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PURITY OF CRYSTAL OR CONDENSATE AS PRODUCTS OF REFINING IN DEPENDENCE ON THE PURITY OF THE REST

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The equation is displayed, which connects the purity of the product of crystallization or distillation refining (of crystal or condensate) with the purity of the rest. The equation does not contain a separation coefficient.

INTRODUCTION

Crystallization and distillation are the main methods for obtaining high-purity substances. Despite the fact that the theory of these processes has been developed and a lot of experience has been accumulated in the application of these methods [1–17], new questions arise, the solution of which can improve the technology of high-purity substances.

These processes are described by equations with an effective separation factor β, which depends on the conditions of the process, including the speed of process and the yield g [8–10, 17]:

$$\frac{C_1}{C_0} = \frac{1-(1-g)^{\beta}}{g}, \tag{1}$$

$$\frac{C_r}{C_0} = r^{\beta-1}, \tag{2}$$

where C_1 is the average impurity concentration in the condensate or in the crystal; C_r is the average impurity concentration in the rest; C_0 is the initial impurity concentration; g is the degree of distillation (the ratio of the mass of the condensate to the initial mass of the distilled substance) or the fraction of crystallized material; r is the fraction of the residue (the ratio of the mass of the residue to the initial mass of the refined substance); β is the effective separation factor or the effective distribution coefficient [7–11]. The process with n-fold repetition, when the starting material of the next operation is the product of the previous operation, is described by the equation:

$$\frac{C_n}{C_0} = \left(\frac{C_1}{C_0}\right)^n = \left[\frac{1-(1-g)^{\beta}}{g}\right]^n, \tag{3}$$

where C_n is the average impurity concentration in production of n-fold refining.

The resulting crystal (often a single crystal) as a product of crystallization refining, and often condensate as a product of evaporative refining (if the distillate is obtained by condensing steam into a solid phase) have an uneven distribution of impurities [1, 4, 12], which complicates the control of its purity – especially in cases where the product has a complex shape. At the same time, the refined substance in the residue during the refining process is under conditions of intense convection mixing, which ensures a uniform composition of the residue.

The purpose of the work is to establish the relationship between the purity of the product of normal directional crystallization or the product of the evaporation process (distillation or sublimation) with the purity of the rest in the refining processes of substances "base-impurity".

THEORETICAL ANALYSIS

Taking into account the fact that $g + r = 1$, equation (3) is transformed to the form:

$$\frac{C_n}{C_0} = \left(\frac{1-r^{\beta}}{1-r}\right)^n, \tag{4}$$

whence it follows:

$$r^{\beta} = 1 - (1-r)\left(\frac{C_n}{C_0}\right)^{1/n}. \tag{5}$$

On the other hand, equation (2) after multiplication by r is transformed to the form:

$$r^{\beta} = r\frac{C_r}{C_0}. \tag{6}$$

Comparing equations (5) and (6), we obtain the dependence C_n/C_0 from C_r/C_0:

$$\frac{C_n}{C_0} = \left(\frac{1-r\frac{C_r}{C_0}}{1-r}\right)^n. \tag{7}$$

In the case of single refining, the equation (7) are simplified to the form:

$$\frac{C_1}{C_0} = \frac{1-r\frac{C_r}{C_0}}{1-r}. \tag{8}$$

Equations (7) and (8) can be represented as inverse relationships C_r/C_0 from C_n/C_0 or C_r/C_0 from C_1/C_0 correspondently:

$$\frac{C_r}{C_0} = \frac{1-(1-r)\left(\frac{C_n}{C_0}\right)^{1/n}}{r}, \tag{9}$$

$$\frac{C_r}{C_0} = \frac{1-(1-r)\frac{C_1}{C_0}}{r}. \quad 10)$$

RESULTS AND DISCUSSION

The main result of the work is equation (7). Equations (7) and (8) are useful for determining the average impurity concentration in products of distillation or crystallization refining (with an uneven distribution of impurities) by simply controlling the purity of the residue from a single refining (with an even distribution of impurities) – without the often undesirable remelting of the product, which can average it out compound. It is important to note that equations (7)–(10), unlike equations (1) and (2), do not contain the separation factor β – the value of which depends both on the properties of the "base-impurity" system being refined, and on a number of technological process parameters such as, for example, process speed. That is, equations (7)–(10) are universal for any refined systems and regardless of the technological features of the processes.

