Control of a Granulation Process Using a Nonlinear MPC Formulation

Justin Gantt and Edward Gatzke[1]
Department of Chemical Engineering, University of South Carolina, Columbia, SC 29208

Abstract

This paper presents a Model Predictive Control (MPC) algorithm capable of controlling the evolution of particle size distributions used in aggregation/breakage processes such as granulation. High-shear wet granulation is an important aggregation/breakage process due to its ability to produce dense, spherical particles in a short amount of time. Problems typically arise in high-shear wet granulation while attempting to control final particle size distributions due to process sensitivity with respect to liquid addition. Thus, advanced control of high shear granulation processes is greatly dependent on a model capable of predicting process transients during particle growth. A Population Balance Equation (PBE) model is implemented to capture process dynamics for the model based controller. A discrete element simulation model will act as the process to be controlled. The model determines the result of particle-particle interactions based on the physics of the process. This highly realistic model will act as a test bed for the newly developed MPC formulation which in the future can be implemented on an actual granulation process. Complexity arises in the MPC algorithm due to the fact that the model used by the controller is nonlinear, the process in question operates in batch, and the non-square nature of this problem.

1 Introduction

Advanced control and modeling of granulation processes presents many challenges. In many industrial granular processes it is preferential to produce granules with consistent product quality indicated by size uniformity, flowability, attrition resistance, break-up rate, etc. These product quality indicators can be related by two granular quantities: particle size distribution and bulk density [16]. In the past, advanced control strategies such as Model Predictive Control (MPC) have been used in granulation processes due to the ability of MPC to accommodate both multivariable systems and systems with process constraints [3, 19]. Research has been performed using MPC to control these fundamental granular quantities when the MPC formulation is applied to continuous granulation processes ([6, 16]).

Typical MPC algorithms formulate an optimization function at discrete time steps to determine the next control move. That control move is applied to the system at the next sampling time and a new process measurement is received. The model is then updated and a new optimization problem is solved. Pottman et al. [16] achieved quality control in a continuous system by adjusting flowrates on a series of spray nozzles that dry powder passes through to be nucleated to control the bulk density of the product as well as the 90th and fifth percentiles of the product. Gatzke and Doyle [6] extended on traditional MPC controllers by presenting soft output constraints and prioritized control moves to the system.

While MPC may be best applied to continuous systems, many granulation processes are performed in batch. Batch processes typically exhibit large variations in operating conditions resulting in an MPC formulation which cannot be optimized by static formulation [4, 13]. In a batch granulation process, the bulk density of the system will be uniform, under the assumption that the system is well mixed. The control strategy must only be concerned with the particle size distribution as it changes with time. Processes operating in the batch mode are usually required to follow a given trajectory determined by model-based optimization or operator experience. Trajectory tracking of batch processes presents difficult control problems for batch processes due to the nonlinearity of the processes and the dynamic nature of the operating points. A highly realistic model of a high shear granulation process based on discrete element simulation will act as the plant to be controlled. This model simulation scheme depends directly on the physics of the process to determine an evolving particle size distribution. This model will act as a test bed until the final nonlinear Model Predictive Controller can be applied to an actual high shear granulation process.

2 Plant Model

A high fidelity model of the process was developed using a discrete element simulation approach. The proposed simulation method is developed from a collection of physically

[1]Corressponding author's email: gatzke@sc.edu

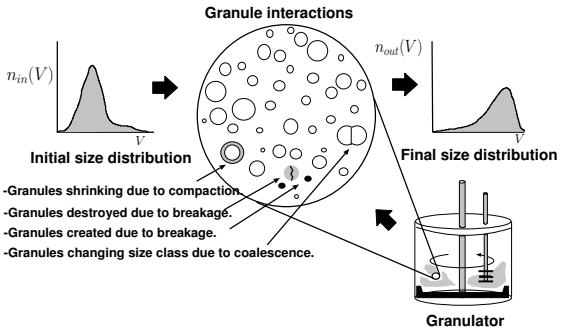

Figure 1: The evolution of the PSD by tracking physical inter-granule changes and interactions.

