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"Giulio Natta"

AN INVESTIGATION INTO THE EFFECT OF BOUND CONTROL

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Preface

This thesis has been carried out thanks to the collaboration between Politecnico di Milano and University College London, in the person of Prof. Dott. Ing. David Bogle, for courtesy of data system and modelling advices.

The thesis' aim is to explore the ability to determine dynamic optimal performances within strict bounds: starting from one of the simplest system, the analysis has been carried out through the use of a Proportional Integral Controller. The main characteristic is working with very tight enclosures. It's important to find out the best trajectory that the system can reach, in order to save resources, reduce time and cost, improve quality and safety. To satisfy this, optimisation problems constrained by ODEs are formulated and some controls are modified.

Ringraziamenti

Vorrei ringraziare innanzitutto il mio relatore Professor Flavio Manenti, per essersi dimostrato sempre disponibile verso qualsiasi mio dubbio o incertezza, per avermi dato la possibilità di svolgere parte del mio lavoro di tesi a Londra, per avermi incoraggiata e per aver avuto fiducia in me.

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Un grazie va anche all'Ing. Francesco Rossi, per essere stato presente durante lo svolgimento di questa tesi, per avermi aiutata, anche a distanza, quando ci son stati problemi e per aver condiviso con me le soddisfazioni.

ABSTRACT

Ordinary differential equations (ODEs) and differential algebraic equations (DAEs) can be used to describe many chemical engineering systems. The optimisation of these dynamic systems has advanced considerably in the last years. The main aim is exploring ability to determine dynamic optimal/performance within strict bounds.

In this thesis, the systems subjected to some disturbances were investigated. They presented uncertainty in some of the system parameters and initial conditions. A controller that is based on proportional and integral action was developed. The approach must satisfy two conditions, namely: the process must operate inside the safety region and with the best stability. The controller was tested on different case studies to evaluate its performance and to demonstrate its effectiveness.

The models for the cases studied were implemented in MATLAB, employing codes in which the proportional-integral controller was defined. C++ was used to find the enclosure that defines the safety bounds.

The simulations demonstrated that the PI controller is able to satisfy the conditions required by the system. It is possible to work along the entire process inside the safety bounds by controlling the manipulated variable and the disturbances. It's important to arrange in the right way the proportional action (proportional gain) and the integral action (integral time) in order to achieve the best stability.

SOMMARIO

Le equazioni differenziali ordinarie e le algebrico-differenziali si possono impiegare per modellare molti processi chimici e/o sistemi di pertinenza dell'ingegneria chimica. L'ottimizzazione di questo tipo di sistemi di equazioni si è evoluta significativamente negli ultimi anni. L'obiettivo principale è di esplorare l'abilità di determinare performance dinamiche ottimali all'interno di limiti ristretti.

In questa tesi, sono stati studiati sistemi soggetti a tipici disturbi di processo. Essi presentano incertezza in alcuni dei valori dei parametri di sistema e condizioni iniziali. È stato sviluppato un controllore basato su azione proporzionale e integrale. L'approccio deve soddisfare due condizioni: il processo deve operare all'interno della regione di sicurezza e con la massima stabilità. Il controllore PI è stato testato su diversi casi studio per valutare la sua performance e per dimostrare la sua efficienza.

I modelli per i casi studio sono stati implementati in MATLAB, impiegando codici in cui è stato definito il controllore PI. È stato utilizzato C++ per trovare l'enclosure che definisce i limiti di sicurezza.

Le simulazioni hanno dimostrato che il controllore PI è capace di soddisfare le condizioni richieste dal sistema. È possibile lavorare lungo l'intero processo all'interno dei limiti di sicurezza controllando le variabili manipolate e i disturbi. È importante trovare un buon compromesso tra i l'azione proporzionale (guadagno proporzionale) e l'azione integrale (tempo integrale) in modo tale da ottenere la migliore stabilità.

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1. INTRODUCTION

1.1.Process Control

Process Control involves numerical methods, process modelling, process simulation and process optimization. It's important to study process control because it is used to manage chemical/power generation plants and it is required everywhere, in particular to the operators that work with distributed control system.

A chemical process is any single processing unit, or combination of processing units, that is used for the conversion of raw materials (through any combination of chemical, physical, mechanical or thermal changes) into finished products.

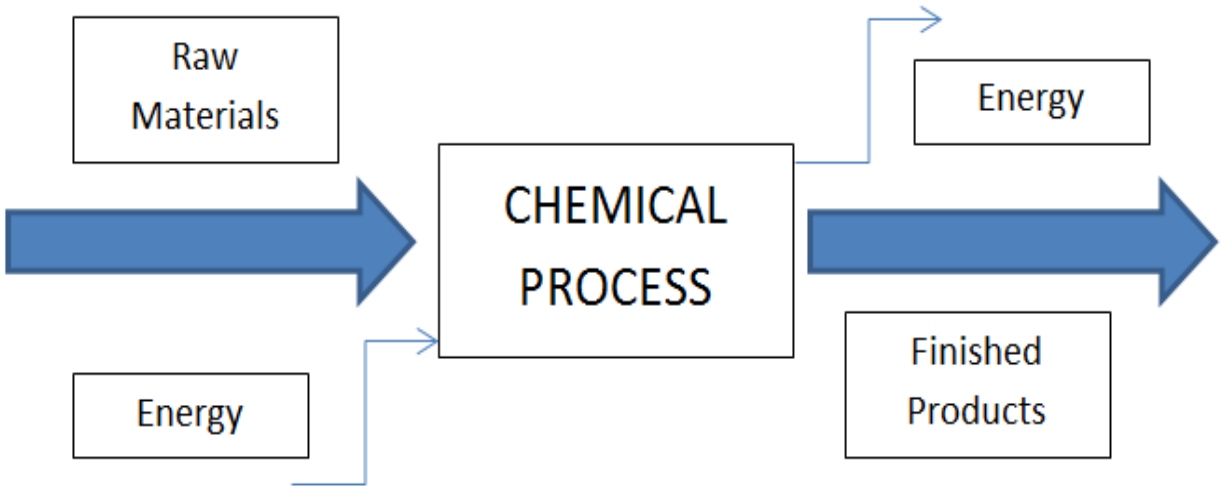


Figure 1.1: Chemical Process

The principles which guide the operation of the processing units of a chemical process are based on the following broad objectives:

- It is advisable to operate the processing units under safety conditions;
- It is necessary to maintain specified production rates;
- It is needed to maintain product quality specifications.

Chemical processes are dynamic: this means that their variables are always changing with time. So, in order to achieve the above noted objectives, there is the need to monitor, and be able to induce change in those key process variables that are related to safety, production rate and product quality. Therefore, the job of the control system is dual: it must be able to monitor certain process condition indicator variables and to induce changes in the appropriate process variables in order to improve process conditions. In other words: process dynamics and control is that aspect of chemical engineering concerned with the analysis, design and implementation of control systems that facilitate the achievement of specified objectives of process safety, production rates and product quality.

The process control system, in a typical chemical process, is the entity that is charged with the responsibility for monitoring outputs, making decisions about how best to manipulate inputs so as to obtain desired output behaviour and effectively implementing such decisions on the process. These tasks can be carried out in different ways, namely: manually by a human operator and, in this case, it is called manual control system; automatically by a machine and this scenario is known as an automatic control system (when the machine involved is a computer then it’s called computer control system).

A process control system can be configured in several different ways:

- Feedback control: it measures the output variable, so it operates by feeding process output information back to the controller; the decisions based on such feedback information are then implemented on the process.

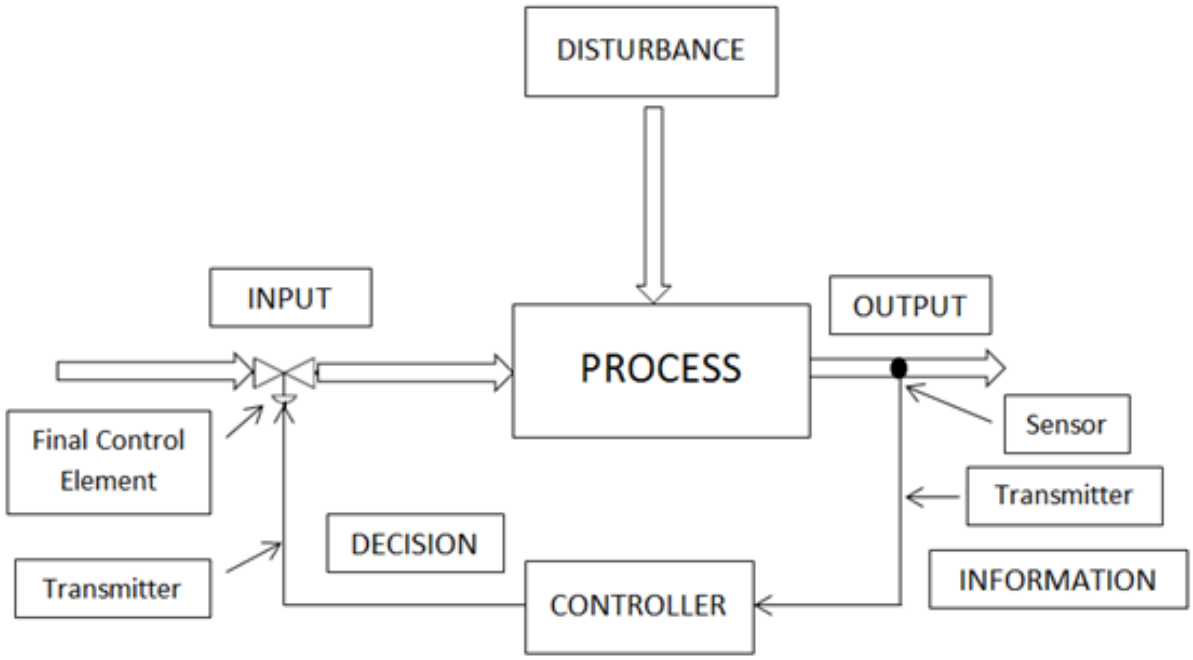


Figure 1.2: The feedback control configuration

- Feedforward control: it measures the disturbance variable (rather than the output variable) that we desired to regulate; therefore, the system has the information about an incoming disturbance that gets directly communicated to the controller.

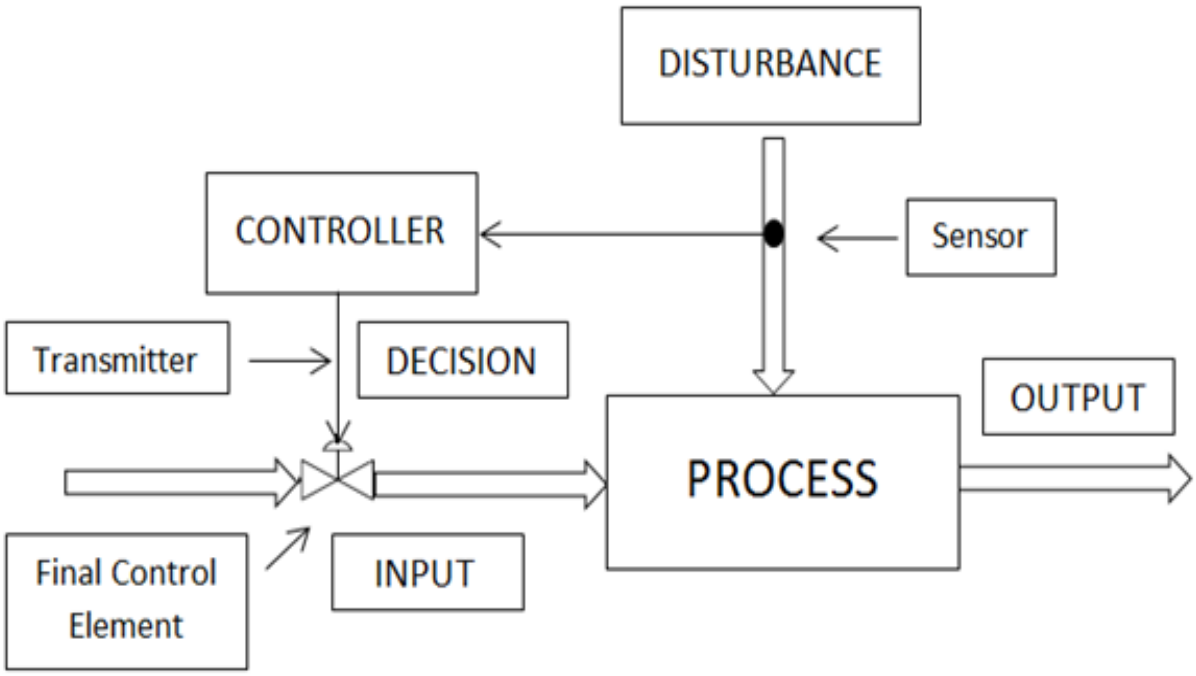


Figure 1.3: The feedforward control configuration

- Open-Loop control: the controller decision is based upon some sort of internally generated strategy; so the controller makes decisions without the advantage of information that close the loop between the output and the input variables of the process.

