrivial. Its solution depends on the number of free variables that should be set in a certain

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manner. Because various free variables can be generally chosen, calculating the material balance becomes a polyvariant task.

Work [10] considers options of setting the free variables when calculating the mass balance of a complex for separating the three-component mixture acetonitrile – isopropyl alcohol – hexane. The structure of its vapor-liquid equilibrium diagram belongs to class 3.3.1-2. This article extends this approach to ternary systems with various structures of the vapor-liquid equilibrium diagram and of the phase separation diagram. Separation of the mixture with use of a special method based on a combination of rectification and phase separation is considered. The separation complex should include a minimum number of rectification columns equal to the number of components (additional restriction).

Theoretical Part

The possibility of separating three-component mixtures in complexes based on a combination of rectification and phase separation is determined by characteristics of the relative position of azeotropes, separatrixes and binodal curves in the phase diagram. If the position is unfavorable, using this method becomes impossible, and it is necessary to apply other special methods [11–13]. These cases are not considered in this article. The position of the above elements is considered to be unfavorable, when the compositions of equilibrium liquid phases (the slopes of liquid–liquid nodes) belong to different areas of continuous rectification.

The article considers a number of ternary systems characterized by various structures of vapor-liquid equilibrium diagrams (classes 3.1.0-1a, 3.1.0-2, 3.2.0-2b, 3.1.1-2, 3.2.1-2b, 3.3.1-2) [14] and phase separation diagrams (areas of two-phase phase separation of the opened and closed type, areas of three-phase separation) [15, 16]. For each system and preset point of original composition F_0 a scheme of separation including three rectification columns and a Florentine vessel (Figures 1–3) is suggested.

The number of free variables required for calculating the material balance is determined as follows:

1. *Determination of the number of variables (M)*

For this purpose it is necessary to determine the number of flows of the scheme. Each flow is characterized by quantity and composition. If a flow contains three components, the composition is determined by two concentrations; if it contains two components, by one concentration. The number of variables (*M*) is equal to the sum of quantities and concentrations of all flows.

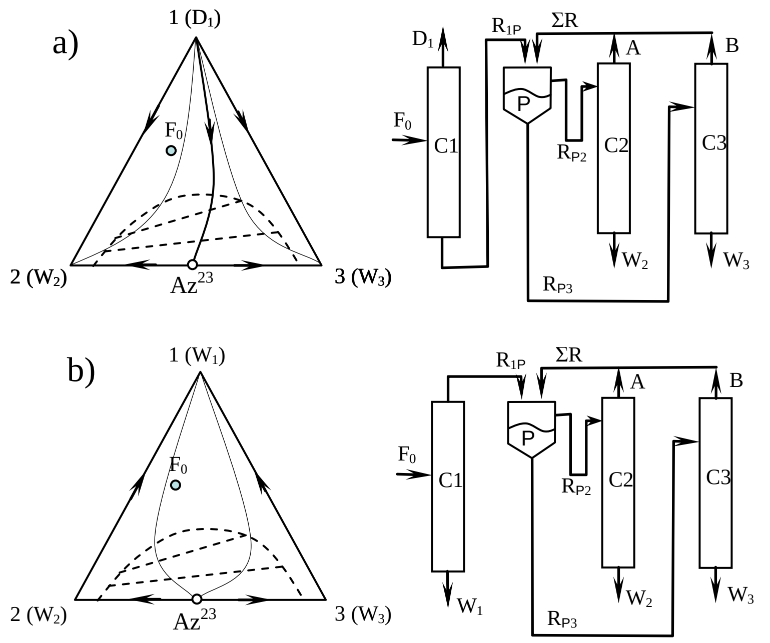


Figure 1. Phase equilibrium diagrams and separation complexes
for systems with one binary azeotrope

