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# Application of extended method of classes for solving population balance equations and optimization study for crystallization process involving dissolution phenomena

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**Abstract.** Crystallization is a well-established chemical process for producing high quality of crystals. Several phenomena such as nucleation, crystal growth and dissolution are involved in producing good crystal's quality. Thus modelling of crystallization process is essential for representing crystal quality as well as for process control and optimization purposes. One of the widely approach to represent crystal quality in terms of crystal size distribution (CSD) and to solve population balance equations (PBE) is by using method of classes (MOC). However, MOC is only applicable for the case of nucleation and crystal growth and thus needs to be extended for the case of dissolution. Therefore, the objective of this paper is to extend MOC for the case of dissolution and demonstrate crystallization process involving dissolution in order to achieve desired CSD with minimum fine crystals. The mathematical model of the process is developed and simulated in Matlab. The optimization algorithm is employed to generate set-point trajectory for Proportional-Integral (PI) controller in the case of with and without dissolution phenomena. Based on the simulations, the MOC have shown comparable results with published literature, which indicates MOC has been successfully extended to solve the PBE and representing CSD for size dependent growth rate system.

## 1. Introduction

Formation of crystals from a supersaturated solution or simply crystallization process is an extremely old unit operation used to produce highly valuable products of pharmaceuticals, bulk chemicals and fertilizer chemicals [1]. These products have to conform certain product specifications with respect to crystal size and shape, purity, percentage of impurities as well as crystal size distribution (CSD) in order to be considered as good quality of crystals. Also, these product properties will determine the types of crystallization process, crystallization mode and types of equipment used for production [1-3]. Therefore, it is necessary to conform to these final specifications in order to avoid unnecessary problem in the downstream processes such as long filtration times and inadequate drying [2-6].

In crystallization process, several phenomena involves in a molecular level such as nucleation, crystal growth, agglomeration, breakage and dissolution. However, in this paper only nucleation, crystal growth and dissolution are discussed in detail as agglomeration and breakage can be neglected due to the weak impact in the solid-liquid systems [7]. Nucleation can be defined as the initial process that occurs in the formation of a crystal from a solution in which small amount of molecules aggregate to become arranged in a pattern characteristic of a crystalline solid, forming a site upon which additional particles are deposited as the crystal grows [8]. Crystal growth refers to the process of progressive addition of the particles to the surface of initial seed crystal causing an increase in crystal size. Crystal growth is a layer-



by-layer process, and only occur at the face of the crystal where the material must be transported to that face from the bulk of solution [9]. Crystal growth along with the nucleation are the most common crystallization phenomena that control the final CSD obtained in a system. In addition, the conditions and rate of crystal growth have a significant impact on the purity and the crystal habit [9]. An understanding of both nucleation and crystal growth theory are imperative in the development of industrial crystallization process.

Other crystallization phenomena, which is dissolution is referred as the reverse process of crystallization where dispersed solid that goes into solution is the solute [10]. As dissolution proceeds, the concentration of the solute increases. Given sufficient time at the fixed conditions, the solute will eventually dissolve up to a maximum solubility where the rate of dissolution equal to the rate of crystallization. Then, the solution is incapable of dissolving any solute under these equilibrium conditions. In cooling crystallization, dissolution may be achieved by simply heating up the solution to a specified temperature in which would cause the solute to dissolve. The alternating cycle of high and low temperature allow the crystal particles grown from seed crystals and fine crystals produced by secondary nucleation to dissolve back during reheating cycle. Therefore, dissolution would become beneficial in terms of dissolving fine crystals produced by secondary nucleation if properly designed into the model [4]. However, there is limited available published literature regarding dissolution model and mostly assume that the kinetic model of dissolution is the inverse of crystal growth model [2-4, 8, 11].