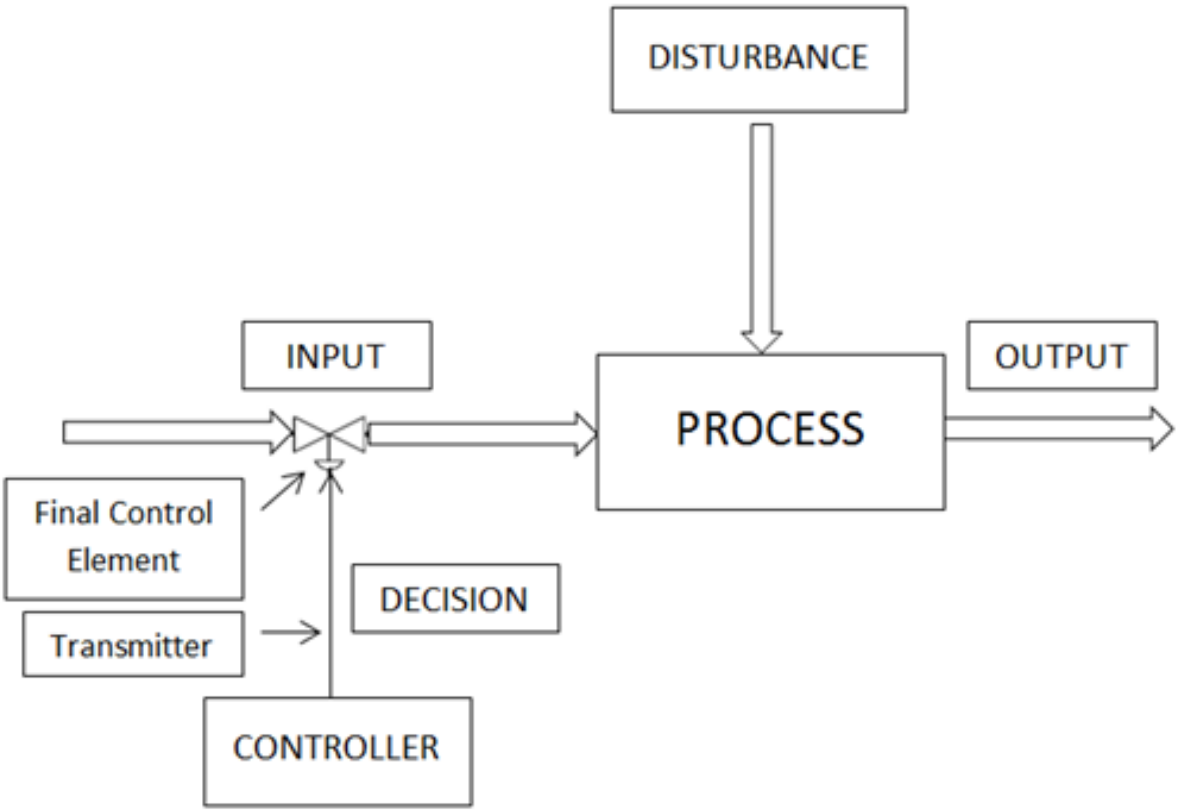


Figure 1.4: The open loop control configuration

The process variables which have been selected to receive the supervision of the control system typically have target values, usually called set-points, at which they are required to be maintained. This is the main objective of the process control system. However, the output variables deviate from their set-points either as a result of the effect of disturbances or because the set-point itself has changed. Depending on the reason why there is the deviation, there are two different type of control: the regulatory control that is used when the task of the control system is that of counteracting the effect of disturbances in order to maintain the output at its set-point; and the servo control which is exploited when the objective is to cause the output to track the changing set-point.

The general principles based on the design of effective control systems, which is the main objective of the process control engineer, are:

- Assess the process and define control objectives;
- Select the process variables to be used in achieving the control objectives;
- Select control structure;
- Design controller.

The last step means that we need to obtain a control law by which, given information about the process, a control decision is determined which the controller implements by adjusting the appropriate manipulated variables accordingly.

The successful of chemical plants depends largely on the design of effective controllers. For this reason and in order to know how process outputs respond to process inputs, it's important to understand both the dynamic and steady state behaviour of the process.

1.2.Global Optimisation

Global Optimisation is a branch of applied mathematics and numerical analysis and it deals with the global optimisation of a function or a set of functions according to some criteria. Typically, a set of bounds is also present and the decision variables are optimized considering also the constraints. The objective is to find the globally best solution of models, in the presence of multiple local optima. In fact, we need to differentiate the local minimum from the global minimum: the first one is a point where the function value is smaller than or equal to the value at nearby points, but possibly greater than at a distant point; the last one is a point where the function value is smaller than or equal to the value at all other feasible points.

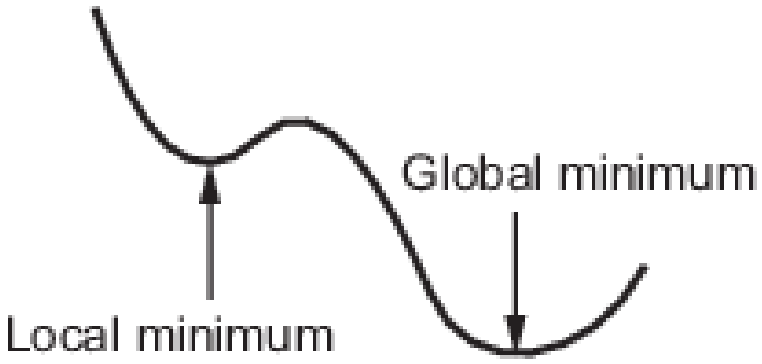


Figure 1.5: The Global and Local minimum

Global optimisation as a field has become more and more important during the past 10 years. Also, the interest in dynamic simulation of chemical processes has increased significantly in process industries. This is because there has been an exponential increasing in the number of publications and success at resolving practical problems that other methods could not. The aforementioned developments have been both theoretical and practical. In fact, process industries are driven by strongly competitive markets and have to face evertighter performance specifications and regulatory limits. Furthermore it is often required that dynamic processes be

operated to satisfy certain safety and/or quality control concerns over their entire operating time. In many cases, in particular in chemical engineering, the phenomena of interest are nonlinear in nature and are described by systems of ordinary differential equations (ODEs), by differential-algebraic equation (DAE) systems or partial differential-algebraic equation (PDAE) systems. These equations describe mass, energy and momentum balances and ensure physical and thermodynamic consistency.

Dynamic optimisation consists of determining values for input/control profiles as well as real valued parameters, initial conditions, and/or boundary conditions of a dynamic system that optimize its performance over some period of time according to a specified metric. The optimisation of a dynamic system is a classical problem in the calculus of variations and its extension by modern optimal control theory. For such problems, a great variety of numerical algorithms have been proposed. They fall into one of two categories: variational (or indirect) methods and discretization (or direct) methods. The first one attempts to find stationary functions via solution of the Euler-Lagrange equations which are necessary for optimality; when an analytical solution can be found, this approach has the advantage of being rigorous, namely the solution is found in the original infinite dimensional space. Instead, the direct methods are based on problem formulations that use discretization to reduce the infinite-dimensional problem to a finite-dimensional one.

These approaches can be further subdivided into two broad categories: the simultaneous (total discretization) and the sequential (control parameterization) methods. In either approach, the objective is to minimize a weighted squared error between the observed values and those predicted by the model. The sequential approach, in which only the decision variables (control parameters) are discretized, involves the use of integration routines to determine the values of

the states for a given set of model parameter values. This in turn allows for the evaluation of the objective function and its gradients. This is more traditional than the other one and it is referred to a sequential algorithm because the optimisation steps and solution of the differential system are performed in a sequential manner. The simultaneous approach, in which both decision and state variables are discretized, involves the conversion of the dynamic system into a set of algebraic equations which are included directly in the formulation. This results in a nonlinear programming (NLP) problem to which standard or specially designed solvers can be applied. Both the sequential and the simultaneous approaches have been successfully applied to a wide range of problems and both approaches are currently used.

There are two categories of algorithms that can be exploited in order to handle the problem of multiple local optima: the stochastic and the deterministic approaches. The stochastic methods are usually based on statistical arguments in order to prove their convergence. The deterministic methods are able to guarantee that the optimal performance has been found and to ensure the location of the global optimum solution within a prespecified tolerance.

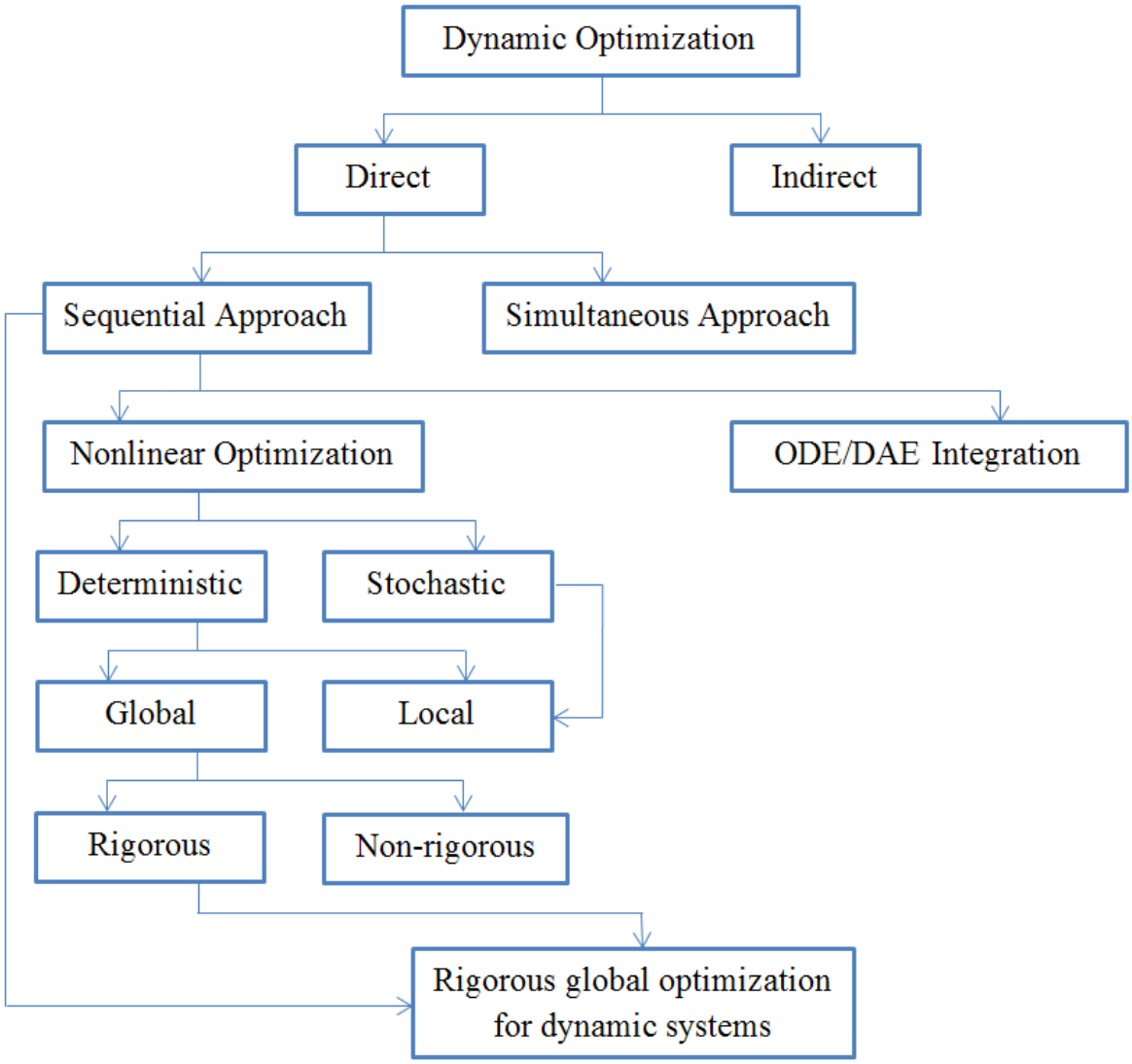


Figure 1.6: Global Optimisation of dynamic system

The dynamic optimisation of most chemical engineering process examines their performance and searches to optimise their behaviour. The systems considered present uncertainty and they are subjected to disturbances.

This work discusses the ability to determine dynamic optimal/performance within strict bounds. Such bounds are useful because they define and delimit the area in which the process can be carried out in safety conditions. At the same time, they can represent a problem because

the profile of the variable of interest must lie inside the enclosure and if it is very tight, respecting the safety condition could be difficult. The objective to find non-conservative bounds was investigated also in the article of Scott and Barton (2013) in which they developed new differential inequalities methods that use physical information to produce greatly improved enclosures at minor additional costs. The enclosures are exploited in many applications such as in controller synthesis (Lygeros, Tomlin, & Sastry, 1999), in state and parameter estimation (Singer & Barton, 2006), and in safety verification and fault detection (Lin & Stadtherr, 2008). The computation of rigorous enclosures can be of general interest for online applications such as robust Model Predictive Control (Limon, Bravo, Alamo & Camacho, 2005). In dynamic optimisation, there can be problems related to the presence of nonconvexities that may lead to multiple local optima. In order to handle this issue, stochastic global optimisation methods can be used. However, this approach is not able to guarantee to find the global optimal. So, an alternative method that involved the use of the deterministic spatial branch and bound global optimization algorithm (Papamichail and Adjiman, 2004; Esposito and Floudas, 2000; Chachuat and Latifi, 2004) in which the global minimum is approached form above and below by generating converging sequences of upper and lower bounds can be exploited.

1.3.The Aim

In this study, we considered the problem of finding a very tight enclosure and of remaining inside the bounds during the entire length of the process. Such enclosure must not be violated: a PI controller has been used for this purpose. We reproduced the bounds and developed the controller for an irreversible series first order reaction and an exothermic batch reactor. In these different systems, the first main step is to arrange the values of the tuning parameters, that are the proportional gain and the integral time, so that the controller can act properly. According to the values assigned to the aforementioned parameters, the results can be different: the profile could reach the upper/lower bound once and in this case the controller will act by maintaining it inside the enclosure (simplest example); the profile could oscillate inside or outside the limits and in this case the controller can act but maybe not in the proper way (if the system continues oscillating). The results depend also from the variables that are controlled and from them that are used as disturbance. For these reasons, one of the key concept is the stability of the system: if this condition is not satisfied, in the presence of a disturbance, maintaining the variable's profile inside the enclosure can be difficult and in certain cases cannot be reached. We don't want to operate in dangerous conditions or with a profile that starting from the beginning is very close to the upper/lower bound. With this study what we want to do is to explore the ability to determine dynamic optimal performance within strict bounds and so we need to study the process control considered in order to be able to manage chemical/power generation plants.

2. ENCLOSURE

2.1. The Interval Analysis

The method of interval analysis exploits closed intervals, that are defined in the following way:

$$[a] = \left[\underline{a}, \overline{a}\right] = \left\{x \in \mathbb{R} | \underline{a} \leq x \leq \overline{a}\right\} \tag{2.1}$$

Defined for intervals, there are operations, like multiplication, division, addition and subtraction, functions, like width, absolute value and midpoint, and set operations, like union and intersection. The interval is called degenerate when the lower bound overlaps the upper one: $[a] = [a, a]$.