based models. It is initially assumed that an array of granules are in a nucleated particle matrix. Each granule is composed of an identical initial pore saturation due to an assumed uniform binder dispersion in the granulator. The binder is assumed to be a compressible Newtonian fluid and the granule is assumed to react as a simple elastic-plastic solid as described by Liu et al. [12]. Given initial positions and velocities, granules move in small increments at each time step. This discrete element simulation method is beneficial in modeling a granulation process because the simulation allows for easy application of phenomenologically based physical changes to the process. Figure 2 shows the basis of this simulation technique. Changes in each granule are tracked to predict the evolution of the PSD.

Granule Position-A number of particles is first chosen, and each particle, i, is randomly given a fixed position, x_i, y_i, z_i, Initial positions are developed in a manner such that no two particles initially overlap. Repeating spatial boundary conditions are used for particles that that move beyond the borders of the simulation.

Granule Composition-Using granule volume as the intrinsic parameter in the simulation, Verkoeijen et al. [17] proposed a method where a particle volume can be described as a vector $\underline{G}$ composed of the granule solid volume s, liquid binder volume l, and air volume a, $\underline{G} = [s \quad l \quad a]^T$ where the total volume of granule i is the sum of the three components $v_i = s_i + l_i + a_i$. Using this initial composition of phases in each granule, internal granule properties such as porosity ε, pore saturation S, moisture fraction w, and liquid fraction L, can be calculated from these quantities.

Granule Velocity-The particles are given a randomly determined velocity in each direction in three dimensional space. Here, the distribution used is a normal distribution with a mean velocity of 3 m/s and a standard deviation of 1 m/s. The mean velocity of the normal distribution is based on the impeller speed of the granulator by: $v_{x_i} = \frac{\omega D}{2}$, where v_{x_i} is the velocity of the i^{th} granule in the x direction, ω is the angular velocity of the impeller $(1/s)$ and D is the diameter of the granulator, (m).

The granule vector, G_i is expanded to include all granule components: position, composition, velocity, porosity, pore saturation, etc. With each of parameters of the granule known in the vector G_i, the simulation progresses incrementally each time step. At each time step, there are many other aspects of the simulation which must be updated. Consolidation is a continuous process updated at each time step.

Consolidation-As granules collide against each other or against walls or impellers in granulators, air is slowly forced out of the granule. Consolidation controls not only the amount of air inside a particle, but also controls the rate that binder is eventually forced out of pores therefore controlling binder layer height on the surface of the particle. Several models for consolidation have been described by an exponential decay relationship for porosity as a function of time [8, 17]:

$$\frac{d\varepsilon}{dt} = -k_c\left(\varepsilon - \varepsilon_{min}\right) \tag{1}$$

where ε_{min} is the minimum porosity attainable and k_c is a consolidation rate constant.

Coalescence-Collisions are detected and conditions for coalescence, rebound, and breakage are calculated. Liu et al. [11] present criteria for coalescence among deformable surface-wet granules. For a full description of the physics of granule coalescence, see references [11, 12]. This criteria was first derived using contact mechanics described by Johnson [9]. Their model assumes that deformation begins when granules are in physical contact, liquid capillary forces are negligible, the interparticle attractive forces are negligible, and fluid cavitation does not occur during rebound. If the kinetic energy caused by a collision of two particles is completely dissipated by the viscous binder layer, these particles coalesce due to Type I coalescence [11]. Once the surfaces touch and rebound begins, if the binder layer is capable of dissipating the energy caused by this rebound force, the particles then coalesce due to Type II coalescence. If the energy caused by the collision is too great to be dissipated by the binder layer, the particles completely separate and rebound occurs. The rate of granule growth is greatly dependent on binder content in a granule. As a granule becomes saturated, the binder layer height increases, causing particles to more readily coalesce via Type I coalescence. As impeller speed increases, particles are less likely to coalesce due to Type I coalescence until the kinetic energy reaches a point where breakage may occur.