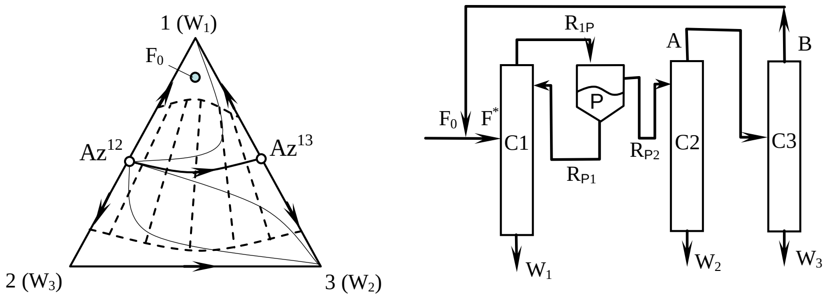


Figure 2. Phase equilibrium diagrams and separation complex
for a system with two binary azeotropes.

2. Determination of the number of independent equations (N)

The number of independent equations (*N*) consists of the number of material balance equations for different space-time contours, requirements to the quality of product flows, initial conditions (quantity and composition of the original mixture), liquid-vapor and liquid-liquid equilibrium conditions (compositions of equilibrium liquid layers in the Florentine vessel). It should be noted that the number of equations of mass balances depends on the number of devices (column, Florentine vessel, mixers) of the flow diagram. For each device of the scheme the overall mass balance and component-by-component balances should be written. The number of the latter is determined by the number of independent concentrations of components in the incoming flow and outgoing flow.

