For continuous melt crystallization process, the crystal size distribution (CSD) of product could be derived from the population balance equation

$$n = n^0 \exp(-L/G\tau) \tag{11.4}$$

where n is the number of crystals per unit volume and size differential, τ is the residence time. The population density of nuclei, n^0, is related to the numerical nucleation rate B^0 and crystal growth rate G, according to

$$B^0 = n^0 G \tag{11.5}$$

Therefore, with CSD data, n^0, G, B^0 could be obtained for continuous melt crystallization process.

11.2.3 Model Description of Melt Crystallization

For the design and optimization of melt crystallization processes, a complete understanding of the process is necessary. To this end, a detailed mathematical model needs to be established to describe the impurity concentration distribution, separation efficiency and product purity during the melt crystallization processes. Nevertheless, limited model theories could be found in the literature, which is mainly caused by the complexity of mass and heat transfer processes in the crystallizers. The non-linear differential equations could only be solved numerically and also require a considerable number of simplifying assumptions.[18–21] In this chapter, a typical model established by Yazdanpanah *et al.* for layer crystallization process is introduced.[22–24]

Figure 11.2 shows the assignment of state variables for the melt crystallization process on cooled surface. T_m is assumed to be constant at the cooled surface, while r_s, T_s and r_f, T_f would change due to the growth of crystal layer. The length of cooled surface in the axial is L.

11.2.3.1 Mass Transfer

The product component mass balance equation in the melt can be represented by Fick's diffusion law:

$$\frac{\partial C}{\partial t} + u(r)\frac{\partial C}{\partial x} = D\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right), r_s \le r \le r_f, 0 \le x \le L \tag{11.6}$$

where C is the product component concentration, $u(r)$ is the fluid velocity, D is the molecular diffusion coefficient, x is the axial distance, r is the radial distance, and L is the total length of cooled surface.

At the solid–liquid surface, the mass flux to the surface is equal to the crystallization rate. Therefore, the initial and boundary conditions for eqn (11.6) are IC:

$t = 0$, $C(r,x,0) = C_0$

$$x = 0, \quad \frac{\mathrm{d}C(r,0,t)}{\mathrm{d}t} = \frac{F(L,t)\left(C_{\text{melt}}(L,t) - C_{\text{melt}}(0,t)\right)}{V_{\text{tank}}}$$