# CONTROL-RELEVANT CHARACTERIZATION OF NONLINEAR CLASSES OF PROCESS SYSTEMS

Nicholas Hernjak<sup>\*</sup> Francis J. Doyle III<sup>\*,1</sup> Ronald K. Pearson<sup>\*\*</sup>

\* Department of Chemical Engineering, University of Delaware, Newark, DE \*\* TICSP, Tampere University of Technology, Tampere, Finland

Abstract: In this work, a nonlinearity measure is used to examine the relative severity of various classes of inherently nonlinear behavior. Using the Optimal Control Structure, the analysis includes a study of how the classes and their properties affect systems' control-relevant nonlinearity. Two chemical reactor systems that demonstrate a wide range of nonlinear behaviors are examined. The results indicate that the nonlinearity measure is able to distinguish between the different categories of nonlinear behavior. The control-relevant analysis indicates that the open-loop behavior may or may not necessarily transfer to the control-relevant setting.

Keywords: Nonlinear control systems, Nonlinear models, Optimal control, Reactor control, Fourier analysis

#### 1. INTRODUCTION

Nonlinear systems are able to display a wide range of substantially different behaviors. General categories of these nonlinear behaviors have been developed along with a qualitative understanding of their relative severity (Pearson, 1999).

A significant amount of effort has been expended of late into developing numerical measures for the degree of nonlinearity of a system. One of the early references to a nonlinearity measure is found in (Desoer and Wang, 1980). The first set of practical, on-line characterization techniques were reported in (Haber, 1985). Since then, several other measures of nonlinearity have been proposed in (Ogunnaike *et al.*, 1993), (Guay, 1996), (Nikolaou and Hanagandi, 1998), and (Allgöwer, 1995), the last of which is employed in the current work. This work was focused on establishing links between the output of the nonlinearity measure and the classification of the types of nonlinearity that the systems exhibit.

With the purpose of controller design for a system, it is the *control-relevant* nonlinearity that needs to be characterized. It is the severity of this effect that dictates the need for nonlinear control in order to obtain optimal closed-loop performance. In (Stack and Doyle III, 1997), the problem is addressed using the Optimal Control Structure (OCS). The OCS is a system that provides the dynamics of an optimal controller for a particular open-loop system model and performance objective. In the current work, the nonlinearity of the OCS is analyzed in the same means as an open-loop plant and comparisons between the open-loop nonlinearity (character and severity) and control-relevant nonlinearity made.

# 2. CATEGORIES OF NONLINEAR BEHAVIOR

Many of the commonly-observed nonlinear behaviors of general dynamic systems can be classified using six categories (Pearson, 1999):

 $<sup>^1</sup>$  Author to whom correspondence should be addressed. E-mail: fdoyle@udel.edu

- (1) Harmonic generation
- (2) Subharmonic generation
- (3) Chaos
- (4) Input-dependent stability
- (5) Asymmetric response
- (6) Steady-state multiplicity(a) Input multiplicity
  - (b) Output multiplicity

Harmonic generation refers to the ability of a nonlinear system to generate harmonics of higher frequency than that of a single-frequency input. Conversely, subharmonic generation refers to the ability of a nonlinear system to generate harmonics of frequency lower than that of the input. Chaos describes a nonperiodic response to a periodic input.

A system displaying input-dependent stability may display both stable and unstable responses depending on the magnitude or character of the system input. This term can also refer to a change in the nature of a *stable* response. For example, certain inputs may result in asymptotically stable responses while others result in responses that are only stable in a bounded sense. Similarly, asymmetric response refers to a process responding differently to symmetric positive and negative inputs, but is usually reserved for the description of stable responses.

Steady-state multiplicity behavior can be divided into two sub-categories. Input multiplicity refers to multiple steady-state input values yielding the same steady-state output. Output multiplicity refers to a single input value yielding multiple possible steady-state outputs.

In terms of severity of nonlinearity, note that item 1 is exhibited by almost all nonlinear systems (see (Doyle III et al., 2001) for one of the rare examples of a nonlinear system that does not generate harmonics) and item 5 is exhibited by all nonlinear systems except for certain structures based on nonlinear functions exhibiting odd symmetry. Similarly, item 6a is characteristic of any system that exhibits an optimum steadystate input level and is also quite common among nonlinear systems. Consequently, items 1, 5, and 6a may be viewed as mild forms of nonlinearity. In contrast, items 2, 3, and 6b impose much stronger restrictions on the structure of the nonlinear system; for example, it is a standard result that continuous-time models must have at least a three-dimensional state space if they are to exhibit chaotic responses to simple inputs (Guckenheimer and Holmes, 1983). Similarly, it can be shown that discrete-time dynamic models exhibiting any one of these three forms of behavior must include nonlinear feedback terms (Pearson, 1999). Consequently, these phenomena may be regarded as strongly nonlinear behavior. Item 4 represents an intermediate form of behavior because, although it is not possible in systems exhibiting feedforward block-oriented structures or, more generally, fading memory behavior (Boyd and Chua, 1985), it is possible in important model classes like bilinear models (Svoronos *et al.*, 1981) which cannot exhibit the strongly nonlinear behavior defined by items 2, 3, and 6b.