Besides, describing crystallization process using model-based approach or population-based modelling is considered as the commonly accepted modelling approach [7]. Generally, crystallization models involve three types of dynamic balance equations which are population, mass and energy. Population balance equation (PBE) is a hyperbolic partial differential equations that is usually coupled with a set of equations describing crystallization phenomena, saturation equilibrium as well as mass and energy balances in the forms of ordinary differential equations (ODEs). This PBE requires complex numerical solution techniques which is characterized by significant computational burden [10]. One of the commonly used PBE numerical solution technique is the standard method of moments [3-4, 12]. The approach of this method is by converting the partial differential equations (PDEs) that represent the population balance into a set of coupled ordinary differential equations (ODEs) for the  $n$ -moments considered. Since the ODE solvers are readily available, many researchers use this method to ease the solution of PBE. Another available method to solve PBE is method of classes (MOC). Method of classes permits the partial differential equations (PDEs) to be sectioned along the size domains into finite classes. This means that the method of classes allows estimation of crystal size distribution (CSD) at any point during crystallization process of either size dependent or size independent growth. This could not be achieved by using standard method of moments due to its limited function of  $n$ -moments. It is worth noting that method of moments capable of characterizing the crystal product only by mean crystal size or mean size diameter. In order to construct CSD, the standard method of moments needs to be extended or modified which increases the complexity of PBE solution. Thus, in this paper applications of method of classes are studied. Other than that, most of the crystallization work found in the literature used method of classes for the case of nucleation and crystal growth only. There is only one research that used method of classes as a solution for generic PBE in the case of including dissolution phenomena [13]. In their work, crystal growth and dissolution models are developed based on the assumptions of size independent rate but no detailed clarification on the construction of CSD is provided in their work. The relationship between method of classes and concentration or energy balances are also not presented.

Therefore, in this paper the study of seeded batch cooling crystallization is demonstrated using extended method of classes for both without and with dissolution phenomena. Potassium nitrate crystallization is chosen as the case study which is adopted from published literature [3]. The mathematical model of potassium nitrate crystallization using extended method of classes is simulated in Matlab software. For both cases of without dissolution and with dissolution phenomena, specified optimization algorithms are employed to generate the temperature trajectory of the system which is then served as the set-point for Proportional-Integral (PI) controller. The performances for both cases are studied and compared with the published literature [3] especially in terms of the construction of CSD for demonstrating the capability of the extended method of classes.

## 2. Extension of Method of Classes

In this section, the population balance model for a batch crystallizer with size dependent growth of the one characteristic length ( $L$ ) adopted from [3] is described as shown in equation (1).

$$\frac{\partial f_n(L,t)}{\partial t} + \frac{\partial G(L,S)f_n(L,t)}{\partial L} = B_{nuc} \quad (1)$$

where  $f_n(L,t)$  is the population density function,  $G(L,S)$  is the size dependent linear crystal growth rate,  $B_{nuc}$  is the nucleation rate and  $t$  is crystallization time. This one-dimensional PBE is solved by using extended method of classes as shown in equations (2)-(7) instead of the conventional standard method of moments. The usage of extended method of classes is to demonstrate the capability of this method to incorporate the dissolution terms and to generate the CSD accurately and similarly as the published literature [3]. Please note that dissolution term,  $D_x$  is used as the relative supersaturation level proceeds lesser than 0 where the relative supersaturation ( $S$ ) is applied as  $S = (c - c_{sat})/c_{sat}$ , where the  $c$  is the concentration of the solute and  $c_{sat}$  is the saturation concentration. The usage of the dissolution term,  $D_x$  is based on the assumption that it is the inverse of crystal growth model.

For  $S > 0$ ,

$$\frac{dN_1}{dt} + \frac{G_{x1}}{2\Delta Cl_2} N_2 + \frac{G_{x1} - G_{x0}}{2\Delta Cl_1} N_1 = B_{nuc}, i=1 \quad (2)$$

$$\frac{dN_i}{dt} + \frac{G_{xi}}{2\Delta Cl_{i+1}} N_{i+1} + \frac{G_{xi} - G_{xi-1}}{2\Delta Cl_i} N_i + \frac{G_{xi-1}}{2\Delta Cl_{i-1}} N_{i-1} = 0, 1 \leq i \leq n \quad (3)$$

$$\frac{dN_n}{dt} + \frac{G_x}{2\Delta Cl} N_n + \frac{G_{x1} - G_{x0}}{2\Delta Cl} N_n = 0, i = n \quad (4)$$

