Passivity based inventory control of particulate systems

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High purity silicon production: µE and PV

Siemens Reactor
Batch Process
1100°C

Fluid Bed Reactor
Continuous Process
Large surface area
650°C

Dense Phase
SiH₄ Decomposition
Particle Growth
Size Distribution

Heterogeneous →
grey, crystalline solid

Homogeneous →
brown, amorphous powder

particle growth = heterogeneous + scavenged powder
Particulate processes

Control Challenges
- Nonlinear, long delays
- Limited measurements
- Few manipulated variables
- Uncertain parameters

Control Techniques
- Linear and nonlinear MPC
- Nonlinear output feedback
- Passivity

Population Balance Equation (PBE)
\[
\frac{\partial n}{\partial t} + \nabla \cdot vn = B - D
\]
- Moment transformation
- Discrete system

External Coordinates: space, time
Internal Coordinates: size, age, composition
Discrete size distribution model

Derive conservation law over discrete size intervals

\[
\frac{dM_i}{dt} = f_{i-1} - f_i + f a_{i}^{IN} - f a_{i}^{OUT} + p_i + \sum_{\gamma} q_{i,\gamma}
\]

Internal flow

Production

External flow

Closure Relationships
- constant average size within interval
- real-valued “number” of particles

\[
f_i = p_i \cdot \frac{m_{i+1}}{m_{i+1} - m_i}
\]

- aggregation proportional to particle concentration (binary collision)

\[
f a_{i,j} = k_{i,j} C_i C_j
\]

System dependent
- reaction
- condensation

System dependent
- seed addition
- product removal
Relationship to continuous population balance

Discrete model:

\[ \frac{dM_i}{dt} = f_{i-1} - f_i + f a_i^{IN} - f a_i^{OUT} + p_i + \sum_{\gamma} q_{i,\gamma} \]

Re-write macroscopic values:

\[ M = \int_{\Omega} \mu d\Omega \]

\[ f_{i-1} - f_i + p_i + \sum_{\gamma} q_{i,\gamma} = \int_{\Omega} v d\Omega \]

\[ f a_i^{IN} - f a_i^{OUT} = \int_{\Omega} (B - D) d\Omega \]

As the number of size intervals approaches infinity:

\[ \frac{dM_i}{dt} = \frac{d}{dt} \int_{\Omega} \mu d\Omega = \int_{\Omega} \frac{\partial}{\partial t} \mu d\Omega = \int_{\Omega} (B - D) d\Omega + \int_{\Omega} v d\Omega \]

\[ \Rightarrow \frac{\partial \mu}{\partial t} + \nabla \cdot v = B - D \]

model is discrete version of PBE
Discrete model solution

Ordinary differential equations for mass in gas and solid phases + Algebraic constitutive equations

MATLAB's ode15s

<table>
<thead>
<tr>
<th>Adjustable Parameters</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{sc}$</td>
<td>Powder scavenging coefficient $0 \leq k_{sc} \leq \frac{R_{hom}}{(C_p \sum A_i)}$</td>
</tr>
<tr>
<td>$k_{i,j}$</td>
<td>Aggregation proportionality constant $0 \leq k_{i,j} \leq 10^{-8}$</td>
</tr>
</tbody>
</table>
Model validation

Silicon in Reactor

Size Distribution

- Experiment
- Model
- With Powder Loss

- Experiment
- Model
- With Aggregation

Silicon Mass

Number of Particles

Silicon Mass Fraction

Size Interval
Observer-based estimator (Dochain, et al.)

Observer theory → estimates of unknown states and parameters

\[
\begin{align*}
\frac{dx_1}{dt} &= F_{11}(x)\theta + F_{21}(x) \\
\frac{dx_2}{dt} &= F_{12}(x)\theta + F_{22}(x)
\end{align*}
\]

Design estimator (similar to Luenberger)

\[
\begin{align*}
\frac{d\hat{x}_1}{dt} &= F_{11}(x)\hat{\theta} + F_{21}(x) - \Omega(x_1 - \hat{x}_1) \\
\frac{d\hat{\theta}}{dt} &= [F_{11}(x)]^T \Gamma (x_1 - \hat{x}_1)
\end{align*}
\]

correction terms

Stable if
1. \(\Omega^T \Gamma + \Gamma \Omega\) negative definite
2. \(F_{11}\) persistently excited

measured or unmeasured \(x_2\) independent of parameter estimation
Parameter estimation for fluidized bed reaction

- How much powder is scavenged (contributes to growth)?
- How much powder is lost?

\[
\frac{dM_i}{dt} = f_{i-1} - f_i + f_a^{IN} - f_a^{OUT} + \sum_\gamma q_{i,\gamma} + p_i
\]

\[
p_i = (R_{het} + R_{sc}) \cdot \frac{A_i}{\sum_i A_i}
\]

\[
R_{sc} = k_{sc} C_p \sum_i A_i, \quad C_p = \text{powder concentration}
\]

Estimation equations:

\[
\frac{d\hat{M}}{dt} = \sum_i r_i + q^{IN} - q^{OUT} - C_1(M - \hat{M})
\]

\[
\frac{dk_{sc}}{dt} = \frac{1}{C_p \sum_i A_i} C_2(M - \hat{M})
\]

- \(C_1, C_2 > 0\) and \(\frac{1}{C_p \sum_i A_i} \neq 0\) \(
\Rightarrow\) stability
Size control during continuous production

Control: mass of specified size $\sum_i M_i$

Manipulate: external flow rates $\sum_i q_i$

Apply inventory control to system:

$\sum_i \frac{dM_i}{dt} = \sum_i g_i + \sum_i q_i = -K \left( \sum_i M_i - M^* \right)$

$\Rightarrow \sum_i q_i = -\sum_i g_i - K \left( \sum_i M_i - M^* \right)$

Constant mass in reactor: $product = -\sum_{i=1}^{N} g_i - K_t \left( \sum_{i=1}^{N} M_i - M^* \right)$

Constant seed mass: $seed = -\sum_{i=1}^{I_s} g_i - K_s \left( \sum_{i=1}^{I_s} M_i - M_s^* \right)$
Passivity

Given storage function $V$:

$$0 \leq V(t) \leq V(0) + \int_0^t u^T y - \beta_0 \int_0^t u^2$$

System is

1. Passive if $\beta_0 = 0$
2. Input strictly passive if $\beta_0 > 0$

Feedback connection of passive system and input strictly passive system of dissipation rate $\beta_0$:

Passive with $\mathcal{L}_2$ gain $= \frac{1}{\beta_0}$

i.e.

$$\int_0^\infty y^2 \leq \frac{1}{\beta_0} \int_0^\infty d^2$$
Input strictly passive controllers

Observer-based estimator: \((M - \tilde{M})\)
- prediction error and persistent excitation \(\rightarrow\) parameter convergence
- estimation stability \(\rightarrow\) closed loop stability

Passivity theory: \((M - M^*)\)
- set point error \(\rightarrow\) (input/output) stability
- parameter parameter convergence?

Proportional
\[ u = Ke \]

PID
\[ u = K \left( e + \frac{1}{\tau I} \int_0^\infty e + \frac{de}{dt} \right) \]

Adaptive
\[ u = Ke + \phi^T \hat{\theta}, \hat{\theta} = -\mu \phi e \]
Control of fluidized bed reactor
Particle size achieved under control
Parameter estimation

- True ksc
- Estimated ksc
Summary

- Discrete population balance model of particle distribution compares well with data
- Observer-based estimator provides parameter convergence
- Passivity based inventory control enables size control
- Further investigation of yield control and zero dynamics of size distribution is required

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