PLANT AND CONTROL-RELEVANT NONLINEARITY ANALYSIS OF A CSTR: A CASE STUDY

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Abstract: Control-relevant nonlinearity analysis has gained importance with the need to control nonlinear processes more tightly. To this effect, the recently proposed closed-loop optimal control law (OCL) nonlinearity measure quantifies the degree of nonlinearity of the optimal state feedback controller for a given control problem. The current paper attempts to gain more insight into the characteristics and behavior of the formulation through a case study using a CSTR model. The multivariate character and the correlation of plant and control-relevant nonlinearity are analyzed with particular focus.

Keywords: Optimal control, Nonlinear systems, System analysis, Reactor control

1. INTRODUCTION

Nonlinear systems have been the most challenging ones for a control engineer. For many of these systems, a linear controller no longer suffices for the desired degree of performance. Regarding the complexity of nonlinear controller design, an answer is needed to the question: in which cases is the effort for nonlinear controller design justified by the resulting performance gain? The first approaches to this question considered the plant nonlinearity to be the determining factor and analysis of the degree of nonlinearity inherent to the system have been made (Guay *et al.*, 1995; Mäkilä and Partington, 2003; Sun and Hoo, 2000; Hahn and Edgar, 2001; Harris *et al.*, 2000). But the first assumption is found to be doubtful as the performance criterion plays an important role as well. This leads to the concept of control-relevant nonlinearity dealing with the assessment of the nonlinearity of a suitable controller (Stack and Doyle III, 1997).

Although an optimal state feedback controller of the form $\mathbf{u}=\mathbf{k}(\mathbf{x})$ is a good control structure for analysis, it is well-known that the derivation of such a controller is mathematically complex and not feasible for many practical systems. To circumvent these difficulties, Stack and Doyle (1997) have proposed the so called Optimal Control Structure (OCS) based on the optimal control theory and an approximation of the exact controller dynamics. Picking on the idea of analyzing the optimal controller, a more rigorous formulation, the closed-loop optimal control law nonlinearity measure has been recently proposed (Schweickhardt *et al.*, 2003) which quantifies the nonlinearity under the condition of closed-loop operation.

In this article this closed-loop optimal control law has been studied on a well-known chemical model of a CSTR. Owing to its interesting system

[1] This work was done while this author was an exchange student at the University of Stuttgart.

dynamics, the work deals with the plant as well as control-relevant nonlinearity studies for better insight. The next section first briefly introduces the general nonlinearity measure, which is the basic tool used for nonlinearity quantification, and then describes the philosophy of the closed-loop optimal control law nonlinearity measure. Section 3 deals with the CSTR case study which includes a short system description, the plant and the control-relevant nonlinearity analysis followed by the interpretation of the results. The last section draws conclusions.

2. THE CLOSED-LOOP OPTIMAL CONTROL LAW NONLINEARITY MEASURE

2.1 General nonlinearity measure

Nonlinearity measures, first proposed by Desoer and Wang (1981), rank various systems by quantifying their nonlinearity. Amongst the various formulations proposed for the nonlinearity measure in literature (Guay *et al.*, 1995; Nikolaou and Hanagandi, 1994; Sourlas and Manousiouthakis, 1992) this work uses the measure proposed by Allgöwer (1995).

Definition of the nonlinearity measure: The nonlinearity measure $\phi_N^{\mathcal{U}}$ of a nonlinear dynamic system $N : \mathcal{U} \rightarrow \mathcal{Y}$ is defined by the non-negative number

$$\phi_N^{\mathcal{U}} := \inf_{G \in \mathcal{G}} \sup_{\mathbf{u}(.) \in \mathcal{U}} \frac{\|G[\mathbf{u}] - N[\mathbf{u}]\|_{L_2}}{\|N[\mathbf{u}]\|_{L_2}} \qquad (1)$$

where $G : \mathcal{U} \rightarrow \mathcal{Y}$ is a linear dynamic operator belonging to the space of linear operators $\mathcal{G}$. $\mathcal{U}$ and $\mathcal{Y}$ are the spaces of admissible inputs and outputs, respectively and $\|.\|$ is a suitable norm in $\mathcal{Y}$. In this work the L_2-norm is used although some other norm can also be used. The measure is bounded between 0 and 1. While a value of zero (practically very close to zero) indicates that the given system is linear, a value of 1 (practically very close to 1) indicates that system is highly nonlinear. For computational purposes, the infinite dimensional min-max problem given by (1) is converted into finite dimensional constrained convex minimization problem. For this work, sinusoidal and step inputs of relevant amplitude and frequency were considered. Simulations and optimization were preformed in MATLAB using standard toolboxes.

