ISSN 1027-5495. Functional Materials, 32, No.1 (2025), p. 157-160
doi:http://dx.doi.org/10.15407/fm32.01.157

Effective separation factor depending on distillation degree and temperature

A.I. Kravchenko, A.I. Zhukov

National Science Center “Kharkov Institute of Physics and Technology”,
Kharkov, Ukraine, Academic st, 1, Kharkov, 61108 Ukraine

Received August 1, 2024

The possibility of plotting the dependence of the effective separation factor β (in a well-known refining equation) on the degree of distillation $_g$ and temperature (for given values of the vapor pressure of the evaporated substance, the Peclet number at the melting temperature, the activation energy of impurity diffusion and the initial separation factor β_0) through building the dependence of the purity of the condensate on g at a given β_0 and at values of the Peclet number corresponding to a number of considered temperatures is shown. An example of calculating this dependence for a model material based on beryllium is given. The patterns of the named dependence are noted.

Keywords: distillation, sublimation, effective separation factor, Peclet number, beryllium.

Ефективний коефіцієнт поділу у залежності від ступеня дистиляції та температури. *О.І. Кравченко, О.І. Жуков*

Показана можливість побудови залежності ефективного коефіцієнта поділу β (у відомому рівнянні рафінування) від ступеня дистиляції g і температури (при заданих значеннях тиску пари речовини, що випаровується, числа Пекле при температурі плавлення, енергії активації дифузії домішки та початкового коефіцієнта поділу β_0) - через побудову залежності чистоти конденсату від g при заданому β_0 і значеннях числа Пекле, відповідних ряду температур, що розглядаються. Наведено приклад розрахунку зазначеної залежності модельного матеріалу на основі берилію.

1. Introduction

Distillation and sublimation are among the main methods for obtaining high-purity substances, and therefore there is interest in their theory [1-10]. In the general case, these processes are described by a system of equations with two parameters: with the initial separation factor β_0 and the Peclet number

$$Pe = \frac{wX}{\rho D}, \qquad (1)$$

where w is the velocity of evaporation of a substance per unit surface, D is the impurity diffusion coefficient, X is the dimensional factor of the evaporated material (for example, the initial thickness of the liquid layer in the crucible), ρ is the density of a substance (β_0 is the ratio of impurity concentration in a pair that leaves the surface of evaporation to impurity concentration in the evaporated substance near the surface of evaporation at the process temperature; in the simplest case, if a substance consisting of two components that do not interact, evaporates in a vacuum, then β_0 is approximately equal to the ratio of vapor pressure of pure components: impurity and basic). Due to the complexity of the equations, their solutions cannot be obtained in an analytical form, but can be found by numerical methods [6-9].

While the temperature dependence $\beta_0(T)$ is weak, the Pe number is highly dependent on T due to the dependences $w(T)$ and $D(T)$ [8, 9]:

$$D = D_m exp\left[\frac{Q}{R}\left(\frac{1}{T_m}-\frac{1}{T}\right)\right], \qquad (2)$$

where Q is the activation energy of impurity diffusion, R is universal gas constant, D and D_m are impurity diffusion coefficients at T and melting point T_m correspondently (the order of magnitude D_m is known: ~ 10^{-6} cm^2/s in solid and ~ 10^{-5} cm^2/s in liquid [11]);

$$w = Kp\left(\frac{T}{M}\right)^{1/2}, \qquad (3)$$

where M is the molecular mass of the evaporating substance, K is proportionality coefficient (Langmuir equation [12]). (Data on the vapor pressure of substances can be taken from reference literature, for example, from [13]).

At the same time, to describe distillation and sublimation, a simple equation is applicable with an effective separation factor β [5, 7]:

$$\frac{C}{C_0} = \frac{1-(1-g)^{\beta}}{g}, \qquad (4)$$

where C is the average impurity concentration in the condensate, C_0 is the initial impurity concentration. If the mixing of the refined liquid is ideal $Pe = 0$ and $\beta = \beta_0$ [7]. Coefficient β is the number in which equation (4) turns in true equality with given values g and $Pe > 0$; $\beta = \beta_0$, if $g = 0$ or 1.

For the correct use of the equation (4) in calculations of distillation and sublimation a clear idea of the dependence of β on g and on the temperature T of the process is necessary. (It can be noted that until recently, it was assumed that β, like β_0, is independent of g, but there is experimental confirmation of the existence of the dependence β(g) [14].) Identification of dependence $\beta(g, T)$ was the aim of work. At the same time, attention was drawn to the fact that the graphs of the dependence of C/C_0 on g [7-10], in fact, demonstrate the discrepancy between β and β_0, which depends on β_0 and Pe.

