Application of a Lyapunov-Based Nonlinear Controller to a Reactor with Highly Exothermic Reactions

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Abstract

This work examines a nonlinear algorithm to control a class of chemical reactors in which a highly exothermic reaction takes place, and gives relevance to the controller's experimental performance in a real application equivalent to what is encountered in industry.

The control objective is to maintain the temperature inside the reactor by manipulating two variables. Several options are available; in this work, we consider as controls the cooling supplied by the jacket and the inlet concentration of one reactant (or, alternatively, the concentration of a homogenous catalyst or promoter of the flow rate of a diluent). These variables are most easily adjusted in the experimental set-up used to test the performance of the Lyapunov-based nonlinear robust controller developed previously.

This work fills a gap caused by the lack of experimental applications of the numerous different nonlinear controller proposals to relevant real life situations. It provides some experimental results, which were obtained in a pilot plant CSTR. The reactor is a pilot plant among the facilities in the laboratories at Imperial College London.

The results obtained are consistent with earlier simulation studies. They strongly suggest the ability of the proposed controller to globally stabilise the closed loop system and to achieve the desired setpoint(s) as long as the control problem is feasible within the available bounded inputs.

1 - Introduction

The literature available presents many aspects of the behaviour of nonlinear processes, but the same is not true for their control. In recent years, many papers dealing with control of nonlinear systems and nonlinear control have become available, clearly indicating that control techniques for such processes are still evolving.

Lyapunov based controllers are attractive because of their recognised ability to globally stabilise a system. These controllers are mainly used when the model description is poor or inaccurate; model based solutions may be preferred otherwise. A simple mathematical controller formulation, like the one

employed in this work, was proposed (Viel *et al.*, 1995; 1997a and 1997b) to stabilise the temperature in a CSTR, in spite of uncertainties in the reaction kinetics and input saturations. The authors focus on an irreversible exothermic reaction taking place in a CSTR – control problem frequently found in the literature. Antonelli and Astolfi (2003) utilises the same type of nonlinear controller and extensively examines chemical reactors stability in the sense of Lyapunov and presents some experimental results for biological systems (Antonelli *et al*., 2003).

In line with these works, Antonelli and Astolfi, (2003) and Luís *et al.* (2004) prove, making use of Lyapunov theory, the capability of a simple mathematical algorithm in globally stabilising a closed loop chemical reactor system where a strongly exothermic reaction takes place. The non-model based mathematical algorithm can be interpreted as an integrator of the error between the setpoint and the actual value of the controlled variable. The regulator performs an online search of the input values that keep the system at the desired setpoint. Moreover, a feature to explicitly deal with input constraints has been added to cope with discontinuous nonlinearities (Slotine and Li, 1991), which are present in all chemical processes.

The resulting regulator (1) is non-model based, therefore robust against poor knowledge of the (generally unknown or uncertain) system parameters, and it only makes use of the output of the system avoiding the difficult-to-quantify controller performance degradation resulting from the introduction of a state observer.

$$\dot{I} = G\left(I - I^{min}\right)\left(I - I^{max}\right)\left(O - O^{sp}\right) \qquad (1)$$

I, *O,* and *G* stand for input, output and controller gain of the closed loop system respectively. The superscripts *min* and *max* indicate the minimum and maximum values input can take and *SP* is the output setpoint.

Recently, there has been an interest to incorporate several techniques for nonlinear systems in the same control strategy (El-Farra at al., 2004a and 2004b; Mhaskar, 2005). The importance of Lyapunov-based strategies in global stabilisation of chemical systems is acknowledged and the benefits of optimality brought by model based control strategies are grasped. These control strategies also known as hybrid controllers, involve the switching between bounded control (essentially robust) and MPC in well-characterised regions of the state space (essentially optimal).

However it is difficult to find in the literature examples of experimental applications of the numerous different nonlinear controller proposals (and modified versions) to relevant real life situations although there has been recommendations in that direction for instance by Bequette (1991). Therefore, the orientation of the present work is to contribute for the understanding of nonlinear controllers in real situations.

2 - Experimental Apparatus

The objective of this section is to provide an overview of the experimental apparatus used to produce the results included and to create an insight on the possibilities that such a reactor offers in controller testing.

