

The parameters for the seed distribution are shown in Table 2.11 below

The mass balance equation needs to be considered which accounts for the changes in solution concentration due to growth and dissolution of both polymorphs.

$$\frac{dC}{dx} = -3 \frac{10^3}{\rho_{\text{soln}}} \sum_i \rho_{c,i} k_{v,i} G_i \mu_{i,2}, i = \alpha, \beta \quad (2.74)$$

The experimentally determined kinetic parameters are taken from Hermanto *et al.*,³⁴ which are listed in Table 2.12.

The inlet concentration is taken as $C = 20$ (g per kg solvent) and an exponentially decaying temperature profile is applied along the crystallizer going from 45°C to 33°C. The resulting PBE is solved using HR FVM. The results are summarized in Figure 2.14. It can be seen that although both the metastable α -form and stable β -form are in the feed, the CSD at the outlet indicates that the stable form has grown in size and metastable form has almost disappeared due to dissolution. The disappearance of the α -form can be further explained with the help of Figure 2.14b where the operating curve in the

Table 2.11 Parameters for seed distribution.

	λ_i	$\sigma_{i,\text{seed}}$ (m)	$\mu_{i,\text{seed}}$ (m)
α	2×10^{10}	2×10^{-6}	30×10^{-6}
β	2×10^{10}	4×10^{-6}	50×10^{-6}

Table 2.12 Kinetic parameters used in this case study.

Parameter (unit of measure)	Value
$k_{b,\alpha}$ (# m ⁻³ s ⁻¹)	exp(17.233)
$k_{g\alpha,0}$ (m s ⁻¹)	exp(1.878)
g_α (-)	1.859
$E_{g\alpha}$ (J mol ⁻¹)	10.671
$k_{d,\alpha}$ (m s ⁻¹)	exp(-10.260)
$k_{b\beta,1}$ (# m ⁻³ s ⁻¹)	exp(15.801)
$k_{b\beta,2}$ (# m ⁻³ s ⁻¹)	exp(20.00)
$k_{g\beta,0}$ (m s ⁻¹)	exp(52.002)
$k_{g\beta,2}$ (m s ⁻¹)	exp(-0.252)
g_β (-)	1.047
$E_{g,\beta}$ (J mol)	exp(12.078)
ρ_{soln} (kg m ⁻³)	990
$\rho_{c,\alpha}$ (kg m ⁻³)	1540
$\rho_{c,\beta}$ (kg m ⁻³)	1540
$k_{v,\alpha}$ (-)	0.480
$k_{v,\beta}$ (-)	0.031
$a_{\alpha,0}$ (g kg ⁻¹)	4.564
$a_{\alpha,1}$ ((g kg ⁻¹) °C ⁻¹)	0.03032
$a_{\alpha,2}$ ((g kg ⁻¹) °C ⁻²)	8.437×10^{-3}
$a_{\beta,0}$ (g kg ⁻¹)	6.622
$a_{\beta,1}$ ((g kg ⁻¹) °C ⁻¹)	-0.1165
$a_{\beta,2}$ ((g kg ⁻¹) °C ⁻²)	7.644×10^{-3}