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EFFICIENCY OF MULTIPLE DISTILLATION OR CRYSTALLIZATION REFINING: ECONOMIC ASPECT

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The expediency of using Φ_n was noted. To assess the efficiency of *n*-fold refining of a substance by simple distillation or normal directional crystallization, taking into account the costs of carrying out the process, it is proposed to use a special criterion $\Phi_n = G/n(C_n/C_0)$ where C_0 and C_n are the initial and final concentration of the impurity, *G* is the process yield. The influence of the refining parameters (separation coefficient and number *n*) on the position of the maximum of the $\Phi_n(G)$ dependence is noted.

INTRODUCTION

Distillation, sublimation and crystallization are the main methods for obtaining high-purity substances, and therefore interest in the theory of these processes is maintained [1–4].

The refining of substances in processes of normal directional crystallization or in simple evaporation processes (excluding rectification) with *n*-fold repetition is described by the equation

$$\frac{C_n}{C_0} = \frac{\left[1-\left(1-G^{1/n}\right)^{\beta}\right]^n}{G}, \qquad (1)$$

where C_0 is the initial concentration of the impurity; C_n is the average concentration of the impurity in the refining product (in the crystal or in the condensate); *G* is the final yield of the process; β is the effective separation coefficient, depending on process conditions, including yield *g* of the process in each unit process [5–8] ($G = g^n$). At $n = 1$ equation (1) takes the form of the well-known equation

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

In the absence of convection in the refining material, the coefficient β is determined by the parameter $v\delta/D$ in crystallization processes [4] or the Peclet number $Pe = vX/D$ and separation factor β_0 in evaporation processes [6–8] (*v* is the linear speed of movement of the crystallization front or evaporation surface; δ – thickness of the diffusion layer; *X* is size factor of the evaporated material; *D* is diffusion coefficient of the impurity: β_0 is the ratio of the concentration of impurities in a pair that leaves the surface of evaporation, to the concentration of impurities in the evaporated substance near the surface of evaporation or in the evaporated substance with its perfect mixing). If $v\delta/D = 0$ or $Pe = 0$, then $\beta = \beta_0$ [6, 7]. For crystallization processes, and often for distillation processes (at not too large *Pe*: from 0 to ~ 10 [9]), the assumption is valid that β is a constant value (independent on g).

Despite the development of theories of the named refining methods, almost no attention was paid to the economic aspect of *n*-fold refining in theoretical developments, but the following can be noted.

To assess the economic efficiency of crystallization refining, a factor

$$\varphi_n \frac{G}{C_n/C_0} \qquad (2)$$

was proposed which is greater, the greater the purity achieved and the greater *G* [9] – with the dependence of C_n/C_0 on *G* according to equation (1). It has been shown that for difficult-to-remove impurities with a separation coefficient β = 0.1...0.9, the best performance of this criterion is achieved with $g \approx 80...90\%$ in each single process. (The feasibility of replacing single refining with multiple refining – but without taking into account the labor costs associated with repeating the process – was discussed in the article [4]).

Meanwhile, this approach (using factor Φ [9]) to the economic assessment of the process does not take into account the fact that in an *n*-fold process, as the number *n* increases, labor costs also increase. The purpose of the work was to consider such a criterion for the economic efficiency of the named processes of refining substances (normal directional crystallization or simple evaporation) with *n*-fold repetition, which takes into account the labor and energy costs associated with their implementation.

THEORETICAL ANALYSIS

To assess the economic efficiency of these refining processes taking into account labor costs, it is proposed to use the factor $\Phi_n = \varphi_n/n$, which, taking into account formulas (1) and (2), can be presented in the form

$$\Phi_n = \frac{G}{n(C_n/C_0)} = \frac{G^2}{n\left[1-\left(1-G^{1/n}\right)^{\beta}\right]^n}, \qquad (3)$$

at

$$\varphi_n = \frac{G}{C_n/C_0} = \frac{G^2}{\left[1-\left(1-G^{1/n}\right)^{\beta}\right]^n}. \qquad (4)$$

In formulas (1) and (2), and consequently in formulas (3) and (4), for simplicity of calculations, it is assumed that β does not depend on *g*.

Factor Φ_n grows not only with an increase in the purity of the product and an increase in the yield of the process (as factor Φ), but also with a decrease in labor costs (If $n = 1$, then $\Phi_n = \varphi_n$).