The PARSEX (**PAR**tially **S**imulated **Ex**othermic) reactor is a pilot plant among the facilities in the laboratories at Imperial College London, which simulates in a realistic way the operation of a CSTR and has already been thoroughly described (Hussain, 1996; Hussain and Kershenbaum, 2000; Kershenbaum, 2000; Kershenbaum and Kittisupakorn, 1994).

Essentially, the core of the PARSEX consists in two main units: a continuous tank “reactor” and a cooler where the reactor contents recirculate and cool down; the plant is represented in Figure 1.

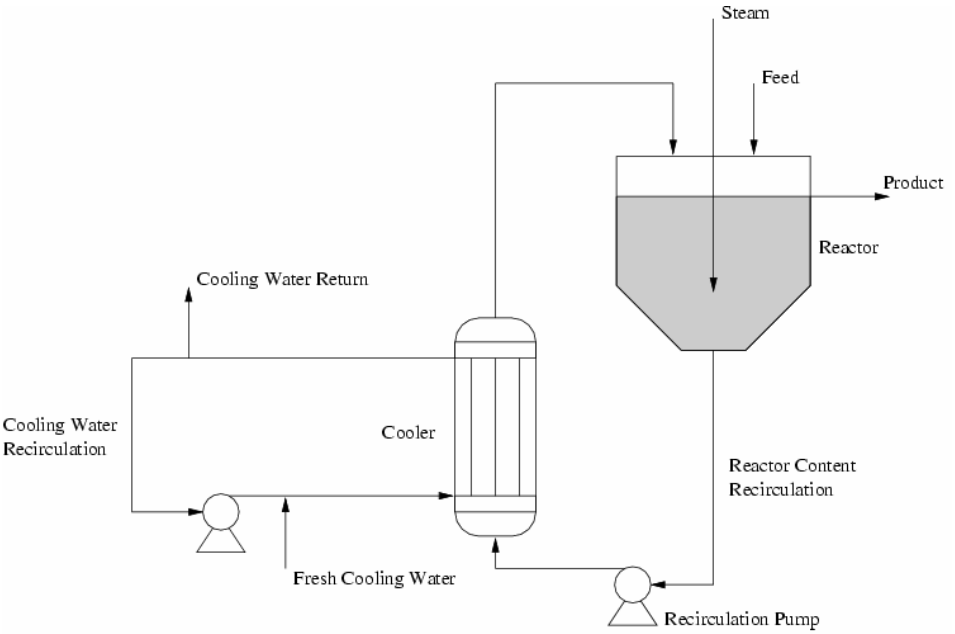

Figure 1 – Simplified schematic of the PARSEX plant.

Mixing in the CSTR is achieved by rapid recirculation rate of the reactor contents. The external cooler that substitutes the jacket in a jacketed reactor is a shell-and-tube heat exchanger with the coolant (water) on the shell side. The most interesting feature of this pilot plant is the way exothermic reactions can be simulated. In fact, the only fluid circulating in the reactor is water. A hypothetical reaction is then implemented on an online simulator (Paragon^{TM} – Scan, Control and Data Acquisition software) that calculates the amount of heat that would have been released in the period of time the simulator takes to complete a run (typically 1 second) and injects an amount of steam corresponding to that heat the reaction

In a typical SISO control scheme the manipulation of the fresh cooling water controls the temperature in the reactor. However, in this work, a MIMO approach was investigated as well, namely the temperatures in the reactor

and in the cooler were controlled via manipulation of the reactant feed (or catalyst) concentration and the fresh cooling water, respectively.

3 - Experimental Results

The PARSEX reactor, like any other chemical reactor, operates within bounds determined by safety and the variable ranges involved in the process. Table 1 summarises the relevant variable ranges that are necessary to define the available region of operating conditions.

Table 1 – Variable ranges to define the operating region.

Variable	Range	Units
F_{feed}	0 – 110	g s^{-1}
T_{feed}	room temp.	^oC
C_{feed}	0.5 – 3.0	kmol m^{-3}
$F_{CW,fresh}$	40 – 110	g s^{-1}
F_{steam}	0 – 14	g s^{-1}

These ranges constraint the choice of reaction simulated by Paragon™. The first-order exothermic reaction used in the experiments had, then, the parameters included in Table 2.

Table 2 – Reaction parameters.

