

Stability and Control of Complex Nonlinear Systems with Application to Chemical Reactors

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Abstract: This paper introduces a robust strategy for stabilizing complex industrial processes exemplified by a complex chemical reactor. The design uses a combination of backstepping methods and Lyapunov-based techniques for implementing a robust feedback controller. A model-reference-like virtual system is proposed to accomplish both asymptotic stability and satisfactory transient performance. The controller is robust in the sense that it accommodates uncertainties inherent in complex industrial processes. The suggested design procedure also has the advantage of being applicable to nonlinear processes without having to carry out linearization approximations. A simulated continuous stirred tank reactor is used to exemplify the suggested technique and the superiority of the controller is demonstrated by comparing its response to a standard PID controller. Practical considerations are addressed to investigate the causality and feasibility of the proposed controller and its applicability to real-time situations. Tradeoffs between stability and performance are carefully studied.

Keywords: Nonlinear Systems, Modeling and Simulation, Chemical Reactors, Control Engineering.

1. INTRODUCTION

The regulation problem of chemical reactors is very important as it finds typical applications in chemical industry, e.g. production of Fertilizers and Petroleum-based industries. The chemical reactor is a very rich example of MIMO systems with complex nonlinear behavior and sensitivity to parameters uncertainty [1-3]. Most systems in actual real-time applications are inherently nonlinear, which establishes a barrier when trying to adopt tracking controllers especially designed for linear systems. Linearization-based techniques have limited success when applied to nonlinear systems that possess model uncertainty and subject to external disturbances, and tend to become unstable when applied to a wide range of operating conditions [4-5]. Introducing virtual reference models in designing model-based control systems has proven to be very efficient for both regulation and tracking problems [6]. Complex MIMO industrial processes that need to operate continuously in real-time are typical candidates for such methods. When using virtual reference models, it is possible to prescribe a target behavior of some or all of the system states and then use some of them as virtual controls to the output [7]. This idea seems to be very appealing, especially when combined with Lyapunov-energy-like functions to design the control law [3, 8].

If either the system to be controlled is in some way ill defined and/or it is not possible to gain access to the internal variables of the system, conventional control systems will probably fail. PID controllers fall under such category although they are the most widely used conventional controllers for industrial processes. The only way to cope with the control of such systems, that are structurally complex, is to transfer the system to a representation with less resolution [9]. Thus the system may be represented at a level of abstraction appropriate to the known characteristics of the system. In this paper an explicit model is used to generate estimates of the system's behavior that can be used to modify the closed-loop time response and satisfy the performance specifications [4, 5, 10].

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Lyapunov-based designs are among the most appealing methods ever used in designing and implementing systems that are capable of controlling unknown plants or adapting to unpredictable changes in the environment. Traditional adaptive schemes may be classified as Lyapunov-based and estimation-based. The distinction between them is very substantial and is indicated in part by the type of parameter update law and the corresponding proof of stability and convergence. Recursive design procedures, referred to as backstepping, extend the applicability of Lyapunov-based designs to nonlinear systems [3, 7, 8, 11]. Backstepping designs are flexible and do not force the designed system to appear linear. They can also avoid cancellation of useful nonlinearities and often introduce additional nonlinear terms to improve transient performance. The idea of backstepping is to recursively design a controller by considering some of the state variables as “virtual controls” and designing for them intermediate control laws. When trying to deal with unknown parameters a conflict will exist between virtual controls and parameter update laws that could be sorted out using adaptive backstepping techniques [11]. The chemical reactor model considered in this paper is assumed to be time-invariant. When time delays and time-dependent disturbances are in effect, flatness-based control, time-varying feedforward, and other adaptive techniques can be used [2-14]. Addressing uncertainties and their effect on the closed-loop performance has been an active area of research that often led to the design of tracking controllers with the purpose of minimizing the effect of these uncertainties on the output. A variety of techniques have been developed such as adaptive nonlinear control [3], nonlinear robust control using Lyapunov-based techniques [2], and model predictive control [15]. Intelligent control methods, based on artificial neural networks and fuzziness, are also found in the literature that rely on black-box modeling in an attempt to capture the nonlinear behavior of the system in terms of look-up tables and/or complex interconnections [16]. State feedback controllers are sometimes not suited for practical applications, as some of the states might not be available for direct measurements. Major contributions to overcome such difficulties are reported that use, some way or another, a controller-observer combination [17-21]. In this paper an attempt is made to make use of the advantages of both backstepping and Lyapunov-based techniques to design a robust controller. In the following, section 2 introduces the model of the system, while section 3 investigates the controller design.

2. MATHEMATICAL MODEL OF A CHEMICAL REACTOR

Fig. 1 shows a continuous stirred tank reactor (CSTR). It's a jacketed-type reactor, and it's assumed that [1]:

1. both the reactor and the jacket are perfectly mixed,
2. volumes and physical properties are constant, and
3. heat losses are neglected.

It is required to control the temperature of the reactor via adjusting the position of the control valve. The reactor is subjected to various kinds of disturbances such as the feed rate and ambient temperature fluctuations. The valve has equal percentage dynamics that adds to the nonlinear behavior of the model.

2.1 Model Equations

The system has a total of four states; x , and a single output; y , given by:

$$X = [x_1 \ x_2 \ x_3 \ x_4]^T = [C_A \ T \ T_c \ b]^T \text{ and } y = [0 \ 1 \ 0 \ 0]X \quad (1)$$

where X is defined in Table 1. The model of the chemical reactor has state variables as well as auxiliary variables that can be calculated. Some of the auxiliary variables are more relevant in analyzing the controller performance than some of the state variables. A complete description of the parameters involved in deriving the mathematical model of the chemical reactor [1], their units, as well as their nominal values is given in Table 1.

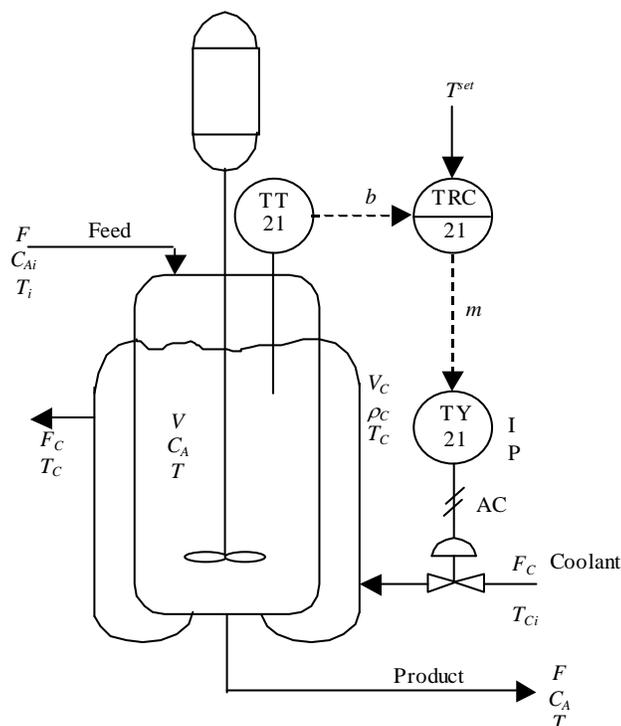


Fig. 1: A Continuous Stirred Tank Reactor

 Table 1
 System Parameters

| # | Parameter | Definition | Value |
|----|--------------|---|----------|
| 1 | C_A | Reactant concentration | |
| 2 | T | Reactor temperature | |
| 3 | T_C | Jacket temperature | |
| 4 | b | Normalized TT signal | |
| 5 | C_{Ai} | Concentration of the reactant in the feed | 2.88 |
| 6 | T_i | Feed temperature | 66 |
| 7 | T_{Ci} | Coolant inlet temperature | 27 |
| 8 | F | Feed rate | 7.5 E-3 |
| 9 | V | Reactor volume | 7.08 |
| 10 | k_0 | Arrhenius frequency parameter | 7.44 E-2 |
| 11 | ΔH_R | Heat reaction | -9.86 E7 |
| 12 | ρ | Reactant density | 19.2 |
| 13 | C_P | Reactant heat capacity | 1.815 E5 |
| 14 | U | Overall heat transfer coefficient | 3.55 E3 |
| 15 | A | Heat transfer area | 5.4 |
| 16 | V_C | Jacket volume | 1.82 |
| 17 | ρ_C | Density of the coolant | 1000 |
| 18 | C_{PC} | Coolant heat capacity | 4.184 E3 |
| 19 | ΔT_T | TT calibrated range | 20 |
| 20 | T_M | Lower limit of TT | 80 |
| 21 | F_C | Coolant rate | |
| 22 | τ_T | TT time constant | 20 |
| 23 | m | Normalized controller output | |
| 24 | F_{Cmax} | Maximum flow through the control valve | 0.02 |
| 25 | α | Valve rangeability parameter | 50 |
| 26 | E | Reaction activation energy | 1.182 E7 |
| 27 | R | Ideal gas law constant | 8314.39 |

In practice the system parameters are obtained from equipment specifications and from piping and instrumentation diagrams. The input variables that affect the operation of the reactor are F , C_{Ai} , T_{Ci} and T_i . These variables may be considered as disturbances and some of them may be uncertain. A robust design should guarantee a satisfactory performance over the whole range of uncertainty. Also, in order for the analysis to be complete, a sensitivity study should be carried out. For practical reasons, both the measured variable; b , and the control signal; m , are calculated in a percentage format such that:

$$0 \leq b, m \leq 1 \quad (2)$$

where 0% indicates fully open position and 100% indicates fully closed position.

