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CALCULATION OF DISTRIBUTION OF IMPURITIES IN SOLIDIFIED CONDENSATE INTO ACCOUNT OF PECLET NUMBER

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The results of calculations of the distribution of impurities in the condensate obtained by condensation of vapor into a solid phase in the process of evaporation of the "base-impurity" substance are presented at the values of the equilibrium separation factor β_0 in the range of 0.001…10 and the values of the diffusion Peclet number (*Pe*) in the range of $0.1…1\cdot10^4$. One can see the influence of both parameters on the formation of the distribution: at given values of β_0 and *Pe*, the condensates have larger or smaller areas with a uniform distribution of impurities. The graphs of the averaged impurity concentration in the condensates are also presented depending on the degree of distillation at the same values of β_0 and *Pe*.

INTRODUCTION

Distillation and sublimation (as well as directional crystallization) are the main methods for obtaining high-purity substances, and therefore there is an interest in the theory and practice of evaporation refining [1–8].

In the general case, the refining of a two-component substance during evaporation is described by a system of equations with two parameters: the equilibrium separation factor β_0 and the Peclet number

$$Pe = wX / \rho D,$$

where w is the rate of evaporation of the substance from a unit surface; D is the diffusion coefficient of the impurity, ρ is the density of the substance; X is the size factor of the evaporated material (for example, the thickness of the material layer in the crucible and the radius of the evaporated ball at sublimation) [4, 5, 8] – Fig. 1.

An idea of the possible values of *Pe* for "base-impurity" substances, when the base is a simple substance, is given by the results of studies [6, 7]. Thus, at the melting temperature of the base, the values of *Pe* at $X = 1$ cm for most substances lie in the range from almost zero to $\sim 10^5$ (for arsenic, under the indicated conditions, $Pe \sim 10^8$).

One of the issues of the theory and practice of evaporative refining processes is the question of the distribution of impurities in the condensate obtained during the condensate of steam into the solid phase. The equation for the distribution of impurities in the condensate was derived [9]

$$C_x / C_0 = \beta(1 - x / L)^{\beta - 1},$$

where C is the impurity concentration in the condensate at a distance x from the substrate; L is the final thickness of the condensate; C_0 is the initial impurity concentration; β is the separation coefficient. The calculations assumed ideal mixing of the evaporated liquid, so equation (1) was used – i.e., in fact, it was assumed that $Pe = 0$. For simplicity of calculations, vapor condensation on a substrate, the area of which is equal to the area of the evaporation surface, was considered.

There is information about the experimental study of the distribution of impurities in a solid condensate [10, 11] – but without discussing the role of diffusion of impurities in the evaporated material in the formation of the named distribution. Meanwhile, it is of practical interest to know the distribution of impurities in the condensate obtained by condensation of steam into a solid phase, in the general case: taking into account the diffusion of impurities in the evaporated material, i. e., at $Pe > 0$.

The aim of the work was the calculation the distribution of impurities in a solid condensate in a wide range of values of parameters β_0 and *Pe* to get an idea of the effect of this parameters on the named distribution.

CALCULATIONS

The calculation of the impurity distribution in the solid condensate was based on the technique developed earlier for calculating the average impurity concentration in the condensate [5]. As in the previous study [9], for simplicity, the evaporation of the material in the form of a flat layer in a cylindrical crucible with vapor condensation into a solid phase on an unheated flat crucible lid (with equal evaporation and condensation surfaces and equal densities of the evaporated substance and condensate) in vacuum was considered.

RESULTS AND DISCUSSION

The results of calculations of the impurity distribution in the condensate obtained during the condensation of steam into a solid phase at various values of β_0 and *Pe* are shown in the form of graphs in Fig. 2. The graphs give an idea of the processes of formation of condensates during the condensation of steam into a solid phase. At certain values of β_0 and *Pe*, the graphs have larger or smaller sections with a uniform distribution of impurities.

