

mediated polymorphic transformation one population is dissolving, the efficient moment based methods are generally not suitable.

2.6.1.2 Solution Mediated Polymorphic Transformation in a PFC

The cooling crystallization of L-glutamic acid is investigated in a PFC with 25 segments. Each of these segments are 60 cm long and with internal diameter of 12.7 mm. The feed at the inlet contains seeds of both the metastable α -form and the stable β -form. However, the temperature of the first segment is such that the feed concentration lies between the metastable and stable solubility curves so that the metastable form dissolves and stable form grows in size. This solution mediated polymorphic transformation is modeled using steady state population balance equation (PBE) where nucleation, growth and dissolution kinetics are considered to account for the transformation.

At steady state, the PBEs describing the crystallization process for supersaturated and undersaturated regions take the forms:

$$u_x \frac{\partial n_i(x,L)}{\partial x} + \frac{\partial [G_i n_i(x,L)]}{\partial L} = B_i \delta(L - L_n), \text{ if } c > c_{\text{sol},i}(T), i = \alpha, \beta \quad (2.70)$$

$$u_x \frac{\partial n_i(x,L)}{\partial x} - \frac{\partial [D_i n_i(x,L)]}{\partial L} = 0, \text{ if } c < c_{\text{sol},i}(T), i = \alpha, \beta \quad (2.71)$$

with the boundary condition $n_i(0,L) = n_{i,\text{seed}}(L)$. Note that Greek letters (α, β) are used interchangeably with the roman numerals (I, II) to distinguish between polymorphic forms. In this case study, the applied kinetic equations for the α and β forms are written as:

$$\begin{aligned} B_\alpha &= k_{b\alpha}(S_\alpha - 1)\mu_{\alpha,3} \\ B_\beta &= k_{b\beta,1}(S_\beta - 1)\mu_{\alpha,3} + k_{b\beta,2}(S_\beta - 1)\mu_{\beta,3} \\ G_\alpha(t) &= k_g(S_\alpha - 1)^{g_\alpha} \\ G_\beta &= k_{g\beta,1}(S_\beta - 1)^{g_\beta} \exp\left(-\frac{k_{g\beta,2}}{S_\beta - 1}\right), \end{aligned} \quad (2.72)$$

$$D_\alpha = k_{d\alpha}(1 - S_\alpha)$$

where the saturation concentration for both polymorphic forms in (g kg^{-1}) as a function of temperature (in $^\circ\text{C}$) is given by the second order power law model eqn (2.35).

The seed crystal size distribution n_i (# per m^2 kg solvent) is given as:

$$n_i(L,0) = n_{\text{seed},i} = \frac{\lambda_i}{\sqrt{2\pi}\sigma_{i,\text{seed}}} \exp\left(-\frac{(L - \mu_{i,\text{seed}})^2}{2\sigma_{i,\text{seed}}^2}\right); i \in \{\alpha, \beta\}. \quad (2.73)$$