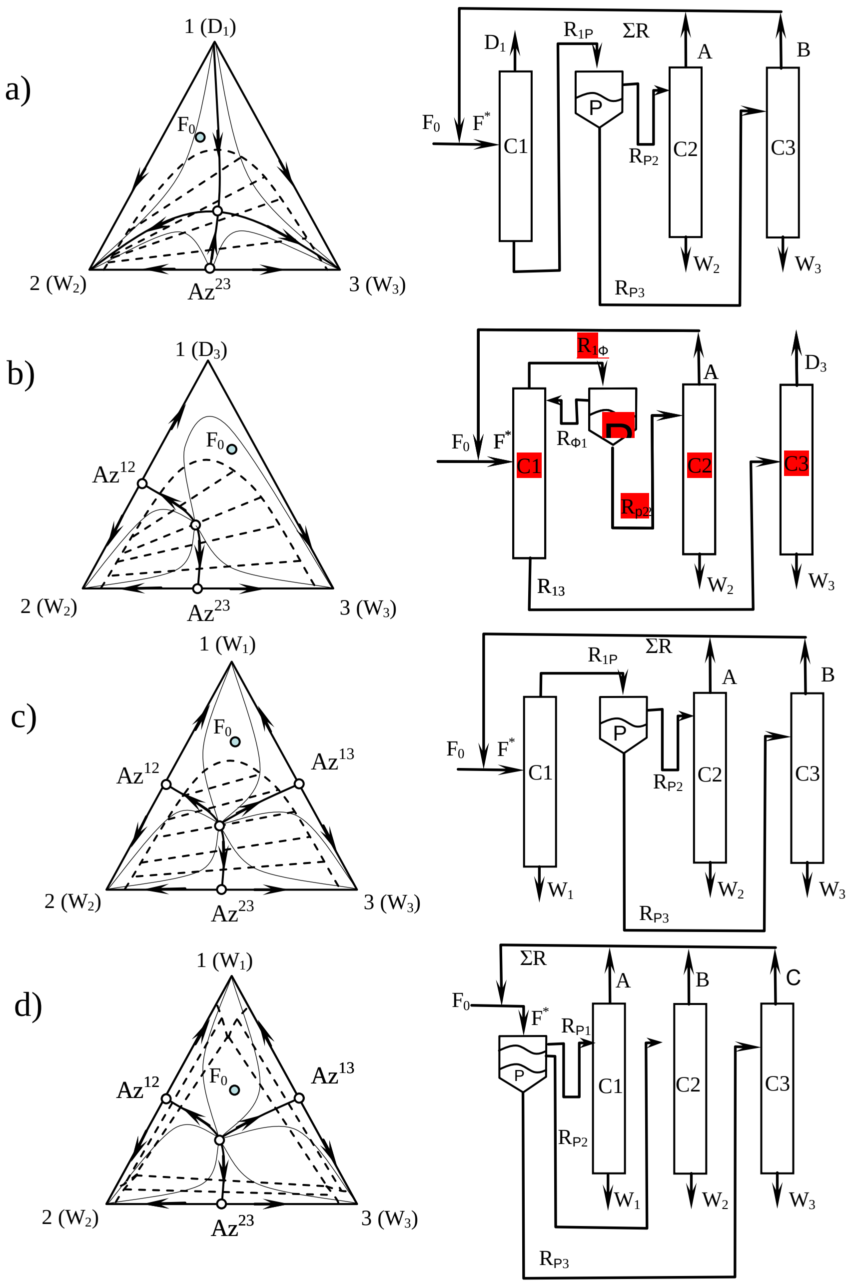


Figure 3. Phase equilibrium diagrams and separation complexes for systems with a ternary azeotrope.

All the listed equations and conditions compose a uniform system of equations describing the balance task. The number of its solutions is determined by the degree of freedom of the scheme (the number of free variables).

3. Determination of the number of free variables (F)

F is equal to the difference of the number of variables *M* and the number of independent equations *N* connecting these variables.

If the number of free variables is equal to zero, the balance task has a single solution. If F is equal to some number $a > 0$, it is necessary to preset a variables for determining the compositions and quantities of all material flows of the scheme, for example, compositions belonging to separatrixes or azeotropes [10]. The number of free variables equal to a makes the solutions of the balance task polyvariant [17]. Each of such solutions is characterized by its volume of recycles, its values of reflux-to-product ratios upon calculation of the rectification process and, finally, its power expenses.

Let us use proof by contradiction in order to explain the essence of the suggested approach. For this purpose let us consider a system and separation complex corresponding to it and presented in Figure 3c. Let us allow limit sharp separations in all the rectification columns. This means that the compositions of the bottoms of the columns correspond to pure components; distillates belong: to the ternary azeotrope, to the separatrix generated by azeotrope 12 and to the separatrix generated by azeotrope 13 for columns C1, C2 and C3, respectively.

The total number of material flows is equal to 11. Taking into account that each flow is characterized by a certain quantity and composition (two concentrations), the number of independent variables is 33. Let us determine the number of independent equations N. The equations of independent material balances for the considered case are given in [10]. Their number is equal to 18.

Let us write the equations of functional connection and the equations following from the initial conditions, from the separation conditions and from the thermodynamic restrictions:

(1) $x_{1,2}^{Rp2}$; $x_{1,2}^{Rp3}$ – known from the liquid–liquid equilibrium condition (4 equations);

(2) $x_1^{W1}=100$; $x_2^{W1}=0$; $x_1^{W2}=0$; $x_2^{W2}=100$; $x_1^{W3}=0$; $x_2^{W3}=0$ % mol – fro the separation condition (6 equations);

(3) F^0; $x_{1,2}^{F0}$ – known from the initial conditions (3 equations).

(4) The distillates of all the columns belong to the boundaries of the distillation regions (3 equations).

So, the number of equations is equal to 34, and, therefore, $F = –1$. If the number of free variables is negative, some equations are excluded (in this case one equation). Equations (1)–(3) cannot be excluded. Therefore, it is necessary to exclude one of three conditions of the belonging of compositions of the distillates in the columns to the boundaries of the distillation regions. Because the compositions of equilibrium liquid layers directly depend on flow R_{1p}, it is necessary to reject the condition of the belonging of the distillate composition in the second (or third) column to the separatrix.

This conclusion allows proving the results obtained in [10], namely: the impossibility of implementing limit sharp separations in all the rectification columns of the considered separation complex.

