



**Figure 2.14** Simulation results for the polymorph transformation. (Top left) Seed and product CSD from the PFC,  $\alpha$ -form completely dissolved at the outlet. (Top right) Operating curve in the phase diagram where starting point lies in between two solubility curves. (Bottom left) Evolution of the  $\beta$ -form along the PFC. (Bottom right) Dissolution of the metastable  $\alpha$ -form in the first segment.

phase diagram is shown. As can be seen, the inlet point lies in between the solubility curves, *i.e.*, supersaturated with respect to the stable form while undersaturated with respect to the metastable form, resulting in dissolution of the metastable crystal form.

## 2.6.2 Modeling Preferential Crystallization of Enantiomers

Chiral molecules or enantiomers are molecules which are non-superimposable mirror images of each other. Chirality is very common in organic molecules, *e.g.*, amino acids. These molecules have identical physical properties, however, their biological activities can be different. For instance, *S* (-)-fluoxetine shows remarkable therapeutic effects in preventing migraines, while the racemic (equimolar mixture of both enantiomers) drug has no effect.<sup>35</sup> Thus, the pharmaceutical regulatory authority demands that the drugs are manufactured in enantiopure form. The enantiomers are typically found in an equimolar mixture known as a racemic mixture. Due to the identical physical properties, separation