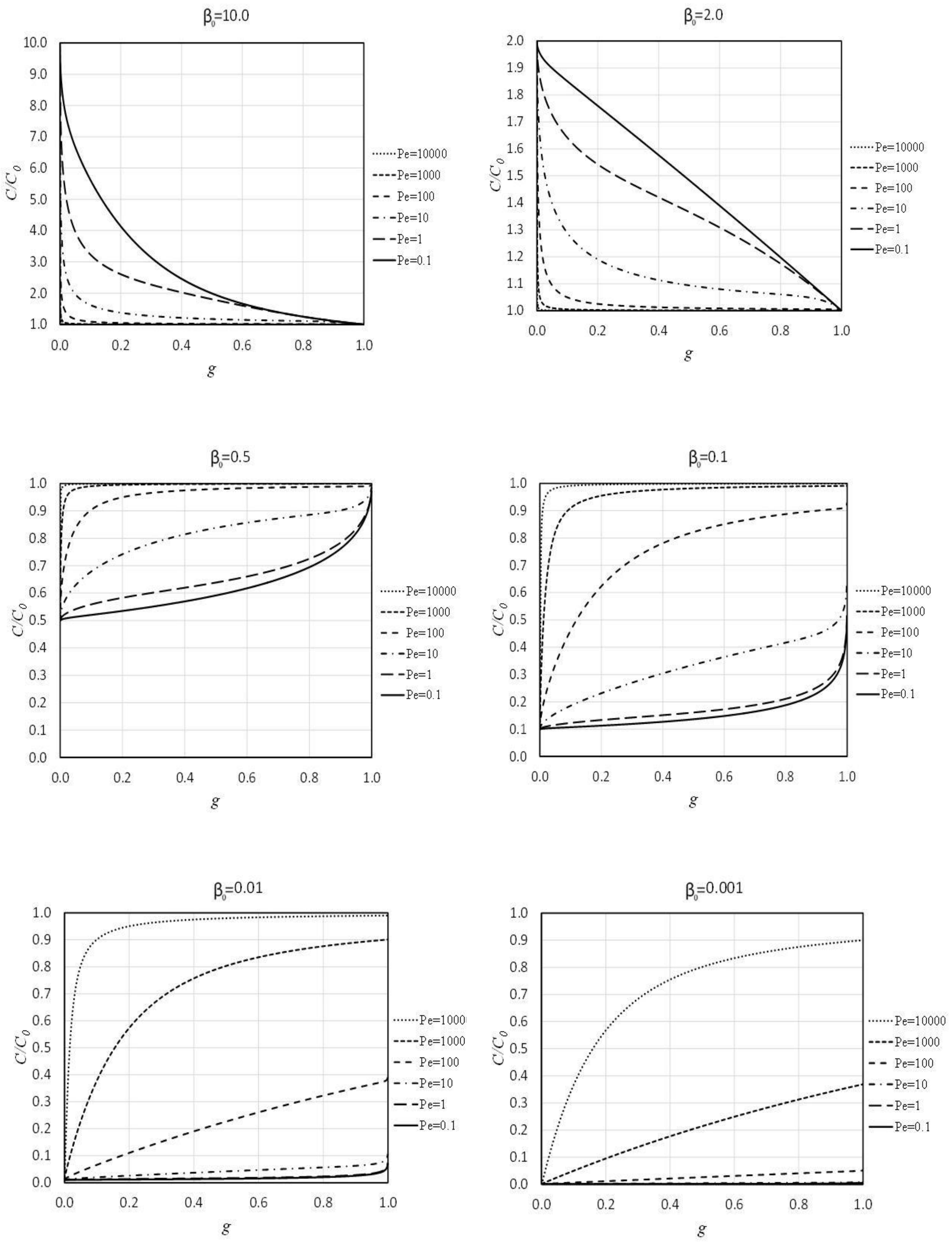

Fig. 1. Dependence of C/C_0 on the degree of distillation g of the material in the form of a flat layer during its one-sided evaporation in vacuum – at different values of β_0 and Pe (C_0 is the relative average impurity concentration in the condensate, C_0 is the initial impurity concentration) [8]