2.2 The closed-loop optimal control law nonlinearity measure

Consider a general nonlinear system governed by the equation

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \qquad (2)$$

where $\mathbf{x}(t) \in R^n$ is the state vector and $\mathbf{u}(t) \in R^p$ is the control vector and the initial condition is given by $\mathbf{x}(t_0) = \mathbf{x_0}$. According to the theory of calculus of variations, for a particular objective function J, the optimal *open-loop* control policy is given by the solution of a two point boundary value problem, while the optimal *feedback law* is determined by the solution of the Hamilton-Jacobi-Bellman PDE (Kirk, 1970). While the open-loop control problem is solvable by numerical methods for practical problems, the feedback controller synthesis is not feasible for most practical problems. But note that, for a given initial condition of the plant, the solution of the open-loop control problem and the application of the optimal feedback law will lead to the same trajectories of the manipulated variable and the system states. The closed-loop optimal control law (OCL) nonlinearity measure assumes the problem to be that of infinite time horizon. In that case the optimal control law is a static state feedback law (Kirk, 1970).

Definition of the closed-loop OCL nonlinearity measure: The closed-loop optimal control law (OCL) nonlinearity measure for a control problem is defined as (Schweickhardt *et al.*, 2003)

$$\hat{\phi}_{N_{OCL}}^{\mathcal{B}} := \inf_{K \in R^{q \times n}} \sup_{\mathbf{x}_0 \in \mathcal{B}} \frac{\|N_{OCL}[\mathbf{x}_{x_0}^*] - K\mathbf{x}_{x_0}^*\|_{L_2}}{\|N_{OCL}[\mathbf{x}_{x_0}^*]\|_{L_2}} \qquad (3)$$

with $N_{OCL}[\mathbf{x}_{x_0}^*] := \mathbf{u}_{x_0}^*$ being the solution of the infinite horizon open-loop optimal control problem for the initial condition x_0. The region $\mathcal{B} \subset R^n$ is the set of considered initial conditions. n is the dimension of the state space of the plant and q is the number of manipulated variables.

The definition is the application of the nonlinearity measure defined previously to the optimal control law with respect to *closed-loop trajectories* where the input signals are parameterized by their corresponding initial conditions. This measure can be efficiently computed by considering a finite set of initial conditions $\mathcal{B}$, because only optimal control *trajectories* need to be computed in order to assess the nonlinearity of the optimal control *law*. The computation is further facilitated by considering static approximations only. This approach is appropriate as the optimal control law is known to be static as well. Computations first involve the generation of optimal trajectories $\mathbf{x}_{x_0}^*$ and $\mathbf{u}_{x_0}^*$ through the boundary value problem solution for different x_0. These trajectories are then used in the optimization scheme to generate a linear approximation using the K matrix. It is important to note that the nonlinearity captured is the input to state nonlinearity and the output

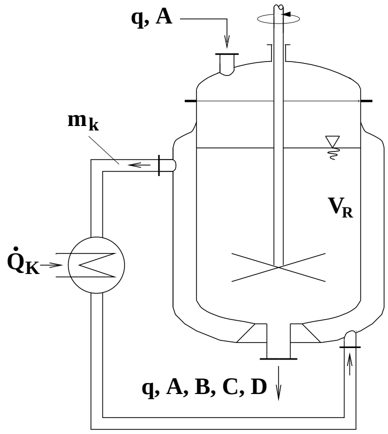

Fig. 1. Schematic of the CSTR.

nonlinearity is not accounted for. It is assumed that all the states are available. The OCL nonlinearity measure is therefore some sort of special application of the general formulation of Sec. 2.1 and is used to quantify the degree of nonlinearity of a suitable controller. The system considered in the OCL formulation is not any system but the solution to an optimal control problem that is known to be a nonlinear algebraic function and the considered class of input functions is the set of closed-loop trajectories.

