Passivity based inventory control of particulate systems

Christy M. White
B. Erik Ydstie

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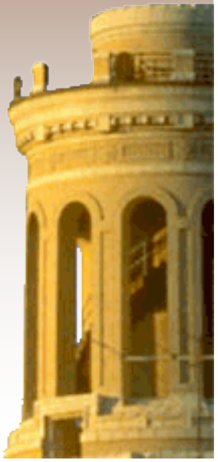
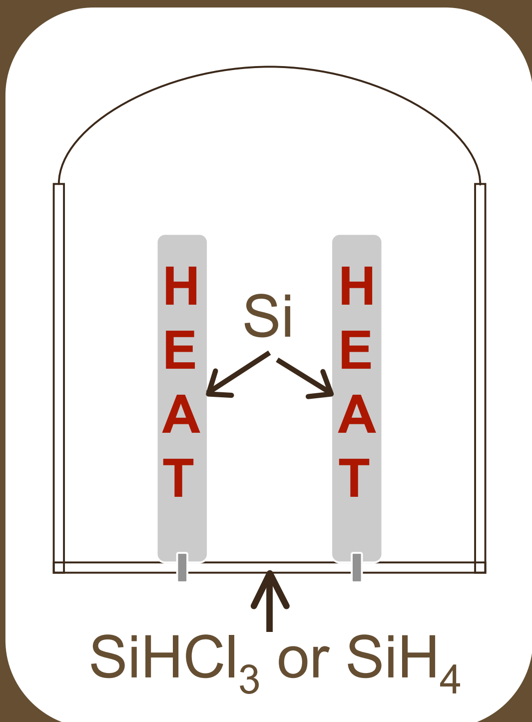
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA

AIChE
AMERICAN INSTITUTE OF CHEMICAL ENGINEERS



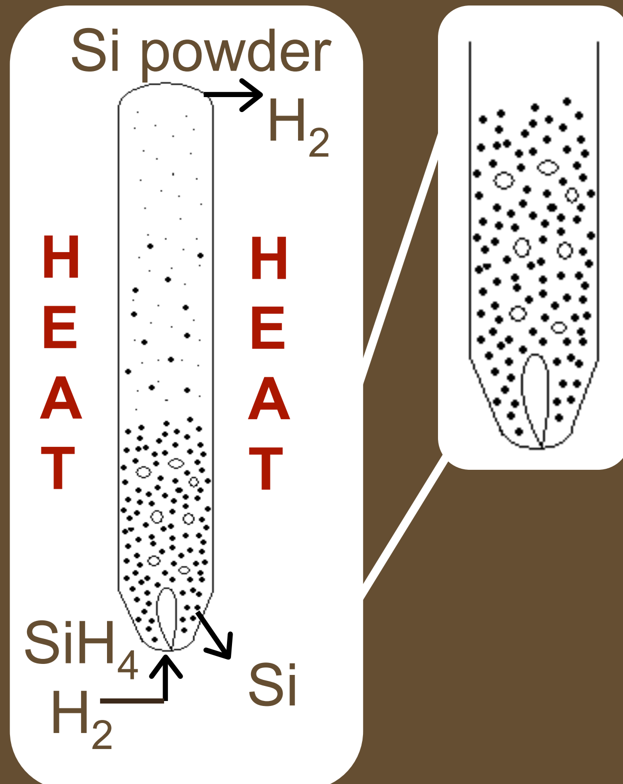
High purity silicon production: μE and PV