Let us consider in detail as an example the case presented in Figure 3b. The separation of a three-component mixture is suggested in a complex, in which the first preset separation is implemented in rectification column C1, i.e., three-component azeotrope 123 is isolated in the distillate. Zeotropic binary mixture 1-3 is formed in the still, and then it is separated in rectification column C3. The flow, the composition of which corresponds to the three-component azeotrope, belongs to the region of two-phase separation and goes to the Florentine vessel. One of the equilibrium liquid layers comes to column C2, in which component 2 is isolated in the still. The second layer from the Florentine vessel is recycled back to the first column.

Let us determine the separation conditions: limit sharp separations are implemented in the columns, i.e., the compositions of the distillates and of the columns stills belong to the boundaries of the distillation regions. The quantity F_0 and composition $x_{1,2}^{F0}$ of the initial mixture are preset.

The number of material flows of the considered scheme is equal to 10. Flows D_3 and W_3 are binary mixtures, the compositions of which are characterized only by one independent concentration. Flow R_{13} also contains a binary mixture (separation conditions). However, it leaves column C1, in which the three-component mixture is separated. Therefore, for this flow it is important to specify that the concentration of the second component is equal to zero. The other flows are characterized by three indicators: quantity and two concentrations. Thus, the number of variables is $2\cdot 2 + 3\cdot 8 = 28$.

Let us determine the number of independent equations (N).

Let us write the equations of the overall and component-by-component material balances for different spatial contours (in time unit) required for determining the quantities of all the flows:

For the scheme in total:

$$F^0 = W_2 + W_3 + D_3; \quad (1a)$$

$$F^0 x_{1,2}^{F0} = W_2 x_{1,2}^{W2} + W_3 x_{1,2}^{W3} + D_3 x_{1,2} D_3; \quad (1b,c)$$

For column 1:

$$F^* + R_{p1} = R_{1p} + R_{13}; \quad (2a)$$

$$F^* x_{1,2}^{F*} + R_{p1} x_{1,2}^{Rp1} + = R_{1p} x_{1,2}^{R1p} + R_{13} x_{1,2}^{R13}; \quad (2b,c)$$

For the Florentine vessel:

$$R_{1p} = R_{p1} + R_{p2}; \quad (3a)$$

$$R_{1p} x_{1,2}^{R1p} = R_{p1} x_{1,2}^{RP1} + R_{p2} x_{1,2}^{RP2}; \quad (3b,c)$$

For column 2:

$$R_{p2} = A + W_2 \tag{4a}$$

$$R_{p2}x_{1,2}^{RP2} = A\, x_{1,2}^{A} + W_2 x_{1,2}^{W2} \tag{4b,c}$$

For column 3:

$$R_{13} = D_3 + W_3 \tag{5a}$$

$$R_{13}x_1^{R13} = D_3 x_1^{D3} + W_3 x_1^{W3} \tag{5b}$$

The total quantity of material balance equations is 14.

The compositions of the liquid phases in the Florentine vessel ($x_{1,2}^{Rp1}$ and $x_{1,2}^{Rp2}$) are known from the liquid–liquid phase equilibrium (the three-component azeotrope is separated).

The quality of the product flows is preset: $x_1^{\mathrm{D3}}=100$; $x_1^{\mathrm{W3}}=0$; $x_1^{W2}=0$; $x_2^{W2}=100\%$ mol; F^0 and $x_{1,2}^{F0}$ are preset. From the condition of the first preset separation in column C1 it is known that $x_1^{\mathrm{R1p}}=x_1^{\mathrm{Az123}}$; $x_2^{\mathrm{R1p}}=x_2^{\mathrm{Az123}}$. The total number of equations is $N = 14+4+4+3+2 = 27$. Thus, the number of degrees of freedom for the considered complex is equal to 1. This means that in order to determine all the material flows it is necessary to preset one variable. This variable can be the concentration of the first component in the distillate of the second column (x_1^{A}). In order to preset the position of the point corresponding to the composition of flow A one concentration is sufficient, because the position of the separatrixes is determined by the vapor-liquid equilibrium diagram and, therefore, this point is situated at the intersection of the separatrix and the section corresponding to concentration x_1^{A}. This variable can be replaced, for example, with the ratio of the flow of the distillate and of the still of the second column.