2. Calculations

The calculations of dependence $\beta(g, T)$ were based on accounting of dependence $Pe(T)$, while the dependence $\beta_0(T)$ was not taken into account.

From the equation (4) it follows that

$$\beta = \frac{ln(1-g\frac{C}{C_0})}{ln(1-g)}. \qquad (5)$$

Taking into account formulas (1)-(3), the following formula is displayed

$$\frac{Pe}{Pe_m} = \frac{p}{p_m}\left(\frac{T_m}{T}\right)^{1/2} exp\left[\frac{Q}{R}\left(\frac{1}{T}-\frac{1}{T_m}\right)\right], \qquad (6)$$

where Pe and Pe_m are Pe numbers at temperatures T and melting point T_m correspondently, p and p_m are vapor pressures of a substance at T and T_m correspondently.

Formula (6) allows to calculate the values of Pe for a number of values T (for given parameter values T_m, p, p_m, Q and Pe_m) and to build the dependence C/C_0 on g at values Pe, corresponding to a given range of values T, using the previously developed calculation method [7]. After this, using formula (5), the values of β can be calculated for given values of T and g, i.e., the dependence $\beta(T, g)$ can be constructed for a given β_0 and given parameters T_m, p, p_m, Q and Pe_m.

Dependence $\beta(g, T)$ was considered using a beryllium-based material as an example with $Q/R = 1{\cdot}10^4$ K. Calculated data for such material are given in Table 1.

3. Results and discussion

Graphs of dependency C/C_0 on g for beryllium-based material at two values of Pe_m (10 and 100) at values Pe corresponding to the temperatures indicated in the Table 1 are shown in

Table 1. Calculation data for beryllium-based material (T_m = 1551 K) at $Q/R = 1{\cdot}10^4$ K

T, K	p, mm Hg [13]	$\frac{p}{p_m}$	$\left(\frac{T_m}{T}\right)^{1/2}$	$e^{\frac{Q}{R}\left(\frac{1}{T_m}-\frac{1}{T}\right)}$	$\frac{Pe}{Pe_m}$
1551	0.03	1	1	1	1
1600	0.06	2.0	0.98	1.22	1.6
1700	0.24	8.0	0.96	1.77	4.3
1800	0.80	26.7	0.93	2.44	10.2
1900	2.32	77.3	0.90	3.29	21.1

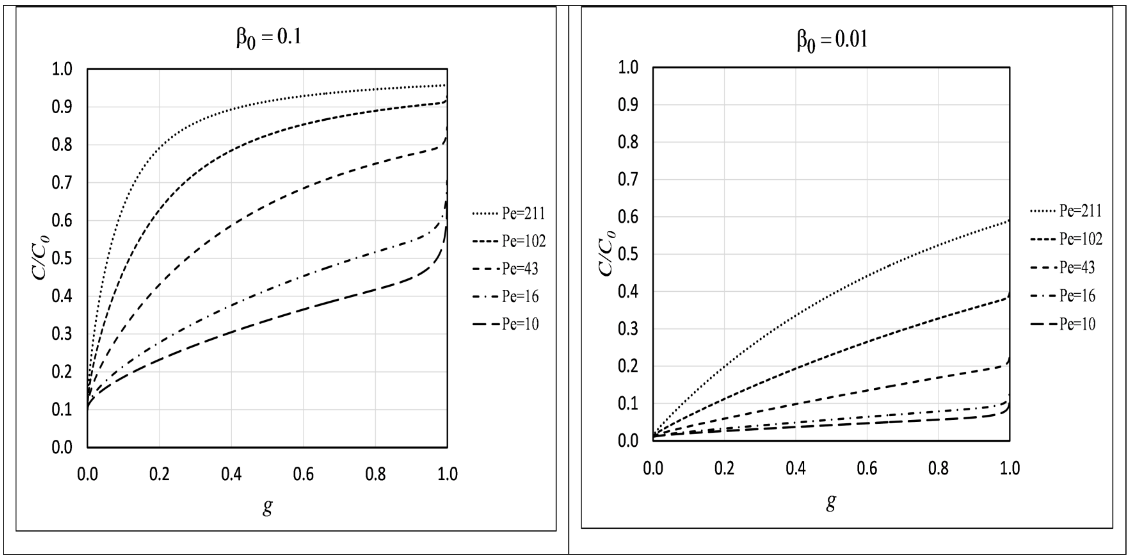

Fig. 1. Dependence of the purity of the condensate on the degree of distillation g in the process with a flat constant surface of evaporation - for two values of β_0 and different values of Pe (C is an average concentration of impurities in condensate, C_0 is the initial concentration of the impurity)