<u>Siemens Reactor</u>

Batch Process

1100°C



<u>Fluid Bed Reactor</u>

Continuous Process

Large surface area

650°C

<u>Dense Phase</u>

SiH_4 Decomposition

Particle Growth

Size Distribution

Heterogeneous → grey, crystalline solid

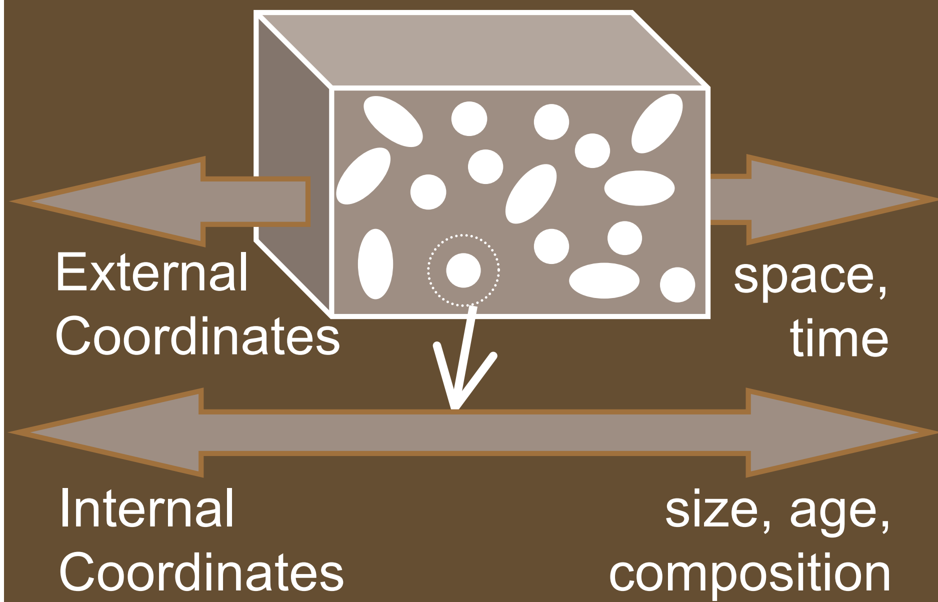
$$SiH_4 \rightarrow Si + H_2$$

Homogeneous → brown, amorphous powder

$$SiH_4 + SiH_4 \rightarrow Si + H_2$$

particle growth = heterogeneous + scavenged powder

Particulate processes



Population Balance Equation (PBE)

$$\underbrace{\partial n/\partial t}_{\text{density distribution}} + \underbrace{\nabla \cdot vn}_{\text{flow}} = \underbrace{B - D}_{\text{birth and death terms}}$$

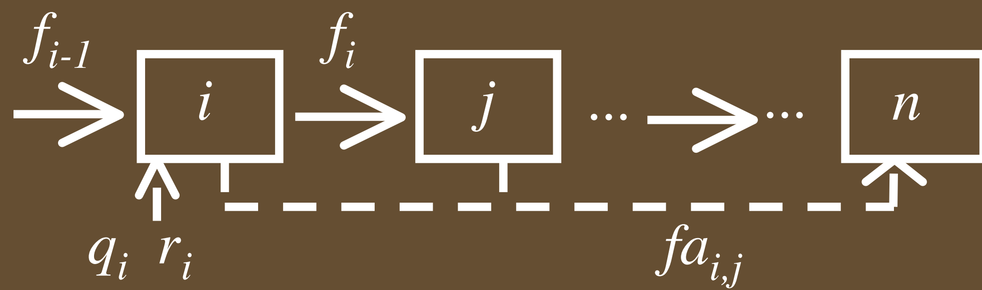
Solution Techniques
- Moment transformation
- Discrete system

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

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

Discrete size distribution model

Derive conservation law over discrete size intervals



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

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)

$$fa_{i,j} = k_{i,j} C_i C_j$$

System dependent
- reaction
- condensation

System dependent
- seed addition
- product removal

→ track particle growth

Relationship to continuous population balance

Discrete model: $$\frac{dM_i}{dt} = f_{i-1} - f_i + fa_i^{IN} - fa_i^{OUT} + p_i + \sum_\gamma q_{i,\gamma}$$