In the interval analysis interval vectors

$$[\boldsymbol{a}] = ([a_1], [a_2], \dots, [a_n])$$

and interval functions

$$f([x]) = \{f(x) | x \in [x]\} \tag{2.2}$$

are investigated; by extending the interval of functions an enclosure of the set $[x]$ can be obtained. In this case, the interval extension means the function achieved by expanded the domain in order to include intervals $[x] = \left[\underline{x}, \overline{x}\right]$ and degenerate intervals $[x] = [x, x]$:

$$f(x) = [f]([x, x])$$

The following equation represents the Taylor model arithmetic able to compute an enclosure

$$\mathcal{T}_{y_{j+1}}(\theta) = \sum_{i=0}^{k-1} h_j^i \mathcal{T}_{f^{[i]}}(\hat{\mathcal{P}}_{y_j}(\theta), \theta) + \left\{\sum_{i=0}^{k-1} h_j^i \mathcal{T}_{\frac{\partial f^{[i]}}{\partial y}}(\mathcal{T}_{y_j}(\theta), \theta)\right\} [\hat{R}_{y_j}] + h_j^k f^{[k]}([\tilde{y}_j], [\theta]) \tag{2.3}$$

2.2.The Overestimation Problem

Working with convex sets means that the true solution is overestimated. This leads to produce results and points that are not included into the true solution set at every time step. So, the overestimation is a problem that need to be solved.

There are different sources that can lead to the overestimation: the cancellation, the dependency problem and the wrapping effect. The first one can arise if there is one or more addition or subtraction in the mathematical expressions. The second one is generated when a variable is repeated twice in the model and it's used as there are two different variables. So, these two problems happen because real arithmetic operations are not directly translated by the interval arithmetic operations. The third one, instead, is due to the depth of a computational graph describing the ODE system and to the repeated enclosure of a solution step by a convex simpler set that accumulates overestimation at every step.

In order to solve the overestimation problem, contractors can be taken into account. They are operators that can lead to replace the domain $[x]$ of the function f with a smaller domain $C([x])$; in this way, the true solution set is not changed.

2.3.Problem Formulation

The ability to represent the solution set with convex sets has been investigated a lot during the past years, because working with these convex sets means that the true solution is overestimated. This leads to produce results and points that are not included and do not belong to the true solution set at every time step. So, the main problem consists on the possibility to obtain overconservative state bounds that can lead to unable to distinguish the true solution. Therefore, there is the need to develop a method that is able to reduce the overestimation.

There are a lot of works in which the aim is to reduce the overestimation of interval evaluated functions and they consist of finding a valid inclusion of the overestimated solution (constraint propagation, fixed-points methods..). According to the thesis of Carlos Perez-Galvan, the Interval Taylor Series method has been exploited. The implementation is quite simple and, in particular, at each iteration of ITS method, he implemented interval contractors (Krawczyk and Newton/Gauss-Seidel) in order to reduce the achieved overestimation.

The aim is to evaluate a proper enclosure suitable for the type of systems analysed that is able to include all the points of the true solution. For this reason, the enclosure considered must be as tight as possible.

The ODE model is described by the vector of state variables y and the vector of system parameters $\boldsymbol{\theta}$: $\dot{\boldsymbol{y}} = \boldsymbol{f}(t, \boldsymbol{y}(t), \boldsymbol{\theta})$. In order to find an enclosure $[\boldsymbol{y}_j] \supseteq \boldsymbol{y}(t_j; t_{0,}[\boldsymbol{y}_0], [\boldsymbol{\theta}]) = \{\boldsymbol{y}(t_j; t_0, \boldsymbol{y}_0, \boldsymbol{\theta}) | \boldsymbol{y}_0 \in [\boldsymbol{y}_0],\ \boldsymbol{\theta} \in [\boldsymbol{\theta}]\}$ it is needed to go on in two steps: the first one is the validation of existence and uniqueness of a solution and the second one consists of the computation of a tighter enclosure. In the first stage, also a suitable a priori enclosure $[\widetilde{\boldsymbol{y}_j}] \supseteq \boldsymbol{y}(t_j; t_{0,}[\boldsymbol{y}_0], [\boldsymbol{\theta}])$ and a time step h_j are produced; they must satisfy the following condition:

$$[\widetilde{\boldsymbol{y}_j}] = [\boldsymbol{y}_i] + \sum_{i=1}^{k-1} [0, h_j]^i \boldsymbol{f}^{[i]}([\boldsymbol{y}_i], [\boldsymbol{\theta}]) + [0, h_j]^k \boldsymbol{f}^{[k]}([\widetilde{\boldsymbol{y}_j}^0], [\boldsymbol{\theta}]) \supseteq [\widetilde{\boldsymbol{y}_j}^0] \quad (2.4)$$

in which $[\boldsymbol{y}_i]$ is the vector of tight enclosures of the solutions with ranges in $[\widetilde{\boldsymbol{y}_j}^0]$, k is the Taylor series expansion's order, $\boldsymbol{f}^{[i]}$ are the Taylor coefficients defined and $[\boldsymbol{\theta}]$ is the system parameters' vector.

Interval analysis is at the base of most verified methods that are used for the solution of Initial Values Problems for ODEs: thanks to these methods, it's possible to define an enclosure that consists of upper and lower bounds in which the true solution of the problem is guaranteed to be contained.

In the second stage, it's possible to evaluate a tight enclosure $[y_{j+1}] \supseteq y(t_{j+1}; t_0, [y_0], [\theta])$ given interval bounds $[y_i]$ at t_j. It works according to the next equation:

$$[\boldsymbol{y}_{j+1}] = \overbrace{\hat{\boldsymbol{y}}_j + \sum_{i=1}^{k-1} h_j^i \boldsymbol{f}^{[i]}(\hat{\boldsymbol{y}}_j, \hat{\boldsymbol{\theta}})}^{\mathbf{u}_{j+1}} + \overbrace{\left\{\mathbf{I} + \sum_{i=1}^{k-1} h_j^i \frac{\partial \boldsymbol{f}^{[i]}}{\partial \boldsymbol{y}}([\boldsymbol{y}_j], [\boldsymbol{\theta}])\right\}}^{[\mathbf{S}_{j+1}^{y}]}([\boldsymbol{y}_j] - \hat{\boldsymbol{y}}_j)$$
$$+ \underbrace{\left\{\sum_{i=1}^{k-1} h_j^i \frac{\partial \boldsymbol{f}^{[i]}}{\partial \boldsymbol{\theta}}([\boldsymbol{y}_j], [\boldsymbol{\theta}])\right\}}_{[\mathbf{S}_{j+1}^{\theta}]}([\boldsymbol{\theta}] - \hat{\boldsymbol{\theta}}) + \underbrace{h_j^k \boldsymbol{f}^{[k]}([\tilde{\boldsymbol{y}}_j], [\boldsymbol{\theta}])}_{[\mathbf{z}_{j+1}]} \tag{2.5}$$

In which $\boldsymbol{I}$ is the identity matrix and $\hat{y}_j = \left(\underline{[y_j]} + \overline{[y_j]}\right)/_2$.

The interval contractors are able to contract the estimated range in an interval evaluated function. In order to apply them it is needed an equation like that:

$$\left(f(y) = 0, y \in [y_j]\right) \tag{2.6}$$

In fact, for this equation, written in a vector form, a constraint satisfaction problem (CSP) can be formulated.

B is the solution set defined as follow:

$$B = \{y \in [y_j] | f(y) = 0\} \tag{2.7}$$

So, it's possible to substitute the domain $[y_j]$ in a smaller one $[y'_j]$ so that $B \subset [y'_j] \subset [y_j]$ that means that the solution set is not changed.

The contractors used are the type suitable for nonlinear functions and the method used is able to predict the effectiveness in the reduction of the overestimation.

The initial formulation

$$g(y) = u_{j+1} + ([S^y_{j+1}]\mathrm{A}_j)[\Gamma_j] + [S^\theta_{j+1}]([\theta] - \hat{\theta}) + [z_{j+1}] - [y_{j+1}] = 0, y \in [y_j] \tag{2.8}$$

Can be reformulated in this

$$g(\hat{y}_j) = \mathrm{A}_{j+1}\Gamma_{j+1}(\hat{y}_j, [\theta]) \tag{2.9}$$

So that the contractors can be implemented because it is the same type of the aforementioned equation (2.9)

The steps that assure to achieved enclosures using contractors are the following:

$$\mathbf{u}_{j+1} = \hat{\mathbf{y}}_j + \sum_{i=1}^{k-1} h_j^i \mathbf{f}^{[i]}(\hat{\mathbf{y}}_j, \hat{\boldsymbol{\theta}})$$
$$[\mathbf{z}_{j+1}] = h_j^k \mathbf{f}^{[k]}([\tilde{\mathbf{y}}_j], [\boldsymbol{\theta}])$$
$$[\mathbf{S}_{j+1}^y] = \mathbf{I} + \sum_{i=1}^{k-1} h_j^i \frac{\partial \mathbf{f}^{[i]}}{\partial \mathbf{y}}([\mathbf{y}_j], [\boldsymbol{\theta}])$$
$$[\mathbf{S}_{j+1}^\theta] = \sum_{i=0}^{k-1} h_j^i \frac{\partial \mathbf{f}^{[i]}}{\partial \boldsymbol{\theta}}([\mathbf{y}_j], [\boldsymbol{\theta}])$$
$$\mathbf{Q}_j \mathbf{R}_j = m([\mathbf{S}_{j+1}^y]\mathbf{A}_j)$$
$$\mathbf{A}_{j+1} = \mathbf{Q}_j$$
$$[\boldsymbol{\Gamma}_{j+1}] = \mathbf{A}_{j+1}^{-1}([\mathbf{z}_{j+1}] - \hat{\mathbf{z}}_{j+1}) + \mathbf{A}_{j+1}^{-1}([\mathbf{S}_{j+1}^y]\mathbf{A}_j)[\boldsymbol{\Gamma}_j] + (\mathbf{A}_{j+1}^{-1}[\mathbf{S}_{j+1}^\theta])([\boldsymbol{\theta}] - \hat{\boldsymbol{\theta}})$$
$$[\mathbf{y}_{j+1}] = \mathbf{u}_{j+1} + ([\mathbf{S}_{j+1}^y]\mathbf{A}_j)[\boldsymbol{\Gamma}_j] + [\mathbf{S}_{j+1}^\theta]([\boldsymbol{\theta}] - \hat{\boldsymbol{\theta}}) + [\mathbf{z}_{j+1}]$$

Newton/Gauss-Seidel contractor:

$$\mathbf{g}(\hat{\mathbf{y}}_j, [\boldsymbol{\theta}]) = \mathbf{A}_{j+1}[\boldsymbol{\Gamma}_{j+1}](\hat{\mathbf{y}}_j, [\boldsymbol{\theta}])$$
$$[\mathbf{y}_{j+1}] \supseteq [\mathbf{y}_{j+1}]_N = \texttt{NGSContractor}([\mathbf{y}_{j+1}], [\mathbf{S}_{j+1}^y], \mathbf{g}(\hat{\mathbf{y}}_j, [\boldsymbol{\theta}]))$$

or

$$[\mathbf{y}_{j+1}] \supseteq [\mathbf{y}_{j+1}]_N = \texttt{KContractor}([\mathbf{y}_{j+1}], [\mathbf{S}_{j+1}^y], \mathbf{g}(\hat{\mathbf{y}}_j, [\boldsymbol{\theta}]))$$
$$[\mathbf{y}_{j+1}] \leftarrow [\mathbf{y}_{j+1}] \cap [\mathbf{y}_{j+1}]_N$$

Since at each time step is possible to implement contractors, at each time step an interval $([y_{j+1}])$ in which is included the solution of the problem is obtained by the interval Taylor series method. The work is carried out with a lot of iterations. The verified method can obtain a new $[y_{j+1}]$, if the reduction achieved is enough, and there is the repetition of the contraction step. If sufficient reduction is not achieved, the algorithm returns the best $[y_{j+1}]$ found so far.

In order to assess the effectiveness of the use of contractors and to provide a comparison in terms of time, their performances can be compared with the one with no contractors. The algorithm has been implemented in C++.

3. DYNAMIC PERFOMANCE WITHIN STRICT BOUNDS

We considered two examples upon which different experiments have been carried out: a first order irreversible series reaction scheme and an exothermic batch reactor where a chemical reaction takes place. The aim is to find out the possible disturbances that could force the trajectories of some key system states to violate their upper/lower bounds, previously computed using interval mathematics, and to find ways to avoid such unwanted using conventional controllers (P, PI, PID).

As first there is the need to define the enclosure, for the example considered, inside of which the profile of the state variable of interest can lie. This implies identification of the behaviour of the lower and the upper limits. This can be realized by exploiting C++ code in which the solver setting and the ODE system are defined. The definition of the enclosure is a very important step: there is the need, in fact, to respect some environmental constraints in order to carry out the process under safety conditions.

Once the enclosure is defined, the next step is to reproduce also the intermediate behaviour of the trajectory on which the disturbance will act. Every parameter could potentially be a disturbance acting on the system: pressure, flowrates, temperature, compositions.. Therefore first we have to define the type of variables present in the system. The input variables are those that independently stimulate the system and can thereby induce change in the internal conditions of the process. They can be classified as manipulated variables and disturbance variables: the first are those input variables that are at our disposal to manipulate freely as we

choose; the last are those over which we have no control. The output variables are those by which we can obtain information about the internal state of the process. They are different from the state variables: these last are that minimum set of variables essential for completely describing the internal state or condition of a process.

