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Bifurcation control of high-dimensional nonlinear chemical processes using an extended washout-filter algorithm

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ABSTRACT

This paper presents a design framework to modify the bifurcation characteristics and stability of high-dimensional, nonlinear, chemical processes within specified operating regions. Portions of solution branches are stabilized and oscillatory process dynamics in the vicinity of Hopf bifurcation points (HBPs) are attenuated. A new optimization algorithm is introduced to circumvent the limitations of traditional washout filters for feedback control. This controller is used to operate a high-dimensional, nitroxide-mediated, radical polymerization (NMRP) in a continuous-stirred-tank reactor (CSTR). The algorithm adjusts the eigenvalues of the model Jacobian matrix to relocate the HBPs. It is shown to permit flexible modifications of the bifurcation characteristics, providing acceptable performance for set-point tracking and disturbance rejection, and stabilizing solution branches in specified regions.

1. Introduction

In nonlinear chemical systems, interesting and troublesome nonlinear dynamics arise routinely in the vicinity of Hopf bifurcation points (HBPs), which are often associated with exothermic processes (Ray and Villa, 2000), diffusion limitations such as gel effects in polymerization reactors (Schmidt and Ray, 1981), or substrate inhibition in bioreactors (Lee et al., 1979, 1980). These nonlinear dynamics include, but are not limited to, undesirable process oscillations associated with HBPs. Ray and co-workers addressed interesting dynamic behaviors and oscillations both theoretically and experimentally in research studies involving the polymerization of ethylene, methylmethacrylate, vinyl acetate, and styrene in CSTRs (Hamer et al., 1981; Ray and Villa, 2000; Pinto, 1995; Schmidt et al., 1984; Schmidt and Ray, 1981; Teymour and Ray, 1989, 1992a, 1992b). Most of the nonlinear structures produce unstable oscillations with stable operations confined to narrow regions (Pinto, 1995).

In fact, these oscillations occasionally occur under traditional static-state feedback and/or adaptive controls. Even worse, local instability and complex dynamical behavior sometimes result from controlled systems (Chen et al., 2000) due to process-model mismatch and undesirable locations of HBPs. In these situations, one or more poles of the closed-loop transfer function move across the stability boundary, leading to unstable operation and even oscillations (Hassouneh et al., 2004).

The development of methods for modifying the bifurcation characteristics of nonlinear chemical processes has been challenging (Ji, 2001; Verduzco and Alvarez, 2006). These methods gain importance when the stability margin (distance from the HBP) is small. Thus far, bifurcation controls have been implemented in experimental systems or tested by numerical simulations for engineering systems (Brandt and Chen, 1997; Chen and Yu, 2005; Wang et al., 2007; Yu and Chen, 2004). In chemical engineering, Chang and Chen (1984) extended linear control theories and utilized conventional PID controllers to stabilize set-points in substrate-inhibition bioreactors (CSTRs), modeled with two ordinary differential equations. However, state feedback and/or adaptive controls often move operating points on steady-state branches, even altering the shapes of these branches. These can counter control efforts to achieve improved equilibrium structures (Levine, 2011) and preferable operating points.

As the theoretical basis of nonlinear analysis, the normal form has been expressed to analyze and modify bifurcations. Recently, Krener and Kang developed an approach to implement bifurcation control for systems having a single uncontrollable mode using normal forms and invariants (Kang, 2000; Krener et al., 2004). However, for bifurcation control, the deviations of normal forms from their central manifolds involve at least two vector fields to be simplified simultaneously, as compared with dynamic systems without control (Chen et al., 2000). Besides, both changes of coordinates and state feedbacks are necessary, which makes its current application

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Nomenclature

Greek letters

ΔH_{R}	heat of polymerization reaction
$\Delta F_{\mathrm{in,tl}}$	maximum off-set tolerance of $F_{\mathrm{in,tl}}$
θ	residence time (s)
$\boldsymbol{\Theta}$	the transformation matrix for $\tilde{\boldsymbol{A}}$ and $\hat{\boldsymbol{A}}$
λ_i	the $k_{deactivation}$ eigenvalue of $\boldsymbol{A}$
λ_p, λ_q	two arbitrary eigenvalues of the coordinates-changed system Jacobian $\hat{\boldsymbol{A}}$
$\boldsymbol{\Lambda}$	$\boldsymbol{V}^{-1}\boldsymbol{A}\boldsymbol{V}$
$\tilde{\boldsymbol{\Lambda}}$	similar matrix of $\tilde{A}$
ρ_{M}	density of the feedsteam ($\mathrm{kg\,L^{-1}}$)
ρ_{c}	density of cooling water ($\mathrm{kg\,L^{-1}}$)