Re-write macroscopic values: $$M = \int_\Omega \mu d\Omega$$

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

$$fa_i^{IN} - fa_i^{OUT} = \int_\Omega (B - D) d\Omega$$

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

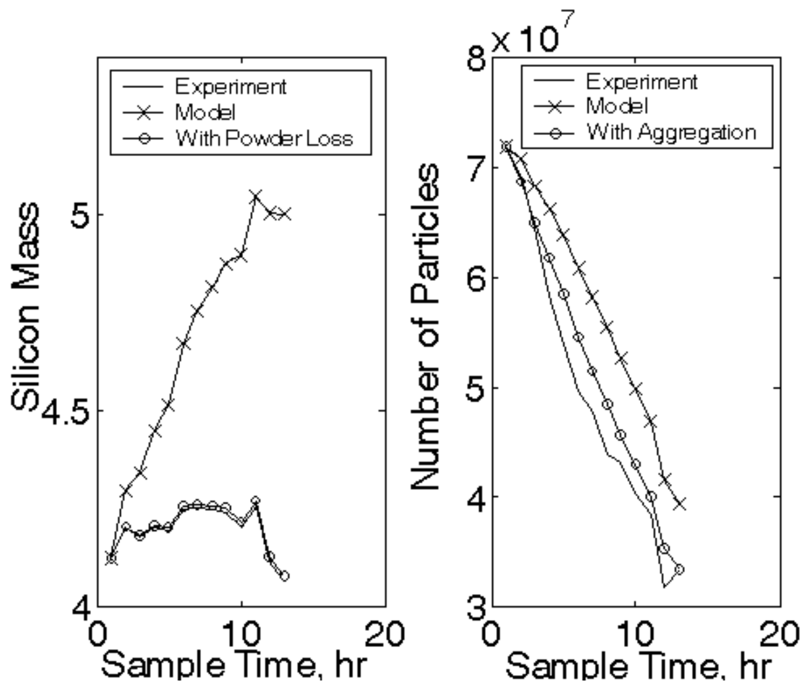
↓

MATLAB's ode15s

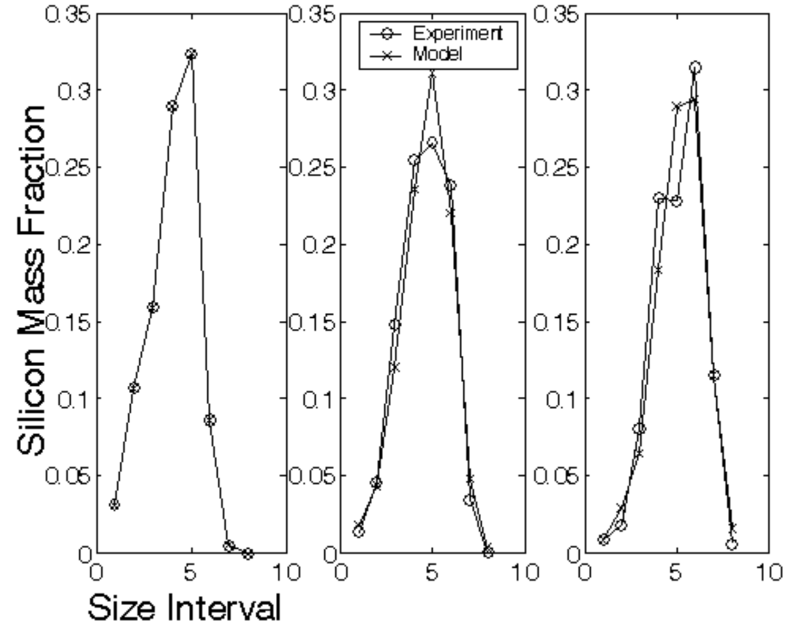
Adjustable Parameters		*Range*
k_{sc}	Powder scavenging coefficient	$0 \leq k_{sc} \leq R_{hom}/(C_p \sum A_i)$
$k_{i,j}$	Aggregation proportionality constant	$0 \leq k_{i,j} \leq 10^{-8}$

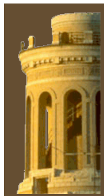
Model validation

Silicon in Reactor



Size Distribution





Observer-based estimator (Dochain, et al.)