Breakage-Breakage occurs in a granulator when the shearing forces of the impeller or chopper are greater than a critical amount of deformation that a granule is able to withstand to remain intact. Breakage can often greatly affect the final particle size distribution, especially in high shear granulators. The criteria was first presented in the form of

the Stokes deformation number criteria as $St_{def} > St^*_{def}$ where St_{def} is the Stokes deformation number, a measure of a granule's impact kinetic energy to the plastic deformation of the granule [18].

3 Population Balance Equation Model

Models based on Population Balance Equations (PBEs) are crucial in the field of particulate process analysis because these models allow for the calculation of size distribution, as well as the determination of controlling granulation mechanisms. Population balances have rate expressions for all granule size changing mechanisms. A common PBE applied to granulation will determine particles that are "born" or that "die" due to coalescence. Particle may also be created from breakage of a mother particle. PBEs also use rate expressions to model particle growth due to layering and particle deterioration caused by consolidation or attrition. PBEs are particularly useful with respect to process control through the use of sensitivity analysis to determine how changes to input conditions effect product quality [2].

Analytical methods of solving PBEs are very difficult, therefore discrete solutions have been found which consider particles of different sizes to exist in groups or "bins" and interact collectively with particles in other groups [7, 10, 1]. These discrete methods are commonly computationally efficient and accurate enough to be an adequate substitution to the analytical model. Verkoeijen et al. [17] proposed a discrete multi-dimensional population balance which uses volume as the intrinsic parameter. Verkoeijen et al. included two main agglomeration mechanisms to their model: coalescence and compaction. This volume-based model tracks the evolution of the volume of solids, volume of liquid, and volume of air of a nucleated granule at each time step in a manner similar to the discrete element simulation model. Models have been established using these intrinsic parameters to calculate granulate parameters such as pore saturation, porosity, and liquid fraction. For a detailed review of this PBE model, see [17]. The continuous coalescence function derived by Verkoeijen et al. is given as:

$$\frac{dq_{sk}}{dt} = \sum_{j=1}^{j=n} \left(\frac{\beta_{ij} q_{si} - \beta_{kj} q_{sk}}{j s_1 N_{tot}} \right) q_{sj} \tag{2}$$

where q_{sk} is the total solid volume of granules in the k^{th} size class, β is the coalescence kernel, and N_{tot} is the total number of granules at time t. The coalescence kernel, β_{ij}, proposed by Verkoeijen et al. defined a criterion which stated that coalescence could only take place once the granule pore saturation, S reached a critical level following consolidation, S^*. This degree of saturation corresponds to the capillary state at which rapid agglomeration begins.

Open-loop results using the discrete element simulation have shown three factors of granules aggregation that need to be captured by a coalescence kernel: (i) an induction behavior is present when granules were not in the capillary state of moisture content, (ii) increased impeller speeds result in less granule growth, (iii) and lastly a promotion of granule growth with an added binded content. The initial proposed coalescence kernel is shown in Eq.3:

$$\beta(u,v) = \begin{cases} \beta_0 (\ln(1.5+\omega))^{2.5} (q_{lt}/q_{lt-1}) \\ 0 \end{cases} \tag{3}$$

$$for\ S \geq S^*\ \&\ \omega > 0$$
$$for\ S < S^*\ or\ \omega = 0$$

where ω is the impeller speed of the mixer, q_{lt} is the total volume of liquid in the granulator at time t, S is the pore saturation, S^* is the critical pore saturation (0.85) and β_0 is the size independent kernel. This hybrid reduced model was run in parallel with the discrete simulation model and has shown to perform very similarly to the full discrete simulation model, yet less computationally intensive and time consuming.

