Chemical Engineering Science 106 (2014) 109–118

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Robust optimization of periodically operated nonlinear uncertain processes

Darya Kastsian, Martin Mönnigmann *

Automatic Control and Systems Theory, Ruhr-Universität Bochum, 44801 Bochum, Germany

AUTHOR-HIGHLIGHTS

- Optimizing autonomously oscillating systems with uncertain parameters.
- Robust stability guarantees for optimal modes of process operation.
- Addressing stability constraints as a system of nonlinear equations.
- Illustration of the method with robust optimization of chemical reaction systems.

ARTICLE INFO

Article history:
Received 5 February 2013
Received in revised form
8 October 2013
Accepted 8 November 2013
Available online 21 November 2013

Keywords:
Optimization
Stability
Nonlinear dynamics
Chemical reactors
Parametric uncertainty
Bifurcation analysis

ABSTRACT

We present a method for determining optimal modes of operation for autonomously oscillating systems with uncertain parameters. In a typical application of the method, a nonlinear dynamical system is optimized with respect to an economic objective function with nonlinear programming methods, and stability is guaranteed for all points in a robustness region around the optimal point. The stability constraints are implemented by imposing a lower bound on the distance between the optimal point and all stability boundaries in its vicinity, where stability boundaries are described with notions from bifurcation theory. We derive the required constraints for a general class of periodically operated processes and show how these bounds can be integrated into standard nonlinear programming methods. We present results of the optimization of two chemical reaction systems for illustration.

1. Introduction

The impact of autonomous oscillations and periodic forcing on economic process performance has been investigated for decades. For example, Douglas and Rippin (1966) demonstrate that the performance of an isothermal continuous stirred-tank reactor (CSTR) may be improved by periodic forcing of the feed. The authors also consider a first order irreversible exothermic reaction in a non-isothermal CSTR. For this case, they show that autonomous oscillations may lead to increased average product concentration compared to steady state operation. Similar investigations have been carried out later by other authors. Jianquiang and Ray (2000) use autonomous oscillations to improve the performance of a bioreactor used for sludge water treatment. Stowers et al. (2009) show that oscillations can increase the product yield in yeast fermentation. Parulekar (2003) demonstrated that the performance of series–parallel reactions can be improved by forced periodic operation. The authors also discuss the benefit of forced periodic operation compared to steady state operation in recombinant cell culture processes. Abashar and Elnashaie (2010) show that periodically forced fermentors provide higher average bioethanol concentrations than fermentors operated in a steady state.

Whenever models of the production process of interest and their economics are available, optimization methods can be used to find an optimal mode of operation. It is known, however, that optimizing a dynamical system may result in a mode of operation that is optimal but unstable (Mönnigmann and Marquardt, 2002; Kastsian and Mönnigmann, 2012). While an unstable mode could be stabilized by feedback control, often stable solutions are preferred due to the additional effort required for controlling unstable states.

We summarize existing methods for the optimization of periodic processes that are able to cope with stability constraints. Mombaur et al. (2005a,b) and Mombaur (2009) consider the optimization of periodic motions with guaranteed stability by solving two-level optimization problems. They optimize the economic objective

* Corresponding author. Tel.: +49 234 3224060; fax: +49 234 3214155.
E-mail addresses: darya.kastsian@rub.de (D. Kastsian), martin.moennigmann@rub.de (M. Mönnigmann).

0009-2509/$ - see front matter
http://dx.doi.org/10.1016/j.ces.2013.11.023

function and minimize the spectral radius at the first and second levels, respectively. The authors guarantee the resulting periodic orbits to be stable by minimizing the spectral radius and forcing all eigenvalues to have moduli strictly smaller than one. Parametric uncertainties in the underlying process models are not considered.

Burke et al. (2003) suggest minimizing the pseudo-spectral radius to guarantee robust stability. The pseudo-spectral radius measures the largest modulus of the eigenvalues of matrices which vary in an ε-neighborhood of the reference matrix. The ε-neighborhood is defined with the standard Euclidean norm. For linear systems it is equivalent to the H_∞ norm (Burke et al., 2003) or linear matrix inequalities (LMI) conditions (Gahinet and Apkarian, 1994). Since the pseudo-spectral radius typically is a nonsmooth function of the corresponding Jacobian entries, Vanbiervliet et al. (2009) and Diehl et al. (2009) proposed to use the smoothed spectral radius. The smoothed spectral radius is based on the H_2-norm and computed by solving relaxed Lyapunov equations.

Chang and Sahinidis (2011) consider parametric uncertainty for optimal steady state solutions and possible extension of the proposed method to oscillating processes. The authors solve semi-infinite programs, where stability constraints are addressed with Hurwitz's criterion. Stability constraints are stated for every point of an uncertainty region. An infinite number of stability constraints are implemented as several relaxation problems that are solved iteratively.

We present an alternative approach for stating constraints for local asymptotic stability while optimizing autonomously oscillating systems with parametric uncertainties. In contrast to Chang and Sahinidis (2011), we ensure stability and robustness by a finite number of nonlinear constraints. Our approach belongs to the class of normal vector methods (Mönnigmann and Marquardt, 2002), which are based on nonlinear programming and applied bifurcation theory. Originally, the normal vector approach was developed to guarantee stability of optimal steady states of ordinary differential equations (ODE) and differential-algebraic (DAE) systems (Mönnigmann and Marquardt, 2002; Mönnigmann et al., 2007). It has been applied to a number of examples from chemical engineering (Mönnigmann and Marquardt, 2003, 2005). Gerhard et al. (2008) and Muñoz et al. (2012) extend the method for robust disturbance rejection and the simultaneous consideration of steady state stability and disturbance rejection, respectively. Kastsian and Mönnigmann (2010) cover the case of fixed points of discrete time systems. In the present paper, we extend the normal vector approach to stability constraints for periodic solutions of ODE systems. Similar but preliminary results are reported in Kastsian and Mönnigmann (2012).