Observer theory → estimates of unknown states and parameters

measured states

$$\frac{dx_1}{dt} = F_{11}(x)\theta + F_{21}(x)$$

$$\frac{dx_2}{dt} = F_{12}(x)\theta + F_{22}(x)$$

unknown parameters

Design estimator (similar to Luenberger)

estimation

$$\frac{d\hat{x}_1}{dt} = F_{11}(x)\hat{\theta} + F_{21}(x) - \Omega(x_1 - \hat{x}_1)$$

$$\frac{d\hat{\theta}}{dt} = [F_{11}(x)]^T \Gamma (x_1 - \hat{x}_1)$$

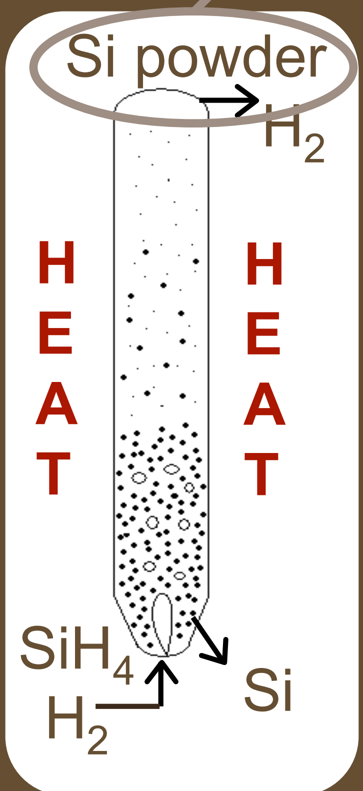
correction terms

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?



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

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

unknown parameter

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

Estimation equations:

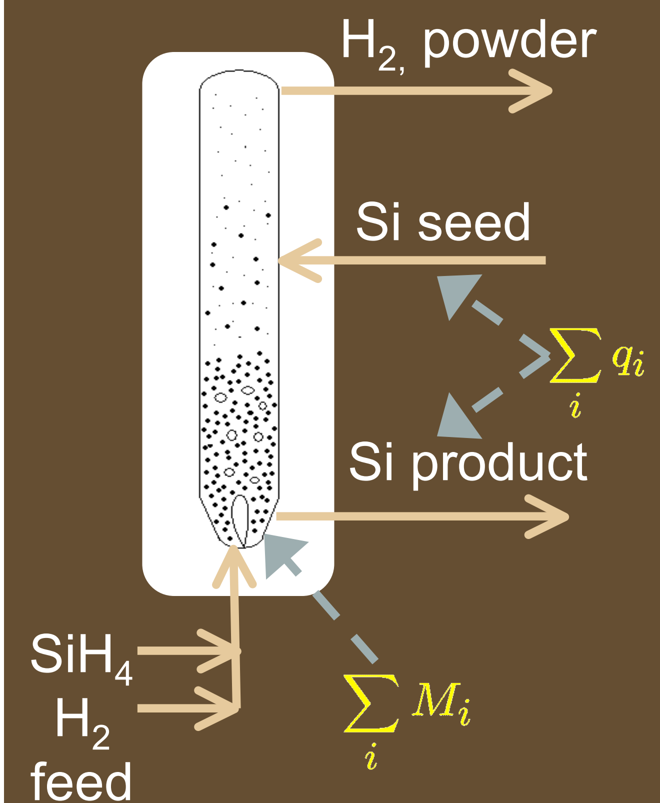
$$\frac{d\widehat{M}}{dt} = \sum_i r_i + q^{IN} - q^{OUT} - C_1(M - \widehat{M})$$

total mass (M) measured

$$\frac{d\widehat{k_{sc}}}{dt} = \frac{1}{C_p \sum_i A_i} C_2 (M - \widehat{M})$$

$$C_1, C_2 > 0 \text{ and } \frac{1}{C_p \sum_i A_i} \neq 0 \;\Rightarrow\; \text{stability}$$