For  $S < 0$ ,

$$\frac{dN_1}{dt} + \frac{D_{x1}}{2\Delta Cl_2} N_2 + \frac{D_{x1} - D_{x0}}{2\Delta Cl_1} N_1 = B_{nuc}, i=1 \quad (5)$$

$$\frac{dN_i}{dt} + \frac{D_{xi}}{2\Delta Cl_{i+1}} N_{i+1} + \frac{D_{xi} - D_{xi-1}}{2\Delta Cl_i} N_i + \frac{D_{xi-1}}{2\Delta Cl_{i-1}} N_{i-1} = 0, 1 \leq i \leq n \quad (6)$$

$$\frac{dN_n}{dt} + \frac{D_x}{2\Delta Cl} N_n + \frac{D_{x1} - D_{x0}}{2\Delta Cl} N_n = 0, i = n \quad (7)$$

where  $N_i$  is the number of crystals per unit suspension for class  $i$ ,  $G_x$  is the crystal growth rate in length direction  $x$  and  $D_x$  is the dissolution rate in length direction  $x$ .

In addition, the overall mass balance and energy balance for potassium nitrate crystallization are shown in equations (8) and (9) respectively.

$$\frac{dc}{dt} = -\frac{\rho_c k_v V}{m_w} \left( \sum_{i=1}^{i=N} S_{xi}^3 \frac{dN_i}{dt} \right) \quad (8)$$

$$\rho V c_p \frac{dT}{dt} = -\Delta H_c \rho_c k_v V \left( \sum_{i=1}^{i=N} S_{xi}^3 \frac{dN_i}{dt} \right) - U_1 A_1 (T - T_w) \quad (9)$$

where  $\rho_c$  is the crystal density,  $k_v$  is the crystal shape factor,  $V$  is the volume of solution,  $m_w$  is the mass of solvent,  $c_p$  is the heat capacity,  $T$  is the temperature of the solution,  $\Delta H_c$  is the heat of crystallization,  $U_1$  is the heat transfer coefficient of internal crystallizer,  $A_1$  is the internal area of crystallizer and  $T_w$  is the cooling water temperature.

Next, the saturation concentration for potassium nitrate is generated and adapted based on the following polynomial expression as the function of solution temperature [3].

$$c_{sat} = 0.129 + 5.88 \times 10^{-3} T - 1.72 \times 10^{-4} T^2 \quad (10)$$

Also, secondary nucleation is assumed while the effect of agitation is neglected in the nucleation, crystal growth and dissolution model equations. It has been assumed that the crystal is grown or dissolved based on size dependent rate. The dissolution rate is set to have the same order of magnitude as the growth rate and a first-order dependence on the degree of under saturation is assumed. The models

for secondary nucleation, crystal growth and dissolution rates in the power law form are shown in equations (11)-(13):

$$B_{nuc} = k_b S^b V \quad (11)$$

For  $S > 0$ ,

$$G_{xi} = k_g S^g (1 + \alpha_g L_{xi})^{\beta_g}, i = 1, 2, 3 \dots n \quad (12)$$

For  $S < 0$ ,

$$D_{xi} = k_d S^d (1 + \alpha_d L_{xi})^{\beta_d}, i = 1, 2, 3 \dots n \quad (13)$$

where  $k_b$ ,  $k_g$ , and  $k_d$  are the kinetic coefficients for nucleation, crystal growth and dissolution respectively.  $b$ ,  $g$  and  $d$  are the nucleation order, crystal growth order and dissolution order respectively.  $\alpha_g$  and  $\beta_g$  are the crystal growth parameters and  $\alpha_d$  and  $\beta_d$  are the dissolution parameters.

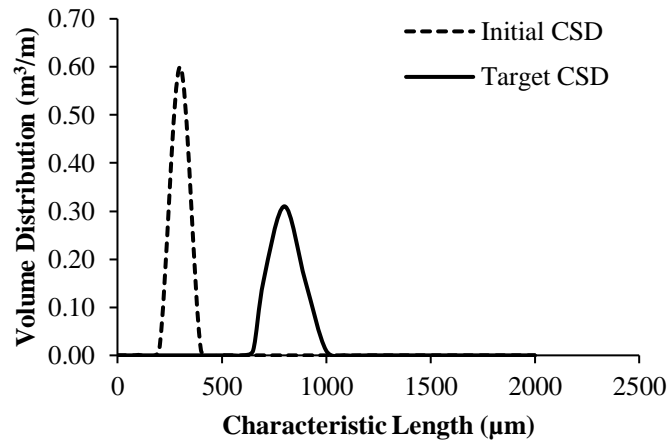
Other than that, the crystal size distribution (CSD) is calculated based on the following equation (14).

$$f_n(L_{xi}) = \frac{N_i / \Delta Cl + N_{i+1} / \Delta Cl}{2} \quad (14)$$

where  $L_{xi}$  is the length of crystal particles and  $\Delta Cl$  is the size of classes where  $\Delta Cl = L_{xi} - L_{xi-1}$ .

