Control of a Granulation Process Using a Nonlinear MPC Formulation

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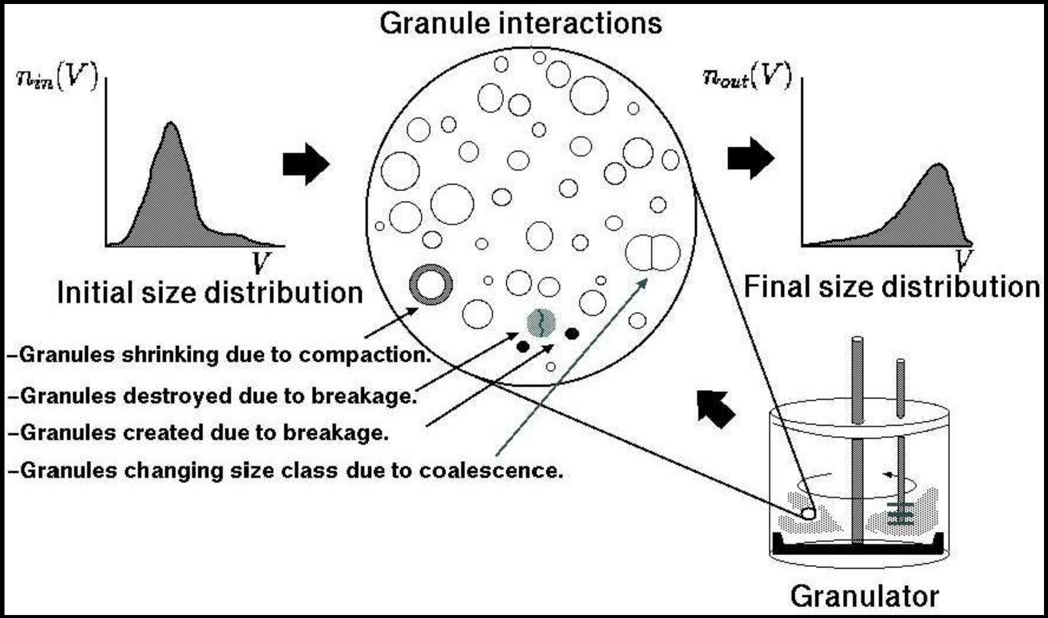
Introduction

- Granulation processes require consistent product quality: size uniformity, proper flowability, attrition resistance, etc.
- Product quality indicators are related to:
  - Particle size distribution
  - Bulk density
- Model Predictive Control (MPC) has been used in granulation processes to control these granular quantities.
- What is MPC?
  - Controller formulates an optimization problem, representing the minimization of an objective function.
  - Continuous MPC vs. Batch (Pottman *et al.* 2000)
  - Nonlinear process concerned with PBEs
  - Nonsquare process

Plant Model

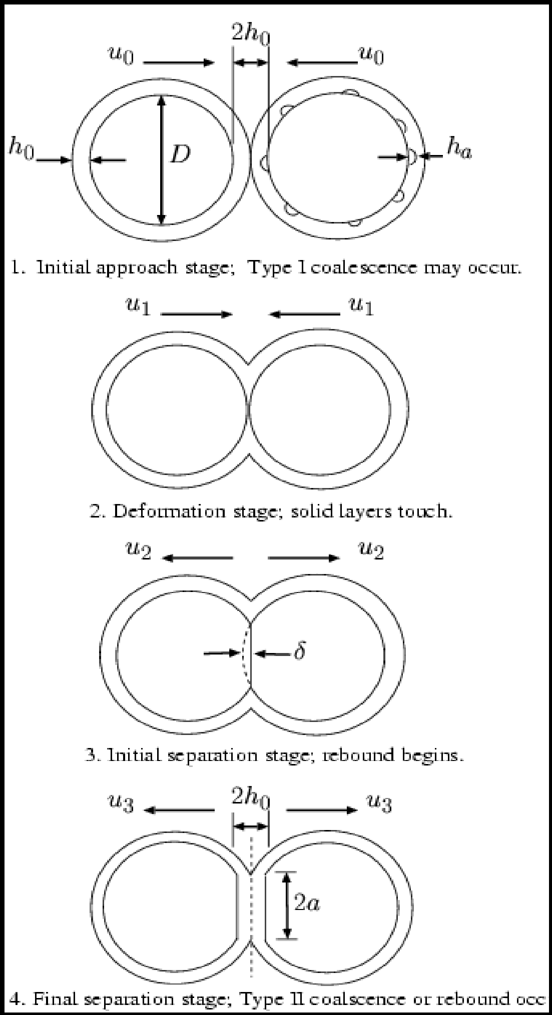
- A high fidelity plant model was derived based on physical models of granular interactions.
- Individual particles are modeled using a DEM approach.
- Due to physical interactions, particles coalesce, consolidate, and break.