2. Derivation of Model Equations

The model equations can be subdivided into five different categories. These categories are described as follows:

- Balance of mass of reactant A:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{Ai} - C_A) - k_0 e^{-\frac{E}{R(T+273.16)}} C_A^2 \quad (3)$$

- Energy balance on reactor contents:

$$\frac{dT}{dt} = \frac{F}{V}(T_i - T) - \frac{\Delta H_R}{\rho C_P} k_0 e^{-\frac{E}{R(T+273.16)}} C_A^2 - \frac{UA}{V\rho C_P}(T - T_C) \quad (4)$$

- Energy balance on jacket:

$$\frac{dT_C}{dt} = \frac{UA}{V_C \rho_C C_{PC}}(T - T_C) - \frac{F_C}{V_C}(T_C - T_{Ci}) \quad (5)$$

- Temperature sensor dynamics:

$$\frac{db}{dt} = \frac{1}{\tau_T} \left(\frac{T - T_m}{\Delta T_T} - b \right) \quad (6)$$

- Valve dynamics:

$$F_C = F_{C_{\max}} \alpha^{-m}, \quad 0 \leq m \leq 1 \quad (7)$$

Thus the system is seen to be fourth order and heavily nonlinear. The idea is to regulate the output to a set point temperature ($T^{set} = 88$) using only one control signal, which is the signal applied to the control valve.

3. CONTROL STRATEGY

It is very obvious, from the model of the chemical reactor, that the system has many parameters, some of them are uncertain. Usually, a PID controller is considered to be a good candidate for such applications because of its simplicity and self-correction mechanism. Unfortunately one PID set will not result in a satisfactory performance for different operating conditions. Backstepping techniques could be used where some of the systems variables could be used as virtual controls [22]. An advantage of this technique is that the system could be forced to

follow prescribed dynamics in a model-reference-like behavior [23]. Also since all the system variables and parameters are easily measured using simple sensors, a feedforward control action could be also incorporated to cancel any unwanted disturbances and to sense any crucial environmental changes. The detailed control strategy is given by:

1. Analyzing the model, and deciding on the equilibrium values assuming the steady state value of the output, T , will asymptotically approach T^{set} . This will involve solving Eq.s (1-5) for the steady state values of C_A , T_C , b and m .
2. Using the results of step one to perform a linear transformation in the states such that the equilibrium point is shifted to the origin, i.e.:

$$\begin{aligned} x_i &\leftarrow x_i - x_{ieq} \quad , \quad e_i = x_i \quad , \quad i = 1, 2, 3, 4 \\ m &\leftarrow m - m_{eq} \quad , \quad u = m \end{aligned} \quad (8)$$

where the subscript “*eq*” stands for equilibrium.

3. Using backstepping, some of the states will be used as virtual controls for the output. The system can be formulated as follows:

$$e_2 = x_2 - x_{2eq} \quad , \quad \text{and} \quad \left\{ \begin{array}{l} x_{ides} = \left(\sum_{j=1}^4 c_{ij} e_j \right) + x_{ieq} \quad , \quad i = 1, 3, 4 \\ e_j = x_j - x_{jdes} \quad , \quad j = 1, 3, 4 \end{array} \right\} \quad (9)$$

where the subscript “*des*” stands for desired, and the c 's are design parameters.

4. Formulating the new system space expressing all the system states in terms of e and \dot{e} by using Eq. (9) to back substituting for all x 's.
5. Constructing a Lyapunov function and its derivative using:

$$V = \frac{1}{2} \sum_{i=1}^4 k_i e_i^2 \quad , \quad k_i > 0 \quad \text{and} \quad \dot{V} = \sum_{i=1}^4 k_i e_i \dot{e}_i \quad (10)$$

6. Solving for the control signal, u , to achieve negative definiteness of \dot{V} in terms of c 's and k 's. Auxiliary design parameters may be added if needed. The overparameterized design should be analyzed carefully to ensure both design simplicity and performance superiority.
7. The designed controller should be compared to a standard PID controller to highlight advantages and disadvantages of the proposed design.

3.1 Equilibrium Conditions

It is required to calculate the initial conditions of the system as well as the equilibrium conditions at steady state. The state equations of the system are given by:

$$\dot{X} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} = \begin{bmatrix} \frac{F}{V}(C_{Ai} - x_1) - k_0 e^{-\frac{E}{R(x_2+273.16)}} x_1^2 \\ \frac{F}{V}(T_i - x_2) - \frac{\Delta H_R}{\rho C_P} k_0 e^{-\frac{E}{R(x_2+273.16)}} x_1^2 - \frac{UA}{V\rho C_P}(x_2 - x_3) \\ \frac{UA}{V_C \rho_C C_{PC}}(x_2 - x_3) - \frac{F_{Cmax}}{V_C} \alpha^{-u}(x_3 - T_{Ci}) \\ \frac{1}{\tau_T} \left(\frac{x_2 - T_m}{\Delta T_T} - x_4 \right) \end{bmatrix} \quad (11)$$

The conditions for equilibrium are given by:

$$\dot{x}_i = 0, \quad i = 1, 2, 3, 4 \quad \text{and} \quad y = x_2 = T_{des} \quad (12)$$

Since it is required to solve for the four states of the system; X , as well as the control signal; u , the following assumption is made in order to have a consistent set of equations:

$$x_2 = T^{set} \quad (13)$$

The following set of equations must be solved in sequence in order to arrive at the correct values of the equilibrium points:

$$x_4 = \frac{x_2 - T_M}{\Delta T_T} = \frac{T^{set} - T_M}{\Delta T_T} \quad (14)$$

First using the following notations:

$$k = k_0 e^{-\frac{E}{R(x_2+273.16)}} \quad \text{and} \quad k_{eq} = k_0 e^{-\frac{E}{R(T^{set}+273.16)}} \quad (15)$$

where, again, “eq” denotes equilibrium, we can arrive at the following, by manipulating Eq. (11):

$$x_1 = \frac{-F + \sqrt{F^2 + 4k_{eq} F V C_{Ai}}}{2k_{eq} V} \quad (16)$$

and:

$$x_3 = \frac{\rho C_P}{UA} \left[\left(F + \frac{UA}{\rho C_P} \right) x_2 - F T_i + \frac{\Delta H_R V}{\rho C_P} k_{eq} x_1^2 \right] \quad (17)$$

In addition, using:

$$F_C = \frac{UA}{\rho_c C_{PC}} \frac{x_2 - x_3}{x_3 - T_{Ci}} \quad (18)$$

we have:

$$u = -\ln\left(\frac{F_C}{F_{C_{\max}}}\right) / \ln(\alpha) \tag{19}$$

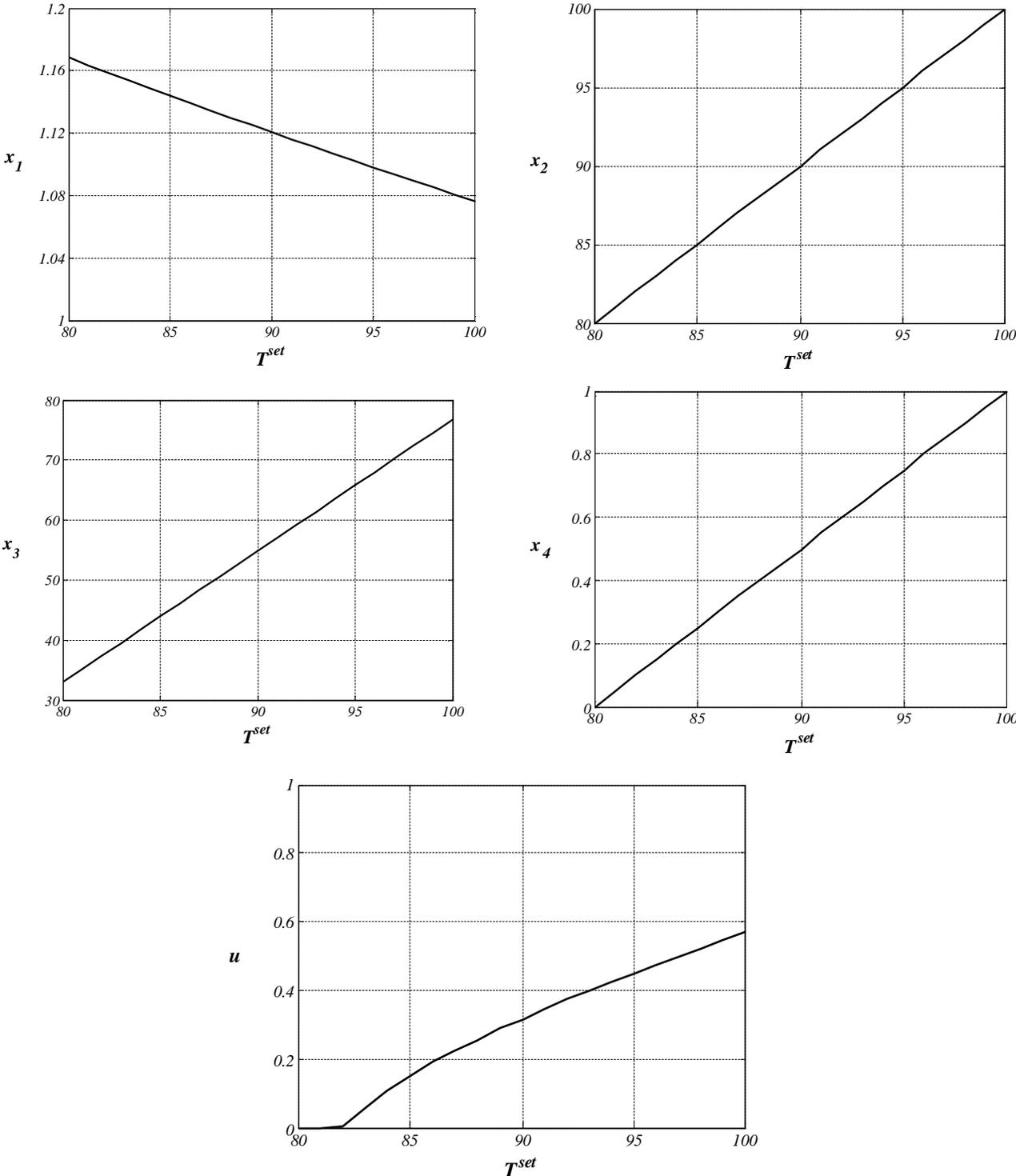


Fig. 2: Equilibrium Conditions

Fig. 2 shows the equilibrium points of the model as a function of the temperature set point; T^{set} . Thus, it is quite obvious that:

1. the system has a smooth transition.
2. no singularities exist
3. the system has a unique equilibrium point for each value of T^{set} .
4. saturation of the control signal can be easily avoided.

The effect of the operation parameters, i.e. F , C_{Ai} , T_{ci} and T_i can be practically neglected since these parameters are easily measured. To ensure system controllability the condition $0 \leq u \leq 1$ must be guaranteed.

3.2 State Transformation

As seen from the previous section, the system has an equilibrium state that does not coincide with the origin of the state space describing the model. Thus it is necessary to shift this point to the origin in order to be able to use a Lyapunov-based design when solving for the control signal; u . Since we are interested in controlling the temperature of the reactor, x_2 will be the most crucial state to deal with. A virtual error is introduced as follows:

$$e_2 = x_2 - x_{2cq} \tag{20}$$

This virtual error will be used as a virtual control in order to drive other states to their equilibrium points. Using:

$$x_{ides} = c_{i2}e_2 + x_{ieq} \quad , \quad i = 1, 2, 3, 4 \quad \text{and} \quad c_{22} = 0 \tag{21}$$

and

$$e_i = x_i - x_{ides} \tag{22}$$

we have:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix} + \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} e_2 + \begin{bmatrix} x_{1eq} \\ x_{2eq} \\ x_{3eq} \\ x_{4eq} \end{bmatrix} \tag{23}$$

From which, the following could be obtained:

$$\begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} - \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} e_2 - \begin{bmatrix} x_{1eq} \\ x_{2eq} \\ x_{3eq} \\ x_{4eq} \end{bmatrix} \tag{24}$$

Thus:

$$\begin{bmatrix} \dot{e}_1 \\ \dot{e}_2 \\ \dot{e}_3 \\ \dot{e}_4 \end{bmatrix} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} - \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} \dot{e}_2 \quad (25)$$

Using Eq.s (11) and (20) an explicit expression for \dot{e}_2 could be obtained as shown in Eq. (26). This expression will be used for the subsequent derivation of the derivatives of the remaining virtual errors.

$$\dot{e}_2 = \dot{x}_2 = \frac{FT_i}{V} - \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) + \frac{UA}{V\rho C_P} (e_3 + c_{32}e_2 + x_{3eq}) - \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \quad (26)$$

Now using Eq.s (11), (21) and (26), we can arrive at the expressions given in Eq.s (27-29).

$$\begin{aligned} \dot{e}_1 = \dot{x}_1 - c_{12}\dot{e}_2 &= \left\{ \frac{FC_{Ai}}{V} - \frac{F}{V} (e_1 + c_{12}e_2 + x_{1eq}) - \bar{k} (e_1 + c_{12}e_2 + x_{1eq})^2 \right\} - c_{12}\dot{e}_2 \\ &= \frac{FC_{Ai}}{V} - \frac{F}{V} (e_1 + c_{12}e_2 + x_{1eq}) - \bar{k} (e_1 + c_{12}e_2 + x_{1eq})^2 - c_{12} \frac{FT_i}{V} + c_{12} \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) \\ &\quad - c_{12} \frac{UA}{V\rho C_P} (e_3 + c_{32}e_2 + x_{3eq}) + c_{12} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \end{aligned} \quad (27)$$

$$\begin{aligned} \dot{e}_3 = \dot{x}_3 - c_{32}\dot{e}_2 &= \left\{ \frac{UA}{V_C \rho C_{Pc}} (e_2 + x_{2eq}) - \frac{UA}{V_C \rho C_{Pc}} (e_3 + c_{32}e_2 + x_{3eq}) - \frac{F_{C_{max}}}{V_C} (e_3 + c_{32} + x_{3eq} - T_{Ci}) \alpha^{-u} \right\} - c_{32}\dot{e}_2 \\ &= \frac{UA}{V_C \rho C_{Pc}} (e_2 + x_{2eq}) - \frac{UA}{V_C \rho C_{Pc}} (e_3 + c_{32} + x_{3eq}) - \frac{F_{C_{max}}}{V_C} (e_3 + c_{32} + x_{3eq} - T_{Ci}) \alpha^{-u} - c_{32} \frac{FT_i}{V} \\ &\quad + c_{32} \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) - c_{32} \frac{UA}{V\rho C_P} (e_3 + c_{32}e_2 + x_{3eq}) + c_{32} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \end{aligned} \quad (28)$$

$$\begin{aligned} \dot{e}_4 = \dot{x}_4 - c_{42}\dot{e}_2 &= \left\{ -\frac{T_M}{\tau_T \Delta T_T} + \frac{1}{\tau_T \Delta T_T} (e_2 + x_{2eq}) - \frac{1}{\tau_T} (e_4 + c_{42}e_2 + x_{4eq}) \right\} - c_{42}\dot{e}_2 \\ &= -\frac{T_M}{\tau_T \Delta T_T} + \frac{1}{\tau_T \Delta T_T} (e_2 + x_{2eq}) - \frac{1}{\tau_T} (e_4 + c_{42}e_2 + x_{4eq}) - c_{42} \frac{FT_i}{V} + c_{42} \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) \\ &\quad - c_{42} \frac{UA}{V\rho C_P} (e_3 + c_{32}e_2 + x_{3eq}) + c_{42} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \end{aligned} \quad (29)$$

where

$$\bar{k} = k_0 e^{-\frac{E}{R(e_2 + x_{2eq}) + 273.16}} \quad (30)$$

Using Eq. (10), we have:

$$\dot{V} = \dot{V}(e_1, e_2, e_3, e_4) = \sum_{i=1}^4 k_i e_i \dot{e}_i \quad (31)$$

or:

$$\begin{aligned} \dot{V} = & k_1 \left\{ \frac{FC_{Ai}}{V} e_1 - \frac{F}{V} e_1 (e_1 + c_{12} e_2 + x_{1eq}) - \bar{k} (e_1 + c_{12} e_2 + x_{1eq})^2 e_1 - c_{12} \frac{FT_i}{V} e_1 + c_{12} e_1 \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) \right\} \\ & - c_{12} \frac{UA}{V\rho C_P} (e_3 + c_{32} e_2 + x_{3eq}) e_1 + c_{12} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12} e_2 + x_{1eq})^2 e_1 \\ & + k_2 \left\{ \frac{FT_i}{V} - \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) + \frac{UA}{V\rho C_P} (e_3 + c_{32} e_2 + x_{3eq}) - \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12} e_2 + x_{1eq})^2 \right\} \\ & + k_3 \left\{ \frac{UA}{V_C \rho C_C C_{Pc}} (e_2 + x_{2eq}) - \frac{UA}{V_C \rho C_C C_{Pc}} (e_3 + c_{32} e_2 + x_{3eq}) - \frac{F_{C_{max}}}{V_C} (e_3 + c_{32} e_2 + x_{3eq} - T_{Ci}) \alpha^{-u} - c_{32} \frac{FT_i}{V} \right\} \\ & + c_{32} \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) - c_{32} \frac{UA}{V\rho C_P} (e_3 + c_{32} e_2 + x_{3eq}) + c_{32} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12} e_2 + x_{1eq})^2 \\ & + k_4 \left\{ -\frac{T_M}{\tau_T \Delta T_T} + \frac{1}{\tau_T \Delta T_T} (e_2 + x_{2eq}) - \frac{1}{\tau_T} (e_4 + c_{42} e_2 + x_{4eq}) - c_{42} \frac{FT_i}{V} + c_{42} \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) (e_2 + x_{2eq}) \right\} \\ & - c_{42} \frac{UA}{V\rho C_P} (e_3 + c_{32} e_2 + x_{3eq}) + c_{42} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12} e_2 + x_{1eq})^2 \end{aligned} \quad (32)$$

As seen from Eq. (32), forcing \dot{V} to be negative definite will not be straightforward due to its very complex structure. Careful analysis of the mathematical expression for \dot{V} reveals that it could be made simpler by canceling some, if not all, the exponential terms. The design parameter c_{12} could serve this purpose by letting the terms containing \bar{k} in the first bracket in Eq. (32) go to zero as illustrated in Eq. (33):

$$k_1 \bar{k} (e_1 + c_{12} e_2 + x_{1eq})^2 e_1 \left[c_{12} \frac{\Delta H_R}{\rho C_P} - 1 \right] = 0 \quad (33)$$