Continuing the study [8] on the advisability of using n-fold refining instead of a single one, a comparison was made of φ_n at some $n > 1$ with the value of φ_n at $n = 1$, i. e. the relation φ_n/φ_1 and the value of Φ_n at some $n > 1$ with the value of Φ_n at $n = 1$, i. e. the relation Φ_n/Φ_1 (with the same values of G and β). Taking into account the equation (2) this relationships can be represented as

$$\frac{\varphi_n}{\varphi_1} = \frac{1-(1-G)^{\beta}}{[1-(1-G^{1/n})^{\beta}]^n}$$

and

$$\frac{\Phi_n}{\Phi_1} = \frac{1-(1-G)^{\beta}}{n[1-(1-G^{1/n})^{\beta}]^n}.$$

RESULTS AND DISCUSSION

The results of constructing the dependence $\Phi_n(G)$ are presented in Figs 1 and 2 and in Tables 1–4. It is noted that the dependences $\varphi_n(G)$ and $\Phi_n(G)$ have a maximums, the position of which depends on β and *n*: as β deviates from unity and *n* increases, the maximums of the dependences $\varphi_n(G)$ and $\Phi_n(G)$ shift towards lower values of *G*. The efficiency of the *n*-fold process on factoe Φ_n is greater or less than the efficiency of the 1-fold process, depending on *n*, β, and *G* (see Table 4) (while $\varphi_n/\varphi_1 \geq 1$ for any *n*, β, and *G*). For given *n* and β, a search can be made of an interval of *G* values in which $\Phi_n/\Phi_1 > 1$ (i.e. interval of *G* outside of which the efficiency by factor Φ_n of *n*-fold refining is less than the efficiency of single refining).

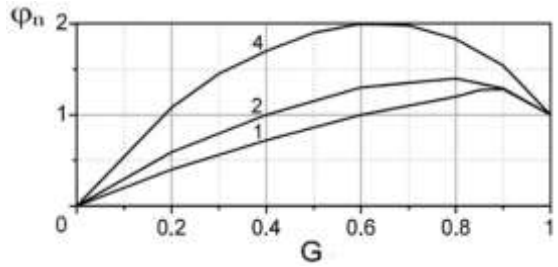
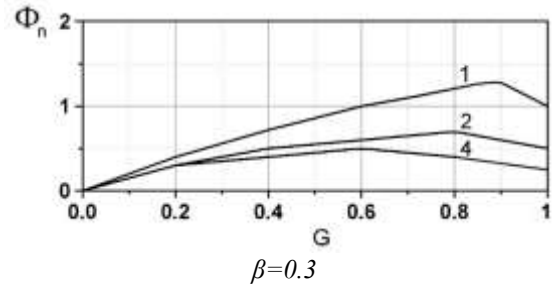


Fig. 1. Dependence $\varphi_n(G)$ at β = 0.5 and n = 1, 2, and 4 β=0.5



β=0.3

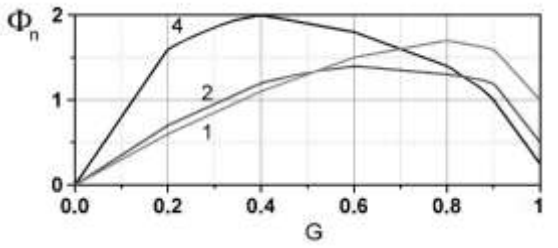


Fig. 2. Dependence $\Phi_n(G)$ at and β = 0.5 and 0.3 and n = 1, 2 and 4

Table 1

Dependence $\varphi_n(G)$ at n = 1 and 2 and β = 0.1 and 0.01

G	$\varphi_n(G)$ at difference *n* and β			
	β = 0.1		β = 0.01	
	n = 1	*n* = 2	*n* = 1	*n* = 2
0.4	3.2	16	16	$1.6\cdot10^3$
0.5	3.6	**25**	25	$1.7\cdot10^3$
0.6	4.0	18	36	$\mathbf{1.8\cdot10^3}$
0.7	**4.5**	16	**49**	$1.6\cdot10^3$
0.8	4.3	13	40	$1.3\cdot10^3$
0.9	3.9	12	35	$0.9\cdot10^3$
1	1	1	1	1

Table 2

Dependence $\Phi_n(G)$ at n = 1 and 2 and β = 0.1 and 0.01

G	Φ_n at different β and *n*			
	β = 0.1		β = 0.01	
	n = 1	*n* = 2	*n* = 1	*n* = 2
0.4	3.2	8	16	$8\cdot10^2$
0.5	3.6	**13**	25	$9\cdot10^2$
0.6	4.0	9	36	$\mathbf{9\cdot10^2}$
0.7	**4.5**	8	**49**	$8\cdot10^2$
0.8	4.3	7	40	$7\cdot10^2$
0.9	3.9	6	35	$5\cdot10^2$
1	1	0.5	1	0.5

