

Research note

Effect of Different Nucleation and Growth Kinetic Terms on Modeling Results of KNO_3 CMSMPR Crystallizer

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Abstract

The aim of this contribution is a survey of different nucleation and growth kinetics terms effects on modeling results of KNO_3 Continuous Mixed Suspension Mixed Product Removal (CMSMPR) crystallizer. By studying the four different states in modeling, results show that, although these terms for similar crystallization system and operating conditions are similar, there is very different dynamic behavior in the results such as Particles Size Distribution (PSD), crystals mean size and relative supersaturation. The main difference in modeling results is oscillating behaviors. It is shown that such behavior strongly depends on kinetics terms sensitivity to supersaturation, especially in nucleation models.

Keywords: *Nucleation, Growth, CMSMPR Crystallizer, PSD, Oscillating Behaviors, Supersaturation*

1. Introduction

Modeling of crystallizer to predict PSD during the process is an important subject for researchers. A commonly accepted concept for the modeling of crystallizer is the population balance approach introduced by Randolph and Larson [1] and Hulburt and Katz [2]. A comprehensive overview on population balance modeling can be found in the review article by Ramkrishna [3] and in the book by the same author [4]. During the past decades many studies have been done on modeling of crystallizers for different crystallization systems. It is clear in all of these researches, growth and nucleation

terms have a considerable effect on the modeling results such as PSD, crystals mean size and etc. Mersmann [5] in his text book refers to some of the various terms. Unfortunately, in spite of the many efforts to understand nucleation and growth mechanisms, [6,7,8], and due to the many complexities and insufficient information about the steps of crystal formation and growth, there are no comprehensive and exact correlations for these terms [7].

Through a survey of researches done on crystallization processes it can be seen that the different models for nucleation and growth kinetic terms have developed in

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similar crystallization systems. The KNO₃ crystallization in aqueous solution is one of the processes in which two different nucleation and growth kinetics terms have been presented for similar operational conditions. One of these kinetics was developed by Miller [9] and the other was developed by Mersmann et al [10]. In this paper, by modeling CMSMPR KNO₃ crystallizer, the effect of these different kinetics on modeling results are discussed.

The article is organized as follows: In the next sections mathematical models of crystallizer based on population balances approach will be developed. Afterwards, the method of governing equation solution will be presented. Finally, by definition of four different states based on Miller [9] and Mersmann [10], nucleation and growth kinetics terms (States 1,2,3 and 4), the effects of these terms on modeling results such as PSD will be discussed.

2. Modeling

According to Fig. 1 modeling of the continuous crystallizer can be divided into two parts. The first is a binary solution in continuous liquid phase L involving dissolved crystals (solute KNO₃ (A)) and solvent H₂O (B). This phase determines nucleation and growth rate of crystals in crystallization process and its properties have a major effect on PSD. The second is dispersed solid phase S consisting of individual crystals. In this phase generated crystals growth corresponds to the degree of super-saturation that is exerted by liquid phase. In the following, mathematical model

of both dispersed phase and liquid phase for CMSMPR will be derived.

2-1. Modeling of dispersed phase

Modeling of PSD in dispersed solid phase needs to make use of population balance approach. For more information concerning this approach the reader is referred to the textbook by Ramkishna [4]. Population balance provides particle size distribution $F(L, t)$ that can be written as follows:

$$\frac{\partial F}{\partial t} = -\frac{\partial(GF)}{\partial L} + \dot{F}_{at}^{\pm} + \dot{F}_{in} - \dot{F}_{out} - \dot{F}_{dis}^{-} \quad (1)$$

In Eq. (1) the term on the left hand side represents the accumulation of crystals with size L. The first term on the right hand side represents the convective transport in the direction of the property coordinates L due to crystal growth, where G is the crystal growth rate. The term denotes source and sink terms due to particle attrition. The terms \dot{F}_{in} and \dot{F}_{out} denote the fluxes of the inlet and outlet particle numbers. Finally, it has to be taken into account that small crystals may dissolve and thus vanish from the population under certain operating conditions. The rate of dissolved particle is denoted by \dot{F}_{dis}^{-} . For solution of Eq. 1 the following conditions are supposed:

1. The term \dot{F}_{at}^{\pm} can be neglected due to low agitation and low concentration of crystal particles.
2. Crystals are not supposed to dissolve in mother liquid. So, the term \dot{F}_{dis}^{-} is assumed to be zero.