Now solving for the required value of c_{12} results in:

$$c_{12} = \frac{\rho C_P}{\Delta H_R} \quad (34)$$

Substituting Eq. (34) in Eq. (32), a more rigorous expression for \dot{V} can be obtained as illustrated in Eq. (35).

$$\begin{aligned}
 \dot{V} = & k_1 \left\{ -e_1^2 \left[\frac{F}{V} \right] + e_1 \left[\frac{F}{V} (C_{Ai} - c_{12}T_i) - \frac{F}{V} (x_{1eq} + c_{12}x_{2eq}) - c_{12} \frac{UA}{V\rho C_P} (x_{2eq} + x_{3eq}) \right] \right\} \\
 & - e_1 e_2 \left[\frac{2F}{V} c_{12} + \frac{UA}{V\rho C_P} (1 + c_{12} + c_{32}) \right] - e_1 e_3 \left[c_{12} \frac{UA}{V\rho C_P} \right] \\
 & + k_2 \left\{ -e_2^2 \left[\frac{F}{V} + \frac{UA}{V\rho C_P} (1 - c_{32}) \right] + e_2 \left[\frac{F}{V} (T_i - x_{2e}) - \frac{UA}{V\rho C_P} (x_{2eq} - x_{3eq}) - \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \right] \right\} \\
 & + e_2 e_3 \left[\frac{UA}{V\rho C_P} \right] \\
 & + k_3 \left\{ -e_3^2 \left[\frac{UA}{V_C \rho_C C_{Pc}} + c_{32} \frac{UA}{V\rho C_P} \right] + e_2 e_3 \left[\frac{UA}{V_C \rho_C C_{Pc}} (1 - c_{32}) + c_{32} \left(\frac{F}{V} + \frac{UA}{V\rho C_P} \right) - c_{32}^2 \left(\frac{UA}{V\rho C_P} \right) \right] \right\} \\
 & - \frac{F_{C_{max}}}{V_C} (e_3 + c_{32}e_2 + x_{3eq} - T_{Ci}) \alpha^{-u} \\
 & + e_3 \left[\frac{UA}{V_C \rho_C C_{Pc}} (x_{2eq} - x_{3eq}) + \frac{F}{V} c_{32} (T_i - x_{2eq}) + \frac{UA}{V\rho C_P} c_{32} (x_{2eq} - x_{3eq}) + c_{32} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \right] \\
 & + k_4 \left\{ -e_4^2 \left(\frac{1}{\tau_T} \right) + e_2 e_4 \left[\frac{1}{\tau_T \Delta T_T} - c_{42} \left(\frac{1}{\tau_T} - \frac{F}{V} \right) + \frac{UA}{V\rho C_P} c_{42} (1 - c_{32}) \right] - e_3 e_4 \left[-\frac{UA}{V\rho C_P} c_{42} \right] \right\} \\
 & + e_4 \left[\frac{1}{\tau_T \Delta T_T} (x_{2eq} - T_M) - \frac{x_{4eq}}{\tau_T} - c_{42} \frac{F}{V} (T_i - x_{2eq}) + \frac{UA}{V\rho C_P} c_{42} (x_{2eq} - x_{3eq}) + c_{42} \frac{\Delta H_R \bar{k}}{\rho C_P} (e_1 + c_{12}e_2 + x_{1eq})^2 \right]
 \end{aligned} \tag{35}$$

Careful analysis of Eq. (35) shows that negative definiteness of \dot{V} could be ensured by making all coefficients of the terms containing e_i^2 , $i = 1, 2, 3$ and 4 , negative and all remaining terms to be non positive. It should be emphasized that this is just one possible solution. In fact the non-uniqueness of a solution for the equation $\dot{V} \leq 0$, that adds more flexibility in choosing the control law, comes at the price of having to experiment many possible solutions to arrive at the best one.

Referring to the term containing e_2^2 in Eq. (35), we must have the following condition to establish negative definiteness of \dot{V} , and hence global stability of the system:

$$\frac{F}{V} + \frac{UA}{\rho C_P} (1 - c_{32}) \geq 0 \tag{36}$$

or

$$\frac{UA}{\rho C_P} c_{32} \leq F + \frac{UA}{\rho C_P} \quad (37)$$

From which:

$$c_{32} < \left(1 + \frac{UA}{\rho C_P} F \right) \quad (38)$$

resulting in:

$$c_{32} \leq 1 + \frac{UA}{\rho C_P} F_{\min} \quad (39)$$

where F_{\min} is the minimum value for the feed rate.

Eq. (39) guarantees robustness of the design as it is shown to be effective for the whole range of expected feed rates for the chemical reactor. Further investigation of Eq. (35) shows that the term $e_2 e_4$ could be made zero as follows:

$$\frac{1}{\tau_T \Delta T_T} - c_{42} \left(\frac{1}{\tau_T} - \frac{F}{V} \right) + \frac{UA}{V \rho C_P} c_{42} (1 - c_{32}) = 0 \quad (40)$$

or

$$\frac{1}{\tau_T \Delta T_T} = c_{42} \left[\left(\frac{1}{\tau_T} - \frac{F}{V} - \frac{UA}{V \rho C_P} \right) + c_{32} \frac{UA}{V \rho C_P} \right] \quad (41)$$

From which the following choice of c_{42} will be necessary to cancel the $e_2 e_4$ term in order to simplify Eq. (35):

$$c_{42} = \frac{1}{\tau_T \Delta T_T \left[\left(\frac{1}{\tau_T} - \frac{F}{V} - \frac{UA}{V \rho C_P} \right) + c_{32} \frac{UA}{V \rho C_P} \right]} \quad (42)$$

Now assuming all the terms containing u and the combination $e_i e_j$, $i \neq j$, $i, j = 1, 2, 3$, and 4 could have minimum effect on the dominant behavior of Eq. (35) and using the maximum value for c_{32} , the following expression is obtained for \dot{v} :

$$\dot{v} = - \left\{ \left[\frac{k_1 F}{C} \right] e_1^2 + \left[\frac{k_2}{V} (F - F_{\min}) \right] e_2^2 + \left[k_3 UA \left(\frac{1}{V_C \rho C_{Pc}} + \frac{c_{32}}{V \rho C_P} \right) \right] e_3^2 + \left[\frac{k_4}{\tau_T} \right] e_4^2 \right\} + \varepsilon(e_1, e_2, e_3, e_4) \quad (43)$$

where $\varepsilon(e_1, e_2, e_3, e_4)$ is a residual function that can be adjusted to have a negligible effect on the first term in Eq. (43) via properly choosing the gains of Eq. (31). In addition, the rate of decay of the individual virtual errors could be adjusted as well.

3.3 Solving for u

There are many ways to solve for the control signal. The only restriction imposed on the design process is to make sure that stability is guaranteed via forcing the gradient of the chosen Lyapunov function to be negative definite. Eq.s (34), (39) and (42) give the desired values for the control parameters c_{12} , c_{32} and c_{42} respectively. These values although simplify the design, waste some degree of flexibility in solving for the control signal as only the k 's values are now left for the sole purpose of having a satisfactory time response. In the following, different attempts are made to solve for u using different approaches. The advantages and disadvantages of each attempt are highlighted in order to arrive at the best technique.

3.3.1 Validating Feasibility of the Control law

Using Eq.s (34), (39), (42) and (43), we can define the following sub-functions in order to simplify the solution of the control signal:

$$f_{11} = f_{11}(k_1, e_1) = k_1 e_1 \left[\frac{F}{V} (C_{Ai} - c_{12} T_i - x_{1eq} - c_{12} x_{2eq}) - c_{12} \frac{UA}{V \rho C_p} (x_{2eq} + x_{3eq}) \right] \quad (44)$$

$$f_{112} = f_{112}(k_1, e_1, e_2) = -k_1 e_1 e_2 \left[\frac{2F}{V} c_{12} + \frac{UA}{V \rho C_p} (1 + c_{12} + c_{32}) \right] \quad (45)$$

$$f_{113} = f_{113}(k_1, e_1, e_3) = -k_1 e_1 e_3 \left[c_{12} \frac{UA}{V \rho C_p} \right] \quad (46)$$

$$f_{22} = f_{22}(k_2, e_2) = k_2 e_2 \left[\frac{F}{V} (T_i - x_{2eq}) - \frac{UA}{V \rho C_p} (x_{2eq} - x_{3eq}) - \frac{\Delta H_R}{\rho C_p} \bar{k} (e_1 + c_{12} e_2 + x_{1eq})^2 \right] \quad (47)$$

$$f_{223} = f_{223}(k_2, e_3) = k_3 e_2 e_3 \left[\frac{UA}{V \rho C_p} \right] \quad (48)$$

$$\begin{aligned} f_{33} &= f_{33}(k_3, e_3) \\ &= k_3 e_3 \left[\frac{UA}{V_C \rho_C C_{pC}} (x_{2eq} - x_{3eq}) - \frac{F}{V} c_{32} (T_i - x_{2eq}) + \frac{UA}{V \rho C_p} c_{32} (x_{2eq} - x_{3eq}) + c_{32} \frac{\Delta H_R}{\rho C_p} \bar{k} (e_1 + c_{12} e_2 + x_{1eq})^2 \right] \end{aligned} \quad (49)$$