4 Controller Formulation

The PBE model of a granulation process can be simplified to the following nonlinear discrete time system:

$$\begin{gathered} x(k+1) = f\left(x(k),\, u_1(k),\, u_2(k)\right), \quad k = 0,\, 1,\, .. \\ y(k) = x(k) \end{gathered} \tag{4}$$

where $x(k) \in \Re^{n_x}$ is the state vector at sample time k, $u \in \Re^{n_u}$ is a vector of inputs, and $y \in \Re^{n_y}$ is a vector of predicted outputs. The states in this discrete process are the total volume of granules, q_i, in size class i, at a discrete time sample time k. The inputs to the process are impeller speed at time sample k and volumetric flowrate of binder at time sample k. In this MPC formulation, a controller is required to calculate a set of control moves that allows the process to operate following a desired setpoint trajectory. These control moves are found by minimizing an objective function, $\Phi(k)$, at each time step k:

$$\begin{aligned} \min_{U(k)} \quad & \Phi(k) = \textstyle\sum_{i=k}^{k+p} e_y^T(i) \Gamma_y e_y(i) \\ & + \sum_{i=0}^{M-1} \Delta u(i)^T \Gamma_u \Delta u(i) \end{aligned} \tag{5}$$

Subject to the constraints:

$$u(i) \in [u_{min},\, u_{max}] \tag{6}$$

where $e_y(i)$ is the model/reference error vector at time i, $\Delta u(i) = u(i) - u(i-1)$, or the difference between the the input at time i and time $i-1$, M is the move horizon, and p is the prediction horizon. Γ_u and Γ_y are diagonal weighting matrices with elements γ_{ui} and γ_{yi}. The error term, $e_y(i) = \Sigma_j^N (y_j(k+i|k) - y_{sj})$ compares the predicted values of the output vectors at each discrete particle size class, j, to the target desired trajectory, y_s, for each size class, j, over N individual size classes.

With a simulation of the process and an efficient model available, it is now possible to formulate a batch NMPC controller which explicitly accounts for process output control objectives. The constraints on this process state: the impeller speed is bound by limits, $0 < u_1(k) < 1000\,rpm$, and volumetric binder flowrate which is a nonnegative value, $u_2(k) > 0$.

$U(k)$ is a vector of all previous input moves, $u_1, \ldots u_{np}$ and future input moves $u(k),\ u(k+1),\ \ldots u(n)$, where np is the previous number of input moves . The objective function, $\Phi(k)$, is minimized over the prediction horizon, p, by applying selected input moves $u(k),\ u(k+1),\ \ldots u(n)$, into $U(k)$. In the formulation of the batch MPC control scheme, a shrinking horizon over which the objective function is minimized is considered [15]. The duration of a given batch is discretized into n time steps, where n spans the entire desired batch trajectory. The vector of input moves, $U(k)$, is then separated into two categories: previous input moves, n_p, and future input moves, n_f, where $n_p + n_f = n$ such that:

$$U(k) = [u_1,\ u_2,\ \ldots u_{np},\ u(k),\ u(k+1),\ \ldots u(n)] \tag{7}$$

Input moves $u(1).\ .\ .u(np)$ are all of the previously calculated input moves over the shrinking horizon, p and thus cannot be altered to minimize Φ. Input moves $u(k)\ .\ .\ .\ u(n)$ consist of the future input moves. The future moves provide a degree of freedom for the controller. The controller then can only choose input moves over the horizon m, for every i greater than $m-1$, such that the input u has identical values: $u(k+m-1) = u(k+m) =.\ .\ .\ = u(n)$.Thus, in choosing a move horizon of one, a vector of uniform future input moves results. The controller chooses the optimum move at each time step using the PBE to calculate the proper input moves over the prediction horizon which will minimizes the objective function at each time step. Only then are these input moves applied to the actual process.