The paper is organized as follows. We begin with a formal problem statement in Section 2 and outline the normal vector method in Section 3. In Section 4 the characterization of the stability boundaries, or more generally critical boundaries, is introduced. The normal vectors to these critical boundaries and the nonlinear programs based on them are discussed in Section 5. The proposed method is illustrated in Section 6. A conclusion is stated in Section 7.

2. System class and optimization problems of interest

We consider dynamic systems described by a set of nonlinear parameterized ordinary differential equations

$$\dot{x}(t) = f(x(t), \alpha), \quad x(0) = x_0, \tag{1}$$

where $x(t) \in \mathbb{R}^{n_x}$ and $\alpha \in \mathbb{R}^{n_\alpha}$ denote state variables and parameters, respectively. The function f maps from some open subset of $\mathbb{R}^{n_x} \times \mathbb{R}^{n_\alpha}$ onto $\mathbb{R}^{n_x}$ and is assumed to be smooth with respect to all variables and parameters.

Let $\varphi(x_0, t, \alpha)$ denote the solution of (1) at time t for the initial condition $x(0) = x_0$. Assume that this solution is a periodic orbit with period T. It therefore satisfies

$$\varphi(x_0, T, \alpha) - x_0 = 0. \tag{2}$$

Without giving details we note that a phase condition is required to identify a periodic orbit uniquely. Essentially, the phase condition is necessary, because the same periodic orbit results if the initial condition is shifted along the orbit. Technically, the phase condition is of the form

$$s(x_0, T, \alpha) = 0, \tag{3}$$

where s maps from a subset of $\mathbb{R}^{n_x} \times \mathbb{R}^{+} \times \mathbb{R}^{n_\alpha}$ onto $\mathbb{R}$ (see, e.g., Kuznetsov, 1998 for details).

The stability of the periodic orbit φ can be investigated with the Jacobian matrix

$$M = \varphi_{x_0}(x_0, T, \alpha). \tag{4}$$

Since this Jacobian is often referred to as the monodromy matrix, we denote it by M for short. We briefly recall that the monodromy matrix has at least one eigenvalue equal to one, and its remaining $n_x - 1$ eigenvalues determine the stability of the periodic orbit. More precisely, let these eigenvalues be denoted by $\lambda_1, \ldots, \lambda_{n_x-1}$. The periodic orbit is locally asymptotically stable, if $|\lambda_i| < 1$ for all $i = 1, \ldots, n_x - 1$ (see, e.g. Kuznetsov, 1998 for details).

The stability of a steady state can be characterized in a similar fashion with the Jacobian f_x. A steady state (x, α) is locally asymptotically stable, if the real parts of all eigenvalues of the Jacobian $f_x(x, \alpha)$ are strictly negative.

We assume that parameters α_i in the model (1) are uncertain and lie in the intervals

$$\alpha_i \in [\alpha_i^{(0)} - \Delta\alpha_i, \alpha_i^{(0)} + \Delta\alpha_i], \quad i = 1, \ldots, n_\alpha, \tag{5}$$

where $\alpha_i^{(0)}$ are the central values of the independent uncertainty intervals and $\Delta\alpha_i$ represent the uncertainties. We are interested in finding steady states or periodic solutions that are optimal with respect to a real valued objective function ϕ, which may represent product concentration, productivity, or economic profit, for example. We seek optimal solutions that are robust in the sense that they are stable for any parameter α in the uncertainty region (5). More precisely, we call a stable periodic orbit or a stable steady state *robust* if

$$S^{(P)}(x_0, T, \alpha) := \begin{cases} 0 = \varphi(x_0, T, \alpha) - x_0, \\ 0 = s(x_0, T, \alpha), \\ |\lambda| \le 1 \quad \forall \lambda \in \sigma(\varphi_{x_0}(x_0, T, \alpha)) \end{cases} \tag{6}$$

respectively

$$S^{(S)}(x, \alpha) := \begin{cases} 0 = f(x, \alpha), \\ \mathrm{Re}(\lambda) \le 0 \quad \forall \lambda \in \sigma(f_x(x, \alpha)) \end{cases} \tag{7}$$

for all $\alpha \in [\alpha^{(0)} - \Delta\alpha, \alpha^{(0)} + \Delta\alpha]$ and in a neighborhood of x_0. In (6) and (7) the symbol $\sigma(\cdot)$ denotes the spectrum of a matrix. The optimization problem of interest for periodic orbits reads

$$\max_{x_0^{(0)}, T^{(0)}, \alpha^{(0)}} \quad \phi(x_0^{(0)}, T^{(0)}, \alpha^{(0)})$$

$$\text{s.t.} \quad 0 = \varphi(x_0^{(0)}, T^{(0)}, \alpha^{(0)}) - x_0^{(0)}, \tag{8a}$$

$$0 = s(x_0^{(0)}, T^{(0)}, \alpha^{(0)}), \tag{8b}$$

$$0 \le h(x_0^{(0)}, T^{(0)}, \alpha^{(0)}), \tag{8c}$$

$$S^{(P)}(x, T, \alpha) \quad \text{or} \quad S^{(S)}(x, \alpha) \qquad \forall \alpha \in [\alpha^{(0)} - \Delta\alpha, \alpha^{(0)} + \Delta\alpha]. \tag{8d}$$