$$f_{323} = f_{323}(k_3, e_2, e_3) = k_3 e_2 e_3 \left[\frac{UA}{V_C \rho_C C_{pC}} (1 - c_{32}) + c_{32} \left(\frac{F}{V} + \frac{UA}{V \rho C_p} \right) - c_{32}^2 \left(\frac{UA}{V \rho C_p} \right) \right] \quad (50)$$

$$\begin{aligned} f_{44} &= f_{44}(k_4, e_4) \\ &= k_4 e_4 \left[\frac{1}{\tau_T \Delta T_T} (x_{2eq} - T_M) - \frac{x_{4eq}}{\tau_T} - c_{42} \frac{F}{V} (T_i - x_{2eq}) + \frac{UA}{V \rho C_p} c_{42} (x_{2eq} - x_{3eq}) + c_{42} \frac{\Delta H_R}{\rho C_p} \bar{k} (e_1 + c_{12} e_2 + x_{1eq})^2 \right] \end{aligned} \quad (51)$$

$$f_{434} = f_{434}(k_4, e_3, e_4) = -k_4 e_3 e_4 \left[-\frac{UA}{V \rho C_p} c_{42} \right] \quad (52)$$

$$f_u = f_u(k_3, e_2, e_3, u) = -k_3 \frac{F_{C_{\max}}}{V_C} (e_3 + c_{32}e_2 + x_{3eq} - T_{Ci}) \quad (53)$$

and finally:

$$f_e = f_{11} + f_{112} + f_{113} + f_{22} + f_{223} + f_{33} + f_{323} + f_{44} + f_{434} \quad (54)$$

Thus, from Eq. (35),

$$f_e + f_u \alpha^{-u} \leq 0 \quad (55)$$

Eq. (55) should now be used in order to solve for the control signal; u . It is clear that a unique solution doesn't exist. One simple and direct solution is given by:

$$u = -\ln\left(-\frac{f_e}{f_u}\right) / \ln(\alpha) \quad (56)$$

However this solution might not always be feasible as non-real values for u could result because of the logarithmic nonlinearity of Eq. (56). One more problem of Eq. (56) is the possibility of singularities when all the virtual errors go to zero. Table 2 illustrates some of the possible scenarios. As indicated from the design analysis, the logarithmic nonlinearity complicates the design and even if the worst-case scenarios don't take place, the control action might be discontinuous causing rapid wear of the control valve and bad performance especially during transients. Also, because the control signal posses saturation nonlinearity, it's possible that u can result in the condition of having the valve always fully open or fully closed with no way to recover from these conditions as the control signal is not directly related to the error as in the case of a PID control. Also, according to the fifth case in Table 2, when all errors cease to zero, the control signal will reach a steady state that might not correspond to the required settling value, causing the errors to swing back and forth making the system unstable. In the following section a systematic methodology is introduced to overcome these problems while still using the same Lyapunov-based approach.

3.3.2 Derivation of the Control Law

By carefully examining the structure of Eq. (35), it's very obvious that we can manipulate the value of the control parameter, c_{32} , from Eq. (39) to arrive at the best results regarding minimizing the values of both f_u and f_e in Eq.s (53-54) respectively. By doing so, we can then decide on the values of the k 's to achieve the required decay rate of the virtual controls. This approach will guarantee the stability of the system as \dot{V} is always negative. The required control signal should always be feasible, hence the following structure of the control signal is proposed:

$$u = u_e + \delta(c, k)e_2 \quad (57)$$

where:

u_e : the equilibrium value of the control signal,

$\delta(c, k)$: a constant that depends on the choice of the design parameters.

It's very obvious that, if $\delta(c, k)$ is chosen to be zero, the controller reduces to the only the steady state value of the I-action of the well-known PID controller. Thus $\delta(c, k)$ acts as an adaptive proportional gain, whose value is chosen according to the required rate of decay of the virtual controls. Thus we can think of this approach as follows:

Table 2
Design Analysis

| Condition | f_e | f_u | Comments on choosing u |
|-----------|-------|-------|---|
| 1 | -ve | -ve | u is not feasible: let $u = u_{old}$, stability is guaranteed |
| 2 | -ve | 0 | u is feasible: let $u = 100\%$, stability is guaranteed |
| 3 | -ve | +ve | u is feasible, but system might be unstable if $f_u > f_e$ |
| 4 | 0 | -ve | u is feasible: let $u = 0\%$, stability is guaranteed |
| 5 | 0 | 0 | u is not feasible: let $u = u_{old}$, stability is guaranteed |
| 6 | 0 | +ve | u is not feasible, system might be unstable if $f_u \gg$ |
| 7 | +ve | -ve | u is feasible, but system might be unstable if $f_e > f_u$ |
| 8 | +ve | 0 | u is not feasible, system might be unstable if $f_e \gg$ |
| 9 | +ve | +ve | u is not feasible: let $u = u_{old}$, stability is not guaranteed |

where $u = u_{old}$ indicates maintaining the control signal at its latest feasibly-calculated value.

1. Propose the required virtual controls,
2. Choose a suitable decay rate for these virtual controls,
3. Use backstepping to control the required system output.

The designed control signal has the same structure as the well-known ($P+MR$) industrial controller. Since the MR value is a function of the system parameters, it is required to have accurate measurements of the uncertain variables. This is quite easy as measuring temperature and flow is very handy in chemical reactors. The following constraint must be considered when designing $\delta(c, k)$:

$$-u_e \leq \delta(c, k)e_2 \leq 1 - u_e \quad (58)$$

otherwise the system will be acting inside the saturation region and Eq. (34) will be no longer valid as a design tool. LMI techniques could then be used to study the sensitivity of the system stability with the control parameters to find out design range for all of them [8, 24]. Fig.s 3-5 show the response of the controlled system assuming the following design parameters:

- $c_{12} = -0.0353$, $c_{32} = 0$, $c_{42} = 0.0519$
- $k_1 = 1$, $k_2 = 1$, $k_3 = 1$, $k_4 = 1$, $\delta(c, k) = -0.005$.

It is quite obvious that the careful choice of the dynamic model for the virtual errors resulted in the zero-overshoot smooth response illustrated in Fig. 4. Thus the virtual system, implicitly introduced by the backstepping design, can also function in a similar way of the well-known model-reference controller which is an added advantage.