Note that the OCS concept used in this work can be interpreted as a relaxed inverse of the original system. From inverse system theory, it is known that some of the nonlinear behaviors present in the original system will appear "reversed" in an inverse system. For example, input multiplicity will become output multiplicity in the system inverse.

# 3. NONLINEARITY MEASURE

To perform the numerical nonlinearity characterization in this work, the nonlinearity measure proposed originally in (Allgöwer, 1995) and elaborated upon in (Helbig *et al.*, 2000) was used:

$$\phi_{N}^{\mathcal{U}} = \inf_{G \in \mathcal{G}} \sup_{\mathbf{u} \in \mathcal{U}} \frac{\|G[\mathbf{u}] - N[\mathbf{u}]\|_{P\mathcal{Y}}}{\|N[\mathbf{u}]\|_{P\mathcal{Y}}} \qquad (1)$$

where  $N : \mathcal{U} \mapsto \mathcal{Y}$  is the actual system operator and  $G : \mathcal{U} \mapsto \mathcal{Y}$  is a linear approximation to N.  $\mathcal{U}$ is the space of admissible input signals,  $\mathcal{Y}$  is the space of admissible output signals, and  $\mathcal{G}$  is the space of linear operators.  $\phi_N^{\mathcal{U}}$  is a number between zero and one where a value of zero indicates the existence of a linear approximation to the system whose output matches the output of the original system over the set of inputs being considered. A value of one indicates a highly nonlinear system.

A computationally efficient lower bound (LB) on (1) can be obtained by limiting the space of admissible inputs to sinusoids of varying amplitude and frequency. Provided that the nonlinear system preserves periodicity, the output can be represented by a Fourier series:

$$y_{ss} = A_o + \sum_{k=1}^{\infty} A_k \cdot \sin(k\omega t + \phi_k) \qquad (2)$$

By choosing an appropriate norm for the system, it can be shown that (1) becomes (Helbig *et al.*, 2000):

$$\chi_N^{\mathcal{U}_s} = \sup_{a \in \mathcal{A}, \omega \in \Omega} \sqrt{1 - \frac{A_1^2(\omega, a)}{2A_o^2(\omega, a) + \sum_{k=1}^{\infty} A_k^2(\omega, a)}} \quad (3)$$

where  $\mathcal{A}, \Omega$  are the sets of input signal amplitudes and frequencies being considered. The calculation problem is thus reduced to determining the Fourier series coefficients for a set of periodic response sequences and then calculating the value of  $\chi_N^{\mathcal{U}_s}$ .

## 4. OPTIMAL CONTROL STRUCTURE

The OCS is an operator that describes the dynamics of the optimal controller for a given open-loop system and performance objective. By characterizing the nonlinearity of the OCS, the open-loop system's degree of control-relevant nonlinearity is obtained (Stack and Doyle III, 1997).

Beginning with an open-loop plant model and performance objective:

$$\dot{x} = f\left(x, u\right) \tag{4}$$

$$I[u(t)] = G(x(t_f)) + \int_{0}^{t} F(x, u) dt \qquad (5)$$

the system's Hamiltonian, H, is given as:

$$H = F(x, u) + \lambda^{T} f(x, u)$$
(6)

From the Hamiltonian, the OCS is given as:

$$\frac{\partial H}{\partial u} = 0, \ \frac{\partial H}{\partial x} = -\dot{\lambda}^T \tag{7}$$

The nonlinearity of the OCS can be characterized by simply treating (7) as a separate dynamic system and applying an open-loop nonlinearity measure.

Note that Equations (7) are equal to the necessary conditions for an extremum trajectory obtained when solving an optimal control problem using Lagrangian optimization. Because the intent is to characterize the nonlinearity of the OCS over a broad domain, Equations (7) are used without solving the two-point boundary value problem that typically results.