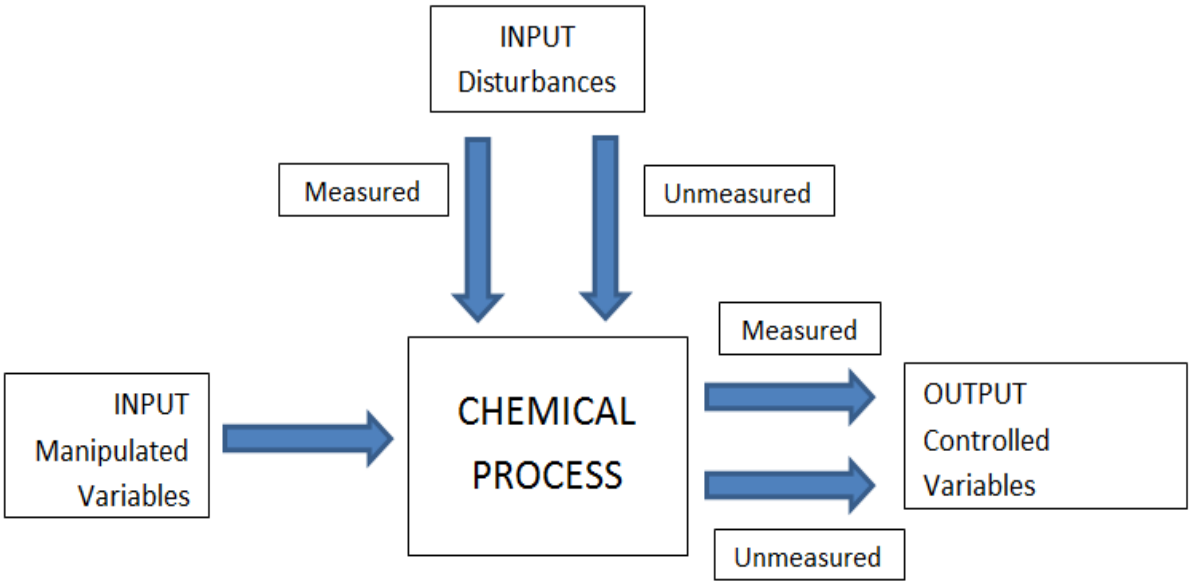


Figure 3.1: The variables of a process

Once the parameter, that acts as a disturbance and creates a change in the shape of the curve, is defined, it is needed to identify which variable we want to change in order to manage the error on the variable of interest. This work can be done by a controller: thanks to it, we try to adjust the error and to keep the curve inside the limits. I used the PID controller; its output signal is a linear combination of three contributions that are a Proportional action, an Integral action and a Derivative action: $C_{PID}(s) = K_p + \frac{K_i}{s} + K_d s, \quad K_p, K_i \in \mathbb{R}$

The control law associated with this type of controller can be written in a synthetic form as follows: $C_{PID}(s) = \frac{K_p s + K_i + K_d s^2}{s} = K_i \frac{1 + \frac{K_p}{K_i} s + \frac{K_d}{K_i} s^2}{s}$ or in this way: $C_{PID}(s) = K_p \left(1 + \frac{1}{sT_i} + T_d s\right)$ where $T_i = \frac{K_p}{K_i}$ represents the time constant of the integral action (integral time) and $T_d = \frac{K_d}{K_i}$ the time constant of the derivative action (derivative time). It is also possible to simplify PID controllers to get a PI controller (with $K_d = 0$), a PD controller (with $K_i = 0$), a P controller (with $K_i = K_d = 0$) or an I controller (with $K_p = K_d = 0$). The integral gain K_i is used to fix the error of the permanent regime to the canonical signal which defines the type.

Type of controller	K_p	T_i	T_d
P	0.5 $K_{p,cr}$	∞	0
PI	0.45 $K_{p,cr}$	0.85 T_{cr}	0
PID	0.6 $K_{p,cr}$	0.5 T_{cr}	0.12 T_{cr}

TABLE 1: PARAMETERS FOR THE PID CONTROLLER ACCORDING TO THE ZIEGLER-NICHOLS METHOD

These types of controllers are typically used to provide feedback control, namely: thanks to an input that defines the current value of the variable of interest, the controller can suggest proper actions aimed at minimizing the error, which is a measure of the distance between the current value of the variable and its set-point. The PID sets the output signal based on:

- The value of the error (proportional action)
- The past values of the errors (integral action)
- The rate of change in the error (derivative action)

In the controller, it is necessary to find a compromise between the number of steps that are analysed and the parameters K_i, K_d and K_p.

4. CASE STUDIES

4.1.Presentation

The first case studied is a *First Order Irreversible Series Reaction scheme*.

Let's consider the kinetic mechanism: $A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C$

Typically, for the latter type of scheme, the associated reaction rates can be expressed in the following form: $\begin{cases} r_1 = k_1 C_A \\ r_2 = k_2 C_B \end{cases}$

The ODE system is represented by the equations that can be obtained from the molar balances on the species A and B under the assumption of constant volume of the reacting system:

$$\frac{dN_k}{dt} = R_k V \quad \overset{constant\ volume}{\Longrightarrow} \quad \frac{dC_k}{dt} = R_k$$

The second case studied is an *Exothermic Batch Reactor*, where a first order irreversible reaction takes place. The initial charge consists of pure A, which is loaded into the reactor, where the reaction takes place. The liquid inside the reactor can be heated or cooled depending on which exercise fluid is used: in the first case steam is fed to the jacket, while in the second scenario cooling water is supplied to the jacket.

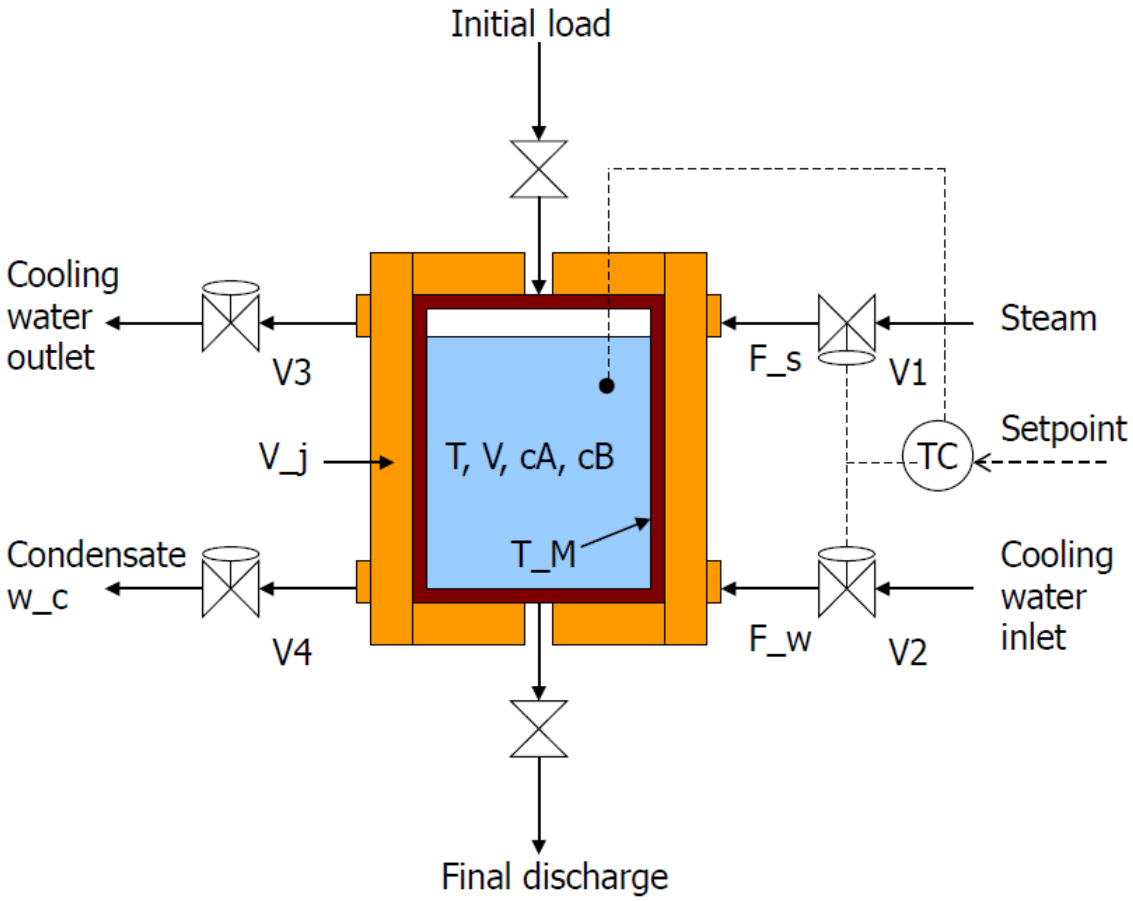


Figure 4.1: The exothermic batch reactor

We are working in Batch mode tracking the optimal temperature profile. The governing equations for a non-isothermal batch reactor are:

$$\begin{cases} \dfrac{dN_j}{dt} = \dot{R}_j V \\ \dfrac{d}{dt}(U + E_K + E_P) = \dot{Q} \end{cases}$$

Usually, for every product, it is defined a specific temperature profile. The ability to ensure the track such profile accurately affects directly the quality of the final product. Moreover, the temperature control allows indirectly managing the chemical reaction inside the reactor. The reactor temperature is usually controlled thanks to the thermal exchange between the reactor itself and the cooling/heating fluid, which is circulated in a serpentine that surrounds the reactor vessel.

The main properties of the cases studied are reported in the following tables:

TABLE 2: ODE SYSTEM AND INITIAL CONDITIONS OF THE CASE STUDIES

CASE STUDIES	ODE SYSTEM	INITIAL CONDITIONS
1. First Order Irreversible Series Reaction	$\frac{dC_A}{dt} = -k_1 C_A$ $\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$	$C_A(0) = 1\ \frac{kmol}{m^3}$ $C_B(0) = 0\ \frac{kmol}{m^3}$
2. Exothermic Batch Reactor (case 1)	$\frac{d\chi}{dt} = (1-\chi)k_0 exp\left(-\frac{E_{att}}{RT}\right)$ $\frac{dT}{dt} = \frac{UA(T_a - T)}{CA_0 VCp} - \frac{\Delta H_R}{Cp}(1-\chi)k_0 exp\left(-\frac{E_{att}}{RT}\right)$	$\chi(0) = 0$ $T(0) = 360\ K$
3. Exothermic Batch Reactor (case 2)	$\frac{d\chi}{dt} = (1-\chi)k_0 exp\left(-\frac{E_{att}}{RT}\right)$ $\frac{dT}{dt} = \frac{UA(T_a - T)}{CA_0 VCp} - \frac{\Delta H_R}{Cp}(1-\chi)k_0 exp\left(-\frac{E_{att}}{RT}\right)$	$\chi(0) = 0$ $T(0) = 360\ K$
4. Exothermic Batch Reactor with balance on the jacket (case 3)	In addition to the previous ones: $\frac{dT_a}{dt} = \frac{F_a}{V_j}(T_a^0 - T_a) + \frac{UA}{V_j \rho_a Cp_a}(T - T_a)$	$\chi(0) = 0$ $T(0) = 360\ K$ $T_a(0) = 300\ K$

TABLE 3: UNCERTAIN AND SYSTEM PARAMETERS

CASE STUDIES	UNCERTAIN PARAMETERS	SYSTEM PARAMETERS
1. First Order Irreversible Series Reaction	$k_1 = [4.5, 5.5]\ s^{-1}$ $k_2 = [0.2, 1.8]\ s^{-1}$	-
2. Exothermic Batch Reactor (case 1)	$T(0) = [310, 410]K$ $T_a = [290,310]\ K$	$T_a = 295\ K,\ \ k_0 = 0.022\ \frac{1}{s},\ \ E_{att} = 6000\ \frac{J}{mol},$ $Cp = 60\ \frac{J}{g\ K},\ \ UA = 3\ \frac{W}{m^2 K}\ m^2$ $CA_0 = 10\ \frac{1}{m^3},\ \ R = 8.314\ \frac{J}{mol\ K}$ $V = 0.1\ m^3,\quad \Delta H_R = -140000\ J$
3. Exothermic Batch Reactor (case 2)	-	$T_a = 310\ K,\ \ k_0 = 0.022\ \frac{1}{s},\ \ E_{att} = 6000\ \frac{J}{mol},$ $Cp = 60\ \frac{J}{g\ K},\ \ UA = 3\ \frac{W}{m^2 K}\ m^2$ $CA_0 = 10\ \frac{1}{m^3},\ \ R = 8.314\ \frac{J}{mol\ K}$ $V = 0.1\ m^3,\quad \Delta H_R = -140000\ \frac{J}{kmol}$
4. Exothermic Batch Reactor with balance on the jacket (case 3)	-	$Cp_a = 4.187\ \frac{J}{kg\ K},\ \rho_a = 1 * 10^6\ \frac{g}{m^3}$ $UA = 1\frac{W}{m^2 K} m^2,\ \ V_j = 0.02\ m^3,\ \ T_a^0 = 310\ K$

In the system parameters k_0 is the rate constant, E_{att} is the activation energy, U is the overall heat transfer coefficient, A is the total Area, χ is the conversion of A, R is the universal gas constant, T is the temperature of the reactor while T_a is the temperature of the cooling/heating fluid, ΔH_R is the enthalpy of reaction, CA_0 is the initial concentration of component A, V is the

total volume of the reactor, Cp is the specific heat capacity of the liquid and V_j is the volume of the metal jacket. F_a, ρ_a and Cp_a are the flow rate, the density and the specific heat capacity of the cooling/heating fluid, respectively. The uncertain parameters are only used to evaluate the enclosure.

4.2.Analysis

There is the need to represent, for each variable of interest, the upper and lower limits, that define the enclosure. The profiles upon which the disturbance will act have been investigated and are shown in the following graphs. The table below represents the variables studied and their bounds, the parameter that acts as disturbance and its value, and the variable that we want to control.