Table 2. Effective separation factor β in process of evaporation of beryllium with impurity (at $Q/R = 1\cdot10^4$ K) at different temperatures (at $Pe_m = 10$ and $Pe_m = 100$) on degrees of distillation g at different values of β_0

β_0	T, K	Pe	C/C_0 at different g					β at different g				
			g=0.2	g=0.4	g=0.6	g=0.8	g=0.9	g=0.2	g=0.4	g=0.6	g=0.8	g=0.9
0.1	1551	10	0.22	0.30	0.36	0.41	0.45	0.19	0.25	0.27	0.25	0.23
	1600	16	0.28	0.37	0.45	0.51	0.55	0.25	0.31	0.34	0.33	0.30
	1700	43	0.42	0.58	0.69	0.75	0.77	0.38	0.52	0.58	0.57	0.51
	1800	102	0.62	0.78	0.85	0.89	0.90	0.57	0.73	0.78	0.77	0.72
	1900	211	0.80	0.90	0.93	0.95	0.99	0.75	0.87	0.94	0.89	0.84
0.01	1551	10	0.02	0.03	0.05	0.06	0.07	0.02	0.02	0.03	0.03	0.03
	1600	16	0.02	0.05	0.07	0.08	0.09	0.02	0.04	0.05	0.04	0.04
	1700	43	0.05	0.10	0.14	0.17	0.19	0.04	0.08	0.10	0.09	0.08
	1800	102	0.11	0.19	0.26	0.32	0.36	0.06	0.16	0.19	0.18	0.17
	1900	211	0.20	0.34	0.44	0.52	0.55	0.18	0.29	0.33	0.33	0.30
0.1	1551	100	0.62	0.78	0.85	0.89	0.90	0.57	0.73	0.78	0.77	0.72
	1800	1020	0.96	0.98	0.99	0.99	0.99	0.91	0.97	0.98	0.98	0.96
0.01	1551	100	0.11	0.19	0.26	0.32	0.36	0.06	0.16	0.19	0.19	0.17
	1800	1020	0.57	0.75	0.83	0.88	0.89	0.52	0.70	0.75	0.76	0.70

Fig. 1, and the results of calculating the dependence β(g, T) are shown in Table 2. (To calculate values C/C_0 at $Pe_m = 100$ и $Pe = 1020$ were used the graphs C/C_0 on g with $Pe = 100$ and $Pe = 1000$ (≈ 1020), correspondently, from [10, 11].) (Obviously, if $g \approx 0$ or $g \approx 1$ then $\beta \approx \beta_0$.) Table 2 data was used to graphically represent the relationship β(g, T) - Fig. 2.

Table 2 and Fig. 2 give an idea of the nature of the dependence β(g, T) with given β_0. The coefficient β increases with increasing g and T. The dependence β(g, T) is more noticeable at a lower value of β_0, a higher temperature and a higher value of Pe_m. One can see the negative impact of increasing the initial thickness X of the liquid layer on the refining efficiency (for beryllium, with T_m = 1551 K, the value Pe_m = 10 corresponds to X ~ 1 cm, and Pe_m = 100 corresponds to X ~ 10 cm at $D_m \sim 10^{-5}$ cm^2/s).

It is possible to pay attention to the dependence of β on Q. As formula (6) shows, an increase in Q reduces the ratio Pe/Pe_m, i.e., it brings closer the graphs of the dependence β(g) plotted at different temperatures at a given β_0.