3. CSTR CASE STUDY

3.1 System description

The system considered in this work for case study is a Continuous Stirred Tank Reactor (CSTR) system shown in figure 1. It consists of a CSTR with a cooling jacket carrying out the van der Vusse reaction scheme described by the following reactions:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
$$2A \xrightarrow{k_3} D$$

Here B is the desired product while C and D are are the undesired byproducts. k_1, k_2 and k_3 are the reaction rate constants. The nonlinear dynamics in the reactor are governed by the following equations:

$$\frac{dc_A}{dt} = \frac{q}{V_R}(c_{A0} - c_A) - k_1(T)c_A - k_3(T)c_A^2 \quad (4)$$

$$\frac{dc_B}{dt} = -\frac{q}{V_R}c_B + k_1(T)c_A - k_2(T)c_B \quad (5)$$

$$\begin{aligned}\frac{dT}{dt} &= \frac{q}{V_R}(T_0 - T) - \frac{1}{\rho C_P}(k_1(T)c_A\Delta H_{R_{AB}} \\ &+ k_2(T)c_B\Delta H_{R_{BC}} + k_3(T)c_A^2\Delta H_{R_{AD}}) \\ &+ \frac{k_W A_R}{\rho C_P V_R}(T_C - T)\end{aligned} \quad (6)$$

$$\frac{dT_c}{dt} = \frac{1}{m_c C_{pc}}(\dot{Q_K} + k_W A_R(T - T_C)) \quad (7)$$

With the reaction rate constants described by

$$k_i = k_{i0}e^{(\frac{E_i}{T})}, i = 1, 2, 3. \quad (8)$$

The concentrations c_A and c_B, reactor temperature T and the coolant temperature T_C constitute the four states of the plant. The heat flow $\dot{Q}_K$ is constant. Two different stable operating points are considered. One is the optimal operating point (OP) characterized by the maximum yield with respect to the desired product B and the other one is a sub-optimal operating point (SP) with a lower yield. Further details about the process and the parameters are available in (Chen *et al.*, 1995).

3.2 Previous results on CSTR nonlinearity

The CSTR has been previously analyzed for nonlinearity at the two operating points in (Helbig *et al.*, 2000). The nonlinearity was calculated between the scaled input flow rate (q/V_R) as input for the plant and concentration of desired product B (c_B) as the output for the plant. The nonlinearity measures reported at the two operating points are:

- Optimal operating point (OP): 1.0
- Sub-optimal operating point (SP): 0.37

The difference in nonlinearity measures is quite significant and interesting. The aim of the control-relevant nonlinearity analysis of this model was thus twofold:

(1) To check the result of the closed-loop OCL nonlinearity measurement on a multi-state model
(2) To check whether the plant nonlinearity values of the CSTR get translated into the control-relevant nonlinearity

3.3 Control-relevant nonlinearity analysis of CSTR

The closed-loop OCL nonlinearity measure of the CSTR was analyzed for the two different operating points using definition (3). The performance criterion used is the quadratic objective functional given by:

$$J[u(\cdot)] = \int_0^\infty \mathbf{x}(t)^T Q\mathbf{x}(t) + \alpha u(t)^2 dt \quad (9)$$

where $\mathbf{x}(t)$ is the state vector, $u(t)$ is the input (scaled input flow rate), α is the controller weighting parameter and Q is the weighting matrix for the states.

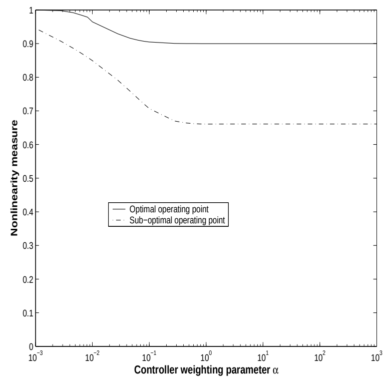

Fig. 2. Variation of OCL nonlinearity measure for the CSTR.

Since OCL nonlinearity gives input to state nonlinearity of the system, for the CSTR with four states, the OCL becomes a four input-one output (MISO) system, i.e. $n = 4$ and $q = 1$ in the definition given in (3). A higher dimension of the plant state results in a larger number of considered initial conditions and translates into an increased number of constraints in the convex optimization framework. The starting conditions x_0 should be in the range of the observed values of physical variable. For the CSTR, the range of starting conditions in terms of the deviation variables were: $c_A = \pm 0.25$, $c_B = \pm 0.10$, $T = \pm 3$ and $T_c = \pm 3$ in $[mol/l]$ and $[K]$ respectively for the sub-optimal operating point and $c_A = \pm 0.5$, $c_B = \pm 0.10$, $T = \pm 3$ and $T_c = \pm 3$ in $[mol/l]$ and $[K]$ respectively for the optimal operating point. The matrix Q in the objective function is a fourth-order identity matrix. The dependence of the OCL nonlinearity on the controller weighting parameter α was sought.