Table 3

φ_n/φ_1 depending on *G* at different *n* and β

G	φ_2/φ_1				φ_4/φ_1	
	β = 0.5	β = 0.3	β = 0.1	β = 0.01	**β = 0.5**	β = 0.3
0.4	**1.5**	2.1	5.0	100	**2.6**	7.0
0.6	**1.4**	1.8	4.5	50	**2.1**	4.9
0.8	**1.2**	1.6	3.0	30	**1.6**	3.1
1.0	**1.0**	1.0	1.0	1.0	**1.0**	1.0

Table 4

Φ_n/Φ_1 depending on *G* at different *n* and β

G	Φ_2/Φ_1				Φ_4/Φ_1	
	β = 0.5	β = 0.3	β= 0.1	β = 0.01	**β = 0.5**	β = 0.3
0.4	**0.7**	1.0	2.5	50	**0.7**	1.8
0.6	**0.7**	0.9	2.3	25	**0.6**	1.2
0.8	**0.6**	0.8	1.6	18	**0.4**	0.8
1.0	**0.5**	0.5	0.5	0.5	**0.25**	0.25

CONCLUSIONS

The expediency of using Φ_n was noted. To assess the efficiency of *n*-fold refining of a substance by simple distillation or normal directional crystallization, taking into account the costs of carrying out the process, it is proposed to use a special criterion $\Phi_n = G/n(C_n/C_0)$ where C_0 and C_n are the initial and final concentration of the impurity, *G* is the process yield. The influence of the refining parameters (separation coefficient and number *n*) on the position of the maximum of the $\Phi_n(G)$ dependence is noted.

REFERENCES

1. C.J. King. *Separation processes* / Second edition. N.Y.: "Dover Publication", 2013.

2. G.G. Devyatykh, Yu.E. Yelliev. *Glubokaya ochistka veshchestv.* M.: "Vysshaya Shkola", 1990 (in Russian).

3. Yu.I. Dytnerskii. *Protsessy i apparaty khemicheskoi tekhnologii:* Uchebnik dlya vuzov. M.: "Himiya", 1995 (in Russian).

4. I. Bartell, E. Burig, K. Haints, L.M. Kuharzh. *Kristallizatsiya is rasplavov:* Cpravochnoe izd. / Per. s nem. M.: "Metallurgiya", 1987, 320 p. (in Russian).

5. A.I. Kravchenko. Efficiency of multiple distillation or crystallization refining with given yield // *Inorganic materials.* 2020, v. 56, N 10, p. 1055-1058; DOI: 10.31857/S0002337X20100085

6. Yu.P. Kirillov, L.A. Kuznetsov, V.A. Shaposhnikov, M.F. Churbanov. Effect of diffusion on the purification of substances by distillation // *Inorganic materials.* 2015, v. 51, N 11, p. 1092-1096; doi 10.1134/S0020168515100088

7. A.I. Zhukov, A.I. Kravchenko. Calculation of sublimation with taking into account of diffusion of impurity // *Inorganic materials.* 2017, v. 53, N 6, p. 648-653; DOI: 10.1134/S0020168517060164

8. A.I. Kravchenko, A.I. Zhukov. Effective separation factor depending on degree of distillation and temperature // *Functional Materials*. 2025, v. 32, N 1, p. 157-160; https://doi.org/10.15407/fm32.01.146

9. A.Ye. Vol'pyan, G.N. Kurdyumov, V.A. Molochko. Optimization of process of multiple directional crystallization // *Teoreticheskiye osnovy khimicheskoy tekhnologii*. 1971, v. 5, N 4, p. 602-604 (in Russian).

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ЕФЕКТИВНІСТЬ БАГАТОРАЗОВОГО ДИСТИЛЯЦІЙНОГО АБО КРИСТАЛІЗАЦІЙНОГО РАФІНУВАННЯ: ЕКОНОМІЧНИЙ АСПЕКТ

О.І. Кравченко, О.А. Даценко

Для оцінки ефективності *n*-кратного рафінування речовини простою перегонкою або нормальною спрямованою кристалізацією з урахуванням витрат на проведення процесу запропоновано застосування спеціального критерію $\Phi_n = G/n(C_n/C_0)$, де C_0 і C_n – початкова та кінцева концентрації домішки, G – вихід процесу. Відзначено вплив параметрів рафінування (коефіцієнта поділу та числа n) на положення максимуму залежності $\Phi_n(G)$.