The other systems and complexes were analyzed similarly. Results are shown in Table 1.

Table 1. The number of free variables that should be preset in order to calculate the material balance

Case	The number of vari-ables (M)	The number of equations					
		of material balances	from the condition of liquid–liquid equilibrium	initial conditions (F_0)	from the conditions of separation (sharp separations)	total number of equations (N)	the number of free variables (F)
1a	**23**	14	2	3	4	**23**	**0**
1b	**23**	14	2	3	4	**23**	**0**
2	**28**	14	4	3	5	**27**	**1**
3a	**33**	18	4	3	6	**31**	**2**
3b	**28**	14	4	3	4	**27***	**1**
3c	**33**	18	4	3	6	**31**	**2**
3d	**36**	18	6	3	6	**33**	**3**

* The total number of equations includes two additional equations ($x_1^{\mathrm{R1p}}=x_1^{\mathrm{Az123}}$; $x_2^{\mathrm{R1p}}=x_2^{\mathrm{Az123}}$) following from the preset separation of the first rectification column.

The systems presented in Figures 1a and 1b differ in the type of binary azeotropes: in case of 1a it is a saddle azeotrope; in case of 1b, an unstable nod. The number of free variables for the suggested separation schemes is equal in both cases to the number of free variables of the complex for the separation of the binary mixture 23 included in them and is equal to zero.

For the systems belonging to the same class (cases 3c and 3d), but characterized by various structures of the phase separation diagram (the existence of a region of two- and three-phase separation) the number of degrees of freedom is different. In case of 3c $F = 2$; in case of 3d $F = 3$. The increase of the number of free variables is due to the emergence of an additional flow (R_{P3}) participating in the recycle.

Analyzing all the cases let us note the following:

– The number of free variables F required for solving the balance task of the linear scheme of separation is always equal to zero.

– The number of free variables F for a scheme containing separation complexes is equal to the number of free variables of the separation complex included in the scheme or to the sum of the numbers of free variables of the separation complexes, if they are several in the scheme.

– The sequence of the arrangement of devices does not affect the number of free variables.

Examples of real three-component mixtures relating to some of the presented cases are considered below. The choice of free variables is shown. The material balances for the preset compositions of the initial mixture are calculated. The working capacity of the separation complexes is proved by calculation of the rectification process and determination of operation conditions of the rectification columns providing products of purity meeting the requirements of the state standard.

Calculation Part

The following systems were chosen as objects of study: methanol – chloroform – water (case 3b), butyl alcohol – water – toluene (case 3c), nitromethane – hexane – water (case 3d). The method of study is mathematical modeling. The following equation of local compositions of NRTL was used for the description of phase equilibriums [18]:

$$\ln\gamma_i = \frac{\sum_j x_i \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right)$$

where $G_{ij} = \exp(-\alpha_{ij}\tau_{il})$; $\tau_{ij} = \alpha_{ij} + \frac{b_{ij}}{T} + e_{ij}\ln T + f_{ij}T$; $\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15K)$; $\tau_{ii} = 0$; $G_{ii} = 1$.

The equation parameters were taken from the software system AspenOne and also estimated independently for components butanol – toluene, methanol – water (Table 2).

Table 2. Parameters of binary interaction

Binary system	a_{ij}	a_{ji}	b_{ij}	b_{ji}	α
methanol (1) – chloroform (2) – water (3)					
1 – 2	0.0000	0.0000	–71.9029	690.0660	0.3
1 – 3	–0.6930	2.7322	172.9871	–617.2687	0.3
2 – 3	–7.3519	8.8436	3240.6875	–1140.1154	0.2
butanol (1) – water (2) – toluene (3)					
1 – 2	0.0	0.0	211.6319	1319.7672	0.4269
1 – 3	10.338	–15.9845	–3895.4223	6471.8186	0.1964
2 – 3	627.0528	–247.879	–27269.355	14759.76	0.2
nitromethane (1) – hexane (2) – water (3)					
1 – 2	0.0	0.0	900.4934	1459.8023	0.3
1 – 3	1.0755	–9.5349	638.607	6692.177	0.2
2 – 3	0.0	0.0	2721.50	5472.00	0.2

Comparing the calculated and experimental characteristics of the azeotropes (Table 3) proves that the description of the phase equilibrium is satisfactory.