### 2.1. Operating scenario

The assumed scenario for crystallizer operation is that initially the crystallizer is loaded with a feed solution whose saturation temperature is  $T_{feed}$ . At the beginning of the batch process, the crystallizer is cooled to a temperature below saturation temperature and then a crystallizer is loaded with an initial seed distribution which is based on the uniform distribution adapted in [3] where it is characterized by the mass  $C_s$ , the average mean size  $L_s$ , and the percentage of width  $w$  of the distribution. The initial mean characteristic length is set to be 300  $\mu\text{m}$  and targeted to grow to 800  $\mu\text{m}$  as shown in figure 1.



**Figure 1.** Initial seed of CSD and targeted CSD.

The temperature then is lowered to  $T_{fin}$  within the time duration  $t_{cool}$ . The specific values of the operating conditions and kinetic parameters are shown in Tables 1 and 2 respectively.

**Table 1.** Operating conditions and major constraints adapted from [4].

| Nomenclature                              |   | Values             |
|---|---|--------------------|
| $T_{feed}$                                | Saturation temperature of feed, °C          | 30.0               |
| $T_{fin}$                                 | Final temperature, °C                       | 20.0               |
| $t_{cool}$                                | Cooling duration, min                       | 120                |
| $t_{batch}$                               | Batch time, min                             | 150                |
| $C_s$                                     | Seed loading ratio, %                       | 0.5                |
| $L_s$                                     | Seed size, $\mu\text{m}$                    | 300                |
| $w$                                       | % Width of distribution, %                  | 10                 |
| $T_s^{\max}$                              | Upper limit of seeding temperature, °C      | 30.0               |
| $T_s^{\min}$                              | Lower limit of seeding temperature, °C      | 27.0               |
| $T_{min}$                                 | Upper limit of crystallizer temperature, °C | 30.5               |
| $T_{max}$                                 | Lower limit of crystallizer temperature, °C | 20.0               |
| $c_0 = c_{sat}(30\text{ }^\circ\text{C})$ | Initial feed concentration, g/g – water     | 0.459              |
| $\rho_c$                                  | Density, $\text{kg/m}^3$                    | $2.11 \times 10^3$ |
| $k_v$                                     | Volumetric shape factor                     | 1                  |

**Table 2.** Kinetic parameters of crystallizer model adapted from [4].

| Parameters                           | Units       | Values                  |
|--------------------------------------|-------------|-------------------------|
| Nucleation parameter ( $k_b$ )       | #/s/g-water | $4.21 \times 10^5$      |
| Nucleation parameter ( $b$ )         | -           | 1.59                    |
| Growth parameter ( $k_g$ )           | m/s         | $1.0741 \times 10^{-4}$ |
| Growth parameter ( $g$ )             | -           | 1.28                    |
| Growth parameter ( $\alpha_g$ )      | 1/m         | 1000                    |
| Growth parameter ( $\beta_g$ )       | -           | 0.5                     |
| Dissolution parameter ( $k_d$ )      | m/s         | $1.19 \times 10^{-4}$   |
| Dissolution parameter ( $d$ )        | -           | 1                       |
| Dissolution parameter ( $\alpha_d$ ) | 1/m         | 1000                    |
| Dissolution parameter ( $\beta_d$ )  | -           | -1.0                    |

### 3. Applications of Extended Method of Classes

The mathematical model for the potassium nitrate crystallization process is developed in Matlab 2014b software and is solved using backward differentiation formula (BDF) method known as ‘ode15s’ solver using the initial conditions in Table 1. Two cases of potassium nitrate crystallization without and with dissolution phenomena are demonstrated in the next subsections 3.1 and 3.2 respectively using specified optimization algorithm to achieve desired target CSD.