Plant Model

- *Granule position:* particles are randomly given a fixed, non-overlapping position in 3D space.
- *Granule composition:* Particles begin in a nucleated matrix of solid powder, trapped air, and liquid binder.
- *Granule velocity:* Particles are assigned a 3D velocity from a normal velocity distribution based on the impeller speed.
- *Consolidation:* As granules collide with each other, air is slowly forced out. As air leaves, more binder is pushed to the surface.
- *Coalescence:* As particles collide, they will coalesce or rebound based on criteria defined by Liu *et al.*

Coalescence of Wet Granules



- Granule growth due to collisions.
- Probability of successful collision is determined by presence of binder layer, *h.*
- Type I coalescence: viscous dissipation of the binder layer is greater than the kinetic energy of the collision.
- Type II coalescence: deformation of collision prevents rebounding of granules.
- Rebound: occurs when the kinetic energy of the collision is great enough to prevent coalescence.

Population Balance Equation Model

- PBE models are used in particulate modeling to calculate size distributions and to determine rate controlling mechanisms.
- PBE's are based on kinetic rate expressions:
  - Birth rate / death rate
  - Growth rate (coalescence) / Attrition and breakage rate
- Batterham *et al.* 1981, Ramkrishna *et al.* 1985, and Hounslow *et al.* 1988 used numerical techniques to solve PBEs.
- Discrete solutions considered particles of different sizes to exist in groups that interacted collectively with particles of different groups.

Population Balance Equation Model

- Verkoeijen *et al.* 2002 proposed a discrete multi-dimensional PBE using volume as the intrinsic parameter. The model tracked evolution of solid, liquid and air volume based on *coalescence* and *consolidation* of granules.
- PBE model: $$\frac{dq_{sk}}{dt} = \sum_{j=1}^{n} \left(\frac{\beta_{ij} q_{si} - \beta_{kj} q_{sk}}{j s_1 N_{tot}} \right) q_{sj}$$
- A coalescence kernel was then created to capture induction behavior, promote granule growth with binder addition and decrease growth due to high impeller speeds.

$$\beta(u,v) = \begin{cases} \beta_0 \left(\ln\left(1.5+\omega\right)\right)^{2.5} \left(q_{lt} / q_{lt-1}\right) & \text{for } S \geq S^* \,\&\, \omega > 0 \\ 0 & \text{for } S < S^* \text{ or } \omega = 0 \end{cases}$$

Controller Formulation

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

$$x(k+1) = f(x(k), u_1(k), u_2(k)), \qquad k = 0,1,\dots n$$
$$y(k) = x(k)$$

x(k): 5 discrete particle size classes

$u_i(k)$: inputs impeller speed and binder volume

- MPC control moves are found by minimizing the objective function:

$$\min_{U(k)} \Phi(k) = \sum_{i=k}^{k+p} e_y(i)^T \Gamma_y e_y(i) + \sum_{i=0}^{M-1} \Delta u(i)^T \Gamma_u \Delta u(i)$$

subject to constraints: $u(i) \in [u_{\min}, u_{\max}]$

Controller Formulation

- Batch MPC concerns:
  - Batch process follow a prescribed trajectory.
  - Error compares the PBE model to the ref. DEM trajectory.

$$e_y(i) = \sum_{j}^{N} \left(y_j(k+i \mid k) - y_{s,j} \right)$$

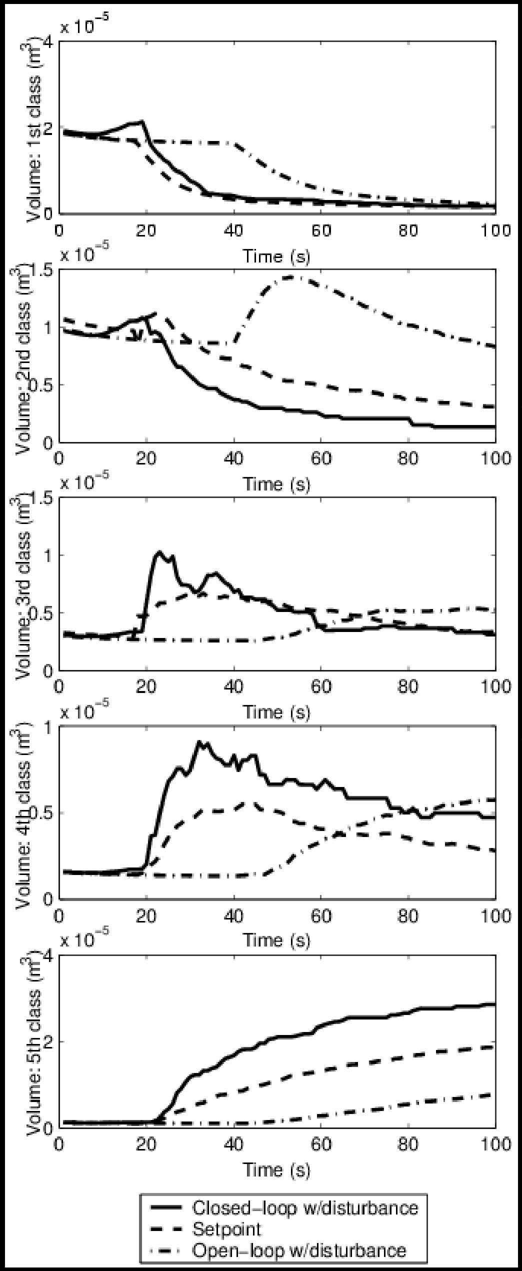
  - Trajectory tracking poses problems due to nonlinearity.
- A shrinking horizon approach is use to minimize the objective function over the duration of the batch.
- *U(k)* is a vector of previous and future input moves.
  - Φ*(k)* is minimized through future input moves over the horizon *m*.