	Parameter	Range	Units
Arrhenius Paramaters	k_0	2.0×10^{11}	s^{-1}
	E/R	10700	K
Heat of Reaction	(-ΔH)	200 000	J mol^{-1}

The steady state analysis of the irreversible reaction A $\rightarrow$ B, considering the feed at 90 g s^{-1} containing an inlet concentration of A of 1.5 kmol m^{-3} and nil concentration of B, leads to an expected operating point for the temperatures in the reactor and in the cooler at around $(T,T_j) \rightarrow (55, 47)^oC$ and approximately 74% conversion of reactant A.

This section includes two sets of typical results obtained on the PARSEX reactor using the proposed controller. The regulator implemented on Matlab® controls the temperature in the reactor T and the temperature in the cooler T_j by manipulating the inlet concentration of reactant $C_{A,in}$ and the flowrate of fresh cooling water $F_{CW,fresh}$,respectively. The MIMO controller is, finally, translated by the equation (2). The gains G_1 and G_2 are set in advance and not altered; other experiments (not shown) have demonstrated that these are not sensitive parameters.

$$\begin{cases} \dot{C}_{A,in} = G_1\left(C_{A,in} - C_{A,in}^{min}\right)\left(C_{A,in} - C_{A,in}^{max}\right)\left(T - T^{sp}\right) \\ \dot{F}_{CW,fresh} = G_2\left(F_{CW,fresh} - F_{CW,fresh}^{min}\right)\left(F_{CW,fresh} - F_{CW,fresh}^{max}\right)\left(T_j - T_j^{sp}\right) \end{cases} \quad (2)$$

In the first experiment a typical setpoint change was performed; Table 3 summarises the operating conditions in the beginning of the experiment.

Table 3 – Setpoint change experiment initial operating conditions.

Variable	Range	Units
T	58.0	^{o}C
T_j	47.0	^{o}C
C_A	0.33	kmol m^{-3}
$C_{A,in}$	1.50	kmol m^{-3}
F_{feed}	90	g s^{-1}
T_{in}	23.1	^{o}C

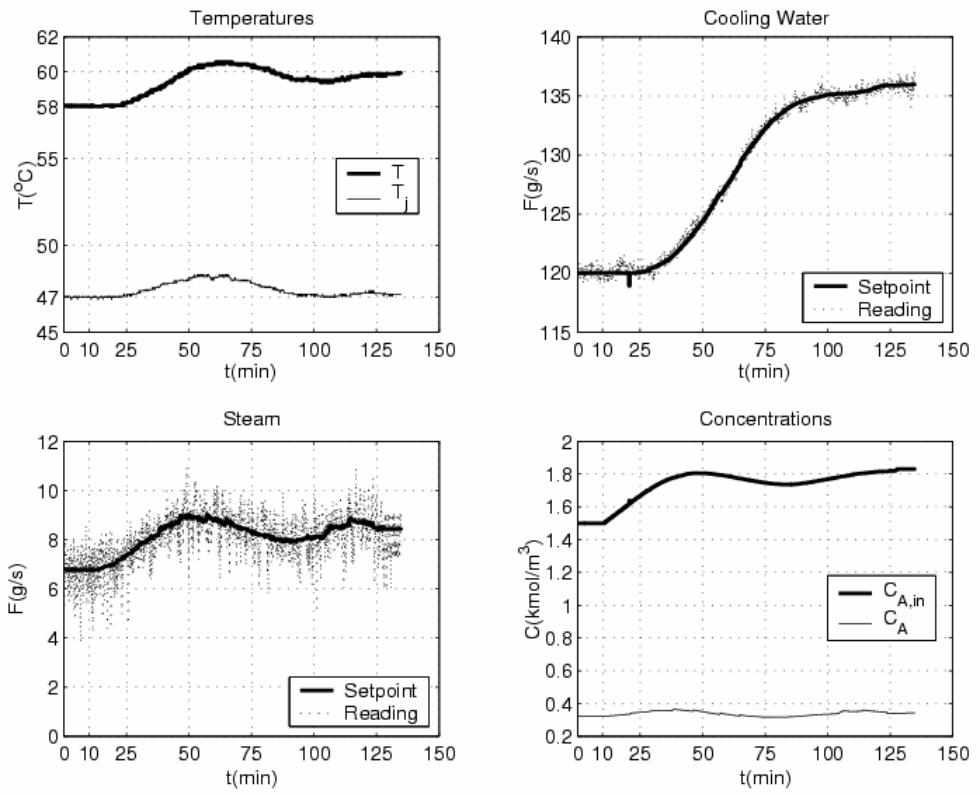

Figure 2 – Reactor temperature setpoint change.