5 Results

The batch NMPC controller was used to stabilize desired steady state operating points for batches simulated with five size classes. The following weights were chosen for the input moves: $\Gamma_{u1} = 0.001$, impeller, and $\Gamma_{u2} = 0.0001$, binder. The weights were sufficiently small enough to allow for a large degree of variation between time steps. It is assumed that the initial particle size distribution in the granulator is known and therefore duplicated for the model. The desired trajectory used as the setpoint is the result of an average of 20 open-loop batch operations without disturbances. At each time step the NMPC controller attempts to minimize the objective function over the entire batch trajectory by altering the inputs (impeller speed, binder addition) into the population balance. Using the population balance

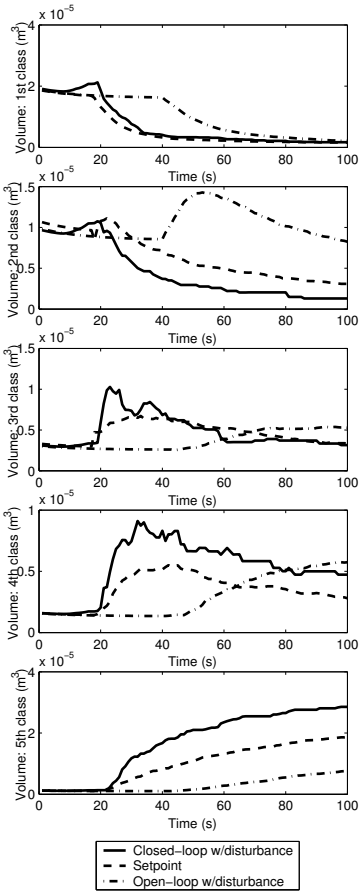

Figure 2: Comparison of desired trajectory with open loop and closed loop trajectory for all five size classes using a batch NMPC controller where the desired particle trajectory had more binder initially present..

model, the batch trajectory can be calculated much more efficiently than using the discrete element approach.The population balance was discretized into five size classes resulting in five individual trajectories in which the NMPC must use only two inputs to control.

Several different trials were examined. In test 1, the initial particle size for the granulator and the model were identical but the granulator particles were nucleated initially with a higher liquid volume fraction. This extra binder present will lead to a decreased induction time and a larger mean particle size according to open loop results [5]. The NMPC controller was applied and the results are shown in Figure 2. The input moves required to reach this setpoint are displayed in Figure 3.

These solutions were found using a shrinking horizon and a move horizon of two. A move horizon less than two produced very undesirable results. This can be attributed to the fact that a controller with a move horizon of one cannot fully accommodate for process disturbances, and instead will average out disturbances over the entire trajectory. A

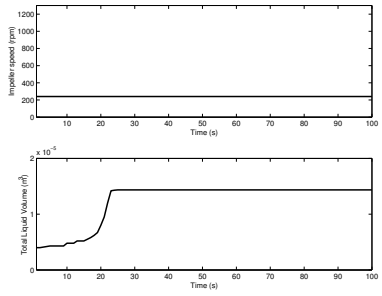

Figure 3: Input moves formulated by the NMPC controller to reach the desired setpoint.

Table 1: Comparison of error from desired trajectory occurring with and without use of the batch NMPC controller for case A.

Size Class	Open loop error $\left(m^3 \times 10^9\right)$	Closed loop error $\left(m^3 \times 10^9\right)$
1	3.583	0.7031
2	2.992	0.6744
3	0.5012	0.1486
4	0.5035	0.8688
5	6.984	5.482
Σ error	14.56	7.877

comparison of the error between the open loop trajectory and the desired trajectory with the closed loop NMPC trajectory and the desired trajectory is given in Table 1. This table clearly shows that despite the fact that the problem is non-square, the controller does provide a closed loop trajectory overall with half as much error than the open loop trajectory. Furthermore, four out of the five particle size trajectories were significantly closer to the desired trajectory using the NMPC controller.

A primary concern with controlling particle size trajectories in granulation processes is the determination of the induction period. For this example, the open-loop trajectory with exhibited an induction time of $40s$ while the setpoint trajectory had an induction time of only $20s$. The difference is attributed to a greater initial binder load for the setpoint trajectory, therefore the granules reach a capillary state of saturation sooner. The NMPC controller was able to predict this necessary addition of binder as shown in Figure 3.