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

Results

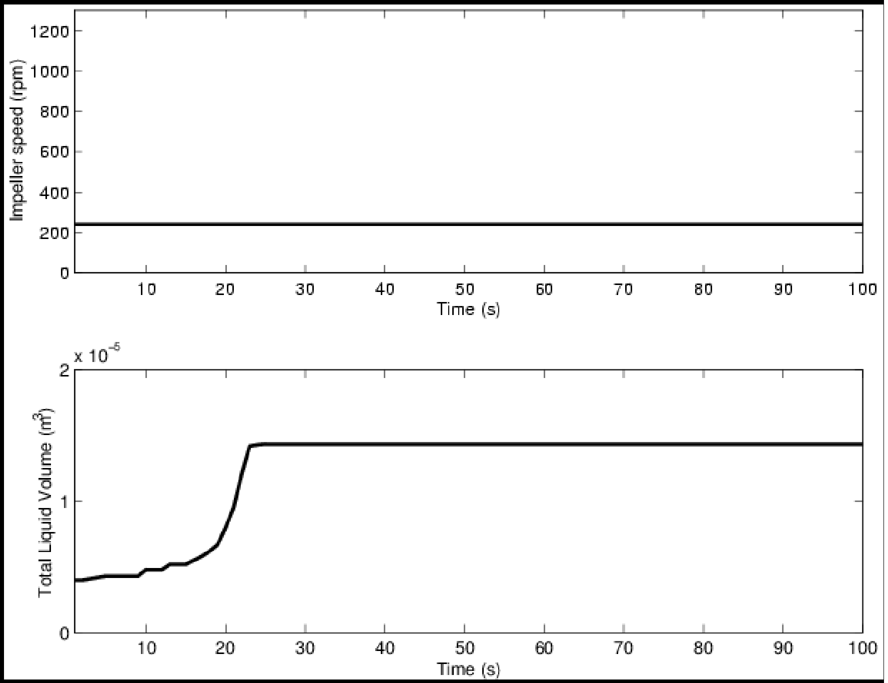
- The following parameters were chosen for the controller:

  $\Gamma_{u1} = 0$, and $\Gamma_{u2} = 0$, and *m*=2.
- The desired trajectory used was an average of 20 open-loop DEM batch results.
- Using the PBE model, a batch trajectory was calculated and compared to the desired DEM averaged trajectory.
- Several different trials were examined:
  - Trial 1: Identical initial PSD for open and closed loop, with the desired trajectory including *more initial binder*.
  - Trial 2: Identical initial PSD for open and closed loop with the desired trajectory including *less initial binder.*

