Inventory control of particulate systems

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Abstract
In this paper inventory control is applied to a particulate system. The performance of inventory control is guaranteed only if the zero dynamics of the closed loop system is stable. Mathematical analysis for the stability of the particulate system is derived to show that the zero dynamics is stable. The approach is illustrated by the application to thermal deposition of silicon in a fluid bed reactor. Simulation results are presented to support the mathematical conclusion.

Keywords: Inventory control, Zero dynamics, Stability analysis, Particulate processes.

1. Introduction
The complexities of particulate processes create challenges for control. The physics of particle processes include nonlinear behavior and distributed parameters. The reaction, growth, or decay mechanisms in particle processes are distributed across both external and internal coordinates. Ray et al. provide a nice review of the nonlinear dynamics that characterize polymerization processes. As Semino and Ray point out, much work has been accomplished to apply and solve the population balance for a variety of particulate systems. In recent years, more groups have developed control theory for a variety of particulate systems. Mantzaris applied nonlinear control techniques to cell growth processes. Diez et al. pointed out that inventory control is a promising method to control particulate systems. Furthermore White et al. showed that inventory control can be applied to the discretized population balance model without model reduction. Du and White demonstrated that only if the zero dynamics of system is stable, the performance of inventory controllers is guaranteed.

In this paper, we present a novel mathematical analysis to show the stability of zero dynamics for the particulate systems. The discretized population balance model developed by White is exploited to represent the particulate system. We show that the discrete population balance with growth from a stable continuous phase is stable without exploiting numerical analysis in section 3. The general results can be applied to various practical problems such as crystallization, granulation and fluidized bed chemical vapor deposition. One example of industrial application about deposition of silicon in a fluidized bed reactor is presented in section 4 to support the analysis results. Inventory control is applied to the complex process and simulation results make a good agreement with those of mathematical analysis. Conclusion is drawn in section 5.

2. Inventory control
Inventory control consists of manipulating process flows such that the inventories follow their setpoints. Inventories are extensive variables which are proportional to the size of the system. The conservation laws used to develop dynamic models of chemical...
processes balance storage, production and flows of inventories in a given control volume. Such balances are written in mathematical form so that:

\[ \frac{dZ}{dt} = p + \phi(m) \tag{1} \]

where the variable \( Z \) represents the inventory at time \( t \) in a sub-section of the process, \( p \) is the rate of production and \( \phi(m) \) is the net flow rate from the surroundings, \( m \) is the control variable.

Farschman et al. proved that for the synthetic input and output pair:

\[ u = p + \phi(m) - \frac{dZ^*}{dt} \]
\[ y = Z - Z^* \tag{2} \]

where \( Z^* \) are arbitrary vector of constant set points, the mapping 

\( (\phi + p) \rightarrow (Z - Z^*) \)

is passive with storage function \( \Psi = \frac{1}{2}(Z - Z^*)^T(Z - Z^*) \).

The inventory controller is in the form of a nonlinear feedback feedforward law:

\[ u = -C(y) = p + \phi(m) - \frac{dZ^*}{dt} \tag{3} \]

The expression \( \phi(m) \) has to be invertible with respect to \( m \) in the domain of interest to implement the control law. If the condition is satisfied then we get the closed loop expression:

\[ \frac{dZ}{dt} = -C(e) + \frac{dZ^*}{dt} \tag{4} \]

If the process model has no model mismatch, a proportional control law is appropriate for inventory control, i.e. \( C(e) = Ke \), where \( K > 0 \) is the proportional gain.

Du et al. demonstrated that only if the zero dynamics of the system are stable, then the overall stability of the system is guaranteed and hence the performance of inventory controller is ensured as well.

3. Mathematical analysis of stability for the particulate systems

Particulate systems can be depicted as a well mixed, two phase contacting system. There are two feeds. One of them may be a disperse mix of solids, immiscible liquids or a catalyst. The other feed may be continuous. The feeds are contacted in a process which encourages reaction and mass transfer from one phase to another. Examples of such processes include crystallization, granulation, polymerization, fluid bed chemical vapor deposition, leaching, fluid bed cracking and combustion of solid particles.