#### 3.1. Potassium nitrate crystallization without dissolution phenomena

The optimization algorithm as shown in equation (15) is employed to generate the supersaturation set-point for the controller to maintain. This objective function adapted from [14] is set to minimize the error between calculated CSD and targeted CSD in order to obtain desired target CSD as shown in figure 1.

$$F_{obj} = \sum_{i=1}^N \left( \frac{f_{n,i} - f_{n,i_{target}}}{f_{n,i_{target}}} \right)^2 \quad (15)$$

Subject to:

$$0 \leq \phi \leq \phi_{\max}$$

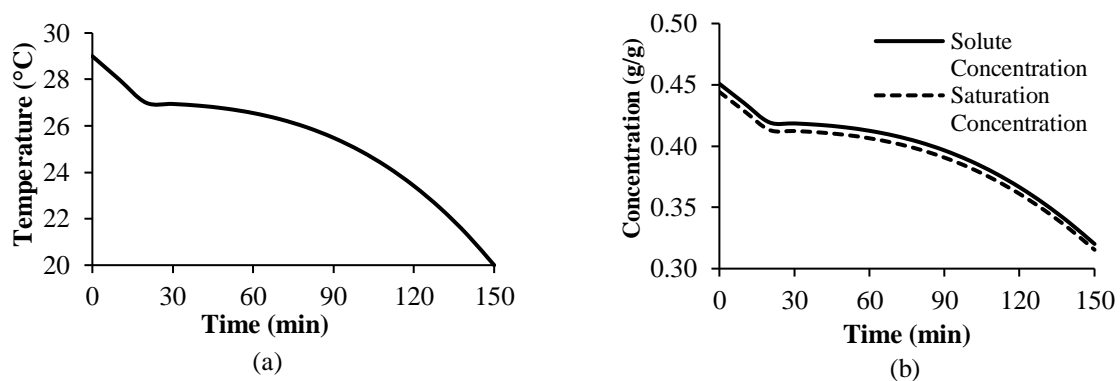
$$t_{\min} \leq t_c \leq t_{\max}$$

$$c_{\text{batch}} \leq c_{f \max}$$

The equation is called as analytical CSD estimator, where  $N$  is the number of discretization points,  $f_{ni}$  is the predicted CSD obtained from mathematical model (equations (2) to (14)) and  $f_{n\text{target}}$  is the desired target CSD.  $\Phi$  is the supersaturation set-point,  $c_{\text{batch}}$  is the expected solute concentration at the end of the batch and  $c_{f\max}$  is the maximum acceptable solute concentration at the end of the process to achieve required yield. This analytical CSD estimator is developed based on the concept of constant supersaturation level throughout the entire crystallization process. Based on the CSD estimator, in order to obtain desired CSD the supersaturation level that needs to be maintained within 150 minutes is 0.015 g/g. Please note that the crystallization time is fixed at 150 minutes in order to allow for model validation with published literature.

Subsequently, the generated supersaturation set-point from equation 15 is used as the set-point for the PI controller in order to achieve desired CSD. Proportional-Integral (PI) controller is used as controller since it is proven to be feasible for maintaining the concentration at its set-point [14]. The temperature of crystallizer is maintained and controlled at its set-point by manipulating the water inlet temperature of the crystallizer using PI controller. The parameters for PI controller is calculated from Internal Model Control (IMC) tuning method where the proportional gain ( $K_c$ ) is 33 and integral time ( $\tau_i$ ) is 2.3.