TABLE 4: LIMITS, DISTURBANCE AND CONTROLLED VARIABLE OF THE CASE STUDIES

CASE STUDIES	LIMITS	DISTURBANCE	CONTROLLED VARIABLE
1. First Order Irreversible Series Reaction	Concentrations of the components A and B	${C_A}^0\ (0.2\frac{kmol}{m^3})$	C_A
2. Exothermic Batch Reactor (case 1)	Conversion and Reactor Temperature	$T^{feed}(430\ K)$	T
3. Exothermic Batch Reactor (case 2)	Conversion and Reactor Temperature	$T^{feed}_{exercise\ fluid}(500\ K)$	T
4. Exothermic Batch Reactor with balance on the jacket (case 3)	Conversion, Reactor and Exercise Fluid Temperature	$T^{feed}_{exercise\ fluid}(350\ K)$	$T_{exercise\ fluid}$

4.2.1 First order irreversible series reaction

What is expected from a first order irreversible series reaction scheme is:

- an exponentially reduction in the concentration of A over time, because this component cannot be produced;
- an initial increment of the concentration of B until it reaches a maximum followed by a subsequent reduction of it in order to lead to the formation of the product C;
- a continuously raising of C with the greatest rate of increase of C occurring where B is a maximum.

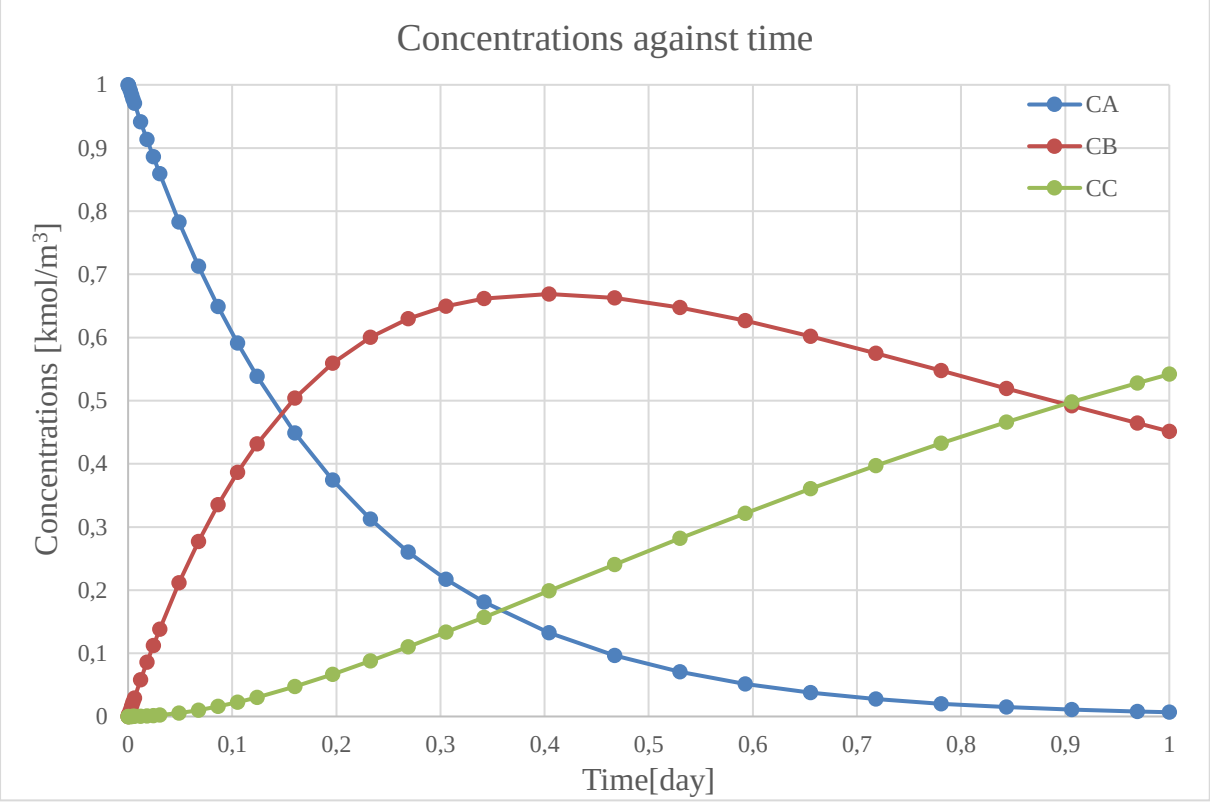
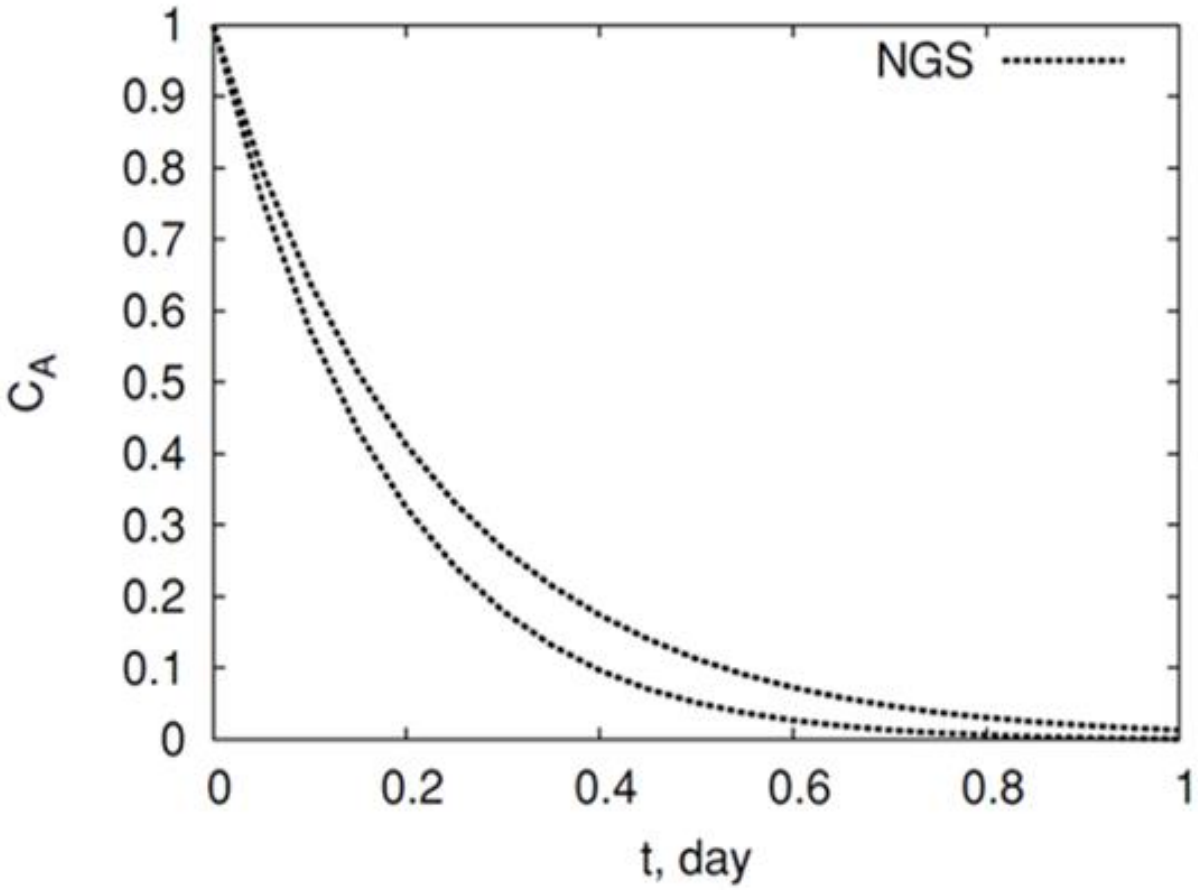
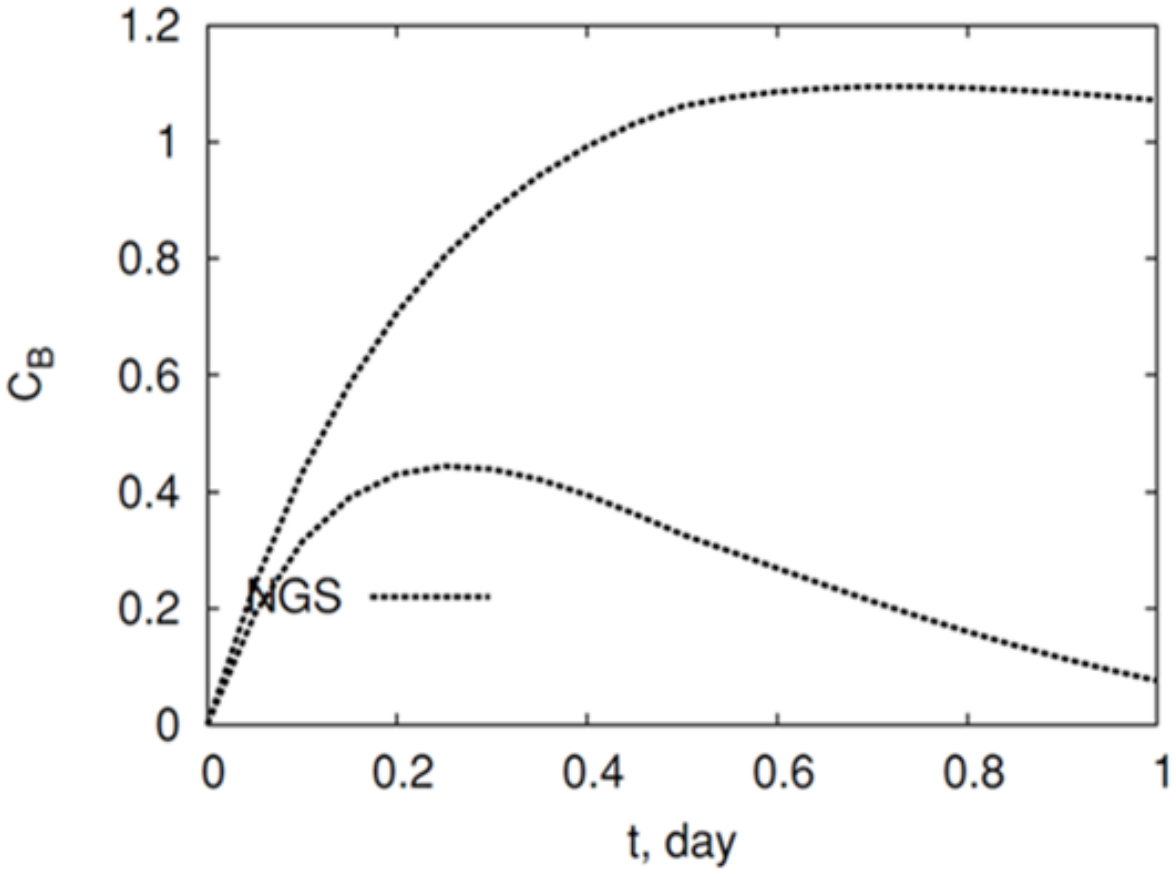


Figure 4.2: Profile of the concentrations against time

In order to find the enclosure inside of which the profiles of the concentrations can lie an enclosure solver can be exploited. The ODE system and the solver setting are used and reported on C++ files so that the upper and the lower limits for the concentration of components *A* and *B* can be obtained; they are represented in figures 3.3 (a) and (b):



(a)



(b)

Figure 4.3: Enclosure of the A concentration (a) and B concentration (b) along time for the first order irreversible series reaction

The intermediate behaviour of C_A has been treated. It is shown in the following graph:

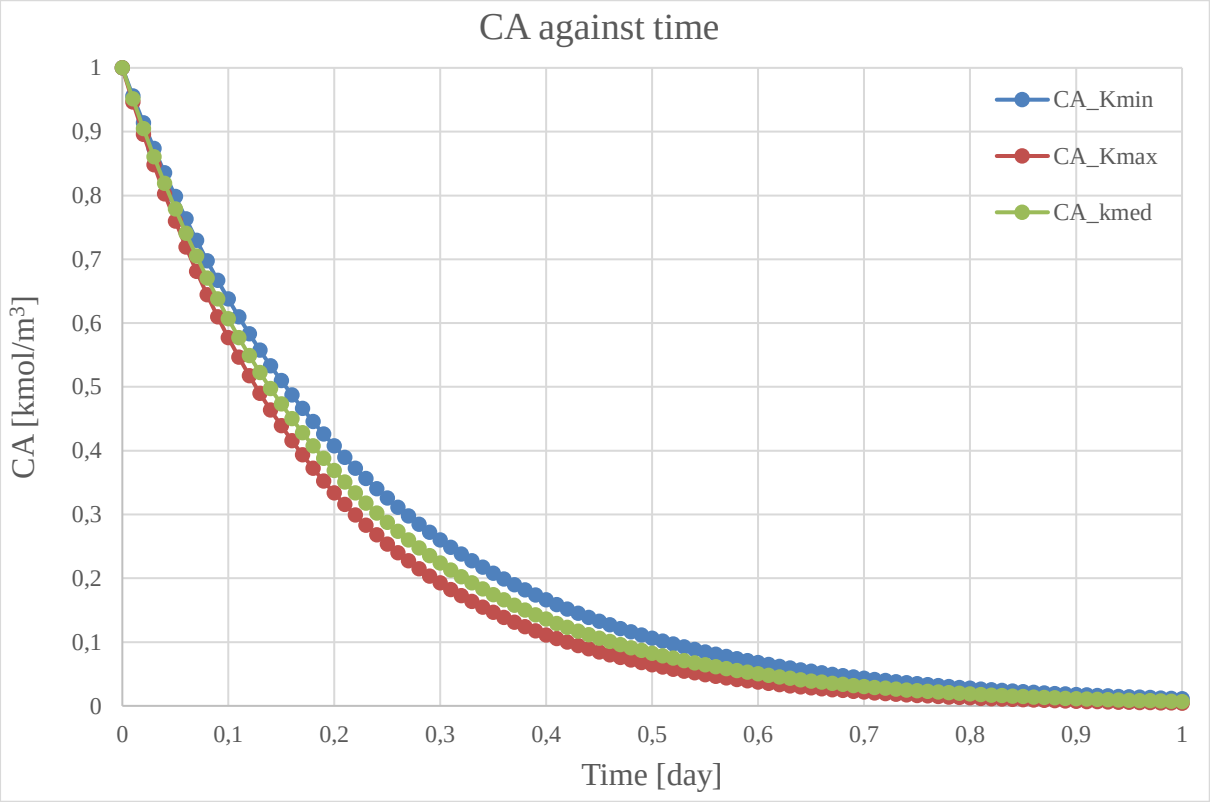


Figure 4.4: Profile of upper and lower limits and intermediate concentration of A component

Now there is the need to find a value of the disturbance that causes the key state of interest to violate the upper/lower bounds. In this case the initial value of the concentration of component A can be used as disturbance in order to see what happens.