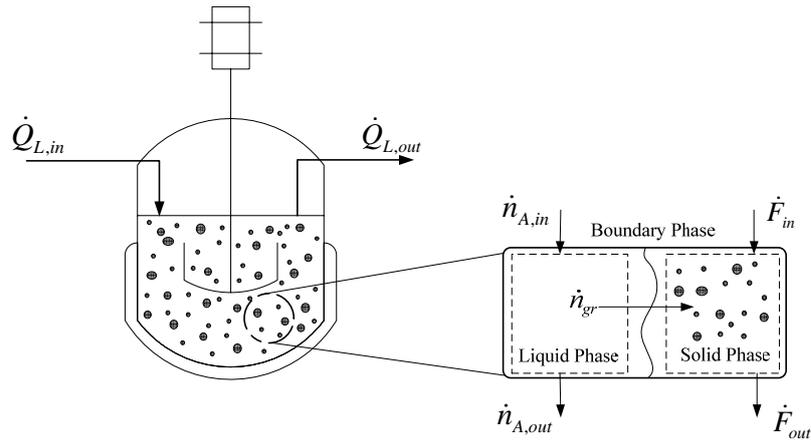


Figure 1. CMSMPR crystallizer and decomposition of crystallizer slurry.

3. Primary nucleation occurs only at $L=0$.
4. There are no crystals in inlet stream, $\dot{F}_{in} = 0$.
5. With the perfect agitation assumption, the values of PSD and component concentration in the withdrawn stream of crystallizer are assumed to be equal inside the crystallizer.

In this study two different growth terms are used for describing G in Eq. 1. The first correlation is developed by Miller [9] and the second is developed by Mersmann et al. [10]. Miller presents G as a function of supersaturation as follows:

$$G = k_g \hat{S}^q$$

$$\hat{S} = \frac{\hat{C}_{L,A} - \hat{C}_{L,A,sat}}{\hat{C}_{L,A,sat}} \quad (2)$$

In this equation k_g and q are constants, \hat{S} is the super-saturation fraction and $\hat{C}_{L,A}$ is the solute concentration A per kg of solvent B, respectively. The solute saturation

concentration A per kg of solvent B, $\hat{C}_{L,A,sat}$, can be evaluated by:

$$\hat{C}_{L,A,sat} = (2.29 + 0.104T_{cr} + 0.00306T_{cr}^2) \times 10^{-2} \quad (3)$$

The second correlation that is quite comprehensive presents G as a function of supersaturation and crystal length as:

$$\frac{G(\Delta c_{L,A}, L)}{2k_d(L)} = \frac{\Delta c_{L,A}}{c_s} + \frac{k_d(L)}{2k_r c_s} - \sqrt{\left(\frac{k_d(L)}{2k_r c_s}\right)^2 + \frac{\Delta c_{L,A} k_d(L)}{c_s 2k_r c_s}} \quad (4)$$

The symbol c_s denotes the molar concentration of the solid phase, k_r is the integration rate constant and k_d is the transfer coefficient. The driving force for crystal growth, $\Delta c_{L,A}$ is defined as the difference between the molar concentration of the solute component A in the liquid phase, $c_{L,A}$ and the molar saturation concentration, by:

$$\Delta c_{L,A} = c_{L,A} - c_{L,A,sat} \quad (5)$$

According to Mersmann et al. [10] the transfer coefficient can be calculated by:

$$k_d(L) = \frac{D_{AB}}{L} \left[0.8 \left(\frac{\bar{\epsilon} L^4}{\nu_L^3} \right)^{1/5} \left(\frac{\nu_L}{D_{AB}} \right)^{1/3} + 2 \right] \quad (6)$$

The symbols D_{AB} , $\bar{\epsilon}$ and ν_L are diffusion coefficient, specified energy dissipation rate and the kinematic viscosity of liquid phase, respectively.

Based on the assumption 5, the following relation holds for the particle number flux due to product removal:

$$\begin{aligned} \dot{F}_{out} &= \frac{F}{\tau} \\ \tau &= \frac{V}{\dot{Q}_{L,out}} \end{aligned} \quad (7)$$

where symbols τ , V and $\dot{Q}_{L,out}$ are the crystallizer residence time, the volume and the outlet liquid flow rate, respectively.

The boundary condition of Eq. (1) is defined on the basis of Miller [9] as follows:

$$F(L=0, t) = \frac{B_{nuc}}{G} \quad (8)$$

where B_{nuc} is the primary nucleation rate that provides total number of nuclei generated at $L=0$. The nucleation models used here are developed by Miller [9] and Mersmann et al. [10]. The first model is:

$$B_{nuc}(T_{cr}, \hat{S}) = k_b \hat{S}^p \hat{\mu}_3 \quad (9)$$

where symbols k_b and p are constants and $\hat{\mu}_3$ is the third moment of crystals per kg of solvent B. The second model is:

$$\begin{aligned} B_{nuc}(T_{cr}, S_{rat}) &= \frac{2}{3} D_{AB} (N_A c_{L,A,sat})^{7/3} S_{rat}^{7/3} V_m \sqrt{C_{het} \frac{\gamma_{sl}}{k_B T_{cr}}} \\ &\times \exp \left[C_{het} \frac{16\pi}{3} V_m^2 \left(\frac{\gamma_{sl}}{k_B T_{cr}} \right)^2 \left(\frac{1}{\ln(S_{rat})} \right)^2 \right] \times V \end{aligned} \quad (10)$$