The more difficult control problem occurs when the desired trajectory has a longer induction time than the process at hand. This is the result of granules with less binder present being used for the desired batch trajectory. In this situation, the NMPC controller is unable to remove liquid from the process. Open-loop tests have shown that increasing impeller speed does effectively hinder granule growth [14]. This is due to the fact that as the kinetic energy of granule collisions increase, the binder layer becomes less ef-

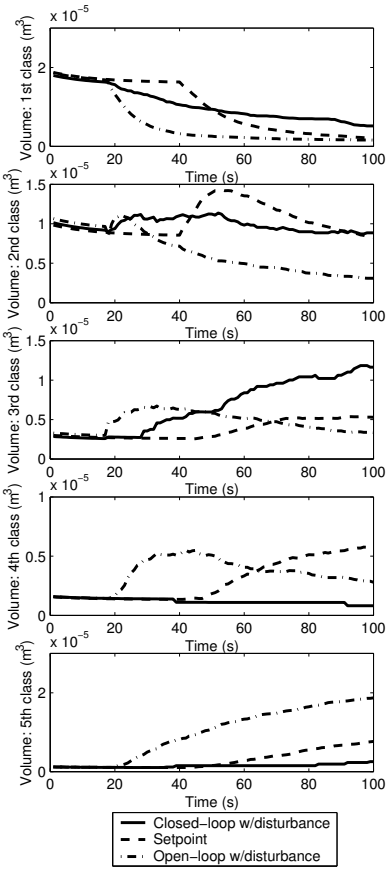

Figure 4: Comparison of desired trajectory with open loop and closed loop trajectory for all five size classes using a batch NMPC controller where the desired particle trajectory had less binder initially present.

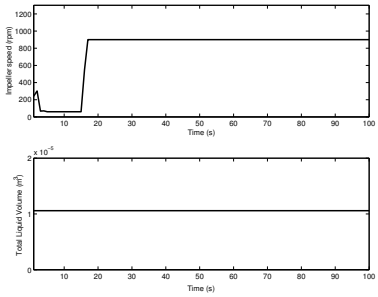

Figure 5: Input moves formulated by the NMPC controller to reach the desired setpoint.

Table 2: Comparison of error from desired trajectory occurring with and without use of the batch NMPC controller fro case B.

Size Class	Open loop error $(m^3 \times 10^9)$	Closed loop error $(m^3 \times 10^9)$
1	3.583	0.9214
2	2.992	0.3673
3	0.5012	1.413
4	0.5035	0.6619
5	6.984	0.5835
Σ error	14.56	3.947

fective in dissipating the resulting force, therefore resulting in more rebounding and less coalescence. In the examples presented in Figure 4, results are shown for particle trajectories of five individual size classes. Figure 5 shows how the controller only changed the impeller speed to decrease the rate of agglomeration of the process. The impeller speed was increased to its saturation point as determined by controller formulation constraints. No binder was added to the process. As can be seen, all five size classes progress in a manner similar to the setpoint. While the induction time could not change, the growth rate was manipulated to find the best solution possible using impeller speed as the only input that could reduce the model/setpoint error. A comparison of the error between the open loop trajectory and closed loop trajectories for this control problem is displayed in Table 2. The controller provides a closed loop over three and a half times closer to the desired setpoint trajectory than the open-loop case. Furthermore, again four out of the five particle size trajectories were significantly closer to the desired trajectory using the NMPC controller.

6 Conclusion

A batch nonlinear MPC controller has been formulated which effectively follows a desired batch output trajectory of a particle size distribution for a simulated granulation process in which five particle size classes are tracked. A discrete element simulation model which determines the result of granular interactions based on physical granular properties was used to simulate the actual granulation process. A population balance equation model in which a new coalescence kernel was determined to minimized plant/model mismatch was used as the model of the process for efficient error determination. The NMPC controller was shown to follow desired particle sized trajectories for five size classes using granulator impeller speed and volume of binder addition as the two input moves. Two differing initial conditions were examined: where the setpoint trajectory had more initial binder present and when it had less initial binder present than the open loop trajectory. Based on the amount of binder present, the induction time of the batch process would vary. Despite this, the NMPC controller showed it could handle either condition. More difficulties arise in the latter situation due to the fact that only impeller speed could be used to change the trajectory. With only one degree of freedom, the controller was able to decrease the error by increasing the impeller speed to its saturation level. More situations will be examined in the future.