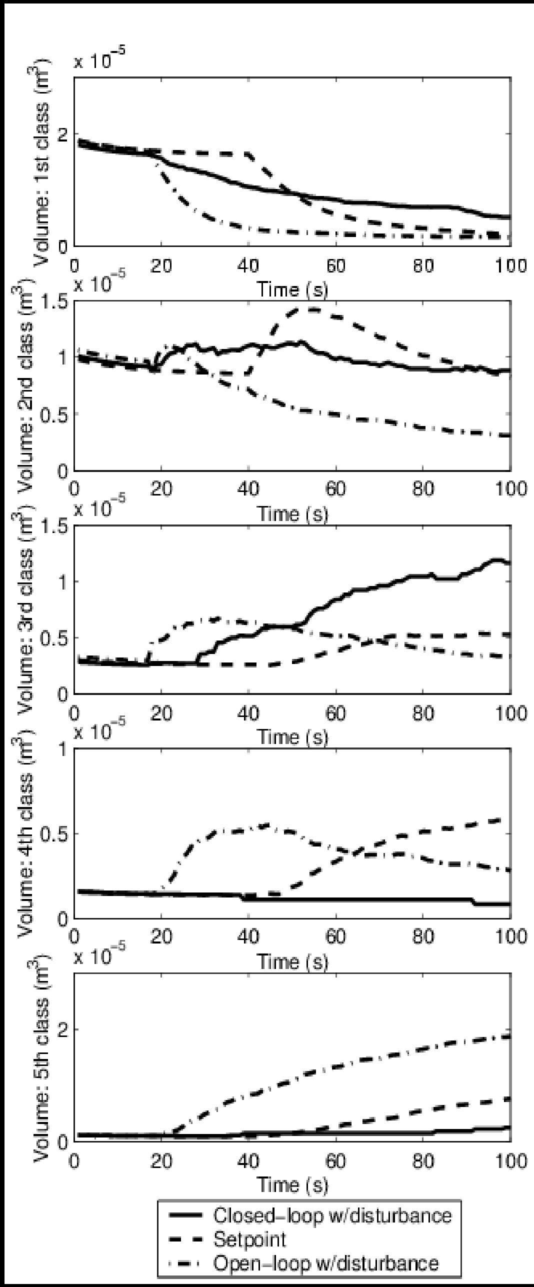


Results: Trial1

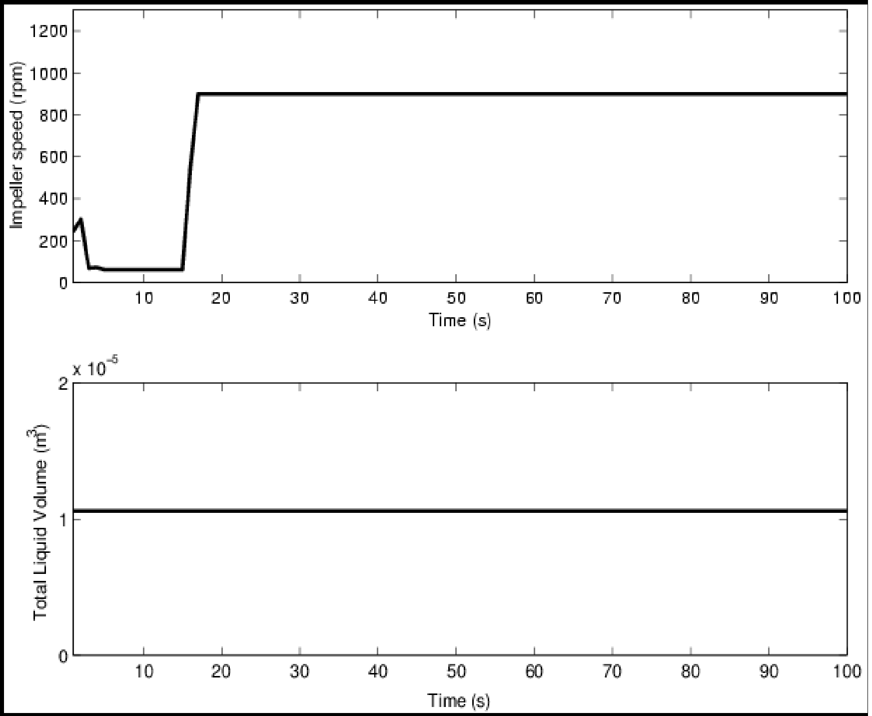
- A move horizon less than 2 produced inadequate results.
- Binder addition was only input move used.



Results: Trial 2



- Test 2 used and open loop trajectory with initially too much binder present.
- Only one degree of freedom: length of induction time could not be altered.
- Increasing impeller speed to saturation was only input move.



Results: Error Comparison Trial 1

Size Class	Open loop error *(m^3 x 10^9)*	Closed loop error *(m^3 x 10^9)*
1	3.583	0.7031
2	2.992	0.6744
3	0.5012	0.1486
4	0.5035	0.8644
5	6.984	5.482
Σ error	14.56	7.877

Results: Error Comparison Trial 2

Size Class	Open loop error *(m^3 x 10^9)*	Closed loop error *(m^3 x 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

Conclusions

- A batch Nonlinear MPC controller has been formulated which follows a batch trajectory for the PSD's of 5 particle size classes in a simulated granulation process.
- The DEM effectively modeled the plant high shear granulator.
- A new coalescence kernel was derived to take account for changes in binder volume and impeller speed when using a PBE model.
- The NMPC controller minimized the error of 5 size classes over the open-loop trajectory for two given circumstances, each with only one degree of freedom.

Future Work

- Model Validation
- Real-time considerations

Acknowledgements

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