#### 5. SYSTEM ANALYSIS

### 5.1 Chemical Reactor with Tunable Nonlinearities

The first system considered is a two-phase isothermal continuous stirred tank reactor (CSTR) for the reaction of a liquid feed of pure component A to component B. A relative volatility model is utilized to represent the components' vapor-liquid equilibrium (VLE) relationship:

$$y_A = \frac{x_A}{\alpha + (1 - \alpha) x_A} \tag{8}$$

where  $x_A$  and  $y_A$  are the mole fractions of component A in the liquid and vapor phases, respectively  $(x_A, y_A \in [0, 1])$  and  $\alpha \in [1.5, 100]$  is the relative volatility of component B relative to component A.

Assuming that the fraction of the feed stream that flashes to vapor is constant, the material balance for component A in terms of its liquid-phase mole fraction is given as:

$$\dot{x}_{A} = -50x_{A}^{\gamma} + u\left(1 - (1 - \beta)x_{A} - \beta y_{A}\right)$$
(9)

where  $y_A$  is given by (8).  $\beta \in [0, 1]$  is the fraction of the inlet molar flow rate that exits in the vapor stream and  $\gamma \in [1/4, 3]$  is the reaction order. By varying  $\alpha, \beta$ , and  $\gamma$ , the nature of the system dynamics can be varied corresponding to different physical characteristics of the system. Implicit in this simplified model is an instantaneous energy balance that yields the amount of heat required to be added to or removed from the system to provide the liquid-vapor split set by  $\beta$  while maintaining isothermal conditions.

Across the space of parameter values investigated, the most dominant classes of nonlinear behavior demonstrated by (9) are asymmetric response and harmonic generation. The effects of varying  $\gamma$  on the severity of the system's asymmetric response with  $\beta = 0$  can be viewed by studying the steady-state loci shown in Figure 1. In the neighborhood of an operating point of  $u_{ss} = 50$  there is an apparent increase in the degree of curvature of the locus as  $\gamma$  is increased leading to greater steady-state asymmetry. About a lower operating point, such as  $u_{ss} = 30$ , an inflection point exists in the loci for low  $\gamma$  thus causing greater asymmetry in the responses from that point.



Fig. 1. Steady-state loci for the tunable CSTR as a function of  $\gamma$  for  $\beta=0$ 

Although Figure 1 was obtained at the particular condition of  $\beta = 0$ , note that it represents a typical family of steady-state loci for (9) in that no steady-state multiplicity is evident. The infeasibility of input multiplicity can be easily noted by considering the steady-state form of (9):

$$u_{ss} = \frac{k x_{A,ss}^{\gamma}}{x_{Af} - (1 - \beta) x_{A,ss} - \beta y_{A,ss}} \quad (10)$$

It follows from (10) that any value of  $x_{A,ss}$  defines one and only one value of  $u_{ss}$ , implying that input multiplicity is not possible. While it is not clear whether more than one physically meaningful  $x_{A,ss}$  is possible corresponding to a single value of  $u_{ss}$ , this behavior was not demonstrated in any of the conditions examined in this work.

The nonlinearity measure (3) was applied to the open-loop system with  $\beta = 0$  and various  $\gamma$  values to investigate its sensitivity to the asymmetric responses discussed above. Figure 2 displays the results at an operating point of  $u_{ss} = 30$  and Figure 3 displays the results at an operating point of  $u_{ss} = 50$  using input sinusoid amplitudes  $\leq 15$ . The results indicate a trend of increasing nonlinearity with increasing  $\gamma$  except at  $\gamma = 1/4$  and  $u_{ss} = 30$  where the effect of the inflection point is seen. Note that all of the results indicate very low nonlinearity (less than 0.25 in all cases). This is consistent with the interpretation that an asymmetric response is considered a mild nonlinearity.



Fig. 2. Results of nonlinearity analysis for the tunable CSTR and its OCS with  $\beta = 0$  at an operating point of  $u_{ss} = 30$ 

To imply an easy separation of the product from the reactant under VLE conditions,  $\alpha$  is taken to be 100 in the following (component B 100 times more volatile than component A). The effect of varying  $\beta$  on the value of the nonlinearity measure for several  $\gamma$  values is shown in Figure 4. Note the general trend of increasing nonlinearity with increasing  $\beta$ , with the highest observed value of the nonlinearity measure for the system occurring at the extreme value of  $\beta = 1$ . Physically, the system with  $\beta = 1$  can be thought of as a reaction taking place in an evaporator (no exiting liquid phase). The step responses for this arrangement with  $\gamma = 2$ , shown in Figure 5, indicate that the system is operating near the physical constraint of  $x_A = 1$  leading to highly asymmetric step



Fig. 3. Results of nonlinearity analysis for the tunable CSTR and its OCS with  $\beta = 0$  at an operating point of  $u_{ss} = 50$ 



Fig. 4. Effect of varying  $\beta$  on the tunable CSTR's open-loop nonlinearity at various  $\gamma$ ,  $\alpha = 100$  and  $u_{ss} = 50$ 



Fig. 5. Step responses of the tunable CSTR with  $\alpha = 100, \ \beta = 1, \ \text{and} \ \gamma = 2 \ \text{at} \ u_{ss} = 50$ 

responses thus increasing the value of the measure at these conditions.