The variables \( F^j_{\text{in}} \) denote input flow and \( F^j_{\text{out}} \) denote output flows. Index \( j = C \) denotes the continuous phase and \( j = D \) the discontinuous (particle) phase. The net flow into each phase is therefore given by

\[ \phi^j = F^j_{\text{in}} - F^j_{\text{out}}, \quad j = C, D \tag{5} \]

The feeds themselves may be disperse so that we can write

\[ F^{i,j}_{\text{in}} = \sum_{i=1}^{N} F^{i,j}_{\text{in}}^{k}, \quad k = \text{in, out} \tag{6} \]

where \( F^{i,j}_{\text{in}}^{k} \) denotes flow of disperse phase from the environment to or from size interval \( i \) and \( N \) is the number of size intervals used to describe the distribution function.
Figure 1. Definition of external flow.  Figure 2. Size interval flow structure.

Figure 2 shows flows between the different size intervals for a system with no agglomeration. Mass transfer between the homogeneous phase and the discontinuous phase is denoted by \( r_i, i = 1, ..., N \). We use the convention that \( r > 0 \) in deposition systems.

White et al. developed a size distribution model for the mass balance of disperse phase as:

\[
\frac{dM_i}{dt} = \phi_i + f_{i-1} - f_i + r_i, \quad i = 1, ..., N
\]  (7)

where \( \phi_i = F_i^{D, in} - F_i^{D, out} \) represents the net effect of external flows distributed over the intervals. The flow between the intervals is related to the deposition rate so that

\[
f_i = r_i \frac{m_{i+1}}{m_{i+1} - m_i}
\]  (8)

The concentration of the active component in the continuous phase is denoted by \( c^C \) whereas the surface concentration on the particles in the disperse phase is denoted by \( c^S_i \). The effective surface concentration may depend on size interval. The rate of mass transfer between the phases for particles in size interval can then be represented by the expression

\[
r_i = A_i \frac{k_i h_i}{r_i} (c^C - c^S_i)
\]  (9)

If \( c^C > c^S \) then mass transfer is from the continuous to the disperse phase where \( k_i \) is the mass transfer coefficient and \( h_i \) is the thickness of the boundary layer. The area available for mass transfer of a spherical particle is given by

\[
A_i = 4\pi R_i^2 N_i
\]  (10)

with \( N_i \) being the number of particles in the size interval and \( R_i \) being the radius of the particles in size interval \( i \). The mass transfer coefficient \( k_i \) and the boundary layer may depend on size and can be expressed as functions of the corresponding dimensionless numbers for mass transfer in turbulent flow.

The mass of the particles in interval \( i \) is related to the radius of the particle so that

\[
M_i = \rho_i \frac{4}{3}\pi R_i^3 N_i
\]  (11)

where \( \rho_i \) is the material density of the disperse phase in interval \( i \). Hence

\[
A_i = \frac{3M_i}{\rho_i R_i^2}
\]  (12)
By combining equations (7) and (8) we can write the mass transfer rate between the intervals so that
\[ f_i = A \frac{k_i}{h_i} (c^C - c^S_i) \frac{m_{i+1}}{m_{i+1} - m_i} \]  
(13)

Hence, using equation (9) we get
\[ f_i = \zeta_i M_i \]  
(14)

where
\[ \zeta_i = \frac{3h_i}{R_{i,0} h_i} (c^C - c^S_i) \frac{m_{i+1}}{m_{i+1} - m_i} \]

The parameters \( \zeta_i \) are constant in the case that the concentration \( c^C \) of the continuous medium is constant. We note that \( \zeta_i > 0 \) if \( c^C > c^S_i \).

We now use equation (4) to write
\[ r_i - f_i = -\mu_i^c \]  
(15)
\[ \mu_i = - \left( 1 - \frac{m_{i+1}}{m_{i+1} - m_i} \right) > 0 \]  
(16)

The last inequality follows as \( m_{i+1} > m_i \). From equation (5) we then have
\[ r_i - f_i = -\frac{k_i}{h_i} A_i (c^C - c^S_i) \mu_i, \quad i = 1, ..., N \]  
(17)

We can therefore write the balance equation for interval \( i \) so that
\[ \frac{dM_i}{dt} = \phi_i + f_{i-1} - \frac{k_i}{h_i} (c^C - c^S_i) \mu_i A_i \]  
(18)

Using equation (8) we can therefore have
\[ \frac{dM_i}{dt} = \phi_i + f_{i-1} - \frac{k_i}{h_i} (c^C - c^S_i) \mu_i \Delta M \]  
(19)

Hence, using equation (10)
\[ \dot{M}_i = \phi_i + \zeta_{i-1} M_{i-1} - \eta_i M_i, \quad i = 1, ..., N \]  
(20)

where
\[ \eta_i = \frac{k_i}{h_i} (c^C - c^S_i) \mu_i \frac{3h_i}{R_{i,0} h_i} \]

The parameters \( \eta_i \) are positive in a deposition process since \( c^C - c^S_i > 0 \) and negative otherwise.