For example, by setting C_A^0 to 0.2 at time equal to 0.4, the trajectory of C_A changes as follows:

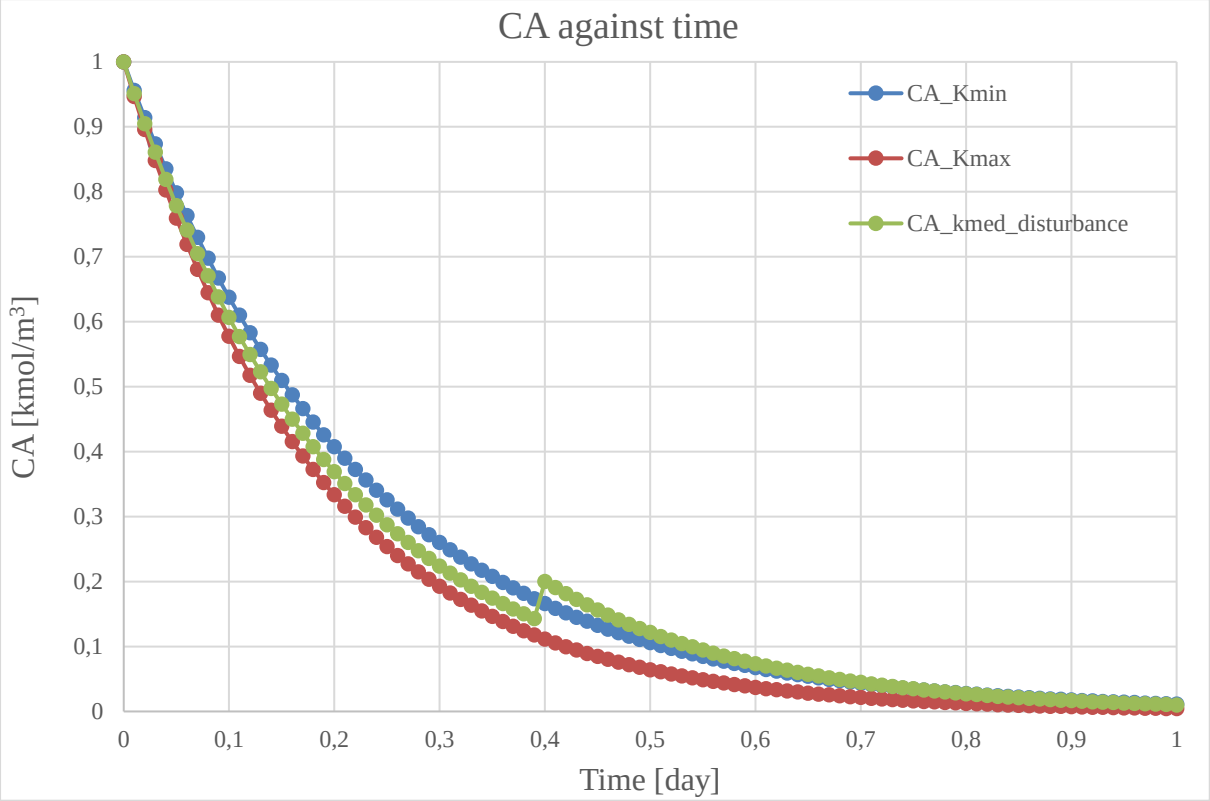


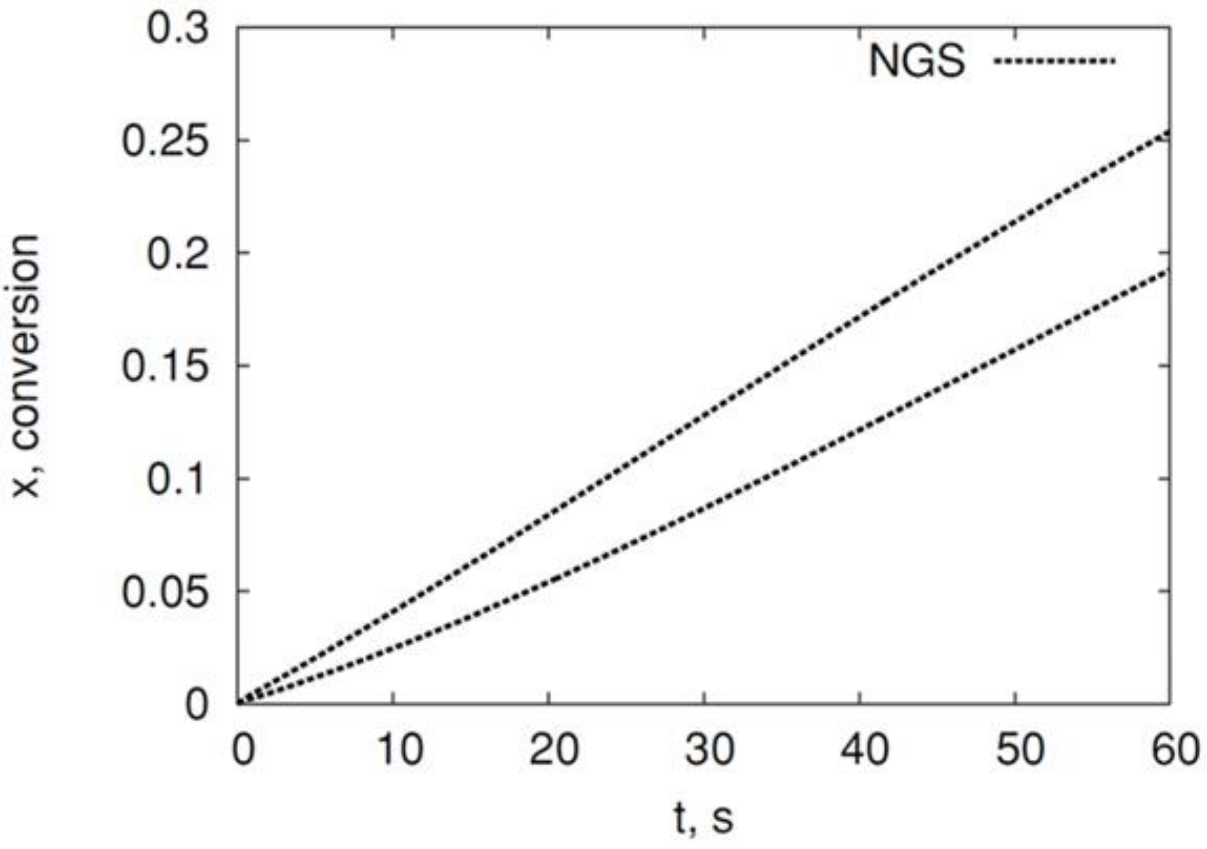
Figure 4.5: A disturbance acts on the A concentration

As shown in the figure, at the point in time where the value of C_A is changed, its curve immediately overshoots the upper limit and remains there until time 1. Therefore, it is needed to find a controller able to keep the curve inside the limit, despite the presence of the disturbance.

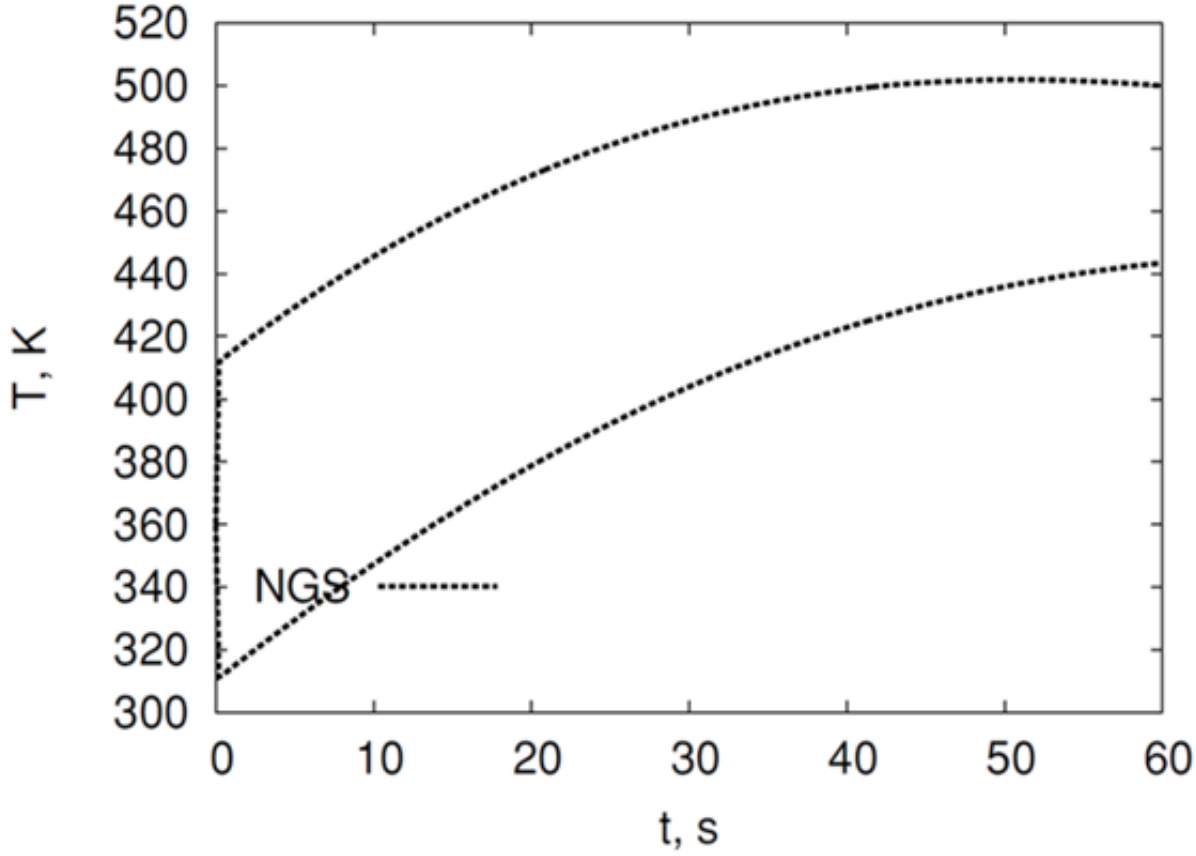
The same approach has been used for the exothermic batch reactor.

4.2.2. Exothermic Batch Reactor

In order to find the enclosure inside of which the curves of the conversion of *A* and the reactor temperature can lie, an enclosure solver can be used. By reporting the system of equation and the solver setting, it is possible to obtain the upper and the lower limits for the conversion of component *A* and the reactor temperature. They are represented in the following figures 3.6 (a) and (b):



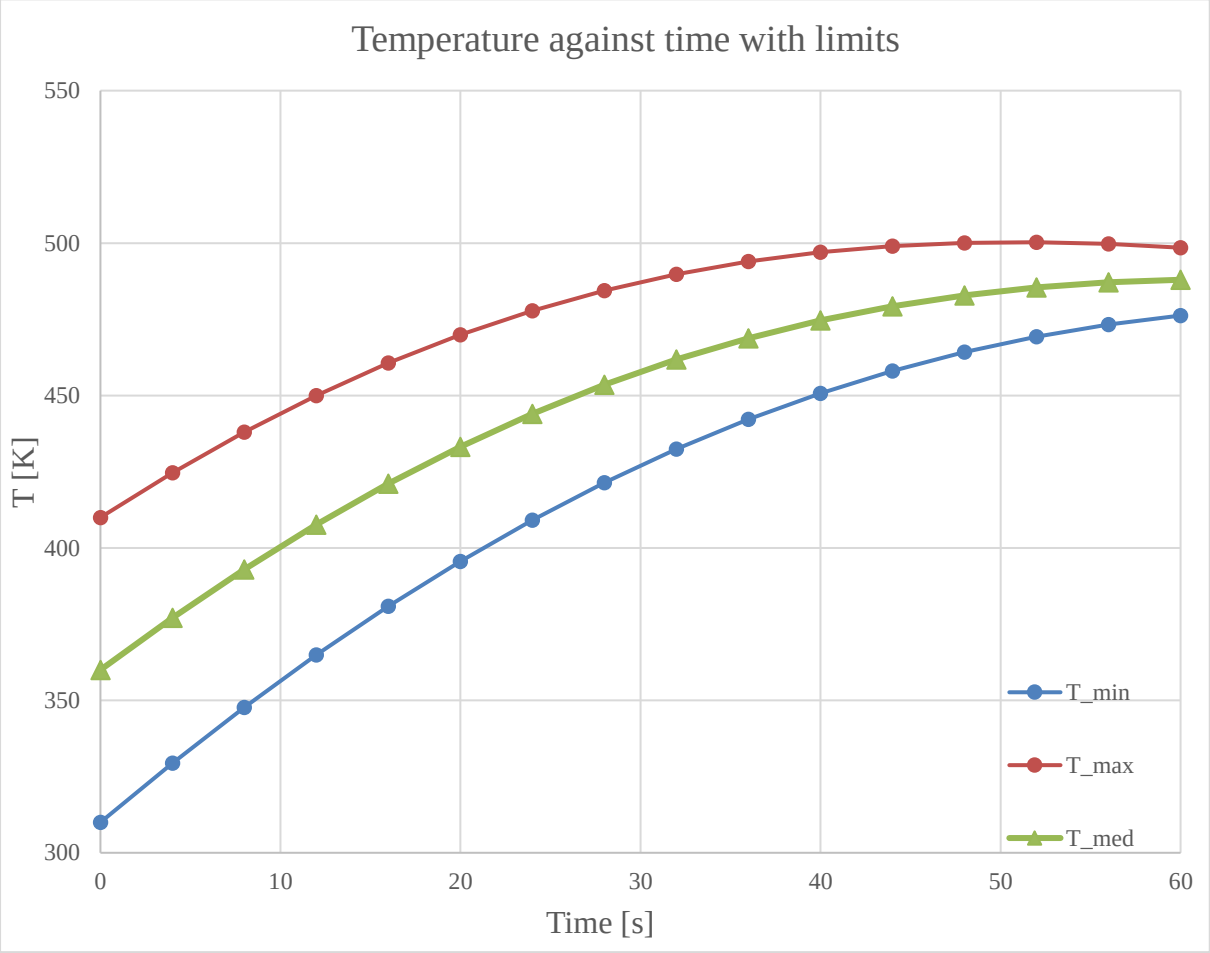
(a)