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:

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

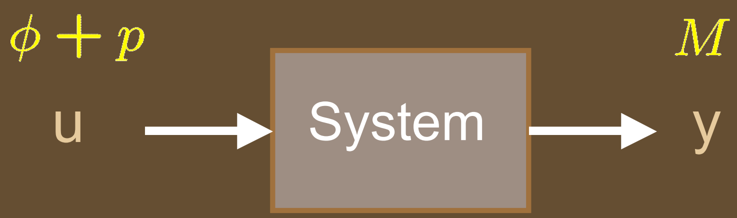
$$\Rightarrow \sum_i q_i = -\sum_i g_i - K\left(\sum_i M_i - M^*\right)$$

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

$$\frac{dM}{dt} = \phi + p$$



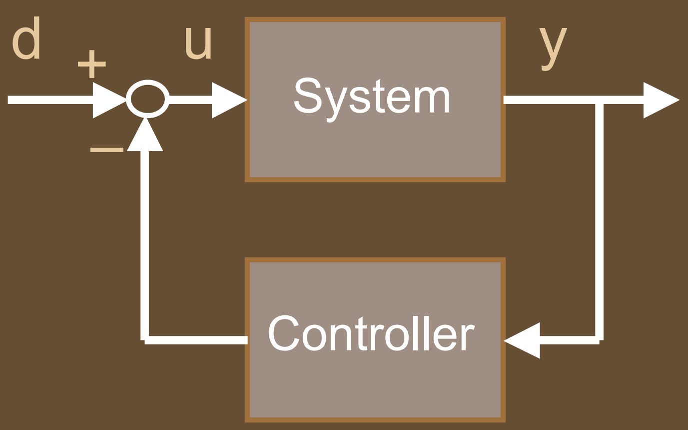
Given storage function V:

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

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 β_0:

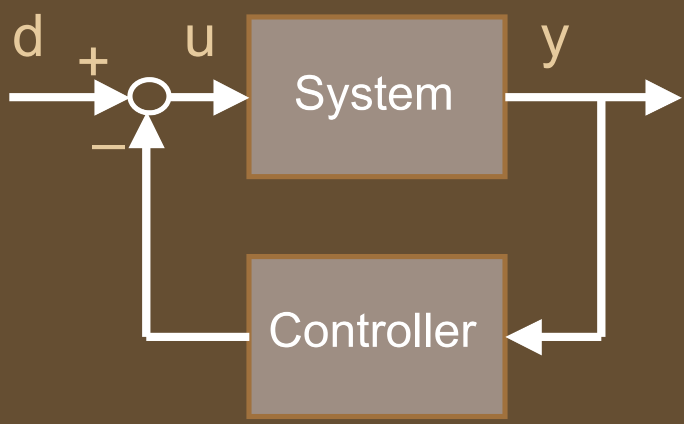


Passive with $\mathcal{L}_2$ gain $=1/\beta_0$

i.e.