In this correlation primary nucleation mainly depends on the surface tension γ_{sl} , the absolute temperature T_{cr} inside the crystallizer and the relative supersaturation S_{rat} . The parameter C_{het} determines the degree of heterogeneity of the primary nucleation and D_{AB} is binary diffusion coefficient. All other parameters are physical constants, like the Avogadro number N_A and the Boltzmann constant k_B or they depend on the chosen chemical system, such as V_m . The surface tension is derived by Mersmann [11] as:

$$\gamma_{sl} = 0.414 k_B T_{cr} \left(\frac{\rho_s N_A}{M_s} \right)^{2/3} \ln \left(\frac{\rho_s}{M_s c_{L,A}} \right) \quad (11)$$

The symbols ρ_s and M_s respectively are density and molar mass of solid phase.

The initial condition of Eq. (1) is defined as:

$$F(L, t=0) = 0 \quad (12)$$

Eqs. (1-12) are mathematical description of the dispersed solid phase S, for continuous crystallizer. The next subsection deals with the modeling of the continuous liquid phase.

2-2. Modeling of continuous phase

The fundamental balance equations for the continuous liquid phase are components mole balance for dissolved crystals (component A) and solvent (component B). During the crystallization it is assumed that the content of liquid phase is ideally mixed and the formed crystals are solvent free (pure component A). Therefore, mole balances for continuous phase are:

$$\begin{aligned} \frac{dn_{L,A}}{dt} &= -\dot{n}_{nuc} - \dot{n}_{gr} + \dot{n}_{A,in} - \dot{n}_{A,out} \rightarrow \text{Solute Balance} \\ \frac{dn_{L,B}}{dt} &= \dot{n}_{B,in} - \dot{n}_{B,out} \rightarrow \text{Solvent Balance} \end{aligned} \quad (13)$$

The first term in the right hand side of solute component balance \dot{n}_{nuc} shows the total molar exchange flux between the solid and the liquid phase due to primary nucleation rate. This term, on the basis of third assumption does not affect balance equation and is put equal to zero. The second term \dot{n}_{gr} shows the total molar exchange flux between the solid and the liquid phase due to growth rate and can be derived as:

$$\dot{n}_{gr} = \frac{3k_v \rho_s}{M_s} \int_0^{L_c} L^2 GF(L, t) dt \quad (14)$$

where symbol k_v is volume shape factor. The terms $\dot{n}_{A,in}$ and $\dot{n}_{B,in}$ are the inlet molar flow rate of components A and B, respectively. The terms $\dot{n}_{A,out}$ and $\dot{n}_{B,out}$ denote the outlet molar flow rate of components A and B and are defined based on the assumption 5 as follows:

$$\begin{aligned} \dot{n}_{A,out} &= \frac{n_{L,A}}{\tau} \\ \dot{n}_{B,out} &= \frac{n_{L,B}}{\tau} \end{aligned} \quad (15)$$

The initial conditions for Eq. (13) are defined as follows:

$$\begin{aligned} n_{L,A}(t=0) &= n_{L,A_0} \\ n_{L,B}(t=0) &= n_{L,B_0} \end{aligned} \quad (16)$$

The symbols n_{L,A_0} and n_{L,B_0} are the initial number of solute and solvent moles in crystallizer, respectively. In crystallization process, because of the dependence of supersaturation on temperature, the exothermic nature of crystallization process, and also the influence of jacket temperature on crystallizer contents temperature, Eq. (1) and Eq. (13) should be coupled with energy balance. In the next section energy balance will be derived as one of the governing equations.

2-3. Energy balance

In crystallization process, product quality depends highly on the amount of nucleation and growth rate. On the other hand, these parameters are severe functions of crystallizer temperature. Thus, temperature behavior should be considered in analysis of processes dynamics. For consideration of crystallizer temperature behavior, energy balance should be coupled with component mole balances and population balance. For CMSMPR crystallizer energy balance is as follows:

$$n_{cr} c_{p,cr} \frac{dT_{cr}}{dt} = -\Delta H_{crystal} \dot{n}_{gr} + c_{p,in} (\dot{n}_{A,in} + \dot{n}_{B,in}) \times (T_{in} - T_{cr}) + Q_{cool} + W_{stirrer} \quad (17)$$

The symbols n_{cr} and $c_{p,cr}$ are total mole numbers and heat capacity of crystallizer contents. The symbol $\Delta H_{crystal}$ in the right hand side is heat produced due to crystallization [9], and is given by:

$$\Delta H_{crystal} = -20484 + 22173.1 \hat{C}_{L,A} + 23881 \hat{C}_{L,A}^2 \quad (18)$$

and $c_{p,in}$ is heat capacity of total inlet components, respectively. In this study because of the low effect of crystals on crystallizer and inlet flow heat capacity, the terms $c_{p,cr}$ and $c_{p,in}$ are considered only as a function of solution heat capacity.