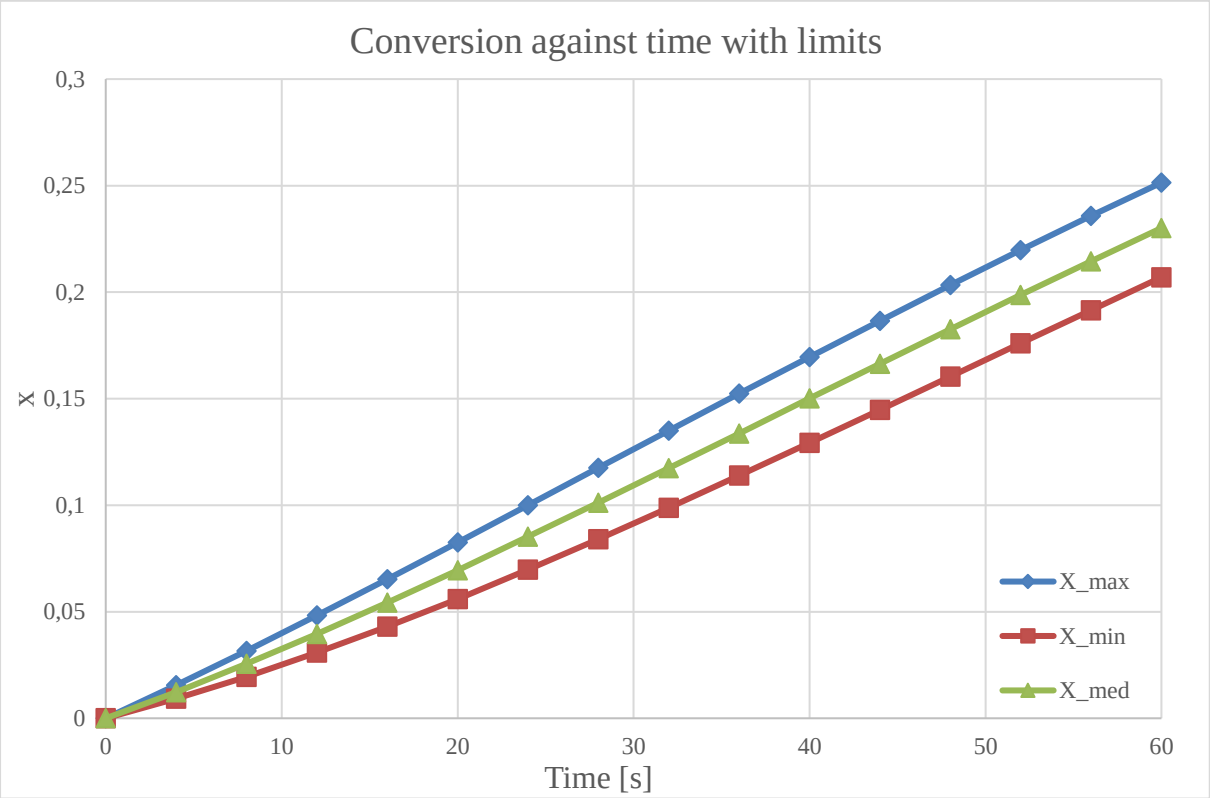
(b)

Figure 4.6: Enclosure of the A conversion and reactor temperature for the exothermic batch reactor

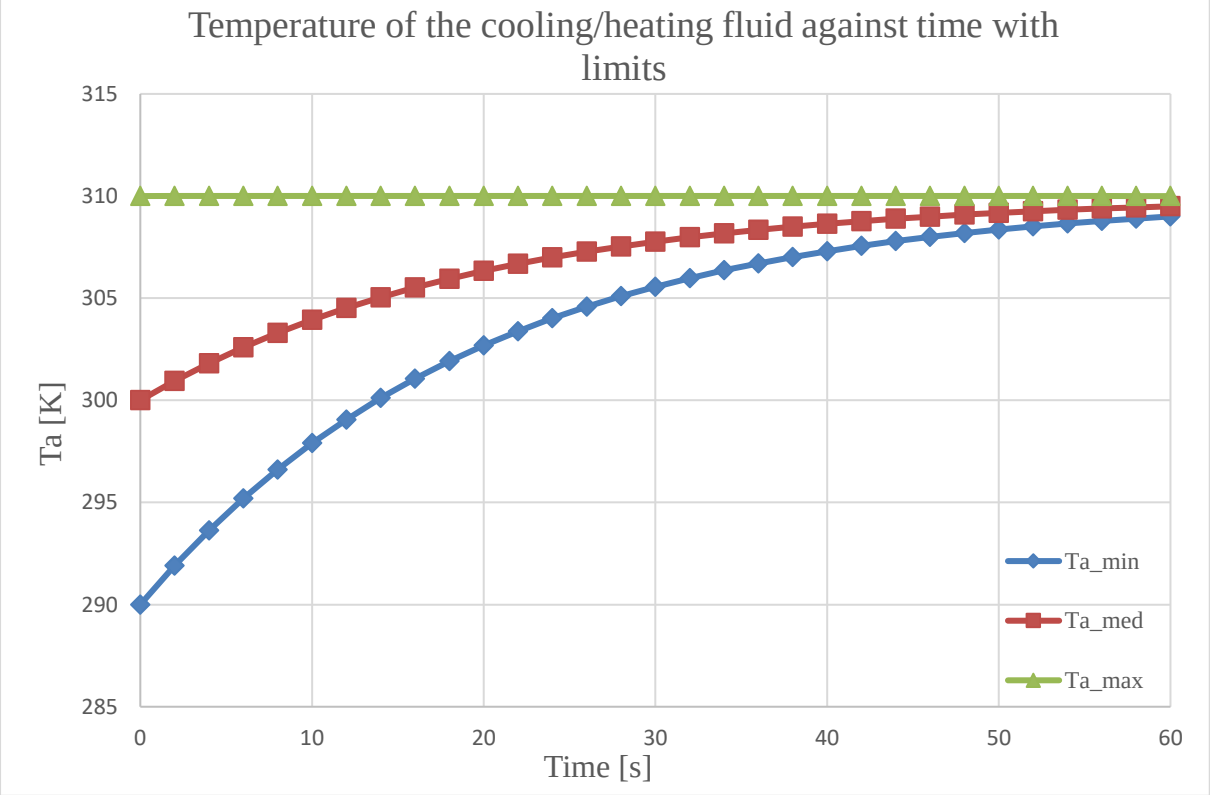
Let's start analysing the intermediate behaviour of the reactor temperature, of the conversion of *A* and of the cooling/heating fluid temperature:



(a)


Conversion against time with limits
X
Time [s]
0,3
0,25
0,2
0,15
0,1
0,05
0
0
10
20
30
40
50
60
X_max
X_min
X_med

(b)


Temperature of the cooling/heating fluid against time with limits
Ta [K]
Time [s]
315
310
305
300
295
290
285
0
10
20
30
40
50
60
Ta_min
Ta_med
Ta_max

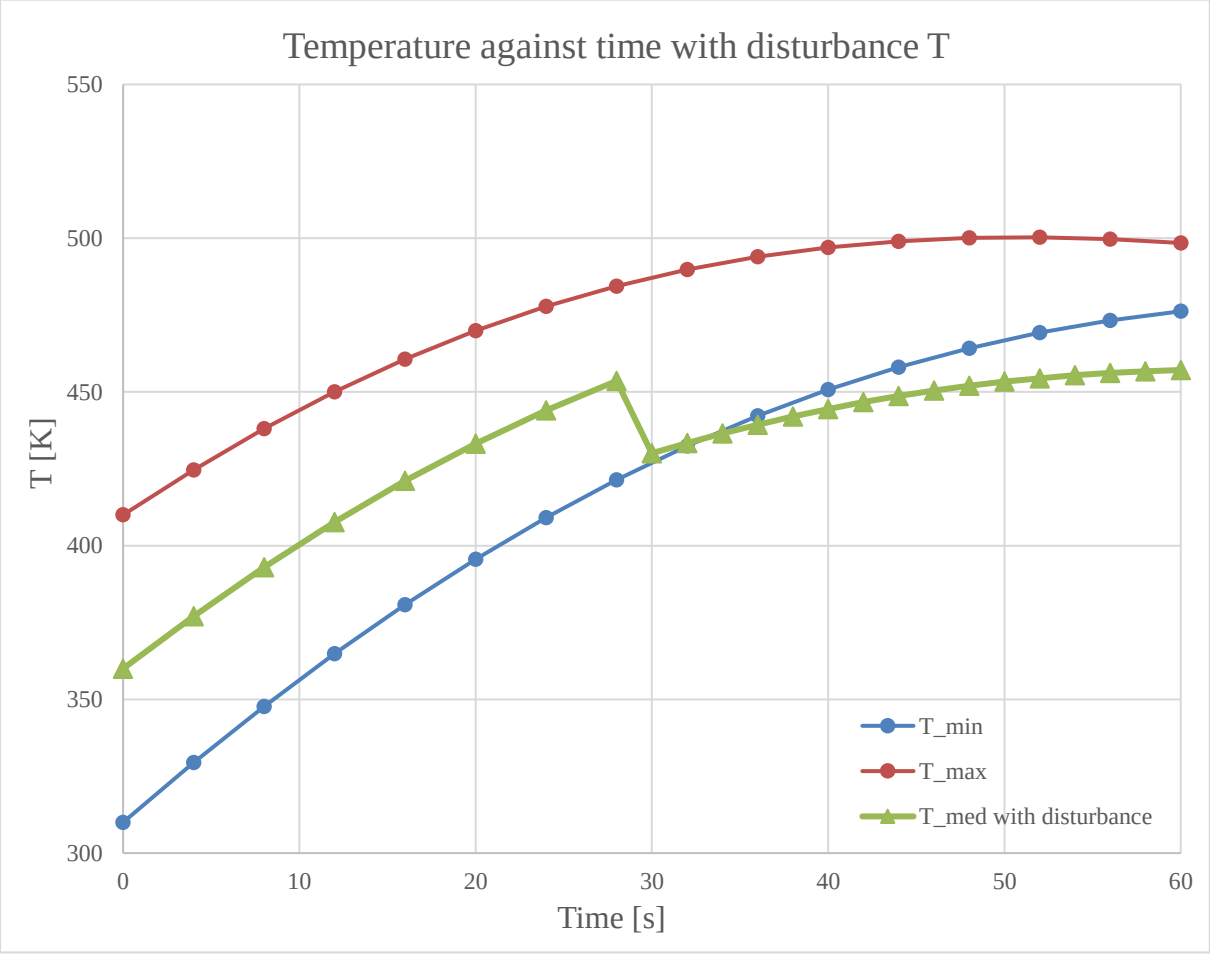
(c)

Figure 4.7: Intermediate profile of the reactor temperature (a), conversion (b) and cooling/heating fluid temperature (c) with respective limits

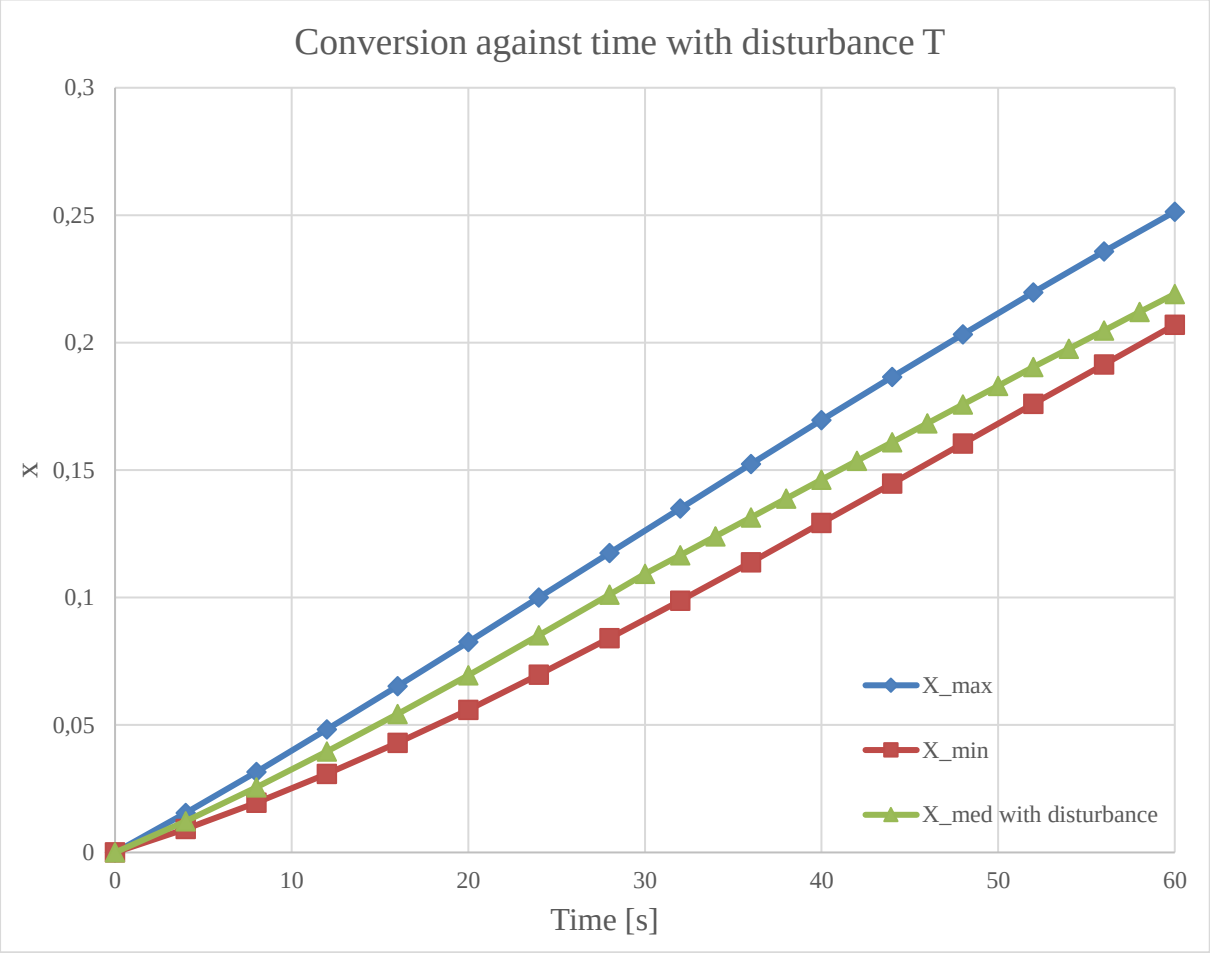
Now, let's find a value of the disturbances that force key system states to violate their lower/upper bounds.