Table 3. Comparing calculated and experimental characteristics of azeotropes (P = 760 mmHg)

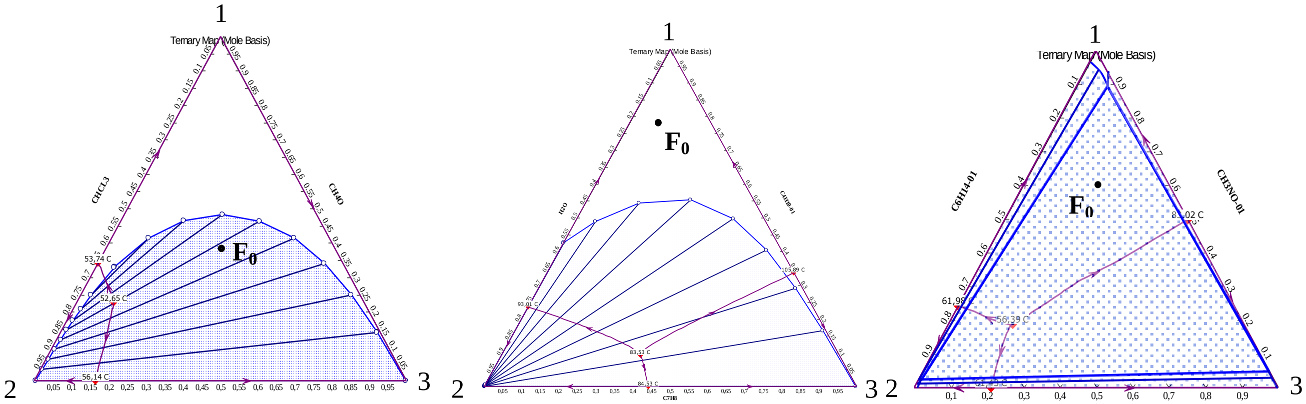
System 1-2-3	Temperature, °C		Concentration, mol %	
	exp. [19]	calc.	exp. [19]	calc.
Methanol – chloroform	53.36–53.5	53.74	65.0–65.35	65.75
Chloroform – water	56.2	56.14	85.2	83.6
Methanol – chloroform – water	52.3	52.65	x_1=23.5 x_2=70.0	x_1=22.77 x_2=67.25
Water – toluene	84.1	84.53	55.5	55.97
Water – butanol	92.7–92.9	93.01	73.7–75.8	76.41
Toluene – butanol	105.5	105.89	66.8 – 67.8	66.30
Water – toluene – butanol	83.3 [20]	85.53	x_1=53.2; x_2=38.8 [20]	x_1=53.46; x_2=38.5
Water – nitromethane	83.75	83.02	51.6	50.2
Water – hexane	61.1	61.4	21.1	21.0
Nitromethane – hexane	62.0	62.0	21.0	24.3
Water – nitromethane – hexane	–	56.4	–	x_1=17.7; x_2=18.8

Experimental and calculated data on solubility also indicating the model adequacy are presented in Table 4.

Table 4. Comparison of experimental [21–24] and calculated data on solubility at 760 mmHg

Binary component	T, °C	Compositions of equilibrium liquid layers			
		Calculated		Experimental	
		x_1', % mol.	x_1'', % mol.	x_1', % mol.	x_1'', % mol.
Water – chloroform	19	0.125	99.56	0.13	99.60
	29	0.12	99.44	0.116	99.41
Water – butanol	25	99.8	0.011	99.9	0.011
Water – toluene	40	98.28	56.51	99.2	56.75
Water – hexane	20	99.99	0.164	99.99	0.06
Water – nitromethane	20	96.8	9.3	98.2	6.4
Nitromethane – hexane	20	97.7	1.1	--	--

Phase equilibrium diagrams of the studied real systems are presented in Figure 4.



methanol (1) – chloroform (2) – water (3)

butanol (1) – water (2) – toluene (3)

nitromethane (1) – hexane (2) – water (3)

Figure 4. Phase equilibrium diagrams of the studied systems at 760 mm Hg

F_0 is the composition of the initial mixture inflowing for separation.