The symbol Q_{cool} is the amount of heat that is transferred between crystallizer and coolant and is calculated as:

$$Q_{cool} = UA (T_{jacket} - T_{cr}) \quad (19)$$

The terms UA and T_{jacket} are the overall heat coefficient and the jacket temperature, respectively. The energy dissipation rate of the stirrer $W_{stirrer}$ is correlated by Gahn and Mersmann [12, 13] and is given by:

$$W_{stirrer} = 0.3 \rho_L \omega_{stirrer}^3 d_{stirrer}^5 \quad (20)$$

where ρ_L , $\omega_{stirrer}$ and $d_{stirrer}$ are liquid density, angular speed and diameter of stirrer. The initial condition for Eq. (17) is:

$$T_{cr}(t=0) = T_{cr_0} \quad (21)$$

where T_{cr_0} is initial crystallizer temperature.

In this contribution we suppose that coolant temperature does not change during the operation. So, the energy balance for coolant is not needed. Eqs. (1-21) are dynamic model description of a CMSMPR system. The next section is concerned with the method of solution of the derived models for governing equations.

3. Model solution

Solution of governing equations in this study is performed by use of finite difference method with order of 6 Adams step discretization. In the case of Miller [9], growth term G is used in governing equations, the moment method to decrease solution time is used, and when Mersmann [10] growth terms are used equations are solved directly. The moment method converts integro-differential PDE form of governing equations to a set of ODE equations and considerably increases solution speed. Shervin et al. [14] suggested this method for population balance models when growth term is either not a function of crystal length nor a first order function of the length. By applying this method to Eq. (1), Eq. (13) and Eq. (17) the governing equations are defined as follows:

$$\begin{aligned} \frac{d\mu_0}{dt} &= (1 - k_v \mu_3) B_{nuc} - \mu_0 / \tau \\ \frac{d\mu_1}{dt} &= G \mu_0 - \mu_1 / \tau \\ \frac{d\mu_2}{dt} &= G \mu_1 - \mu_2 / \tau \\ \frac{d\mu_3}{dt} &= G \mu_2 - \mu_3 / \tau \\ \frac{dn_{A,L}}{dt} &= -\frac{3k_v \rho_s}{M_s} G \mu_2 + \dot{n}_{A,in} - \dot{n}_{A,out} \end{aligned} \quad (22)$$

$$n_{cr} c_{p,cr} \frac{dT_{cr}}{dt} = -\Delta H_{crystal} \left(\frac{3k_V \rho_s}{M_s} G \mu_2 \right) + c_{p,in} (\dot{n}_{A,in} + \dot{n}_{B,in}) (T_{in} - T_{cr}) + Q_{cool} + W_{stirrer}$$

where is μ_i the i^{th} moment and is described by:

$$\mu_i(t) = \int_0^{L_c} L^i F(t, L) dL \quad (23)$$

The main problem in the moment method is evaluation of PSD. Moment method does not provide PSD directly. So in this contribution Log-Normal (L-N) distribution function has been used for calculation of PSD. This function provides a reliable model for prediction of size distribution on the basis of moments values, Sun et al. [15]. The Log-Normal distribution function is described by:

$$F_{L-N}(t, L) = \frac{\mu_0}{\sqrt{2\pi L \ln(\sigma)}} \times \exp\left(-\frac{(\ln(L) - \ln(u))^2}{2(\ln(\sigma))^2}\right) \quad (24)$$

Where u is the geometric mean number and σ is the geometric standard deviation. Applying the L-N distribution to the moment equations, Eq. (23), the moments value can be calculated by:

$$\mu_i = u^i \exp\left(\frac{i^2}{2} (\ln(\sigma))^2\right) \quad (25)$$

The characteristic parameters u and σ of L-N distribution can be derived by use of first order and second order moments as:

$$u(t) = \frac{\mu_1^2}{\mu_2} \quad (26)$$

$$\sigma(t) = \exp\left(\sqrt{\ln\left(\frac{\mu_2}{\mu_1^2}\right)}\right)$$

By evaluation of u and σ , L-N distribution function can be obtained. All used constants values in this modeling are listed in Table. 1. The next section is concerned with modeling results on the basis of nucleation and growth models.

