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Inventory control of particulate processes

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Abstract

In this work we address the problem of designing model-based controllers for particulate processes described by population balance (PB) models. We focus on PB models that are solved by numerical discretization, for which many standard control methodologies are not suitable due to the high order of these models. We interpret discretized PB models as chemical reaction networks and suggest to combine inventory control with techniques of stability of chemical reaction networks to design the controller. Inventory control is based on the idea of manipulating process flows so that certain extensive variables defining the system, called inventories, follow their setpoints. The whole system is stabilized by controlling the dominant inventories. The discretized PB is exploited in all aspects of controller design, from determining the controlled inventories to the final implementation of the control law. The methodology is illustrated with an industrial leaching reactor, the *Silgrain*® process. We show that the discretized PB model takes the form of a Feinberg–Horn–Jackson zero-deficiency network, allowing us to prove stabilization of the whole system. The performance of standard inventory control and robust inventory control are investigated by simulation, with satisfactory results even in the presence of modeling errors.

Keywords: Particulate processes; Population balance; Numerical discretization; Nonlinear control; Multivariable control

1. Introduction

Particulate processes, i.e. processes involving a set of entities that differ from each other in the values of certain distributed properties, are encountered in almost any branch of the process industries (such as in the petrochemical, pharmaceutical, and metallurgical branches). Although the term "particulate processes" comprises unit operations that are different in their nature such as crystallization, emulsification, leaching, etc…, there are certain basic mechanisms that are shared by all particulate processes. Hence, a unified approach to build mechanistic models of particulate processes has been possible: the so-called population balance (PB) approach. The main ideas behind the PB can be traced back to Fisher's work in statistics, and to the work by Flory in polymer growth modeling (Flory, 1953). However, in its modern and unified form, the PB equation was developed in the 1960s by two groups of researchers studying crystal nucleation and growth (Hulburt & Katz, 1964; Randolph, 1964). Since then, extensive research has been carried out on PB modeling of particulate processes. There are conferences and journal issues exclusively dedicated to particulate processes and to the PB. Moreover, detailed models for a considerable number of particulate processes are available in the literature, see for example the review article by Ramkrishna (1985), and the book by the same author (Ramkrishna, 2000).

Despite the rapid and remarkable advances in modeling, numerical solution, and simulation of PB, the field of automatic control of particulate processes has not developed as much as could be expected. Examples of advanced control strategies implemented in real industrial settings are scarce. Some of the reasons that explain the lack of advanced controllers for particulate processes are: the nonlinear and multivariable

Abbreviations: CV, controlled variable; DAE, differential and algebraic equations; HR, first leaching reactor (from '*hovedreaktor*' = main reactor); MPC, model predictive control; MV, manipulated variable; ODE, ordinary differential equations; PB, population balance equation; PSD, particle size distribution; SP, setpoint; UR, second leaching reactor (from '*utlutningsreaktor*' = leaching reactor)

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Nomenclature

a	particle *breakage frequency* function
A	stoichiometric matrix
b	birth probability distribution function
B	birth rate
c_p	heat capacity
C	mole concentration
$\mathbf{C}$	controller operator
C_D	discharge coefficient
d	modelled disturbance
D	death rate
D_cut	cut size
D_p	particle diameter
e	error
E	activation energy (kinetic rate)
g	acceleration of gravity
H	specific enthalpy
k	preexponential factor (kinetic rate)
l	linkage classes
m	manipulated variable
m_j	jth moment
M	mass
$\dot{M}$	mass flow rate
M_w	molecular weight
n_c	set of complexes
n_s	set of chemical species
$\dot{N}$	molar flow rate
p	production term (balance law)
P	pressure
q	volumetric flow rate
Q	heat loss
r	reaction rate
s	rank of reaction network
S	switching surface
t	time
T	temperature
u_sup	superficial velocity
U	internal energy
v	inventory
$V_{(x)}$	storage function
V	volume
w	component weight fraction
W	component mass
W_t	matrix of weighting factors
$\dot{W}$	component mass flow rate
x	controlled inventories
y	uncontrolled inventories
z	intensive variables

Greek symbols

α	measure of conversion
β	fraction of reaction via HCl
γ	reaction order (kinetic rate)
$\boldsymbol{\delta}$	delta dirac function
δ	deficiency of reaction network
Δ	lumped uncertainty
ΔH_r	reaction enthalpy
ε	void bed fraction
ζ	*internal* coordinate in the PB
ζ	size of *mother* particle (disintegration)
ρ	density
Σ	surface to volume ratio
ϕ	transport term (balance law)
Φ	discrete density distribution function
$\dot{\Phi}$	discrete density distribution function flow
ψ	*intensive* population density distribution
Ψ	*extensive* population density distribution
$\dot{\Psi}$	population density distribution *flow*

Subscripts

acid	relative to the acid and/or acid compound
feed	relative to the inlet of the HR
in	relative to the inlet flow of a compartment
Me	metallic component, i.e. Fe, Al, and Ca
RI	relative to the disintegration region of the HR
RII	relative to the storage region of the HR
RIII	relative to the sedimentation region of the UR
RIV	relative to the dissolution region of the UR
out	relative to the outflow from the reactor
overflow	relative to the overflow of the UR
sediment	relative to the sedimentation flow in the UR
solid	relative to the particulate phase
surroundings	relative to the surroundings
tapping	relative to a tapping flow

input-output behavior of such processes, the distributed nature of the PB models (i.e. infinite number of internal states), limited instrumentation (it remains difficult to measure the distribution of properties), insufficient degrees of freedom or manipulated variables, and batch or semibatch operation. Nonlinear and multivariable control approaches would thus be desirable for many particulate processes, but they are also harder to implement than linear single-input single-output approaches.

Some review papers on the status of certain branches of particulate processes include sections on the status of automatic control, such as the papers by Rawlings et al. (1993) and Braatz (2002) dealing with crystallization; the papers by Wang and Cameron (2002) and Cameron, Wang, Immanuel, and Stepanek (2005) dealing with granulation. As regards theoretical control-related issues, one of the first references is the controllability analysis suggested in Semino and Ray (1995a, 1995b).

The most extensive work on design of nonlinear controllers for particulate processes is probably a series of papers coauthored by Christofides and a book by the same author (Christofides, 2002). Their approach, nonlinear output feedback control, was tested on a crystallization process (Chiu & Christofides, 1999, 2000), and an aerosol flow reactor (Chiu & Christofides, 2000). The effect of input constraints was discussed