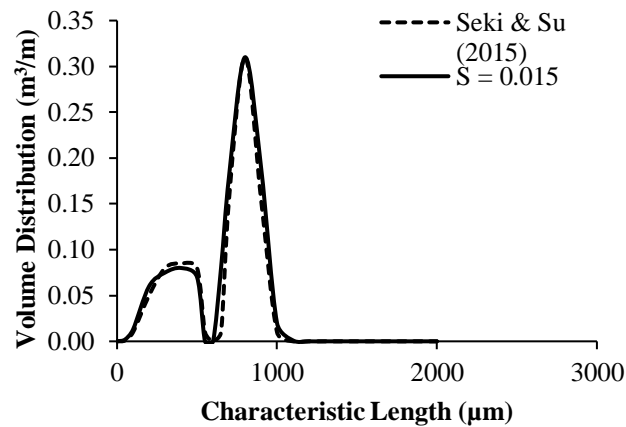
Meanwhile, figure 2 shows the closed-loop simulation results using PI controller for temperature profile of potassium nitrate crystallization with constant supersaturation level at 0.015. It can be seen that the temperature profile in figure 2 (a) drops consistently from 29 °C to 20 °C. Similarly, the solute concentration drops steadily from 0.45 g/g to 0.32 g/g until the end of operational time at 150 minutes. Figure 2 (b) shows there is a constant gap between solute concentration and saturation concentration indicating that the supersaturation level is successfully kept constant to induce high crystal growth and nucleation rate. Nevertheless, sharp drop from 0 to 30 minutes is observed on temperature profile which is mainly due to the compensation of high supersaturation at the beginning of the process in order to keep constant supersaturation level throughout the batch crystallization. It is noted that the solute concentration is operated above the saturation line which indicates that there will be no dissolution for this case study. Both temperature and concentration profiles have similar trend due to concentration profile is temperature dependent as shown in equation (10).



**Figure 2.** (a) Temperature and (b) concentration profiles without dissolution phenomena.

Next, figure 3 shows the CSD profile of the seed crystals is grown from mean crystal size of 300  $\mu\text{m}$  to 800  $\mu\text{m}$  as the result of specified level of supersaturation. As shown in figure 3, high supersaturation level at 0.015 g/g results in high nucleation and crystal growth rate which contributes to the higher secondary nucleation that distributes below 500  $\mu\text{m}$  although the targeted CSD adapted from [3] is successfully achieved. The distribution of the initial seed is divided into two peaks which is desired CSD target and undesirable peak of secondary nucleation. Large size of crystals has been obtained but the amount of fine crystals is also significant. These fine crystals may cause difficulties in the downstream

processing equipment such as filtration and drying whereby longer filtration time and drying is needed [2-6]. The disperse distribution is due to the size dependent crystal growth properties whereby large crystals have high crystal growth rate and vice versa at the selected process conditions. The distribution of the initial seed is decreasing from  $0.6 \text{ m}^3/\text{m}$  to  $0.3 \text{ m}^3/\text{m}$ . This is due to the fact that the low supersaturation would lead to low crystal growth rate that contributes to the low value of the mean crystal size [10]. In summary, desired target CSD is able to achieve but there is significant amount of fine crystals at the end of crystallization process. The simulation of mathematical model of potassium nitrate crystallization process employing method of classes without dissolution case has been successfully performed in this work under closed-loop simulation. The CSD profile obtained through employing method of class is similar to the published literature as shown in figure 3 which proves that the method of classes is capable for achieving similar results for the case of without dissolution.



**Figure 3.** CSD profile based on supersaturation set-point at 0.015.

### 3.2. Potassium nitrate crystallization with dissolution phenomena

Since the fine crystals in the case of without dissolution step is high despite achieving the desired target CSD, the optimization algorithm adapted from [3] as shown in equation (16) is employed to further minimize the CSD that fall under the size of  $500 \mu\text{m}$  by implying the effect of temperature swing (dissolution steps).

$$F_{obj} = \min_{\theta} f_n(500\mu\text{m}) \quad (16)$$

Subject to:

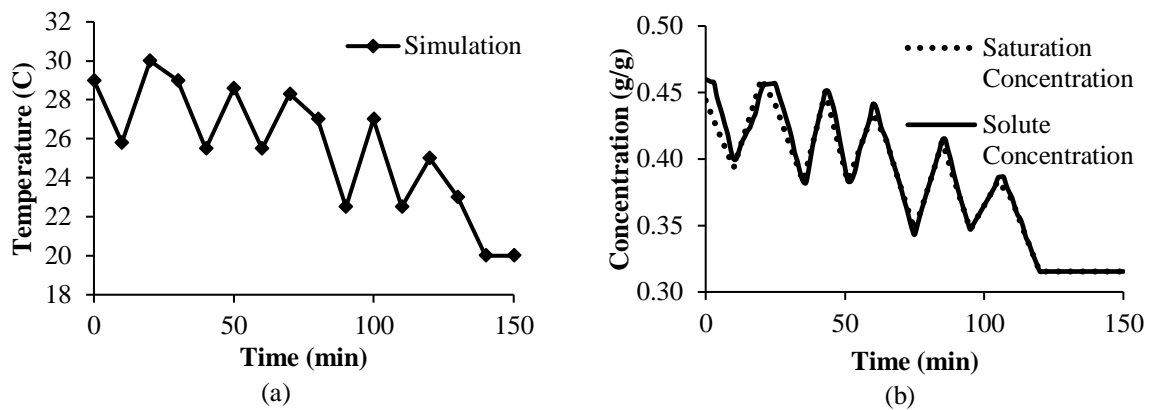
$$\dot{T}_{min} \leq \dot{T}(t) \leq \dot{T}_{max}$$

$$T_s^{min} \leq T(0) \leq T_s^{max}$$

$$T_{min} \leq T(t) \leq T_{max}$$

where the lower limit for the rate of crystallizer temperature change,  $\dot{T}_{min}$  and the upper limit for rate of crystallizer temperature change,  $\dot{T}_{max}$  are set to be  $-0.5 \text{ }^\circ\text{C}/\text{min}$  and  $0.5 \text{ }^\circ\text{C}/\text{min}$  and the values of each  $T_s$  and  $T$  limits are as shown in the Table 1. The temperature trajectory generated by equation (16) is shown in figure 4 where it is served as temperature set-point for PI controller. The temperature of crystallizer is maintained at its set-point by manipulating the water inlet temperature of the crystallizer. The controller parameters which are calculated from IMC tuning method are set to be 33 for proportional gain ( $K_c$ ) and 2.3 for integral time ( $\tau_i$ ).

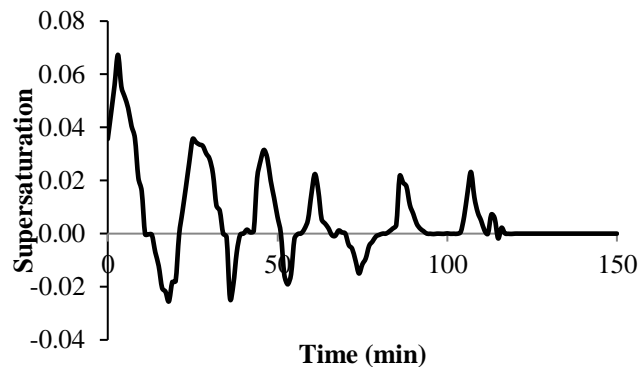




**Figure 4.** (a) Temperature and (b) concentration profiles for dissolution case.

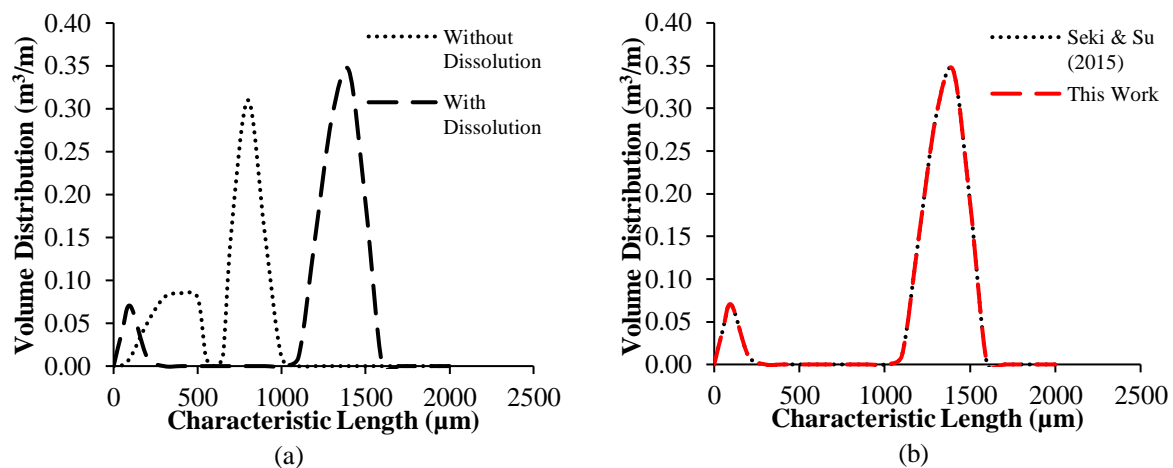
Figure 4 (a) shows temperature profile of potassium nitrate crystallization process with temperature swing (dissolution) where it can be seen that the solution is repetitively being cooled and heated from 29 °C to 20 °C until the end of the batch crystallization operation. The same trend can be seen from figure 4 (b) where concentration profile of potassium nitrate in this case is zigzagged from 0.46 g/g to 0.32 g/g following the temperature swing profile. The crystallization take place as the process begins at operational time of 0 minute due to the first concentration dropped following the first temperature dropped. As consequence, there are huge distance between solute concentration and saturation concentration whereby this condition promotes nucleation and crystal growth phenomena. The solution is further cooled, heated and re-cooled to create multiple supersaturation conditions where the crystal nuclei start to grow following the crystal growth rate model and dissolve following the dissolution rate model. Due to the crystallization kinetics' properties of size dependent growth, fine crystals have smaller growth rate to be compared with large crystals. Therefore, when dissolution takes place fine crystals would dissolve faster due to the fact that small size of particles have higher surface area than big size of particles. The temperature profile is designed and optimized based on this theory.

