

$$r = r_s, -D_{\text{imp}} \frac{\partial C_{\text{imp}}}{\partial r} = -G \left(C_{\text{imp}} - K \frac{C_{\text{imp}}}{C} \rho \right)$$

where $C_{\text{imp, melt}}$ is the average concentration of impurity, K is the distribution coefficient and ρ is the density of crystal.

The definition^{1,8,23,25} for K , the distribution coefficient, is the ratio of the impurity concentration (C_{imp}) to product component concentration (C) in the crystal phase divided by that ratio in the melt phase, calculated as:

$$K = \frac{(C_{\text{imp}}/C)_{\text{crystal}}}{(C_{\text{imp}}/C)_{\text{melt}}} \quad (11.8)$$

A K close to 1 means almost no separation effect, while a K close to 0 means complete separation. Therefore, K is normally used to characterize the separation efficiency of melt crystallization.

11.2.3.2 Heat Transfer

In melt crystallization processes, supersaturation is created by supercooling and tiny temperature changes in the melt could lead to fast crystallization. Therefore, heat transfer processes could play a significant role in melt crystallization.^{17,25} Similar to the mass transfer equation, the heat transfer equation with the initial and boundary conditions is defined as:

$$\frac{\partial T}{\partial t} + u(r) \frac{\partial T}{\partial x} = \alpha \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right), r_s \leq r \leq r_f, 0 \leq x \leq L \quad (11.9)$$

IC:

$$t = 0, T(r, x, 0) = T_m$$

$$x = 0, T(r, 0, t) = T_{\text{tank}}$$

BC:

$$r = r_f, -k_{\text{melt}} \frac{\partial T}{\partial r} = 0$$

$$r = r_s, -k_{\text{melt}} \frac{\partial T}{\partial r} = U(T_m - T_s)$$

where T is the temperature, α is the thermal diffusivity, k_{melt} is the thermal conductivity of the solution, T_m is the temperature of cooled surface and U is the overall heat transfer coefficient.

By solving the mass and heat transfer equations together, the product purity, distribution coefficient, yield and temperature profile of the melt crystallization process could be predicted and further insights could be gained to optimize the crystallization process.