The system's OCS is considered next. Note that (9) is of the form  $\dot{x} = f(x) + g(x)u$ . If a standard quadratic performance objective is assumed:

$$I = \frac{1}{2} \int_{0}^{t_f} \left[ (x - x_{ss})^2 + \eta \left( u - u_{ss} \right)^2 \right] dt \quad (11)$$



Fig. 6. Effect of move suppression parameter  $\eta$  on OCS nonlinearity for  $\gamma = 2$ ,  $\alpha = 5$ , and two  $\beta$  values

where  $\eta$  is the move suppression parameter, the OCS can be shown to be of the form:

$$\dot{u} = \frac{1}{\eta}g(x)(x - x_{ss}) + (u - u_{ss})\left[\frac{f(x)}{g(x)}\frac{dg}{dx} - \frac{df}{dx}\right]$$
(12)

To remove the effects of  $\eta$  on the nonlinearity characterization results, the amplitudes chosen for the input sinusoids to the OCS were taken to equal the lesser of the two steady-state openloop output deviations when the reactor input was set to  $u_{ss} \pm 15$ . Given this amplitude space, the trends in OCS nonlinearity as a function of the system parameters qualitatively matched those of the open-loop analysis, but were typically higher. For example, Figures 2 and 3 also indicate the results of the OCS analysis given the conditions of the open-loop analysis.

It was reported in (Stack and Doyle III, 1997) that the proper way to observe the effect of  $\eta$  on the OCS nonlinearity is to select an OCS input region for characterization that drives the OCS output to the constraints on the input to the open-loop system. Figure 6 displays results of this type of analysis at  $u_{ss} = 50$ ,  $\gamma = 2$ ,  $\alpha = 5$  and two values of  $\beta$ . Note that the plateaus at higher  $\eta$  values correspond to conditions where the OCS output could not be forced to either  $\pm 15$  while keeping the input within its constrained values. The results indicate a trend of increasing nonlinearity with increased  $\eta$ . In other words, as the penalty on controller moves is increased, the system's controlrelevant nonlinearity also increases.

The results in Figure 6 can be construed as counter-intuitive as one normally considers the act of increasing move suppression with detuning of a controller. As shown in (Stack and Doyle III, 1999) with examples of internal model control, detuning of a nonlinear controller leads to a decrease in its measured nonlinearity. The effect in this case is attributable to the role of  $\eta$  in the OCS. A linearization of (12) indicates that  $\eta$  affects only the gain on the OCS. As  $\eta$  is increased, the effective controller gain decreases thus mandating a larger OCS input to drive the output to the constraints. A larger input region allows the measure a greater domain to analyze thus increasing the resulting value of the measure.

### 5.2 Nonisothermal CSTR

The second system investigated is a nonisothermal CSTR found in (Seborg and Henson, 1997):

$$\dot{C}_{A} = \frac{q}{V} \left( C_{Af} - C_{A} \right) - k_{0} \exp \left( -\frac{E}{RT} \right) C_{A}$$
$$\dot{T} = \frac{q}{V} \left( T_{f} - T \right) + \frac{\left( -\Delta H \right)}{\rho C_{p}} k_{0} \exp \left( -\frac{E}{RT} \right) C_{A}$$
$$+ \frac{UA}{V \rho C_{p}} \left( T_{c} - T \right)$$
(13)

In this example, the input is taken to be the coolant temperature,  $T_c$ , and the output is the reactor temperature, T. The steady-state locus for this system has the classical S-shape expected of a nonisothermal CSTR thus leading to the presence of output multiplicity. A peculiar feature of this particular choice of parameters is that both of the top two branches of the steady-state locus are unstable and that there is limit cycle behavior in the approximate range  $303.25 \leq T_c \leq 305$ , just beyond the multiplicity region. This type of behavior has been demonstrated previously in (Uppal *et al.*, 1974).