$$\int_0^\infty y^2 \leq \frac{1}{\beta_0} \int_0^\infty d^2$$

Input strictly passive controllers



Proportional $u = Ke$

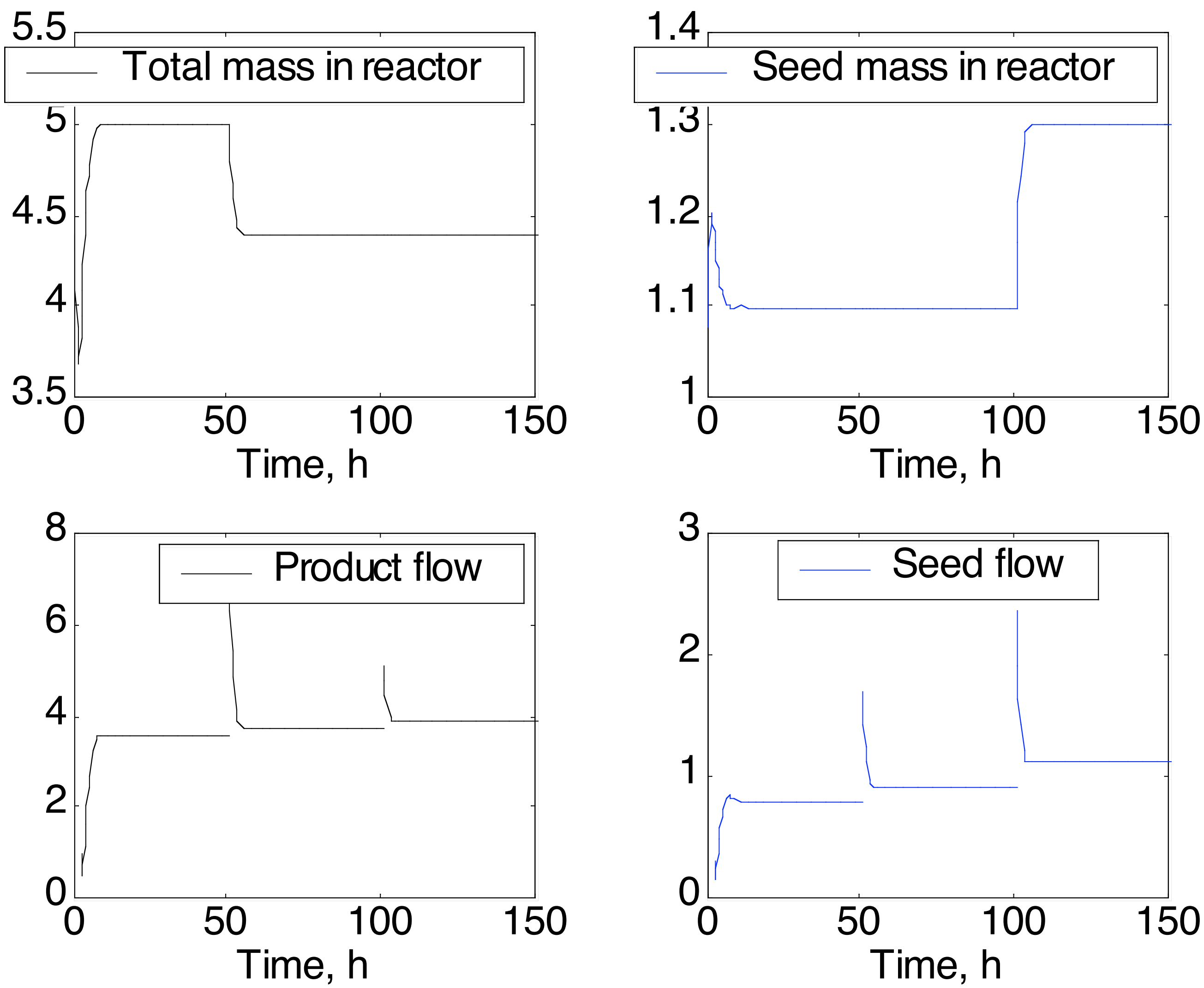
PID $u = K\left(e + \frac{1}{\tau_I}\int_0^\infty e + \frac{de}{dt}\right)$