To illustrate these ideas we firstly consider a system with only two size intervals. Small particles are fed to interval 1 at rate \( F_{in}^1 \). Material is deposited at rate \( r_1 \) and a flow of particles is established to interval 2 where the deposition process continues with the rate \( r_2 \). The particles are then harvested at the rate \( F_{out}^2 = f_2 \). The objective is to prove that the system is stable.

Writing the balance equations (15) for the two intervals and using the assumptions above we get
\[ \frac{dM_1}{dt} = -\eta_1 M_1 + F_{in}^1 \]  
(20.1)
\[ \frac{dM_2}{dt} = \zeta_1 M_1 - \eta_2 M_2 \]  
(20.2)

These equations can be written on the vector matrix form
\[ \frac{dX}{dt} = \left( \begin{array}{c} -\eta_1 \\ \zeta_1 \\ \eta_2 \end{array} \right) X + \left( \begin{array}{c} 1 \\ 0 \end{array} \right) U \]  
(21)
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where the state and control variables are defined so that

\[ X = (M_1, M_2)^T, \quad q = F^{\text{in}} \]

The eigenvalues of the matrix are both negative. The cascaded structure therefore ensures exponential stability of the open-loop system.

The system can be augmented with a measurements used for feedback control, for example,

\[ C = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \]

in the case that we measure the seed-mass and the total mass. Inventory control is trivially stable since we control the entire state vector.

We now generalize to systems with \( N \) intervals using the state vector with \( X = (M_1, \ldots, M_N)^T \) so that:

\[ A = \begin{pmatrix} -\eta_1 & 0 & 0 & 0 \\ \zeta_1 & -\eta_2 & 0 & \vdots \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \zeta_{N-1} & -\eta_N \end{pmatrix}, \quad B = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \]

This structure corresponds to seeding or nucleation of particles in the first size interval, no agglomeration or break-up, and withdrawal of the largest particles at the rate they are generated. The eigenvalue corresponding to the zero dynamics is given by

\[ \lambda_i = -\eta_i, \; i = 2, \ldots, N \]

These are all negative so the zero dynamics are stable. Other measurement and control configurations are easy to determine and stability follows as long as the cascaded structure of the matrix is retained.

In the case of inventory control using the first three intervals to control the seed distribution, we get the measurement structure

\[ C = \begin{pmatrix} 1 & 1 & 1 & 0 & \cdot & 0 \end{pmatrix} \]

4. Application and simulation results

Solar grade silicon production in a fluidized bed reactor is one example of the particular systems discussed in the previous section. Thermal decomposition of silane (SiH4) takes place in a fluidized bed reactor. Silane and hydrogen gases enter at the bottom of the reactor with sufficient velocity to fluidize the silicon particles. When silane gas is heated by wall heaters, it decomposes to silicon and hydrogen gas. Most of the silicon deposits on the surface of the particles which cause particles to grow. The gas exits at the top of the reactor together with solar silicon dust. Total mass hold up is maintained constant via inventory control to keep the change of volume of solid phase as zero.

Proportional control law is performed over all size intervals (1 to \( N \)) to derive the product flow rate \( \dot{P} \) required to maintain a constant hold-up in the reactor \( M^{\text{total}}_0 \), meanwhile proportional inventory controller is implemented to control the seed addition rate \( \dot{S} \) to maintain a constant seed hold-up \( S^{\text{total}}_0 \). The simulation results based on such inventory controllers are shown in Figure 6. The simulation results support the mathematical analysis achieved before.
5. Conclusion

In this paper we showed that the discrete population balance with growth from a stable continuous phase is stable without using numerical analysis. The new result was obtained by using classical eigenvalue analysis. This method is easy to apply to systems with cascaded, linear structure, and it can be generalized to systems with agglomeration. Growth due to agglomeration perturbs terms below the diagonal and does not cause instability. Similar results are easy to develop for systems that dissolve via combination of mass transfer and break-up.

References