DETERMINATION OF OPTIMAL COOLING PROFILE OF BATCH COOLING CRYSTALLIZER

Josip Sacher*, Marko Sejdić, Matea Gavran, Nenad Bolf, Željka Ujević Andrijić, Nikola Rimac, Srečko Herceg

Faculty of Chemical Engineering and Technology, University of Zagreb, Zagreb, Croatia

** Corresponding author: jsacher@fkit.hr*

Introduction

The batch cooling crystallization is widely used unit operation for separation and purification of a compound in a single step. It is widely applied in pharmaceutical, fine chemicals and food industry among the others. In pharmaceutical industry a large number of products (or intermediates) requires crystallization in at least one step of the process. A number of problems can occur due to excessive formation of fine crystals during the process (long filtering times, clogging of the equipment, cake compression) and because of that crystals generated by nucleation are considered undesirable.

Simulation study

In this work we developed a program in Matlab using moment transformation of population balance as the process model. Crystallization kinetics for potassium sulphate was taken from literature because of good quality data and certain kinetics. An optimization problem was formulated to minimize ratio of the third moment of nucleation generated crystals to third moment of seed grown crystal. In addition, constraints were added in order to limit the duration of the process and ensure that appropriate yield is achieved at the end of the process. Optimization was performed first with genetic algorithm in order to find a solution which is near to the optimal solution. Afterwards, a sequential quadratic programming algorithm was applied to further improve the profile obtained by genetic algorithm.

Results

Seed crystals moments:

$$\mu_{0,\mathrm{s}} = \text{const.}$$

$$\frac{d\mu_{1,\mathrm{s}}}{dt} = 1 \cdot \mu_{0,\mathrm{s}} \cdot k_\mathrm{g} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{g}$$

$$\frac{d\mu_{2,\mathrm{s}}}{dt} = 2 \cdot \mu_{1,\mathrm{s}} \cdot k_\mathrm{g} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{g}$$

$$\frac{d\mu_{3,\mathrm{s}}}{dt} = 3 \cdot \mu_{2,\mathrm{s}} \cdot k_\mathrm{g} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{g}$$

Nucleation generated crystals moments:

- $\frac{d\mu_{0,\mathrm{n}}}{dt} = k_\mathrm{b} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{b} \cdot (\mu_{3,\mathrm{s}} + \mu_{3,\mathrm{n}})$
- $\frac{d\mu_{1,\mathrm{n}}}{dt} = 1 \cdot \mu_{0,\mathrm{n}} \cdot k_\mathrm{g} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{g}$
- $\frac{d\mu_{2,\mathrm{n}}}{dt} = 2 \cdot \mu_{1,\mathrm{n}} \cdot k_\mathrm{g} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{g}$
- $\frac{d\mu_{3,\mathrm{n}}}{dt} = 1 \cdot \mu_{2,\mathrm{n}} \cdot k_\mathrm{g} \cdot e^{-\frac{E_\mathrm{g}}{RT}} \cdot S^\mathrm{g}$