The variation at the two different operating points is plotted in figure 2. From the graph, it can be seen that the OCL nonlinearity at OP is very high which is in agreement with the high plant nonlinearity at this operating point. The nonlinearity measure is seen to vary between 0.9999 and 0.8997 for the considered range of α. But for the sub-optimal operating point (SP), the OCL nonlinearity is found to vary between 0.9454 and 0.6609 and is decreasing with increasing value of α. This result is somewhat unexpected as reported plant nonlinearity is 0.37 and so the control-relevant nonlinearity is significantly higher.

This observed difference between the plant and control-relevant nonlinearity measures was postulated to be arising from their differing analytical setups. For the CSTR plant analysis, the nonlinearity measure gives the relationship between input q/V_R and output c_B. On the other hand, the OCL nonlinearity measure, being input to state, describes a relationship between all four states of the plant and the solitary input (corresponding to four inputs and one output of the optimal control law) and thus considers dynamics between all the input-output pairs. In order to verify this hypothesis and shed more light on it, following two different kinds of analysis were carried out at both the operating points.

- Plant nonlinearity measurement for other three states as output and also considering all outputs simultaneously in a single input multi output (SIMO) setup
- OCL nonlinearity measurement using weighted states i.e. giving importance to a particular state in the objective function

3.4 Nonlinearity analysis of CSTR in a modified setup

The nonlinearity measure calculation of the CSTR model with the other three states as outputs is very similar to the previous case, with change only in the output vector considered for analysis. The measurement was carried out using sinusoidal and step inputs of amplitude up to $\pm 11 hr^{-1}$ and maximum frequency (for sinusoidal inputs) of 100 Hz. The results, values of nonlinearity measures at both operating points, are reported in Table 1 where the previous values, with c_B as output are also reported for the sake of comparison.

The nonlinearity measure was also calculated considering all the states as outputs simultaneously i.e. calculation in single input multi output (SIMO) setup. The implementation of the nonlinearity measure definition for the multi output case is logically straight forward but becomes computationally more demanding due to increased dimensionality. The output, which previously was a scalar function of time, is now a vector function of time. The dynamics between different input-output combinations are approximated by different linear systems. Thus, the computational load grows linearly to the number of outputs of the plant (that are here identical to the states). Care must be taken during computation to scale the outputs to the same range so as to avoid masking of linear/nonlinear behavior due to differing ranges. The values of the nonlinearity measure for this case are also reported in table 1. The values in the table will be referred to in the next section for discussion.

3.5 OCL nonlinearity measure of CSTR in a modified setup

The previous nonlinearity analysis for the closed-loop optimal control law in Sec. 3.3 was done using an identity weighting matrix Q i.e. equal weighting given to all the four states in the objective

Table 1. Plant nonlinearity measures of the CSTR at the suboptimal operating point considering different outputs.

Output	Nonlinearity measure at OP	Nonlinearity measure at SP
c_A	0.2478	0.2524
c_B	0.9912	0.3045
T	0.9921	0.5987
T_c	0.9957	0.5988
All	0.9695	0.5877

function. As reported in the previous subsection, the (open-loop) plant nonlinearity measure depends on the input-output pairing. The aim of this section is to perform a similar analysis which will report control-relevant nonlinearity assessment focussing on single states. The optimal control law (OCL) has four states as the four inputs and the plant input q/V_R as its output. The concept of varying only one of the four inputs (states) at a time through different starting conditions does not fit in the realms of optimal control theory as the four states are dynamically highly interconnected and such a situation will never arise in actual closed loop operation. Another way to relate the results of the previous section to OCL nonlinearity measurement is to vary the weights on different states in the objective function. By doing so, different states will dominate the objective and hence the degree of nonlinearity of the optimal control law. There are thus four different cases generated by modifying the weighting matrix Q such that at any time all but one of the diagonal elements are zero, the only non-zero element being equal to one.

Using this setup, the nonlinearity measure calculation for the OCL was carried out at both operating points. Apart from the weighting scheme, all the other aspects of the computation remain the same. The plots for various cases are given in Figure 3 and Figure 4 for the optimal (OP) and sub-optimal (SP) operating points respectively. The plots for the first case with diagonal weighting matrix are also included in the figure for the sake of comparison (labelled as "all states"). These plots will be used to draw conclusions in the next section.