Figure 2 includes the results of the experiment that imposed a 2^{o}C setpoint change in the reactor temperature at 10 min. The new operating temperature T was reached after about 110 min of operation (note that the residence time in the reactor is approximately 34 min). It is interesting to verify that, as expected, the derivative of the input paired with the reactor temperature becomes zero consistently when the controlled variable crosses (at 50 and approx. 85 min) or reaches at the end the new setpoint.

A second experiment simulates a sharp catalyst deactivation. The catalyst activity is always expected to decay throughout the operation of the chemical reactor, yet it is not likely to occur as it was enforced in this case. Nevertheless, an instantaneous deactivation of 40% represents is dramatically challenging situation for the controller.

Table 4 – Catalyst deactivation experiment initial operating conditions.

Variable	Range	Units
T	58.3	^{o}C
T_j	47.0	^{o}C
C_A	0.32	kmol m^{-3}
$C_{A,in}$	1.50	kmol m^{-3}
F_{feed}	90	g s^{-1}
T_{in}	24.9	^{o}C

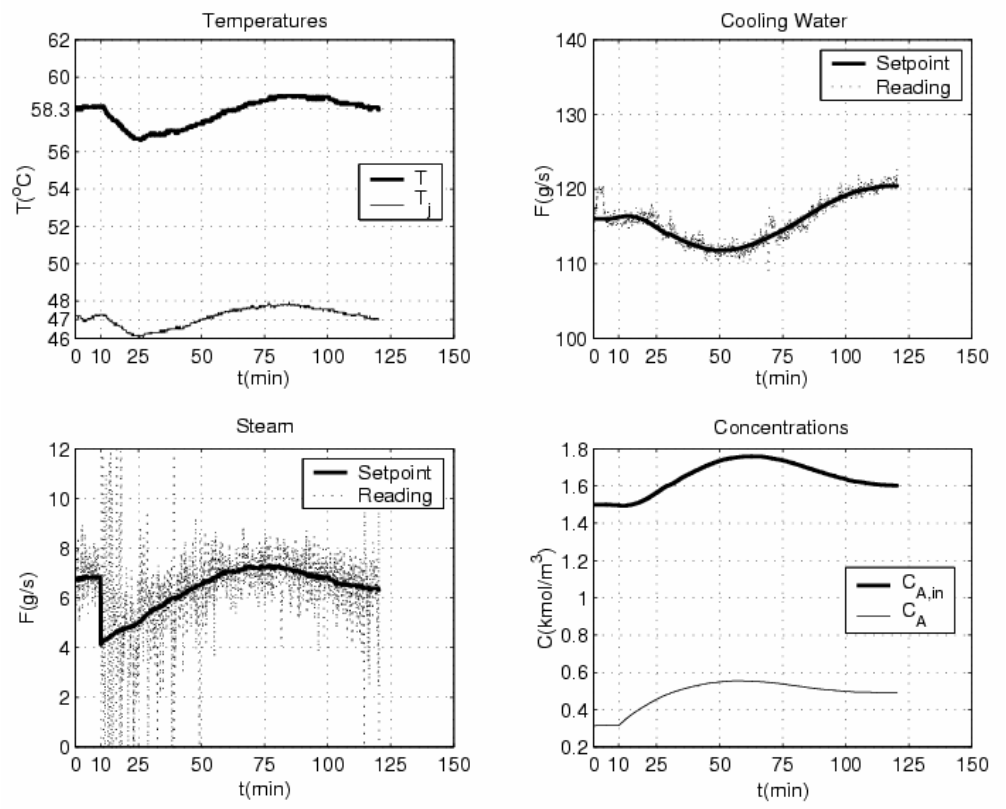

Figure 3 – Catalyst deactivation.

Table 4 presents the initial operating conditions of the experiment; at time = 10 min the pre-exponential Arrhenius parameter k_0 is decrease from 2.0×10^{11} s^{-1} to 1.2×10^{11} s^{-1}.