Table 1. Constants values

Parameter	Value	Unit
C_{het}	0.02	-
k_V	$\pi / 6$	-
v_L	$8.01e^{-10}$	m^2 / sec
M_A, M_S	$101.103e^{-3}$	kg/mol
M_B	$18.015e^{-3}$	kg/mol
V, V_m	$7.5e^{-3}, 4.16e^{-29}$	m^3
UA	200	J/s
D_{AB}	$1.89e^{-9}$	m^2 / sec
ρ_B, ρ_s	987, 2109	kg / m^3
$\omega_{stirrer}$	7.91	$1/s$
$\bar{\epsilon}$	0.5	W/kg
$d_{stirrer}$	0.1	m
n_{L,A_0}, n_{L,B_0}	5.42, 58.82	mol
$\dot{n}_{A,in}, \dot{n}_{B,in}$	$9.68e^{-4}, 1.32e^{-2}$	mol/s
$T_{in}, T_{cr_0}, T_{jacket}$	305	K

4. Results and discussion

In this section modeling results for CMSMPR KNO_3 crystallizer on the basis of different nucleation and growth terms will be presented. For studying these terms the effect on modeling results of four states is regarded as follows:

- State 1: Miller [9], Nucleation and Growth terms.
- State 2: Mersmann [11], Nucleation and Growth terms.
- State 3: Miller [9], Nucleation and Mersmann [11] Growth terms.
- State 4: Mersmann [11], Nucleation and Miller [9] Growth terms.

Governing equations in States 2 and 4 because of independency of growth terms to crystal length are solved by Moment method and other states are solved directly. Fig. 2. shows mean crystal size L_{mean} evaluated by Sauter-mean method during the crystallizer operation time. It can be seen when Mersmann [11] terms for nucleation and growth are used, (State 1) L_{mean} shows oscillating behavior with respect to Miller [9] models. Also, this kind of behavior with less oscillation and different periods can be achieved by combining Miller [9] and Mersmann [11] models, States 3 and 4. (for more information about oscillating behavior

in crystallizers readers can refer to Randolph and Larson [1]). In Fig. 3 similar behavior can be seen in super saturation S_{rat} values. By comparison of L_{mean} and S_{rat} behavior it can be concluded Mersmann [10] nucleation and growth terms have high sensitivity to amount of supersaturation and cause oscillating behavior in the crystallizer. The amplitude and period of oscillations show that nucleation term has the main role in such behaviors.

Survey of L_{mean} behavior in States 1 and 4, Fig. 3, shows when Miller [9] growth term is used in modeling, L_{mean} it takes greater values with respect to the two other states at steady state condition. It can be inferred that rate of crystals growth for Miller [9] growth term is higher than Mersmann [10] model. Evidently the effect of nucleation terms in initial condition is high but when crystallizer shows steady behavior at time around 25000 sec, nucleation does not have a significant effect on maximum length of crystals.

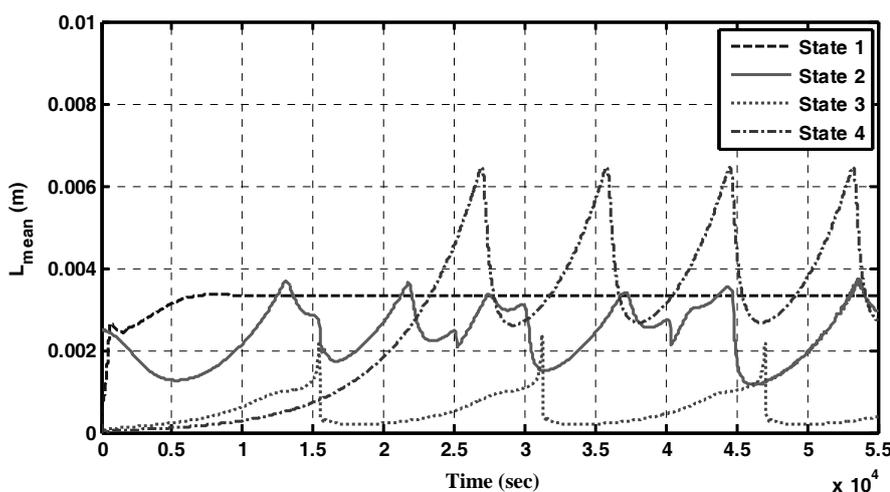


Figure 2. L_{mean} behavior in States 1-4 conditions.