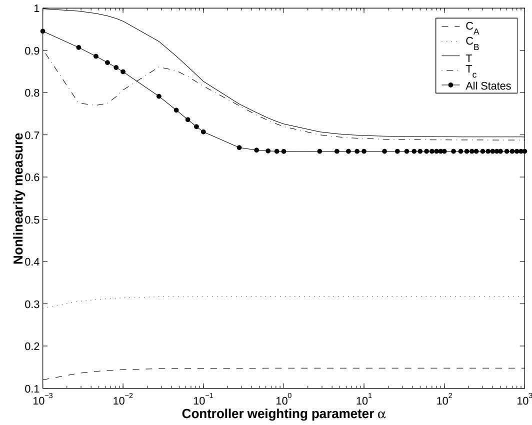

Fig. 3. Comparison of weighted OCL nonlinearities of CSTR model at sub-optimal operating point.

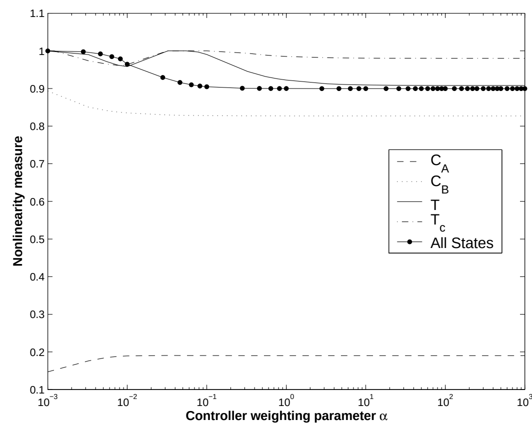

Fig. 4. Comparison of weighted OCL nonlinearities of CSTR model at optimal operating point.

3.6 Discussion

From Table 1, most obvious observation for both the operating points is that the nonlinearity measures with respect to the two temperatures (reactor and coolant) are significantly high whereas the nonlinearity with respect to the concentration of A, is quite low. The previously reported (Helbig *et al.*, 2000) difference in the nonlinearity with respect to the concentration of B, is also observed. In both cases, the overall nonlinearity measure is also very close to that for the temperatures indicating that the overall nonlinearity (in a multi output setup) is dominated by the temperature nonlinearities. This result leads to the conclusion that the temperature nonlinearities pose problems in the regulation of both systems (SP and OP). But the regulation of concentration of B is operating point dependent. But the results also stress the importance to consider all possible dynamic relationships within a system to draw a picture of the nonlinearity of the system as a whole.

The nonlinearity measure variation of the OCL shows a similar qualitative behavior. From the graphs it can be concluded that from control point of view also, the nonlinearity with respect to the two temperatures is always dominant. Another interesting thing to observe is that the difference in the plant nonlinearity with respect to the concentration of B is nicely reflected in the OCL nonlinearity. Not only does the qualitative behavior agree, but quantitatively also the two sets of values are close. Given these results, one can conclude that for this particular system the plant nonlinearity is getting translated into equivalent control-relevant nonlinearity for all dynamic paths of the system. The OCL nonlinearity further shows that the need for nonlinear control does not strongly depend on the cost of control action in this particular example (expressed by the weak dependence on α). But both, plant and OCL nonlinearity values show that the variable to be controlled plays an important role.

Two types of computations are involved in the determination of the OCL nonlinearity measure: first, a finite number of optimal open-loop control problems have to be solved, equivalent to two point boundary value problems. Then the best linear approximation K for the state feedback controller is determined by convex optimization. The computational demand of the optimal control problem solution certainly strongly depends on the specific plant and performance requirements at hand. For the example system, it was observed that for singular Q matrices and very low values of α (less than 0.1) the boundary value problem solution poses accuracy problems. Not surprisingly, the problem is more severe at OP where the system is highly nonlinear. The accuracy problems for the temperatures at OP could not be completely eliminated at low values of α. As a result, the somewhat fluctuating behavior at low α can possibly be due to numerical problems. The computation of the optimal K matrix poses no problem and can be completed very efficiently even for high dimensional systems with multiple inputs.

4. CONCLUSIONS

Nonlinearity analysis of an example CSTR has been done using a general and a control-relevant nonlinearity measure, the optimal control law (OCL) nonlinearity measure. Under similar conditions, the two methods show consistent results. The results suggest that at both operating points, a nonlinear controller would be necessary to control the system temperatures and a linear controller would suffice for concentration of A. The controller requirement for concentration of B though is operating point dependent. This result is in accordance to the working experience that concentration of B at sub-optimal operating point is controller by a PI controller while at the optimal operating point a linear control is not feasible.

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