In the absence of information about the dependence $\beta_0(T)$, relying on indirect signs that this dependence is not strong, the calcula-

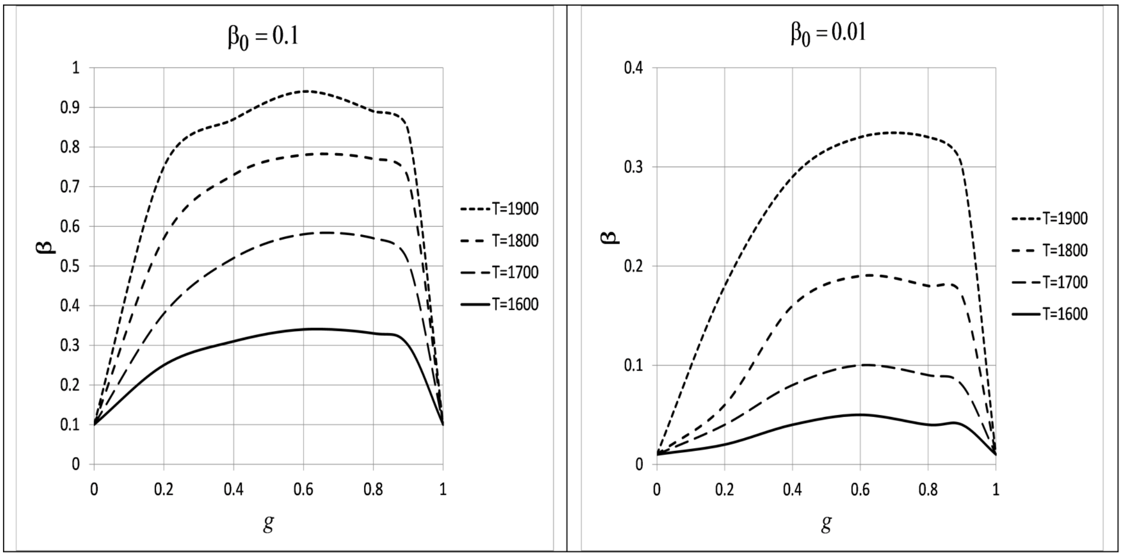

Fig. 2. Dependence β(*g*) at various β_0 and *T* for beryllium-based material at $Q/R = 1\cdot10^4$ K and $Pe_m = 10$ ($X \sim 1$ cm)

tions of the dependence β(*g*, *T*) are made with constant β_0. But if in a certain substance β_0 changes notably to the side to one with growth *T*, then the dependence β(*g*, *T*) becomes more pronounced (see Fig. 2).

4. Conclusion

Using the example of a model material from a "base-impurity" substance with given parameters (T_m, p, p_m, Q, Pe_m и β_0), the possibility of constructing the dependence β(*g*, *T*) using the previously constructed dependence of condensate purity on *g* for a given β_0 and values of the Peclet number corresponding to the range of temperatures under consideration. The nature of this dependence has been revealed.

References

1. C.J. King Separation processes – Second edition. Dover Publication, N.Y. (2013).
2. G.G. Devyatykh, Yelliev Yu.E. Ultrapurification of Substancers. Vysshaya Shkola, Moscow (1990) [in Russian].
3. Yu.I. Dytnerskii. Processes and apparatus of chemical technology: Textbook for high schools. Ed. 2. In two books. P. 2. Mass exchange processes and apparatus. Himiya, Moscow (1995) [in Russian].
4. L.A. Nisel'son, A.G. Yaroshevskii. Interphase separation factors. Nauka, Moscow (1992) [in Russian].
5. A.I. Kravchenko. *Inorganic materials*, **54**, 1. 501 (2018).
6. Yu.P. Kirillov, L.A. Kuznetsov, V.A. Shaposhnikov, M.F. Churbanov. *Inorganic materials*, **51**, 11. 1092 (2015).
7. A.I. Zhukov, A.I. Kravchenko. *Inorganic materials*, **53**. 6. 648 (2017).
8. A.I. Kravchenko, A.I. Zhukov. *Inorganic materials*, **57**. 7. 753 (2021).
9. A.I. Kravchenko, A.I. Zhukov, O.A. Datsenko. *Problems of atomic science and technology*, **1**. 13 (2022).
10. A.I. Zhukov, A.I. Kravchenko. *Problems of atomic science and technology*, **1**. 25 (2024).
11. B.S. Bokshtein, A.B. Yaroslavtsev. Diffusion of atoms and ions in solids. MISiS, Moscow (2005) [in Russian].
12. V.A. Pazukhin, A.Ya. Fisher. Separation and refining of metals in Vacuum. Metallurgiya, Moscow (1969) [in Russian].
13. A.N. Nesmeyanov. Vapor Pressure of Chemical Elements. Akad. Nauk SSSR, Moscow (1961).
14. A.I. Kravchenko. *Problems of atomic science and technology*, **1**, 29 (2024).