Notations

$\boldsymbol{A}$	the Jacobian of the original system
$\hat{\boldsymbol{A}}$	the Jacobian of the augmented system
$\tilde{\boldsymbol{A}}$	the Jacobian of the coordinates-changed system
$\left(\boldsymbol{A}^T\right)_k$	the kth column of $\boldsymbol{A}^T$
A_{k_d}	pre-exponential factor of deactivation reaction ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
$A_{k_{d,nv}}$	nominal pre-exponential factor for deactivation reaction ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
$A_{\mathrm{k_d}}^{\mathrm{U}}$	upper bound of pre-exponential factor of deactivation reaction ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
$A_{\mathrm{k_d}}^{\mathrm{L}}$	lower bound of pre-exponential factor of deactivation reaction ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
A_{h}	heat transfer area ($\mathrm{m^2}$)
$\boldsymbol{B}$	input matrix
$\hat{\boldsymbol{B}}$	$\hat{\boldsymbol{B}} \in \mathbb{R}^{n\times n}$ and has $\boldsymbol{Bw}$ in the kth column
b_k	the kth element of $\boldsymbol{Bw}$
$\boldsymbol{C}_{\mathrm{pen}}$	penalty factor
$C_{\mathrm{p,M}}$	heat capacity of feedstream ($\mathrm{J\,kg^{-1}\,K^{-1}}$)
$C_{\mathrm{p,c}}$	heat capacity of cooling water ($\mathrm{J\,kg^{-1}\,K^{-1}}$)
D_{pert}	diameter of eigenvalue perturbation
d	reciprocal of the filter time constant
D	dimer
$D^{\bullet}$	dimer radical
$F_{\mathrm{c,in}}$	cooling water flow rate (L/s)
F_{in}	feed stream flow rate (L/s)
$\boldsymbol{F}$	ODEs for state variables $\boldsymbol{x}, \dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}, \boldsymbol{u}), \boldsymbol{F}: \mathbb{R}^n \times \mathbb{R}^l \to \mathbb{R}^n$
k_i	rate constant for thermal initiation ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{dim}	rate constant for Mayo dimerization ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_p	rate constant for propagation ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{td}	rate constant for termination by disproportionation ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{tc}	rate constant for termination by combination ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{trm}	rate constant for monomer transfer ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{trd}	rate constant for dimer transfer ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{h_3}	rate constant for rate enhancement ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{decomp}	rate constant for alkoxyamine decomposition (L/s)
k_a	rate constant for activation of dormant species (L/s)
k_d	rate constant for deactivation of dormant species ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
k_{a2}	rate constant for activation of the NO_E species (L/s)
k_{d2}	rate constant for deactivation of the NO_E species ($\mathrm{L\,mol^{-1}\,s^{-1}}$)
$\mathrm{M_{ON_x}}$	monomeric alkoxyamine
$\mathrm{NO_E}$	nitroxyl ether
$\mathrm{NO}_x^{\bullet}$	stable nitroxyl radical
$\mathrm{P}_r^{\bullet}$ and $\mathrm{P}_n^{\bullet}$	propagating living radical with r and n monomer units
$\mathrm{P}_r\mathrm{ON}_x$ and $\mathrm{P}_n\mathrm{ON}_x$	dead polymer with r and n monomer units
$\mathrm{R}^{\bullet}$	primary radical
t	time (s)
T	reactor temperature (K)
T_0	feed stream temperature (K)
$T_{0,nom}$	nominal feed stream temperature (K)
T_{c}	cooling water temperature (K)
$T_{\mathrm{c,0}}$	cooling jacket feed temperature (K)
$\boldsymbol{u}$	input vector
$\boldsymbol{v}$	reference input vector
$\boldsymbol{V}$	the similarity transformation matrix of $\boldsymbol{A}$
$\tilde{\boldsymbol{V}}$	the similarity transformation matrix of $\tilde{\boldsymbol{A}}$
V	reactor volume (L)
V_{c}	cooling jacket volume (L)
$\boldsymbol{w}$	controller parameter
$\boldsymbol{x}$	state variables, $\boldsymbol{x} \in \mathbb{R}^n$
$\dot{\boldsymbol{x}}$	$\boldsymbol{x}$ differentiated by time
y	output of the washout filter
$\mathrm{Y_0}$	0th moment of the living-radical distribution
$\mathrm{Y_1}$	1st moment of the living-radical distribution
$\mathrm{Y_2}$	2nd moment of the living-radical distribution
$\mathrm{Z_0}$	0th moment of the dormant species distribution
$\mathrm{Z_1}$	1st moment of the dormant species distribution
$\mathrm{Z_2}$	2nd moment of the dormant species distribution
$\mathrm{Q_0}$	0th moment of the dead-polymer distribution
$\mathrm{Q_1}$	1st moment of the dead-polymer distribution
$\mathrm{Q_2}$	2nd moment of the dead-polymer distribution

Acronyms

h.o.t	higher-order terms
MWD	molecular-weight distribution
NMRP	nitroxide-mediated radical polymerization
ODEs	ordinary differential equations
PDI	polydispersity index

limited only for theoretic systems, such as Van der Pol oscillators, the three-dimensional Rössler system, and the Lorenz system.

Abed and co-workers (Abed et al., 1992; Abed, 1988a, 1988b; Abed and Fu, 1986, 1987; Lee and Abed, 1991; Wang and Abed, 1995) were among the first to analyze bifurcation control using washout-filter-aided dynamic controllers where the desired operating points are uncertain (Hassouneh et al., 2004). Although washout filters were used successfully in many control applications, no systematic ways of choosing their constants and control parameters existed. To overcome this, Mönnigmann and Marquardt (2002) introduced an approach to calculate directly the controller parameters of a washout filter, introducing a HBP for a polymerization process having a single uncontrollable mode (process Jacobian matrix having only one eigenvalue with a positive real part). Their approach required that the input matrix be invertible, with the number of manipulated inputs equal to the number of state variables – significantly limiting its practical application. Subsequently, they stabilized a multi-input, parameterized nonlinear system (Laiou et al., 2004) by introducing a Hopf bifurcation using washout-filter-aided controllers – allowing the replacement of a pair of unstable complex conjugate eigenvalues. But, to replace both single- and dual-unstable eigenvalues, four conditions (C1 to C4) must be satisfied to insure nontrivial solutions of the $\boldsymbol{w}$ vector of the washout-filter-aided controller (defined in Eq. (8)). To illustrate their approach, an exothermic, irreversible reaction, A → B, which satisfies their four conditions, is used.