References

[1] R. J. Batterham, J. S. Hall, and G. Barton. Pelletizing kinetics and simulation of full scale balling circuits. *Proceedings of the 3rd International Symposium on Agglomeration*, Nurnberg, W. Germany:A136, 1981.

[2] B. J. Ennis and J. D. Litster. *Perry's Chemical Engineers' Handbook*, chapter Particle size enlargement, pages 20–56–20–89. McGraw Hill, 7th edition, 1997.

[3] A. Faure, P. York, and R. C. Rowe. Process control and scale-up of pharmaceutical wet granulation processes: a review. *European Journal of Pharmaceutics and Biopharmaceutics*, 52:269–277, 2001.

[4] B. Foss, T. Johansen, and A. Sorensen. Nonlinear predictive control using local models-applied to a batch process. To appear in Int. Journal of Control 1994, 1994.

[5] J. A. Gantt and E. P. Gatzke. High-shear granulation modeling using a discrete element simulation approach. *Submitted to Powder Technology (9/03)*, 2003.

[6] E. Gatzke and F. Doyle III. Model predictive control of a granulation system using soft output constraints and prioritized control objectives. *Powder Technology*, 121:149–158, 2001.

[7] M. J. Hounslow, R. L. Ryall, and V. R. Marshall. A discetized population balance for nucleation, growth and aggregation. *AIChE Journal*, 34(11):1821–1832, 1988.

[8] S. Iveson, J. Litster, and B. Ennis. Fundamental studies of granule consolidation. part 1: effects of binder content and binder viscosity. *Powder Technology*, 88:15–20, 1996.

[9] K. L. Johnson. *Contact Mechanics*. Cambridge University Press, 1987.

[10] S. Kumar and D. Ramkrishna. On the solution of population balance equations by discretization-i. a fixed pivot technique. *Chemical Engineering Science*, 51:1311–1332, 1996.

[11] L. X. Liu and J. D. Litster. Coalescence of deformable granules in wet granulation processes. *AIChE Journal*, 46(3):529–539, March 2000.

[12] L. X. Liu and J. D. Litster. Population balance modeling of granulation with a physically based coalescence kernel. *Chemical Engineering Science*, 57:2183–2191, 2002.

[13] Z. Nagy and R. Braatz. Robust nonlinear control of batch processes. *AIChE Journal*, 49:1776–1786, 2003.

[14] D. Oulahna, F. Cordier, L. Galet, and J. A. Dodds. Wet granulation: the effect of shear on granule properties. *Powder Technology*, 130:238–246, 2003.

[15] Y. Pan and J. Lee. Recursive data-based prediction and control of product quality for a pmma batch process. *Chemical Engineering Science*, 58:3215–3221, 2003.

[16] M. Pottman, B. A. Ogunnaike, A. A. Adetayo, and B. J. Ennis. Model based control of a granulation system. *Powder Technology*, 108:192–201, 2000.

[17] G. A. Pouw, D. Verkoeijen, G. M. H. Meesters, and B. Scarlett. Population balances for particulate processes-avolume approach. *Chemical Engineering Science*, 57:2287–2303, 2002.

[18] G. Tardos, M. I. Khan, and P. R. Mort. Critical parameters limiting conditions in binder granulation of fine powders. *Powder Technology*, 94:245–258, 1997.

[19] S. Watano, T. Numa, I. Koizumi, and Y. Osako. Feedback control in high shear granulation of pharmaceutical powders. *European Journal of Pharmaceuticals and Biopharamceuticals*, 52:337–345, 2001.