The data of the phase equilibrium diagram completely agree with the diagrams of the model systems presented in Figure 3. Therefore, the complexes suggested in the theoretical part of this article can be used for separation. (The sequence of isolating the components remains unchanged.)

In order to calculate the material balance it is necessary to preset the corresponding variables. For system methanol – chloroform – water (*F* = 1) the concentration of methanol in the distillate of the second column will be preset; for system butanol – water – toluene (*F* = 2) – the concentration of butanol in the distillate of the first column corresponding to the three-component azeotrope, as well as the concentration of butanol in the distillate of the third column; for system water – nitromethane – hexane (*F* = 3) – the concentration of water in the distillates of the three rectification columns.

The compositions of the equilibrium liquid layers corresponding to the compositions of the three-component azeotrope are presented in Table 5.

Table 5. Compositions of equilibrium liquid layers corresponding to the compositions of the three-component azeotropes

System	Compositions of equilibrium liquid layers, mol %		
	x'	*x*''	*x*'''
methanol	46.7	15.0	--
chloroform	16.9	83.5	
water	36.4	1.50	
butanol	0.1	24.3	--
water	99.9	1.3	
toluene	0.0	74.4	
nitromethane	1.10	89.5	3.1
hexane	98.7	1.80	0.0
water	0.20	8.70	96.9

The quantities and compositions of the material flows of the schematic diagrams of separation are presented in Table 6. Calculation of the material balance was carried out for 1 kmol / h of the initial mixture.

Table 6. Material balance of schemes for separating three-component mixtures

Device	Inflow			Outflow		
	Flow	Quantity	Composition x_1 / x_2	Flow	Quantity	Composition x_1 / x_2
Methanol (x_1) – chloroform (x_2) – water						
C1	F_0	1	40.0 / 30.0	R_{1p}	0.771	22.8 / 67.3
	R_{P1}	0.188	46.7 / 16.9	R_{13}	0.7	57.1 / 42.9
	A	0.283	31.0 / 66.0			
P	R_{1p}	0.771	22.8 / 67.3	R_{P1}	0.188	46.7 / 16.9
				R_{P2}		
C2	R_{P2}	0.583	15.0 / 83.5	A	0.283	31.0 / 66.0
				W_2	0.3	0.0 / 1.0
C3	R_{13}	0.7	57.1 / 42.9	D_3	0.4	1.0 / 0.0
				W_3	0.3	0.0 / 0.0
Butanol (x_1) – water (x_2) – toluene						
C1	F_0	1	78.2 / 15.0	R_{1p}	0.637	12.1 / 51.3
	A	0.172	0.3 / 99.7	W_1	0.782	1.0 / 0.0
	B	0.247	31.0 / 2.0			
P	R_{1p}	0.637	12.1 / 51.3	R_{P2}	0.322	0.1 / 99.9
				R_{P3}	0.315	24.3 / 1.3
C2	R_{P2}	0.322	0.1 / 99.9	A	0.172	0.3 / 99.7
				W_2	0.15	0.0 / 1.0
C3	R_{P3}	0.315	24.3 / 1.3	B	0.247	31.0 / 2.0
				W_3	0.068	0.0 / 0.0
Nitromethane (x_1) – hexane (x_2) – water						
P	F_0	1	60.0 / 20.0	R_{P1}	0.219	1.1 / 98.7
	A	0.019	25.0 / 73.0	R_{P2}	0.748	89.5 / 1.8
	B	0.148	44.0 / 10.0	R_{P3}	0.213	3.1 / 0.0
	C	0.013	49.8 / 0.0			
C1	R_{P1}	0.219	1.1 / 98.7	A	0.019	25.0 / 73.0
				W_1	0.2	0.0 / 1.0
C2	R_{P2}	0.748	89.5 / 1.8	B	0.148	44.0 / 10.0
				W_2	0.6	1.0 / 0.0
C3	R_{P3}	0.213	3.1 / 0.0	C	0.013	49.8 / 0.0
				W_3	0.2	0.0 / 0.0

Note: the flow amount is indicated in kmol/h, the composition, in mol %.