By considering the step responses in Figure 7, it is obvious that the reactor exhibits strongly asymmetric response, but note that there is also evidence of input-dependent stability. For the +5step, limit cycle behavior results implying only bounded-input, bounded-output stability for this input. For all other step responses shown, the reactor displays asymptotic stability. In summary, the nonisothermal CSTR exhibits behavior representative of each of the three levels of severity discussed in Section 2.

Although the value of (3) is only a single number obtained after the maximization is performed, it is informative for this example to study the amplitude dependence of the function at low frequency. Figure 8 shows that as the input amplitude becomes large enough to drive the system off of the lower branch of the steady-state locus and into the limit cycle region the function value jumps sharply. Note that the maximum value of the measure is 0.783 - indicating severe nonlinearity thus corresponding to the relative severity of the classes of nonlinear behavior displayed by the reactor.



Fig. 7. Step responses for the nonisothermal CSTR beginning at  $T_c = 300$  on the lower, stable branch. Note carefully the differing scales on the ordinates



Fig. 8. Open-loop nonlinearity results as a function of input sinusoid amplitude at a frequency of 0.5 rad/s

Assuming a quadratic performance objective, this system's OCS maintains the stability properties of the multiple open-loop steady-states investigated. For the stable operating point, the OCS nonlinearity obtained by choosing the OCS input range to equal the minimum constrained values of the open-loop output is 0.751. The OCS nonlinearity at the stable operating point increased monotonically for increasing amplitude suggesting that the limit cycle region does not transfer to the OCS.

### 6. CONCLUSION

Through the study of two chemical reactor systems, comparisons were made between the nonlinear characteristics of the open-loop systems and the results of analysis of both open-loop and control-relevant systems using a lower bound on a nonlinearity measure. The results indicate that existing understanding of the relative severity of the behavior categorizations transfers well to the numerical results of the measure. Analysis of the control-relevant nonlinearity of the systems show that open-loop nonlinear behavior may or may not appear in the control-relevant analysis.

## 7. REFERENCES

- Allgöwer, F.A. (1995). Definition and computation of a nonlinearity measure and application to approximate I/O-linearization. Technical Report 95-1. Stuttgart University.
- Boyd, S. and L. O. Chua (1985). Fading memory and the problem of approximating nonlinear operators with Volterra series. *IEEE Trans. Cir. Sys.* CAS-32(11), 1150–1161.
- Desoer, C. A. and Y. Wang (1980). Foundations of feedback theory for nonlinear systems. *IEEE Trans. Circ. Syst.* CAS-27(2), 104–123.
- Doyle III, F.J., R.K. Pearson and B.A. Ogunnaike (2001). Indentification and Control Using Volterra Models. Springer-Verlag.
- Guay, M. (1996). Measurement of Nonlinearity in Chemical Process Control. PhD thesis. Queen's University at Kingston, ON.
- Guckenheimer, J. and P. Holmes (1983). Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vector Fields. Springer-Verlag, New York, NY.
- Haber, R. (1985). Nonlinearity test for dynamic processes. In: Proceedings of the IFAC Identification and System Parameter Estimation Symposium. pp. 409–414.
- Helbig, A., W. Marquardt and F. Allgöwer (2000). Nonlinearity measures: Definition, computation and applications. J. Proc. Con. 10, 113– 123.
- Nikolaou, M. and V. Hanagandi (1998). Nonlinear quantification and its application to nonlinear system identification. *Chem. Eng. Commun.* 166, 1–33.
- Ogunnaike, B. A., R. K. Pearson and F. J. Doyle III (1993). Chemical process characterization: With applications in the rational selection of control strategies. In: *Proceedings of the European Control Conference*. Gronigen, The Netherlands. pp. 1067–1071.
- Pearson, R. K. (1999). Discrete-Time Dynamic Models. Oxford.
- Seborg, D. and M. Henson (1997). Introduction. In: Nonlinear Process Control (M. Henson and D. Seborg, Eds.). Chap. 1, pp. 1–9. Prentice Hall.
- Stack, A. J. and F. J. Doyle III (1997). The optimal control structure approach to measuring control-relevant nonlinearity. *Comput. Chem. Eng.* 21, 998–1009.
- Stack, A. J. and F. J. Doyle III (1999). Local nonlinear performance assessment for single controller design. In: *Proc. IFAC World Congress.* Beijing. pp. 111–117.
- Svoronos, S., G. Stephanopoulos and R. Aris (1981). On bilinear estimation and control. *Int. J. Control* 34, 651–684.
- Uppal, A., W. H. Ray and A. B. Poore (1974). On the dynamic behavior of continuous stirred tanks. *Chem. Eng. Sci.* 29, 967–985.