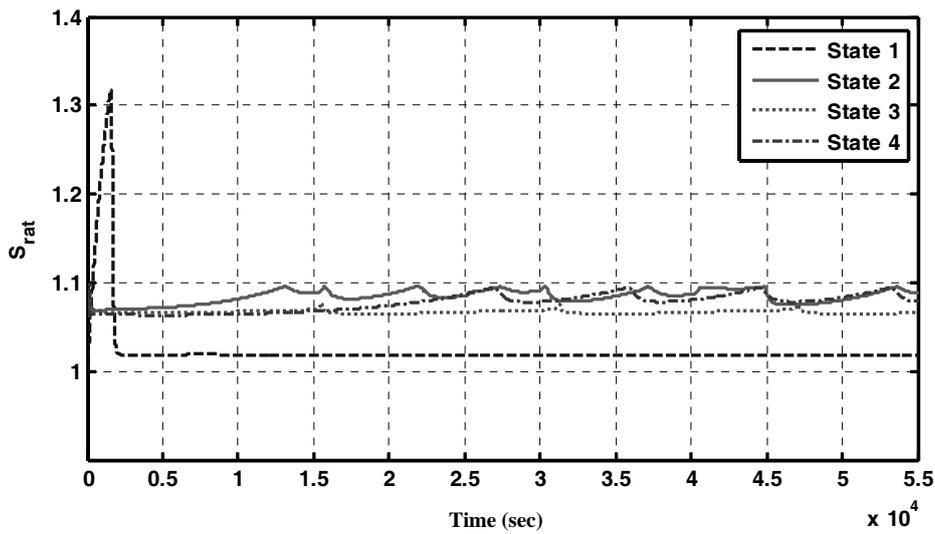


Figure 3. S_{rat} behavior in States 1-4 conditions.

In Fig. 4 total number of crystals μ_0 is depicted for States 1 and 2. This figure shows significant difference between the behaviors at initial time of crystallizer operation in these states. At this time, with an increase of supersaturation degree in the crystallizer by supersaturated stream in the inlet feed, nucleation terms estimate the first

crystals that appear in the crystallizer. Rate of new nuclei generation strongly depend on supersaturation degree to nucleation term. So it can be concluded that Mersmann [10] nucleation term with respect to Miller [9], estimates a greater number of crystals at low supersaturation degrees.

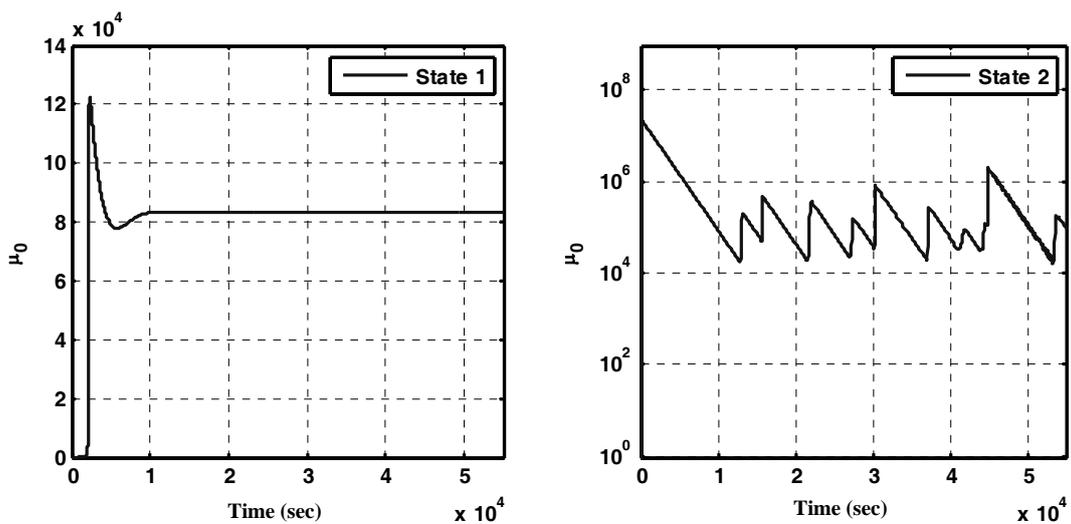


Figure 4. μ_0 behavior in States 1 and 2 conditions.

In Fig. 5 effects of States 1-4 conditions on PSD are depicted. This figure shows very different PSD behavior for the considered States with respect to each other. As discussed above such behaviors strongly depend on nucleation and growth terms that are used in modeling. It should be taken into account that the difference between PSDs are mainly affected by the influence of nucleation terms that cause a periodic peak during the crystallizer operation.

5. Conclusions

The main focus of this paper is the survey of different nucleation and growth terms effects

on modeling of KNO_3 CMSMPR crystallizer as a case study. The results show that, depending on which terms are regarded for modeling States 1-4, different behavior occurs in modeling results during the crystallizer operating time such as L_{mean} , PSD and etc.

The reasons for the difference in results for the studied crystallization system depends strongly on the following subject:

- Sensitivity degree of nucleation and growth terms to supersaturation.
- Independency of Miller [9] growth term to length of crystals.