The working capacity of the schemes for all the cases should be proved by calculating the rectification process (Table 7).

Table 7. Static parameters of the operation of the rectification columns of the complex

Column	TPN	FP	R	Composition of the distillate, % mol.	B.p. (D), °C	Composition of the still residue, % mol.	B.p. (W), °C
Methanol – chloroform – water							
1	8	2	0.001	x_1= 23.0 x_2= 67.3	52.16	x_1= 56.9 x_2= 0.0	71.53
2	10	7	1.7	x_1= 31.0 x_2= 66.1	53.27	x_1= 0.5 x_2= 99.5	60.40
3	13	9	2.1	x_1= 99.5 x_2= 0.0	64.52	x_1= 0.2 x_2= 0.0	99.65
Butanol – water – toluene							
1	17	11	1.1	x_1= 12.1 x_2= 51.2	72.4	x_1= 99.1 x_2= 0.0	117.23
2	3	2	0.01	x_1= 0.5 x_2= 99.5	99.6	x_1= 0.01 x_2= 99.99	100.0
3	15	4	1.0	x_1= 30.8 x_2= 1.7	94.17	x_1= 0.6 x_2= 0.0	110.43
Nitromethane (1) – hexane (2) – water (3)							
1	10	4	2.0	x_1= 14.0 x_2= 83.2	58.57	x_1= 0.3 x_2= 99.7	68.6
2	7	2	0.7	x_1= 46.8 x_2= 9.2	75.81	x_1= 99.96 x_2= 0.0	101.1
3	8	3	0.9	x_1= 49.9 x_2= 0.0	81.72	x_1= 0.04 x_2= 0.0	100.0

Note: TPN – theoretical plate number, FP – feed plate; pressure in all the columns is 760 mmHg.

It can be seen that, when separating butanol – water – toluene mixture (Figure 3c), the equilibrium water layer (flow R_{P2}) can be isolated as an independent product flow requiring further separation. Thus, the column for isolating water can be excluded. The recycle flow contains only the distillate of the third column. The number of free variables in this case is equal to 1 ($F = 24 – 23 = 1$), i.e., in order to calculate the material balance it is necessary to preset only one variable, namely, the concentration of one of the components in the distillate of the third column.

For this case calculation of the rectification process was not carried out separately. The operation parameters of the rectification columns will be little different from the parameters of the initial scheme with three columns, because the quantity of flow A is small in comparison with the quantity of flow B. The latter mostly forms the total recycle flow ∑R.

Conclusion

The thermodynamic restrictions of the vapor-liquid balance and the features of the separatrixes arrangement with respect to the liquid-liquid equilibrium nodes, the implementation of sharp separations not only determine the possibility in principle of separating the mixture into pure components or fractions of the preset composition, but also affect the scheme energy consumption. As shown above, the balance task can be polyvariant in separation schemes containing one or more separating complexes, when the number of free variables F is other than zero.

When creating a balance network of a scheme for separating a particular mixture, we often allow limit sharp modes of separation in each of rectification columns. In addition, the position of balance lines in the concentration simplex should be in full accordance with the course of separatrixes and the slope of the liquid-liquid nodes providing implementation of the principle of redistribution of concentration fields. At the same time, in case of fixing the number of variables exceeding F it is impossible to create a balance network making physical sense. However, also the choice of variables can be limited, which is due to the impossibility of implementing limit sharp separations in one or several rectification columns.

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