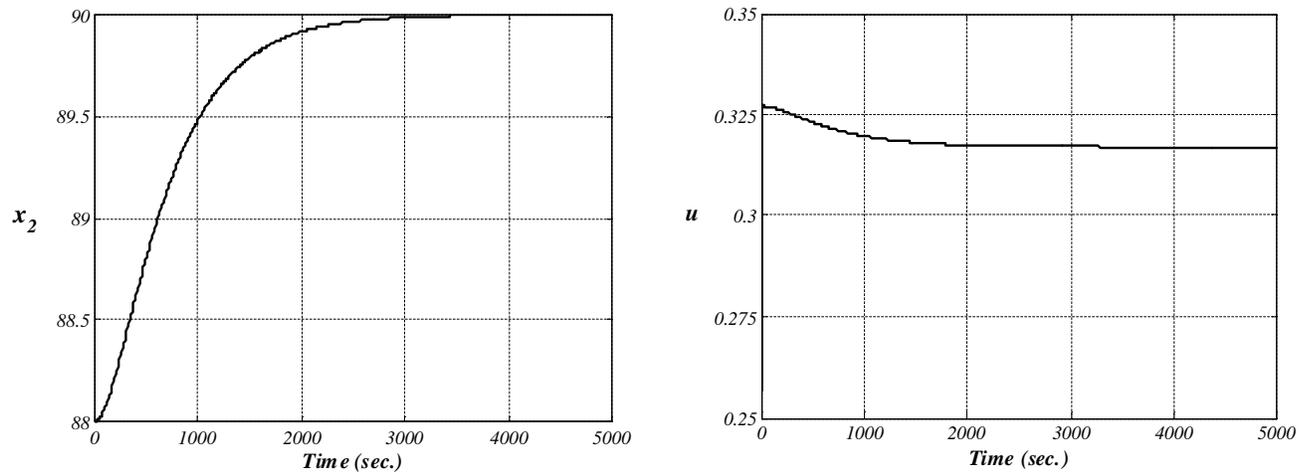


Fig. 3: Response Using the Backstepping Controller

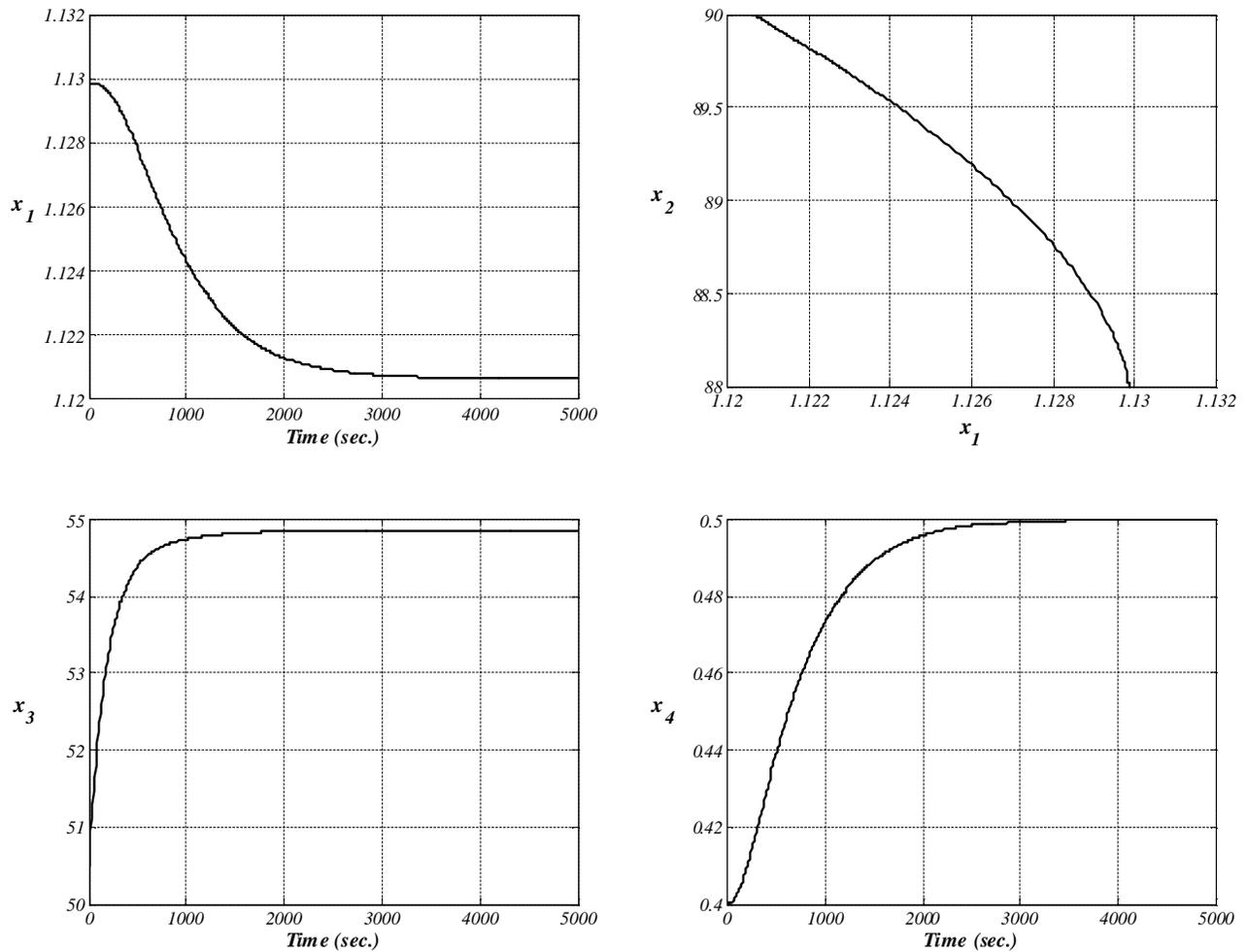


Fig. 4: The System States Using the Backstepping Controller

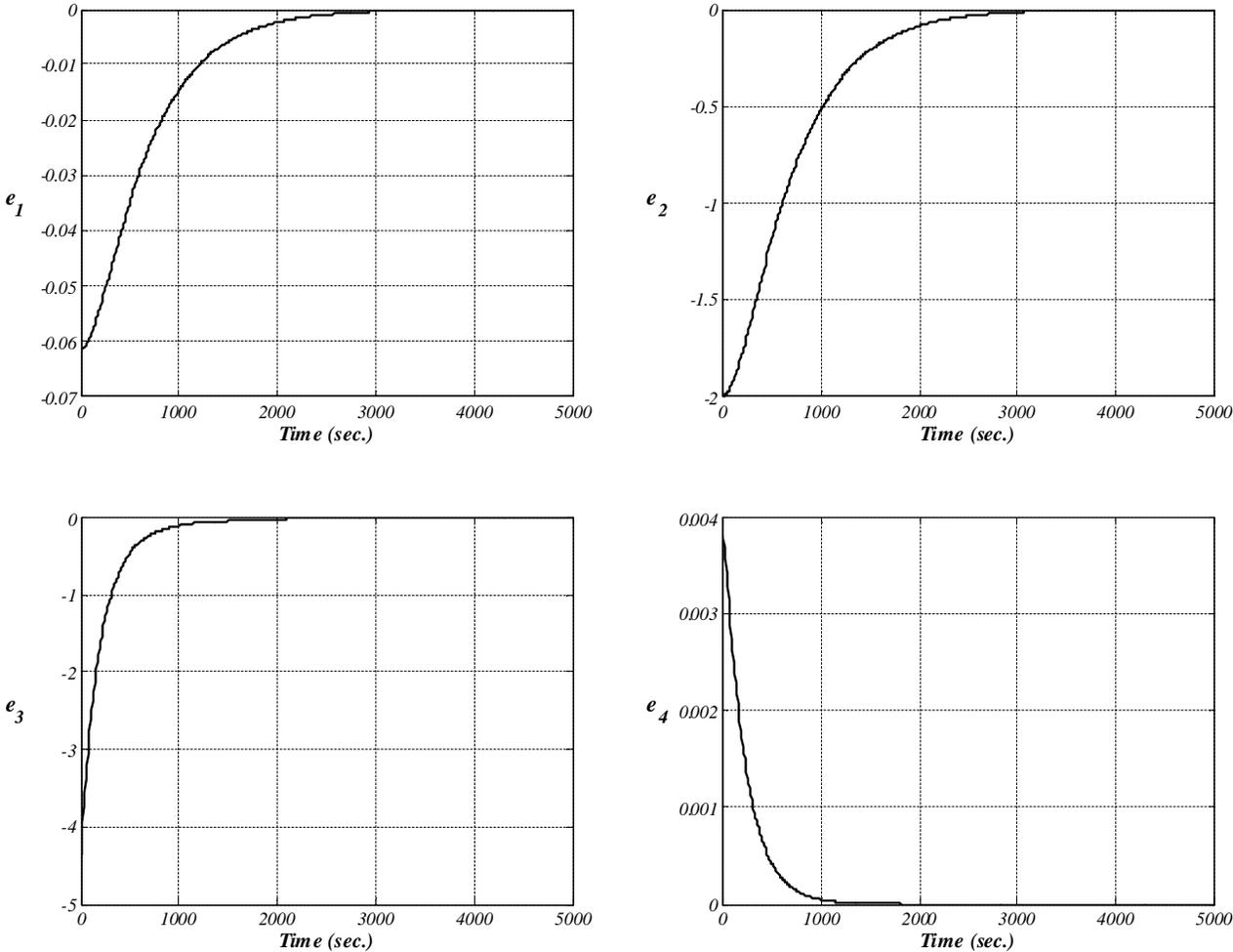


Fig. 5: Virtual Errors Using the Backstepping Controller

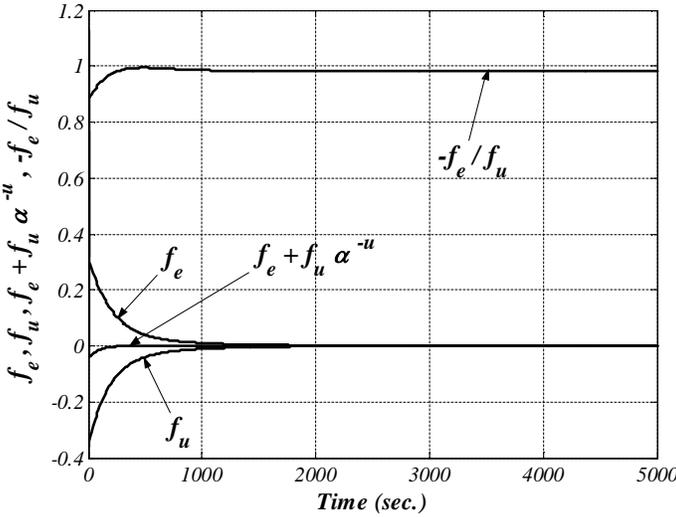


Fig. 6: Illustrations of the Lyapunov Sub-functions, f_e and f_u

Fig. 6 shows both f_u and f_e as given by Eq.s (53-54) respectively. It's quite obvious that:

$$f_e + f_u \alpha^{-u} \leq 0$$

$$0 < -\frac{f_e}{f_u} < 1$$

which implies that the design is successful as u is feasible and \dot{V} is negative definite.

Finally a sketch of both V and \dot{V} as functions of time is given in Fig. 7 which clearly shows that both of them are monotonous.