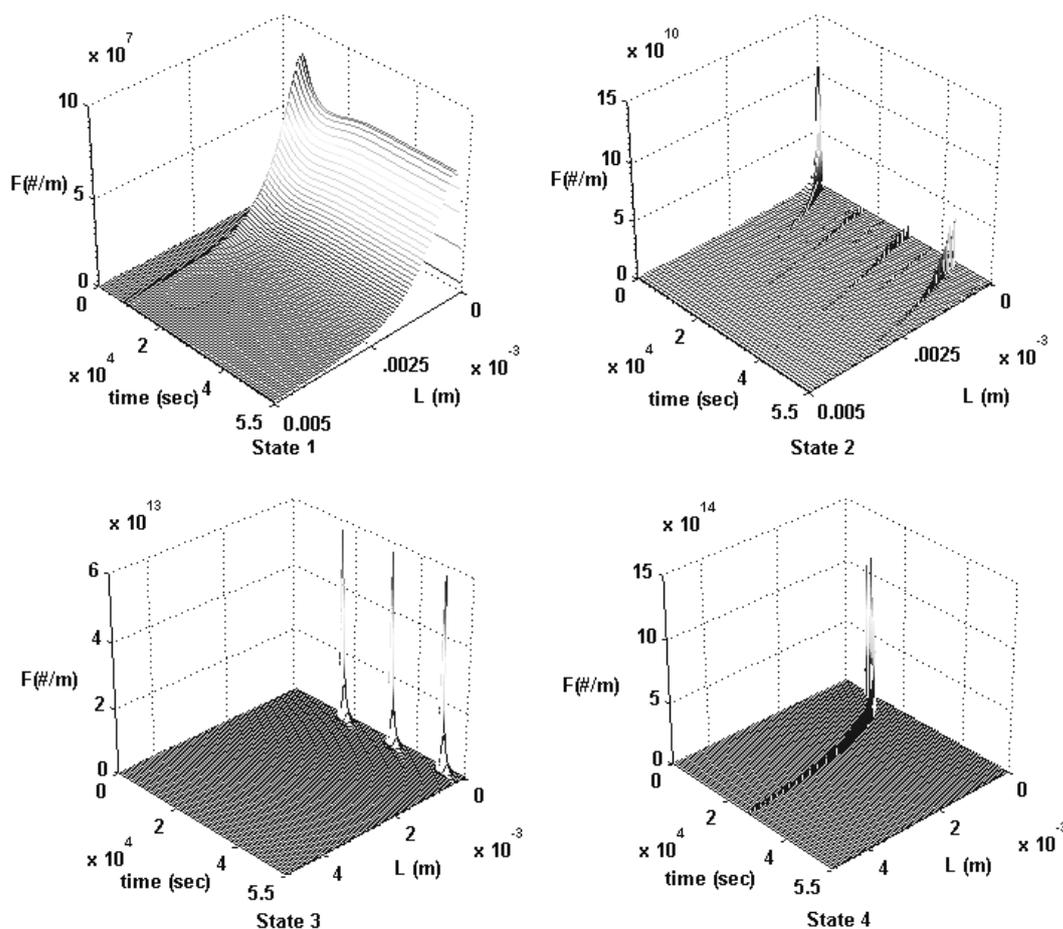


Figure 5. PSD behavior in States 1-4 conditions.

The main problems of such different behaviors in modelling results of states 1,2,3 and 4 are complication in process design, restriction of reliability of modeling, effect on downstream process design and especially, control troubles. So it seems revision in crystallization processes that have such noticeable differences in their kinetics models can help to overcome these problems and increase dependability of modeling and simulation works.

Nomenclature

B_{nuc}	primary nucleation rate, 1/sec
$C_{p,cr}$	crystallizer contents heat capacity, J/mol K
$C_{p,in}$	heat capacity of total inlet components, J/mol K
C_s	molar concentration of the solid phase, mol/m ³
$\Delta C_{L,A}$	driving force for crystal growth, mol/m ³
C_{net}	degree of heterogeneity, dimensionless
$C_{L,A}$	solute concentration (component A), mol/m ³
$C_{L,A,sat}$	solute saturation concentration (component A), mol/m ³
$\hat{C}_{L,A}$	solute concentration A per kg of solvent B, dimensionless
$\hat{C}_{L,A,sat}$	solute saturation concentration A per kg of solvent B, dimensionless
$C_{L,B}$	solvent concentration (component B), mol/m ³
$d_{stirrer}$	diameter of stirrer, m
D_{AB}	diffusion coefficient, m ² /sec
F	particle size distribution, 1/m

