Functional Materials 13, No.3 (2006)

Equation of impurity distribution in a solid distillate

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Received January 23, 2006

An equation has been derived describing the distribution of an impurity in a distillate obtained by vapor condensation into solid phase at a low impurity content and under ideal mixing of the substance being distilled.

Выведено уравнение распределения примеси в дистилляте, полученном конденсацией пара в твёрдую фазу, при малом содержании примеси и идеальном перемешивании дистиллируемого вещества.

Distillation belongs to main purification methods for high purity substances. The known distillation equations [1–5] provide calculation of the averaged impurity concentration as a function of the distilled fraction and are useful when considering the vapor condensation into a liquid. However, the distillation can be performed so that the vapor condenses into a solid phase and forms an elongated cylinder. In the device shown in Fig. 1 [6], the condensate is pulled out of the device (providing a temperature) gradient at a rate providing that the lower condensate surface temperature is retained at a value ensuring the predominant condensation of the main component. (In the course of distillation, the condensate can be further purified by zone crystallization at incomplete melting [7]). In this connection, it is reasonable to calculate the impurity distribution in the solid distillate.

The relation between the compositions of vapor and of liquid in equilibrium therewith is defined by the separation factor α:

$$\alpha = \frac{N'_A}{N'_B} \Big/ \frac{N_A}{N_B} = \frac{C'_A}{C'_B} \Big/ \frac{C_A}{C_B}, \qquad (1)$$

where N_A and N_A' are molar fractions of the component A; C_A and C_A', mass concentrations of the component A in liquid and vapor, respectively. Or,

$$\alpha = \frac{C'}{1 - C'} \Big/ \frac{C}{1 - C}, \qquad (2)$$

where C and C' are the impurity mass concentrations in liquid and vapor, respectively. It follows therefrom that

$$C' = \frac{\alpha C}{1 + (\alpha - 1)C} = \frac{\alpha \frac{C}{C_0}}{\frac{1}{C_0} + (\alpha - 1)\frac{C}{C_0}}, \qquad (3)$$

where C_0 is the initial impurity concentration in the melt. On the other hand, the melt composition at a low impurity content is defined by the equation

$$\frac{C}{C_0} = \left(\frac{G}{G_0}\right)^{\alpha - 1}, \qquad (4)$$

where G and G_0 are the melt mass and the initial melt mass, respectively [3, 4]. Taking (4) into account, let (3) be transformed to

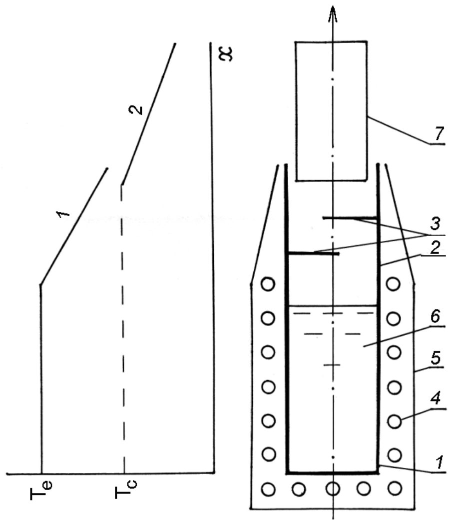

Fig. 1. Distillation device and temperature distribution therein over its height. *1*, crucible; *2*, vapor guide; *3*, baffles; *4*, heater; *5*, heat shield; *6*; material under distillation; *7*, condensate. Curve 1 is the temperature distribution over the crucible and vapor guide height; curve *2*, the temperature distribution over the crystal height. T_e is the evaporation temperature; T_c, temperature of predominated condensation of the main component.

$$C' = \frac{\alpha\left(\frac{G}{G_0}\right)^{\alpha-1}}{\frac{1}{C_0} + (\alpha - 1)\left(\frac{G}{G_0}\right)^{\alpha-1}}. \quad (5)$$

By substituting $G/G_0 = 1 - G_C/G_0$ and $G_C/G_0 = x/L$, where G_C is the condensate mass; x, the condensate height at a certain time moment; L, the same when the melt is fully evaporated (or the initial melt height in the crucible if the condensate diameter is equal to that of the crucible), the Eq.(5) takes the form

$$C' = \frac{\alpha\left(1 - \frac{x}{L}\right)^{\alpha-1}}{\frac{1}{C_0} + (\alpha - 1)\left(1 - \frac{x}{L}\right)^{\alpha-1}}. \quad (6)$$

Fig. 2 presents the Eq.(6) graphically at $C_0 = 0.01$.

When C_0 is small and α differs from unity not too significantly, the denominator in Eq.(6) is approximately equal to $1/C_0$, so Eq.(6) can be simplified to

$$\frac{C}{C_0} = \alpha\left(1 - \frac{x}{L}\right)^{\alpha-1}. \quad (7)$$

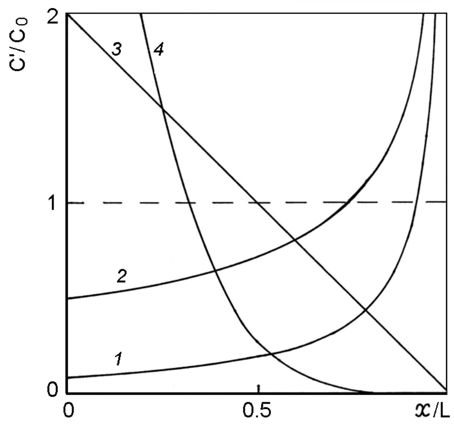

Fig. 2. Impurity gistribution over the condensate height at α values: 0.1 (*1*); 0.5 (*2*); 2.0 (*3*); 5.0 (*4*). C_0=0.01.

Note that if α is replaced by *k* (distribution factor at crystallization), Eq.(7) becomes transformed into the known equation of the impurity distribution in a crystal grown by Czochralski technique [1, 11, 12].

Thus, Eq.(6) describes the impurity distribution in a solid distillate. It is valid at a small impurity content and is derived under assumption of ideal mixing of the substance being crystallized. If α differs from unity not too significantly, the Eq.(6) is simplified to (7). The equations (6) and (7) do not take into account the possible purification of the condensate due to re-evaporation of the vapor particles. So, the distillation in the device shown in Fig. 1 is accompanied by the re-evaporation of condensed vapor particles both in the vapor guide and from the condensate surface. As a result, the purification of some substances from high-volatile impurities may be several tens times more efficient than that by simple distillation. In the case of low-volatile impurities, the efficiency improvement factor may be 2 to 10 [5, 8–10]. Nevertheless, Eqs.(6) and (7) can be useful in consideration of processes related to distillation.

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Рівняння розподілу домішки у твердому дистиляті

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Виведено рівняння розподілу домішки у дистиляті, одержаному шляхом конденсації пари у тверду фазу, для низького вмісту домішки та ідеального перемішування речовини, що дистилюється.