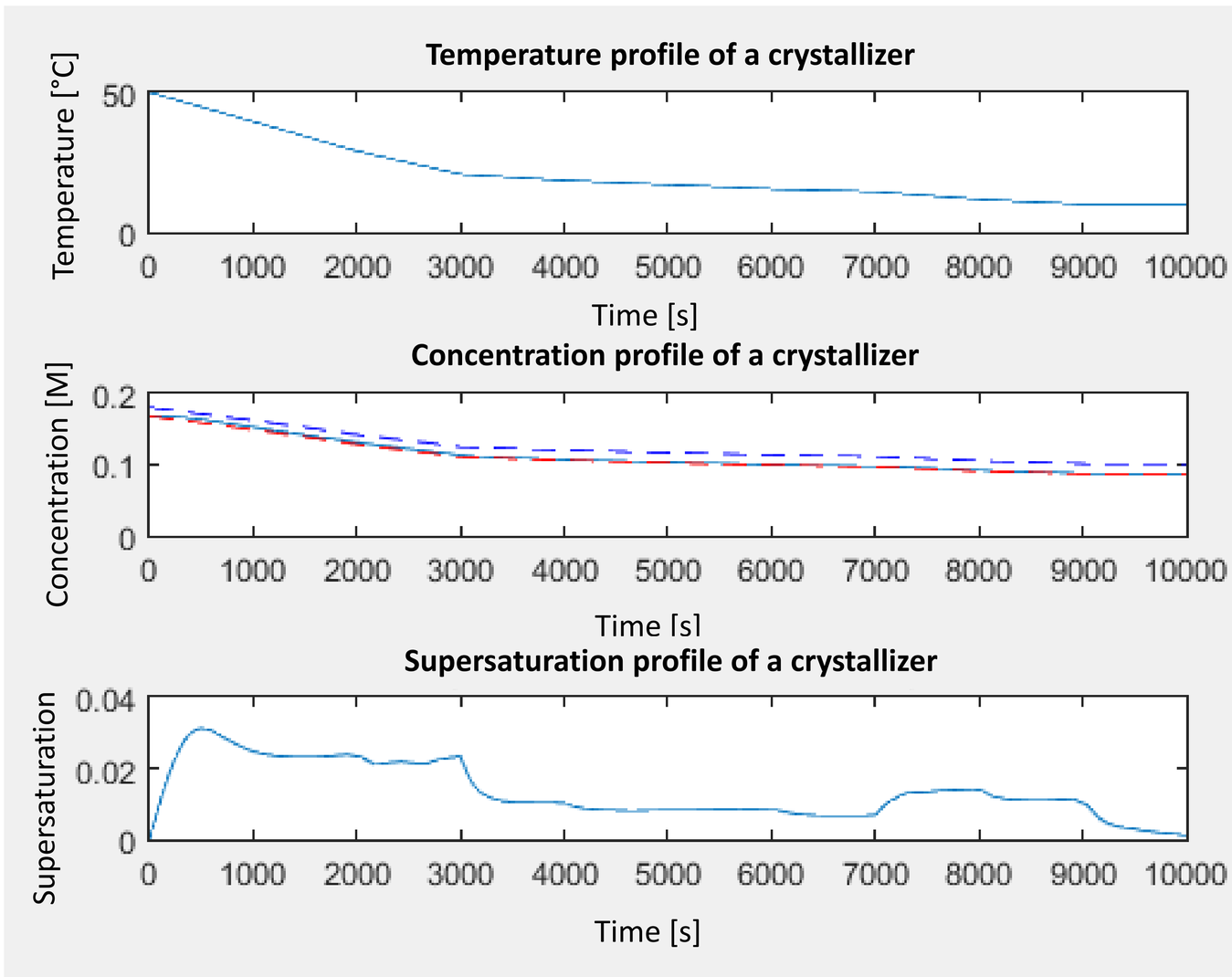
Concentration mass balance:

$$\frac{dC}{dt} = -3\rho_c k_v G(t) \cdot \mu_{2,\mathrm{s}}$$

Objective function: $\mathrm{f} = \frac{\mu_{3,\mathrm{n}}}{\mu_{3,\mathrm{s}}}$

Kinetic parameters and initial values:

Parameters	Value
b	1,45
k_b	$2{,}85 \cdot 10^{20}$ $(\mathrm{s\ m^3})^{-1}$
E_b/R	7517,0 K
k_v	1,5
ρ_c	2660,0 kg $\mathrm{m^{-3}}$
V	0,015 $\mathrm{m^3}$
g	1,5
k_g	$1{,}44 \cdot 10^{2}$ $\mathrm{ms^{-1}}$
Eg/R	4859,0 K
t_f	90,0 min
m	1,2 kg
$T(0)$	323 K



Conclusion

The solution obtained by sequential use of algorithms proves to be stable and satisfies conditions set by constraints. Therefore, the developed program can be used for calculation of the optimal temperature profile of batch crystallizer if the kinetics of the crystallizing compound is known.

Acknowledgments

This research is funded by European Structural and Investment Funds, grant number KK.01.1.1.07.0017 (CrystAPC – Crystallization Advanced Process Control).

međunarodni znanstveno-stručni skup
19. Ružičkini dani
DANAS ZNANOST – SUTRA INDUSTRIJA
21. – 23. rujna 2022. | Vukovar, Hrvatska