Figure 3 reveals that the catalyst changed its activity at instant 10 min. The temperature in the reactor reached the lowest temperature during the experiment corresponding to 1.7°C of displacement from the objective; T_j accompanied this tendency. The controller responded by firstly decreasing $F_{CW,fresh}$ and increasing $C_{A,in}$. The first action appears to have been excessive driving the temperature in the reactor to overshoot (0.7°C) and therefore, further correction was necessary. Then, $F_{CW,fresh}$ was incremented stabilising at around 120 g s^{-1} and $C_{A,in}$ reduced to the steady state value of 1.6 kmol m^{-3} making the reactor stabilise at the desired output setpoints.

It should be noted that these, and many other, experimental results follow the trends predicted by earlier simulation studies (Luís *et al.*, 2004b).

4 - Conclusions

Stability of the closed loop system can be guaranteed in the sense of Lyapunov for the object of this study. It presupposes conditions that were derived elsewhere (Luís *et al.*, 2004a) and that the desired operating conditions can be achieved within the available ranges of the inputs, in other words, as long as the control problem is feasible within the bounded inputs.

Once more, the PARSEX reactor revealed to be suitable to recreate real industrial conditions very closely, adding extra significance to the results obtained.

The results show the ability of the proposed controller to globally stabilise the closed loop system and to achieve the desired setpoint(s) even in the extreme case of rapid catalyst deactivation.

A more detailed set of results will be presented in a forthcoming paper (Luís *et al.*, 2006).

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References

R. Antonelli and A. Astolfi. Continuous stirred tank reactors: easy to stabilise? *Automatica*, 39:1817-1827, 2003.

R. Antonelli, J. Harmand, J.-P. Steyer, and A. Astolfi. Set-point regulation of an anaerobic digestion process with bounded output feedback. *IEEE Trans. Control Systems Technology*, 11(4):495-504, 2003.

B.W. Bequette. Nonlinear control of chemical processes: A review. *Ind. Eng. Chem. Res.*, 30:1391-1413, 1991.

N.H. El-Farra. P. Mhaskar, and P.D. Christofides. Hybrid predictive control of nonlinear systems: method and applications to chemical reactors. *Int. Journal of Robust and Nonlinear Control*, 14:199-225, 2004a.

N.H. El-Farra. P. Mhaskar, and P.D. Christofides. Uniting bounded control and mpc for stabilization of constrained linear systems. *Automatica*, 40:101-110, 2004b.

M.A. Hussain. *Inverse model control strategies using neural network: analysis, simulation and on-line implementation.* PhD dissertation, Imperial College of Science, Technology and Medicine, London, July 1996.

M.A. Hussain and L.S. Kershenbaum. Implementation of an inverse-model-based control strategy using neural networks on a partially simulated exothermic reactor. *Trans. IChemE*, 78, Part A:299-311, 2000.

L. Kershenbaum. Experimental testing of advanced algorithms for process control: when is it worth the effort? *Trans. IChemE*, 78, PartA:509-521, 2000.

L. Kershenbaum and P. Kittisupakorn. The use of partially simulated exothermic (PARSEX) reactor for experimental testing of control algorithm. *Trans. IChemE*, 72, Part A:55-63, 1994.

D. Luís, A. Astolfi, and L. Kershenbaum. Design of a nonlinear robust controller for an exothermic reaction system. *Proceedings of the ESCAPE14,* Elsevier Science B.V., 2004a.

D. Luís, A. Astolfi, and L. Kershenbaum. Design and Implementation of Nonlinear Robust Controllers for Reactors with Strongly Exothermic Reactions. *AIChE Annual Meeting*, 2004b.

D. Luís, A. Astolfi, and L. Kershenbaum. *In preparation*. 2006.

P. Mhaskar, N.H. El-Farra, and P.D. Christofides. Robust hybrid predictive control of nonlinear systems. *Automatica*, 41:209-217, 2005

J.J.E. Slotine and W. Li. *Applied nonlinear control.* Prentice-Hall International Editions, New Jersey, 1991

F. Viel, F. Jadot, and G. Bastin. Robust stabilisation of chemical reactors. *Proceedings of the 34th Conference on Decision & Control, IEEE*, pages 941-984, 1995.

F. Viel, F. Jadot, and G. Bastin. Global stabilization of exothermic chemical reactors under input constraints. *Automatica,* 33(8):1437-1448, 1997a.

F. Viel, F. Jadot, and G. Bastin. Robust feedback stabilization of chemical reactors. *IEEE Trans. Autom. Control*, 42(4):473-481, 1997b.