Based on figure 5, the supersaturation profile has multiple peaks reacting to the temperature swing profile. As the process frequently proceeds far from the saturation concentration and recurrently become undersaturated, the supersaturation concentration is optimized where the growth of seed crystals is favoured instead of the secondary nucleation of the fine crystals. In each cooling cycle as the solute concentration is higher than saturation concentration, the nucleation and crystal growth rate are further enhanced. This condition fortifies the growth of the crystal particles that did not dissolve when heating cycle and production of new crystals. However, in each heating cycle as the nucleation and crystal growth rate drop, crystal particles are forced to stop growing and dissolve. Small crystals formed by secondary nucleation dissolve faster than those of bigger crystals grown from the seed crystals due to the fact that small size of particles have higher surface area than big size of particles. This disappearance of crystals or dissolution phenomena benefits in reducing the fine crystals. This can be confirmed by figure 6 where the generation of small fines is significantly reduced in the case of operating with temperature swing (dissolution). In overall, the supersaturation profile involves both positive and negative values which indirectly mean that both crystal growth and dissolution take place accordingly.



**Figure 5.** Supersaturation profile for dissolution case.

Other than that, figure 6 (a) shows the generation of crystal fines has been considerably reduced when the process involves dissolution phenomena through multiple dissolution steps. This shows that dissolution enables small crystals to dissolve and accelerate growth for the remaining crystals for the next cooling cycle. Apart from that, the mean crystal size for temperature swing case is larger than that of no dissolution step, from 300  $\mu\text{m}$  of seed mean crystal size grown to approximately 1250  $\mu\text{m}$  of mean crystal size which is 56.2% bigger than targeted mean crystal size. The significant difference of crystal size from the seed crystals clearly explains that the dissolution step provides more room for crystals to grow compare to the case with no dissolution. These findings are also supported by the conclusion made by [3] where the final product CSD is significantly improved and the generation of small fines is considerably reduced. Also, figure 6 (b) shows that the simulation of mathematical model of potassium nitrate crystallization process employing extended method of classes which is performed in this work under closed-loop simulation is successfully implemented. The CSD profile generated using method of classes shows similar results with the method employed by published literature [3].



**Figure 6.** (a) Performance comparison for with and without dissolution phenomena and (b) CSD comparison obtained from extended method of classes and published literature [4].

#### 4. Conclusion

Simulation of seeded batch cooling crystallization for potassium nitrate case study is successfully demonstrated for both with and without dissolution phenomena. In this work, the method of classes has been extended and simulated under closed-loop simulation using PI controller. By using extended method of classes, the CSD profiles obtained from both with and without dissolution case are similar and comparable with experimental data indicating a reliability of the extended method. The desired target CSD is successfully achieved for both cases and better performances with 56.2% larger mean

characteristic length than target CSD with dissolution case is obtained. Also, the amount of crystal fines has been reduced by employing dissolution steps in the process.

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