Adaptive $u = Ke + \phi^T\hat{\theta},\ \dot{\hat{\theta}} = -\mu\phi e$

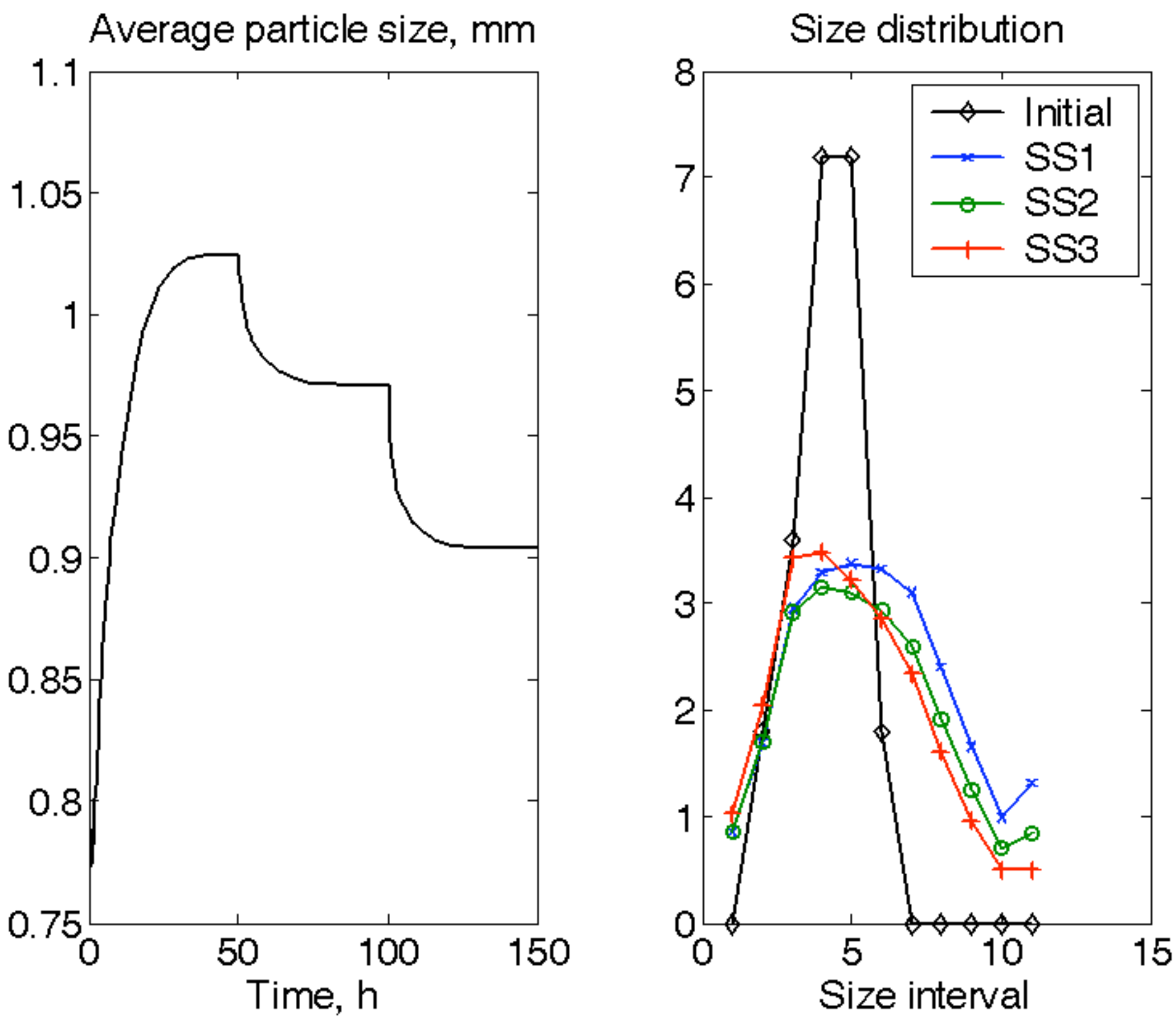
Observer-based estimator: $(M - \hat{M})$
prediction error and persistent excitation → parameter convergence
estimation stability → closed loop stability