Table, that constructed using equations (9) and (10), gives an idea of the possible values of C_r/C_0. Detection sensitivity of C_n/C_0 by value of C_r/C_0 increases with a decrease of r and with an increase of n and decreases with an increase in the purity of the product. In the limit, if $C_n/C_0 = 0$, then $C_r/C_0 = 1/r$.

Correlation between C_r/C_0 and C_n/C_0 in the n-fold refining process at different values of r

C_n/C_0	C_r/C_0 at $n = 1$			C_r/C_0 at $n = 2$			C_r/C_0 at $n = 10$		
	$r = 0.2$	$r = 0.1$	$r = 0.05$	$r = 0.2$	$r = 0.1$	$r = 0.05$	$r = 0.2$	$r = 0.1$	$r = 0.05$
0.5	3.0	5.5	10.5	2.2	3.6	6.6	1.3	1.6	2.3
0.1	4.6	9.1	18.1	3.7	7.2	14.0	1.8	2.9	4.9
0.05	4.8	9.55	19.05	4.1	8.0	15.8	2.0	3.3	5.9
0.01	4.96	9.91	19.81	4.6	9.1	18.1	2.5	4.3	8.0

According to the definition of the separation factor, with ideal mixing of the evaporating or crystallizing liquid, $\beta = C_x/C_r$, where C_x is the impurity concentration in crystal near the crystallization front or in the condensate on the condensation surface. Or:

$$\frac{C_r}{C_0} = \beta^{-1}\frac{C_x}{C_0}. \quad (11)$$

If β does not depend on r (or on g), then the equation (7) can be represented as:

$$\frac{C_n}{C_0} = \left(\frac{1-r\beta^{-1}\frac{C_x}{C_0}}{1-r}\right)^n. \quad (12)$$

The equation (12) allows you to control the average impurity concentration in the product by impurity concentration C_x in the final part of the product, if the value of $\beta = const$ is known.

It can be noted that the union of formula (11) with equation (2) (taking into account the fact that $g + r = 1$ and $g = x/L$, where x is the distance along the crystal from its beginning or the distance in the solid condensate from the substrate, and L is the length of the crystal with a completely crystallized liquid or the initial liquid level in the crucible), – easily leads to the well-known equation for the distribution of impurity concentration C_x over the length of the crystal [1, 4, 5] or over the thickness of the condensate obtained by condensation of vapor into the solid phase [12]:

$$\frac{C_x}{C_0} = \beta\left(1 - \frac{x}{L}\right)^{\beta-1}.$$

CONCLUSIONS

For the processes of crystallization or distillation refining of substances the analytical form of the dependence of the average impurity concentration in the crystal or in the condensate on the impurity concentration in the rest is established. The knowledge of this dependence makes it possible to replace the control of the purity of the refining product with an uneven distribution of impurities by a simpler control of the purity of the residue with a uniform impurity concentration. The derived equation (7) does not contain the separation coefficient β, therefore it is universal for any refined systems and regardless of the technological features of the processes affecting β.

A simple derivation of the equation for the distribution of an impurity in a crystal or in a condensate is also presented.

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ЧИСТОТА КРИСТАЛА ЧИ КОНДЕНСАТУ ЯК ПРОДУКТІВ РАФІНУВАННЯ ЗАЛЕЖНО ВІД ЧИСТОТИ ЗАЛИШКУ

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Встановлено рівняння, яке з'єднує чистоту продукту кристалізаційного або дистиляційного рафінування (кристала або дистиляту) з чистотою залишку. Рівняння не містить коефіцієнта поділу.