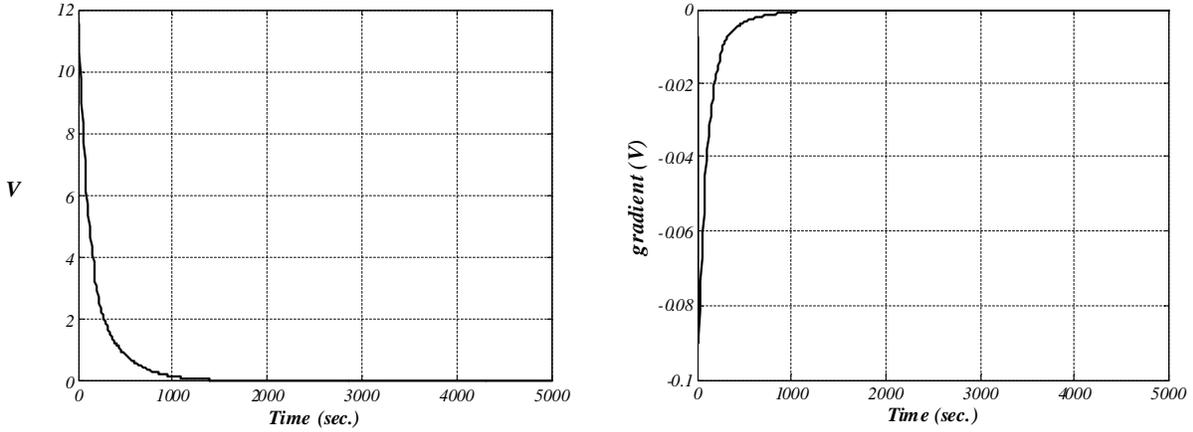


Fig. 7: Illustrations of the Lyapunov functions, V and \dot{V}

3.3.3 How to Choose $\mathcal{X}(c,k)$

By carefully inspecting the virtual errors illustrated in Fig. 5, we can arrive at the conclusion that e_2 and e_3 are the predominant ones as both e_1 and e_4 are very small. Since c_{22} is zero, c_{32} will be the most crucial design parameters assuming that the k 's will have these values:

$$k_1 = k_2 = 1000 \quad k_3 = k_4 = k \tag{59}$$

Thus with reference to Eq.s (34), (39) and (40), and the sample run simulated in Fig.s 3-7, we can propose the following:

$$\delta(c, k) = -0.04 \frac{c_{32}}{\sum_{i=1}^4 k} \tag{60}$$

where c_{32} is used to scale the adaptive proportional gain up, and k is used to compensate its effect, while maintaining k_3 at a comparatively small value to minimize the effect of e_3 and hence, avoiding oscillatory performance.

3.4 Conventional PID Control

In order to test the robustness of the controller designed in the previous section, a comparative study is made with a conventional PID controller assuming the following two conditions:

1. Ideal case (all model parameters are exact)

2. Disturbed case: some fluctuations in the model parameters, e.g.:

$$\beta_1 \leq \frac{F}{F_{nominal}}, \frac{C_{Ai}}{C_{Ai_{nominal}}}, \frac{T_{Ci}}{T_{Ci_{nominal}}}, \frac{T_i}{T_{i_{nominal}}} \leq \beta_2$$

$$0 \leq \beta_1 \leq 1, 1 \leq \beta_2 \leq 2$$
(61)

The following error signal is formulated between the desired set point, T^{set} , and the measured value, $b(t)$:

$$e(t) = \left(\frac{T^{set} - T_M}{\Delta T_T} \right) - b(t) = \left(\frac{T^{set} - T_M}{\Delta T_T} \right) - x_4(t)$$
(62)

Using only the proportional and integral actions, the control signal takes the standard form:

$$u(t) = K_P \left[e(t) + \frac{1}{\tau_I} \int_0^t e(t) dt \right]$$
(63)

The auxiliary state, $x(5)$, is now introduced in order to avoid having to deal with the integral term directly:

$$x_5 = \frac{K_P}{\tau_I} \int_0^t e(t) dt = \frac{K_P}{\tau_I} \int_0^t \left[\left(\frac{T^{set} - T_M}{\Delta T_T} \right) - x_4(t) \right] dt$$
(64)

This has the effect of increasing the overall order of the system. Eq. (65) is introduced to augment the state space representation of the system, hence raising its order to five:

$$\dot{x}_5 = \frac{K_P}{\tau_I} \left[\left(\frac{T^{set} - T_M}{\Delta T_T} \right) - x_4(t) \right]$$
(65)

This results in the following control signal:

$$u = \tau_I \dot{x}_5 + x_5$$
(66)

Hence, the complete system is given by:

$$\dot{X} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ \dot{x}_5 \end{bmatrix} = \begin{bmatrix} \frac{F}{V}(C_{Ai} - x_1) - \bar{k}x_1^2 \\ \frac{F}{V}(T_i - x_2) - \frac{\Delta H_R}{\rho C_P} \bar{k}x_1^2 - \frac{UA}{V\rho C_P}(x_2 - x_3) \\ \frac{UA}{V_C \rho_C C_{PC}}(x_2 - x_3) - \frac{F_{Cmax}}{V_C} \alpha^{-u}(x_3 - T_{Ci}) \\ \frac{1}{\tau_T} \left(\frac{x_2 - T_m}{\Delta T_T} - x_4 \right) \\ \frac{K_P}{\tau_I} \left[\left(\frac{T^{set} - T_M}{\Delta T_T} \right) - x_4(t) \right] \end{bmatrix}$$
(67)

3.4.1 Ideal Case

Using trial and error, or any of the available PID tuning methods, e.g. Ziegler-Nichols tuning method, the controller parameters, K_p and τ_p , could be found. Fig. 8 shows the complete response for the ideal case when the set point is raised from 88 °C to 90 °C in the absence of any disturbances. As shown in Fig. 8, the system has a satisfactory response with a 25% overshoot and settling time of approximately 30 minutes. The control signal is seen to be very smooth with no saturation ensuring both the causality of the control law and the durability of the control valve.

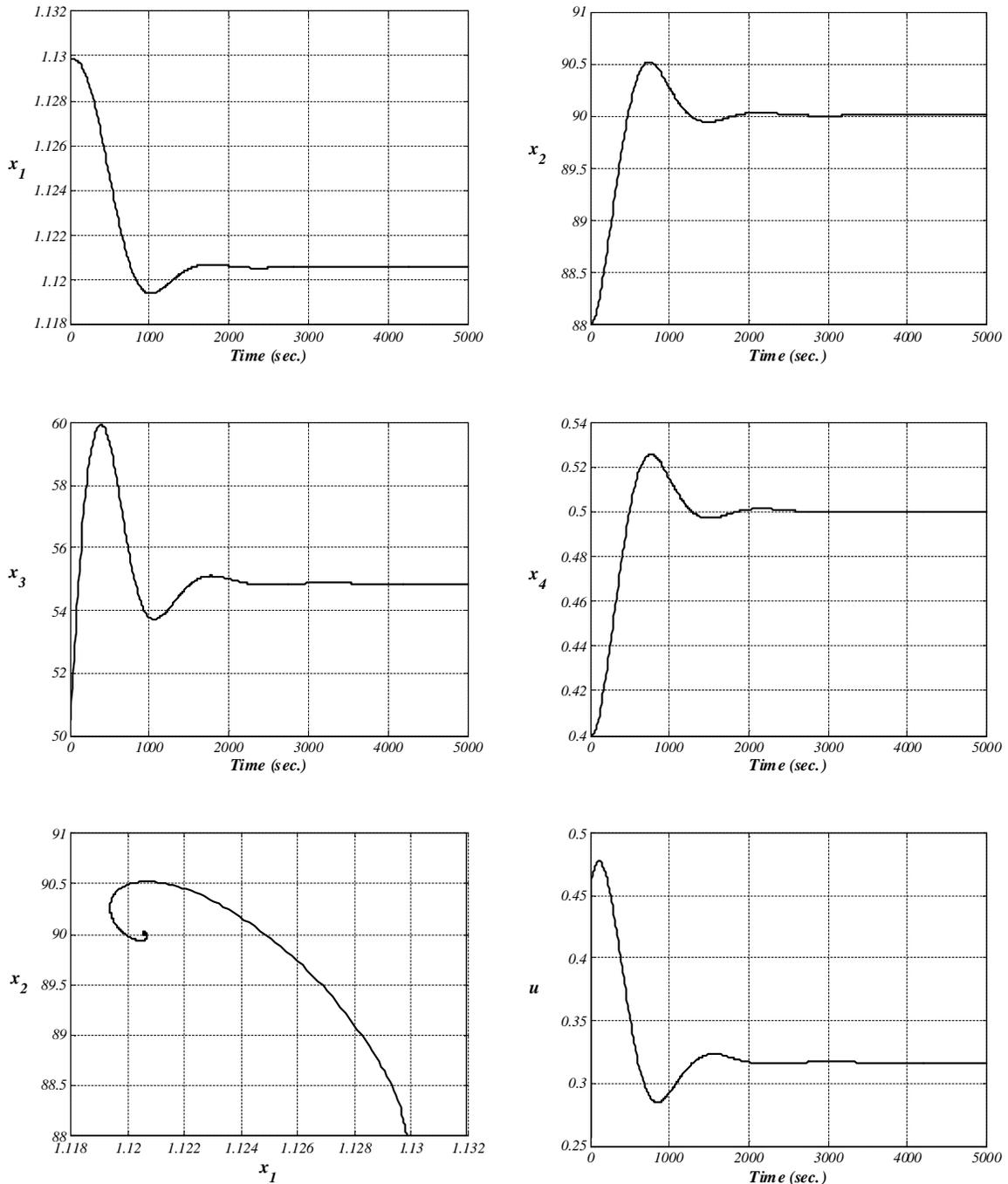


Fig. 8: PID Control Response ($K_p = 2$, $t_i = 600$) – Ideal Case

Although there exist tuning algorithms that can be used to obtain the PID controller parameters, they are very difficult to be used on practice because of the requirement to interactively experiment with the process [8]. A process operating in real-time is very difficult to be stopped or even interrupted, just to try a new parameters set for the controller. Ziegler-Nichols method, for example, requires either an open-loop test to capture the process signature or a closed-loop test to test the critical stability of the process. This is always a very difficult, if not impossible requirement that is always opposed by plant supervisors. Thus, we need to use virtual engineering to accomplish such task [6].