F_{L-N}	Log-Normal particle size distribution, 1/m
\dot{F}_{at}^{\pm}	source and sink term due to attrition, 1/sec
\dot{F}_{dis}^{-}	flux of dissolve crystals, 1/sec
$\dot{F}_{in}, \dot{F}_{out}$	fluxes of the inlet and outlet particle numbers, 1/sec
G	growth rate, m/s
$\Delta H_{crystal}$	heat of crystallization, J/mol
k_b	Constant, kg solvent/(m ³ sec)
k_B	Boltzmann constant, J/K
k_d	transfer coefficient, m/s
k_g	constant, m/sec
k_r	integration rate constant, m ⁴ /mol s
k_v	volume shape factor, dimensionless
p	constant, dimensionless
k_r	rate constant, mol ⁴ /m ³ .s
k_v	volume shape factor, dimensionless
L	crystal size, m
n_{cr}	total mole numbers in the crystallizer, mol
\dot{n}_{gr}	total molar flux due to growth rate, mol/s
$n_{L,A}, n_{L,A}$	mole and initial mol of solute A, mol
$n_{L,B}, n_{L,B}$	mole and initial mol of solute B, mol
$\dot{n}_{A,in}, \dot{n}_{A,out}$	Inlet and outlet molar flow rate of components A, mol/s
$\dot{n}_{B,in}, \dot{n}_{B,out}$	Inlet and outlet molar flow rate of components B, mol/s
\dot{n}_{nuc}	total molar flux due to primary nucleation rate, mol/s
N_A	Avogadro number, 1/mol
M_s	molar mass of solid phase, kg/mol

q	Constant, dimensionless
Q_{cool}	heat that transfers between crystallizer and coolant, W
$\dot{Q}_{L,out}$	liquid flow rate, m ³ /sec
S_{rat}	relative supersaturation, $C_{L,A,sat} / C_{L,A}$, dimensionless
\hat{S}	super-saturation fraction, dimensionless
t	time, sec
T_{cr}	crystallizer temperature, K
T_{cr}	initial crystallizer temperature, K
T_{in}	inlet temperature, K
T_{jacket}	jacket temperature, K
u	geometric mean number
UA	overall heat coefficient, J/K
V	crystallizer volume, m ³
V_m	molecular volume, m ³
$W_{stirrer}$	energy dissipation rate, J

Greek Letters

γSL	surface tension, J/m ²
$\bar{\epsilon}$	specified energy dissipation rate, W/kg
μ_i	i th moment
$\hat{\mu}_3$	third moment of crystals per kg of solvent B
σ	geometric standard deviation
τ	residence time, sec
ν_L	kinematic viscosity, m ² /sec
ρ_s	density solid phase, kg/m ³
ρ_L	liquid density, kg/m ³
$\omega_{stirrer}$	angular speed, 1/sec

References

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|---|---|
| [1] Randolph, A. D. and Larson, M. A., Theory of particulate processes: | [12] Gahn, C. and Mersmann, A., "Brittle fracture in crystallization processes, |
|---|---|

Analysis and techniques of continuous crystallization, 2nd ed., Academic Press, Orlando, (1988).

- | | |
|--|--|
| [2] Hulburt, H. M. and Katz, S., "Some problems in particle technology. A statistical mechanical formulation", Chemical Engineering Science, 19 (8), (1964). | [3] Ramkrishna, D., "Status of population balances", Reviews in Chemical Engineering, 3 (1), (1985). |
| [4] Ramkrishna, D., Population balances: Theory and applications to particulate systems in engineering, Academic, San Diego, Calif., London, (2000). | [5] Mersmann, A., Crystallization technology handbook, 2 nd ed., Dekker, New York, (2001). |
| [6] Scheel, H. J. and Capper, P., Crystal growth technology: From fundamentals and simulation to large-scale production, Wiley-VCH, Weinheim, (2008). | [7] Mullin, J. W., Crystallization, 4 th ed., Butterworth-Heinemann, Oxford, (2001). |
| [8] Pamplin, B. R., Crystal growth, 2 nd ed., Pergamon, Oxford, (1980). | [9] Miller, M. S., Modelling and quality control strategies for batch cooling crystallizers, In: Cemical engineering, Texas University, Austin, USA, (1993). |
| [10] Mersmann, A., Angerhöfer, M., Gutwald, T., Sangl, R. and Wang, S., "General prediction of median crystal sizes", Separations Technology, 2 (2), (1992). | [11] Mersmann, A., "Calculation of interfacial tensions", Journal of Crystal Growth, 102 (4), (1990). |

- Part A. Attrition and abrasion of brittle solids", *Chemical Engineering Science*, 54 (9), (1999).
- [13] Gahn, C. and Mersmann, A., "Brittle fracture in crystallization processes, Part B. Growth of fragments and scale-up of suspension crystallizers", *Chemical Engineering Science*, 54 (9), (1999).
- [14] Sherwin, M. B., Shinnar, R. and Katz, S., "Dynamic behavior of the well-mixed isothermal crystallizer", *AIChE Journal*, 13 (6), (1967).
- [15] Sun, X. G., Tang, H. and Dai, J. M., "Retrieval of particle size distribution in the dependent model using the moment method", *Opt Express*, 15 (18), (2007).