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

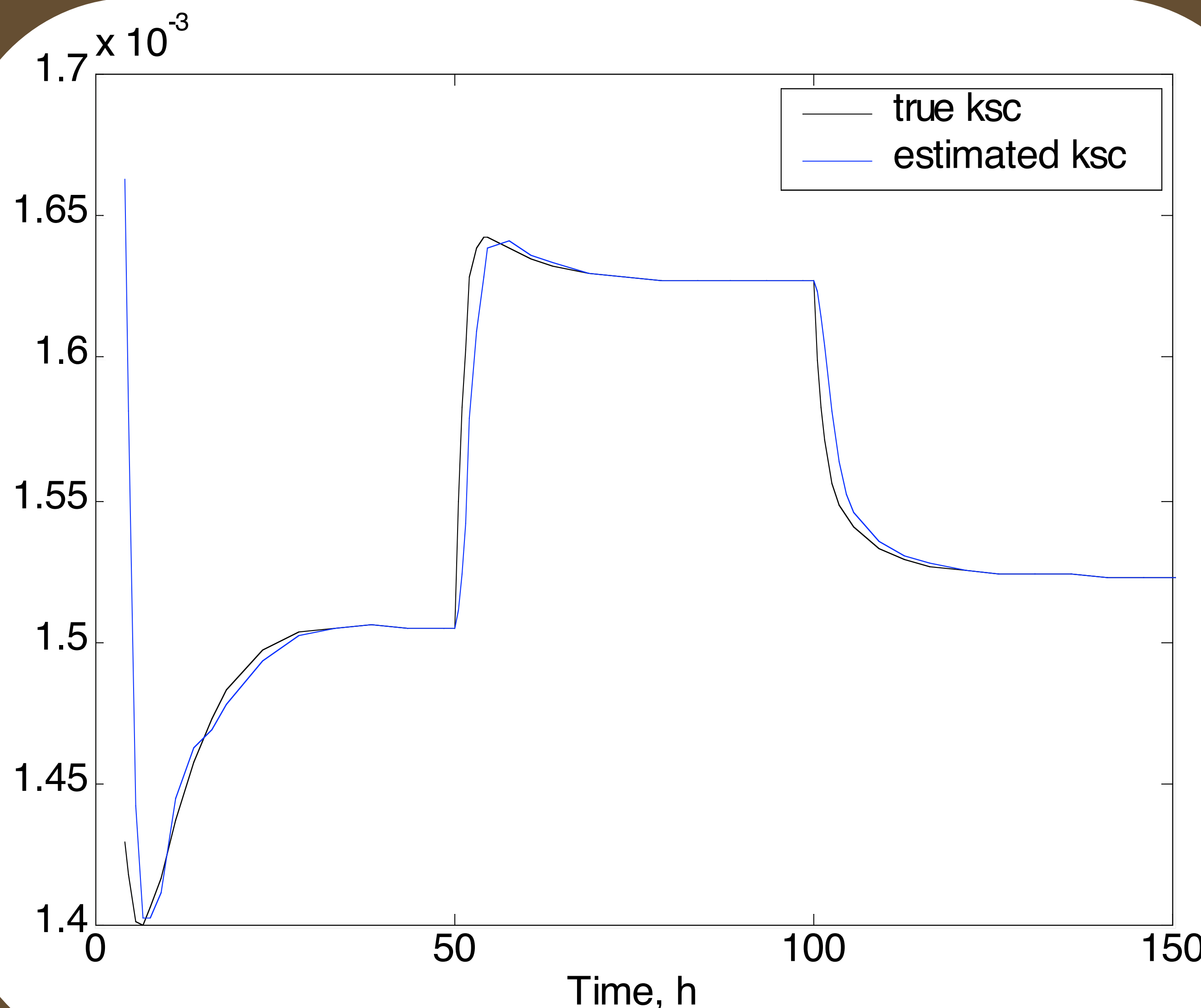
Control of fluidized bed reactor



Particle size achieved under control



Parameter estimation



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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