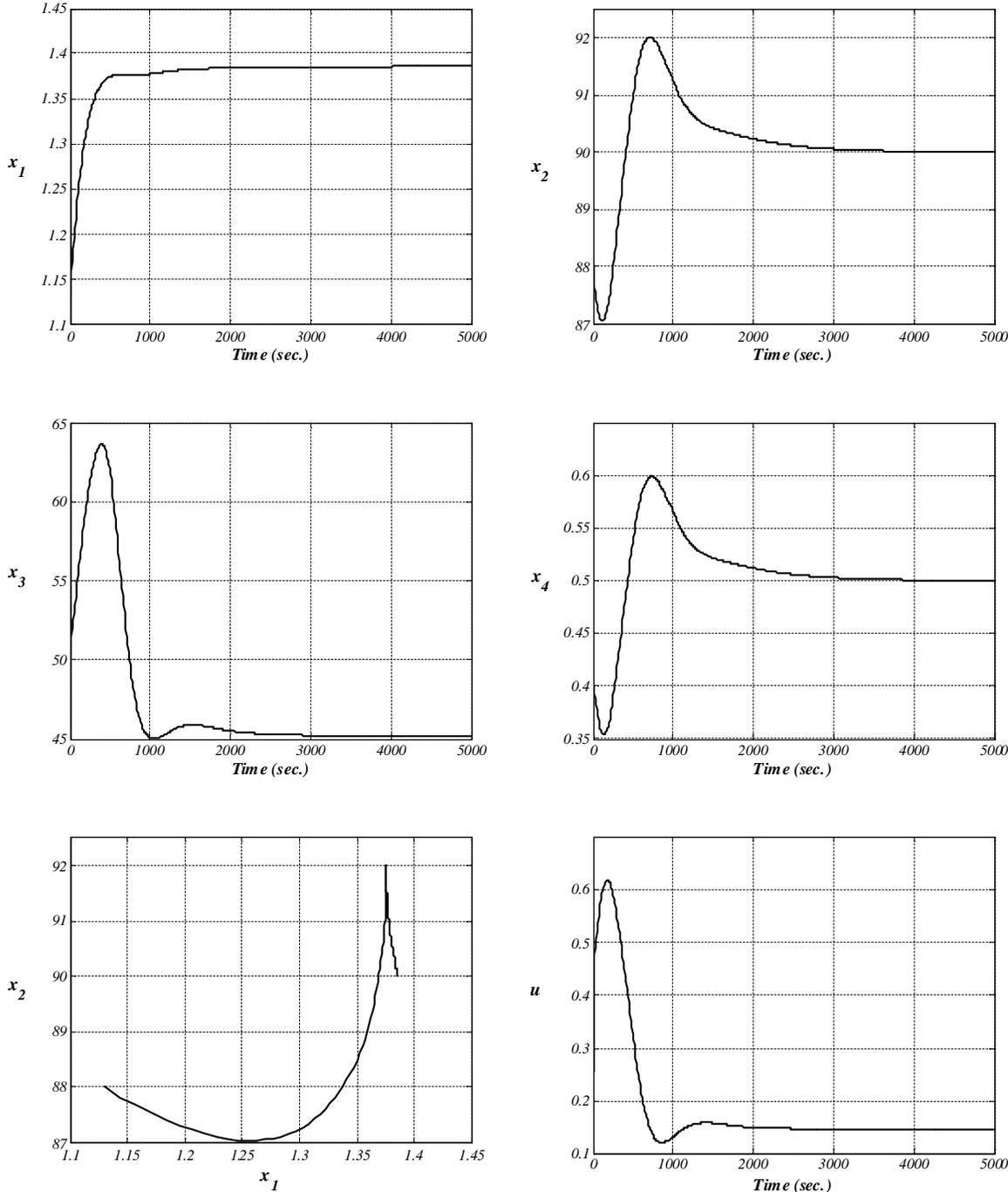


Fig. 9: PID Control Response ($K_p = 2, t_i = 600$) – Disturbed Case

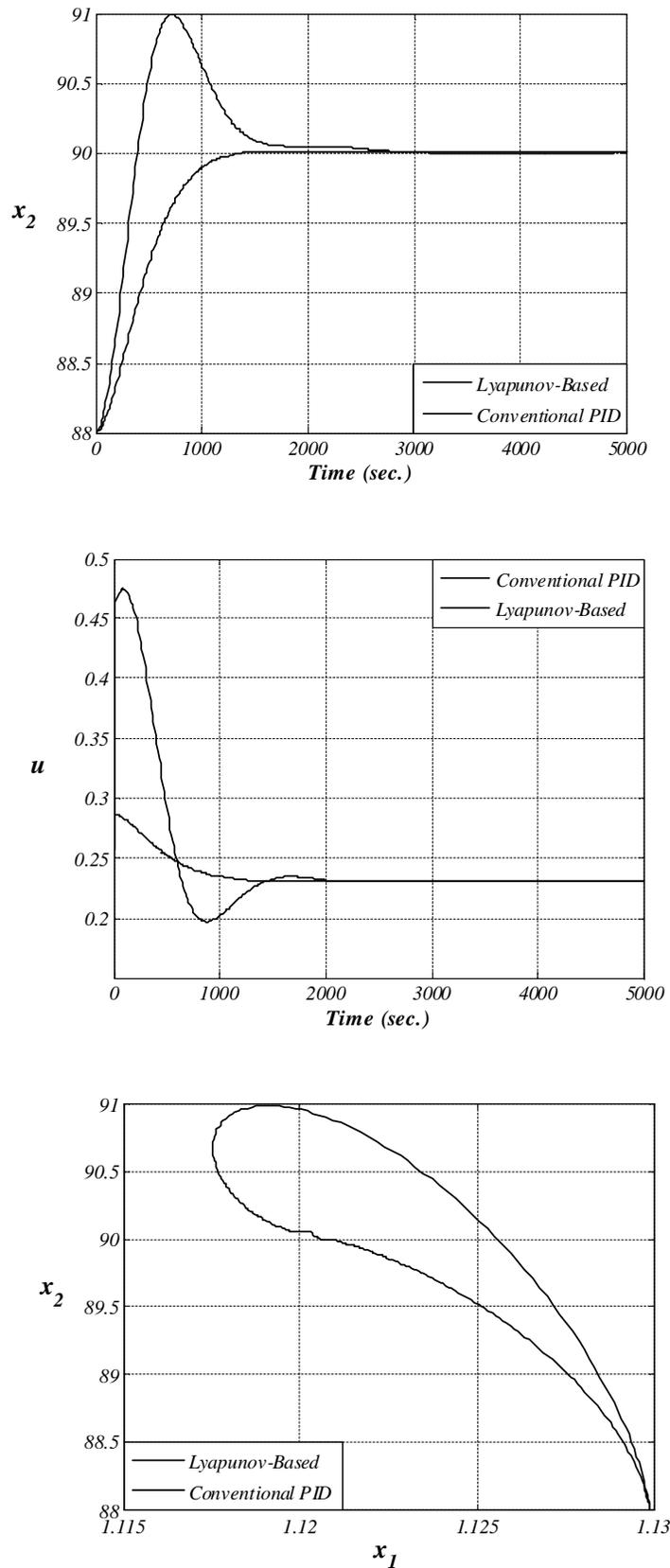


Fig. 10: Comparison – Disturbed Case ($T_{ci} = 35^\circ\text{C}$)

The results of the PID controller, illustrated so far, are seen to be very satisfactory and adequate for the task of process control. Another added advantage of PID controllers is that they require little or no knowledge at all of the underlying process, besides their availability in both electronic and pneumatic forms. Modern industrial PID controllers, e.g. Honeywell 6000 series, incorporate adaptive capabilities for online tuning; however they have very limited success when applied to complex multi-loop processes operating in real-time. This necessitates the need to use other versatile techniques that can robustify the design. The following section supports this idea.

3.4.2 Disturbed Case

To investigate the robustness of the conventional PID controller, a disturbance in the feed rate, F , is now applied such that $F = 0.8 * F_{nominal}$. As shown in Fig. 9, the response is severely deteriorated as the overshoot increased to 100% and the settling time to one hour. This result was expected, as one tuning set for the PID controller can't offer a satisfactory response for wide changes in the operating conditions.

3.4.3 Comparison

Fig. 10 shows a comparison between the designed Lyapunov-based controller and the conventional PID controller when a disturbance is applied to the ambient temperature; T_{Ci} , which is raised to 35 °C instead of the nominal value of 27 °C.

4. CONCLUSION

Although PID controllers are known to be the most standard controllers ever used in industry, they lack the ability to adapt to different operating conditions due to the fact of using a constant parameters set while tuning them to a given setpoint. In this paper we demonstrated the effective use of virtual control laws to design a model-based controller for complex industrial processes, for which PID controllers will not exhibit a robust performance. A combination of model-reference-like and Lyapunov-based designs were augmented, where some of the system states were used as virtual controls for which given dynamics are prescribed. By feeding forward sensitive system variables through direct and easy measurements it was possible to design a PI-like controller that relies on backstepping techniques. The resulting controller has an adaptive proportional gain that uses a changing set of variables that are self-tuned to changing operating conditions. Direct simulations showed the superiority of the proposed controller over conventional PID controllers. The overparameterized structure of the proposed controller adds versatility to the design as it solves the dilemma of maintaining stability, while guarantying a satisfactory performance. The proposed design also proved to be effective as a tuning tool for PID controllers operating under challenging situations.

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