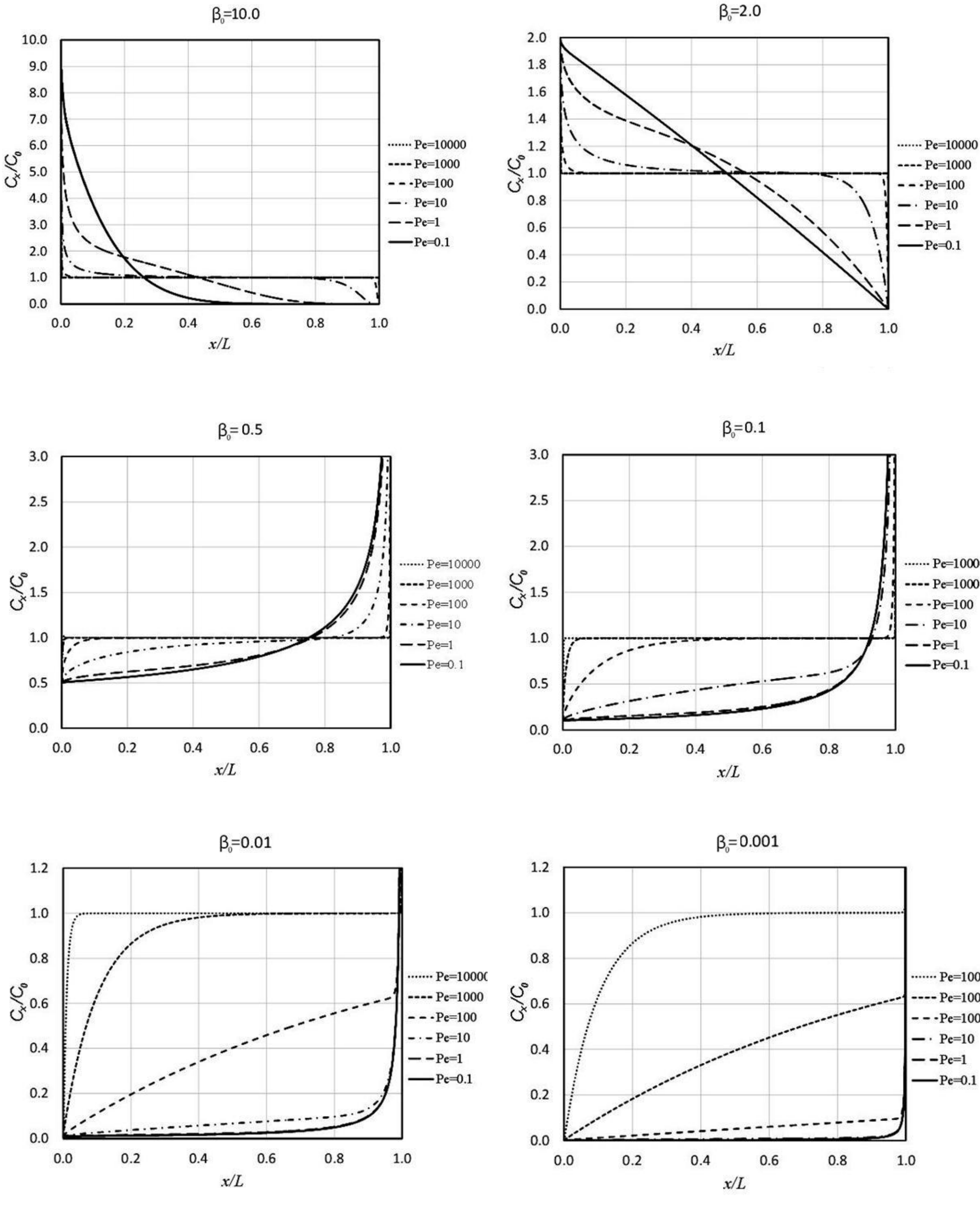

Fig. 2. Dependence of C_x/C_0 on x/L in the condensate obtained by condensation of vapor into a solid phase during one-sided evaporation of a flat layer of material in vacuum – for various values of β_0 and Pe (C_x is the impurity concentration in the condensate at a distance x from the substrate, C_0 is initial impurity concentration in the evaporated substance, L is the final thickness of the condensate)

CONCLUSIONS

The graphs of the distribution of impurities in the condensate obtained by condensation of vapor into a solid phase in the process of evaporation of the "base-impurity" substance are presented for the values of the equilibrium separation factor β_0 in the range of 0.001…10 (assuming that β_0 is constant throughout the entire evaporation process of the substance under consideration) and the values of the Peclet diffusion number (*Pe*) in the range $0.1…1{\cdot}10^4$. The influence of both parameters on the formation of the named distribution is seen. At certain values of β_0 and *Pe*, the graphs have larger or smaller sections with a uniform distribution of impurities.

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РОЗРАХУНОК РОЗПОДІЛУ ДОМІШОК У ТВЕРДОМУ КОНДЕНСАТІ З ОБЛІКОМ ЧИСЛА ПЕКЛЕ

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Представлені результати розрахунків розподілу домішок у конденсаті, отриманому конденсацією пари в тверду фазу у процесі випаровування речовини «основа–домішка» при значеннях рівноважного коефіцієнта поділу в інтервалі 0,001…10 і значеннях дифузійного числа Пекле (*Pe*) в інтервалі 0,1…$1\cdot10^4$. Видно вплив обох параметрів на формування розподілу. При заданих значеннях β_0 і *Pe* в конденсатах є більші або менші ділянки з рівномірним розподілом домішок. Також представлені графіки усередненої концентрації домішки в коденсаті за тих же значень β_0 і *Pe*.