4.2.2.1. Case 1) T^{feed} used as disturbance and T used as controlled variable

In this case, there can be temperature bound violation in order to see what happens.



(a)



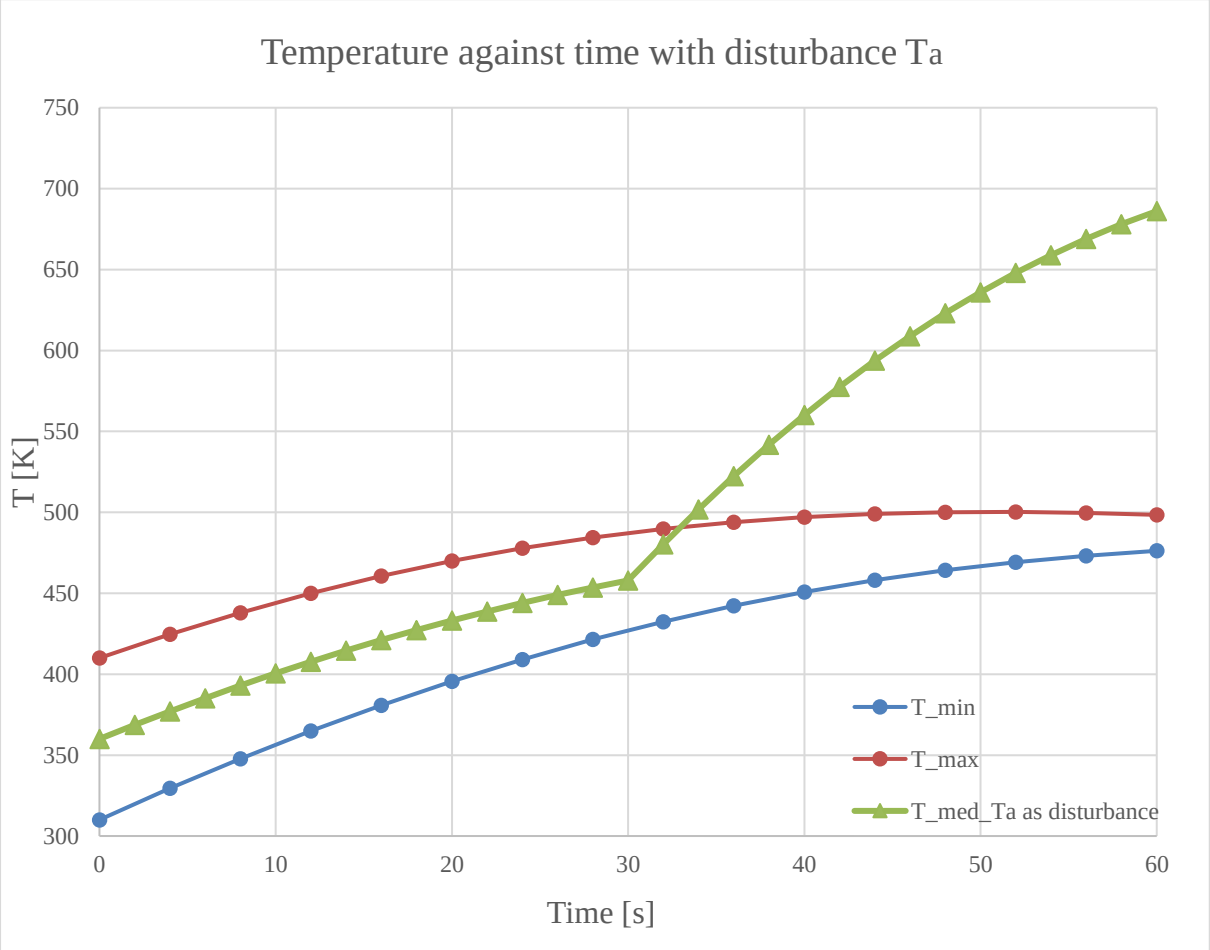
(b)

Figure 4.8: Results in terms of reactor temperature (a) and A conversion (b) if a disturbance acts on the initial temperature profile

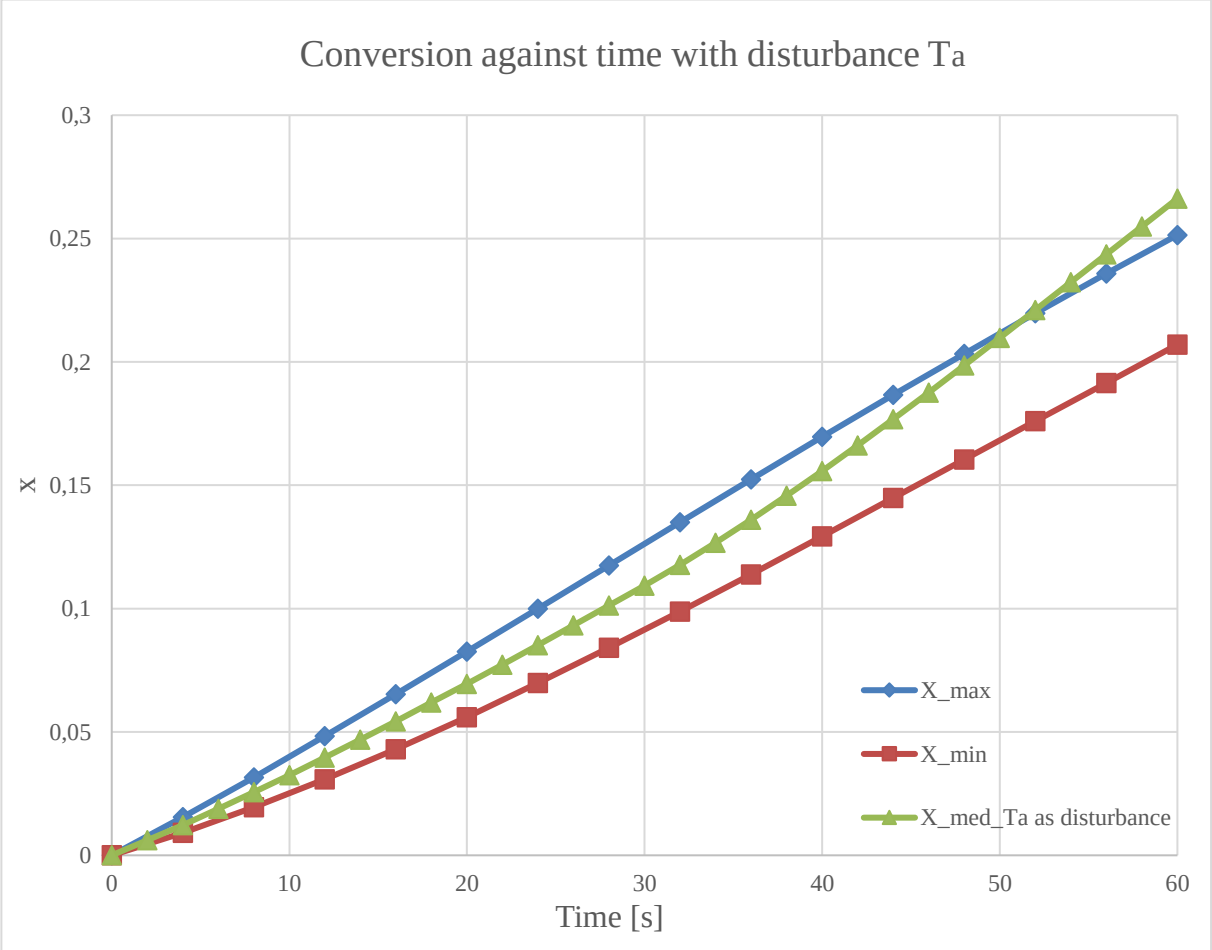
The initial value of the reactor temperature has been changed to 430 K at time equal to 30s. As expected, the curve of the temperature reaches the lower bound, and undershoots it. Therefore, there is the need of a controller able to keep the curve inside the limit. Instead, the conversion profile remains inside the bounds.

4.2.2.2. Case 2) T_a^{feed} used as disturbance and T as controlled variable

The initial temperature of the cooling/heating fluid can be used as a disturbance and the reactor temperature as the manipulated variable. At $t = 30s$ the value of T_a^{feed} has been changed from $310\ K$ to $500\ K$, the results in terms of reactor temperature and conversion of A are shown below.



(a)



(b)

Figure 4.9: A disturbance acts on T_a profile modifying reactor temperature profile (a) and A conversion (b)

As shown in the figure, at the point of time where the value of T_a^{feed} is modified, the curve of the reactor temperature immediately violates the upper limit and qualitatively changes its trend. It remains outside until the end of the batch cycle. Conversely, the curve of the conversion is not too affected by the disturbance and only towards the end of the batch slightly violates the upper bound.

4.2.2.3. Case 3) T_a^{feed} used as disturbance and T_a used as controlled variable

Thanks to the previous equation, the profile of the cooling/heating fluid temperature can be evaluated and correlated to the reactor temperature: it is possible in fact to control T_a in order to maintain T inside its enclosure. In this case T_a^{feed} has been changed from $300\ K$ to $500\ K$ when it reaches $t = 30s$. The result is shown in the following graph.

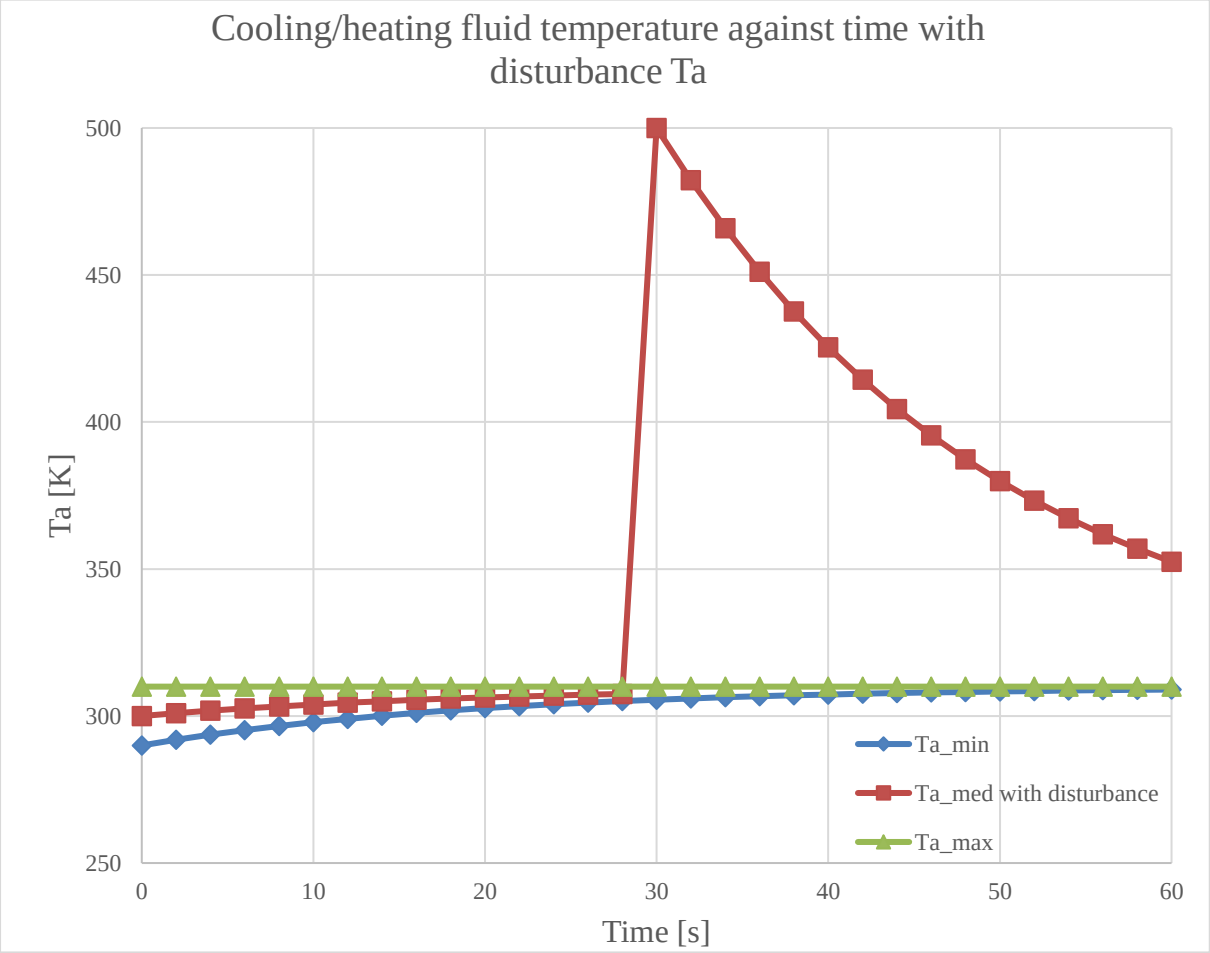
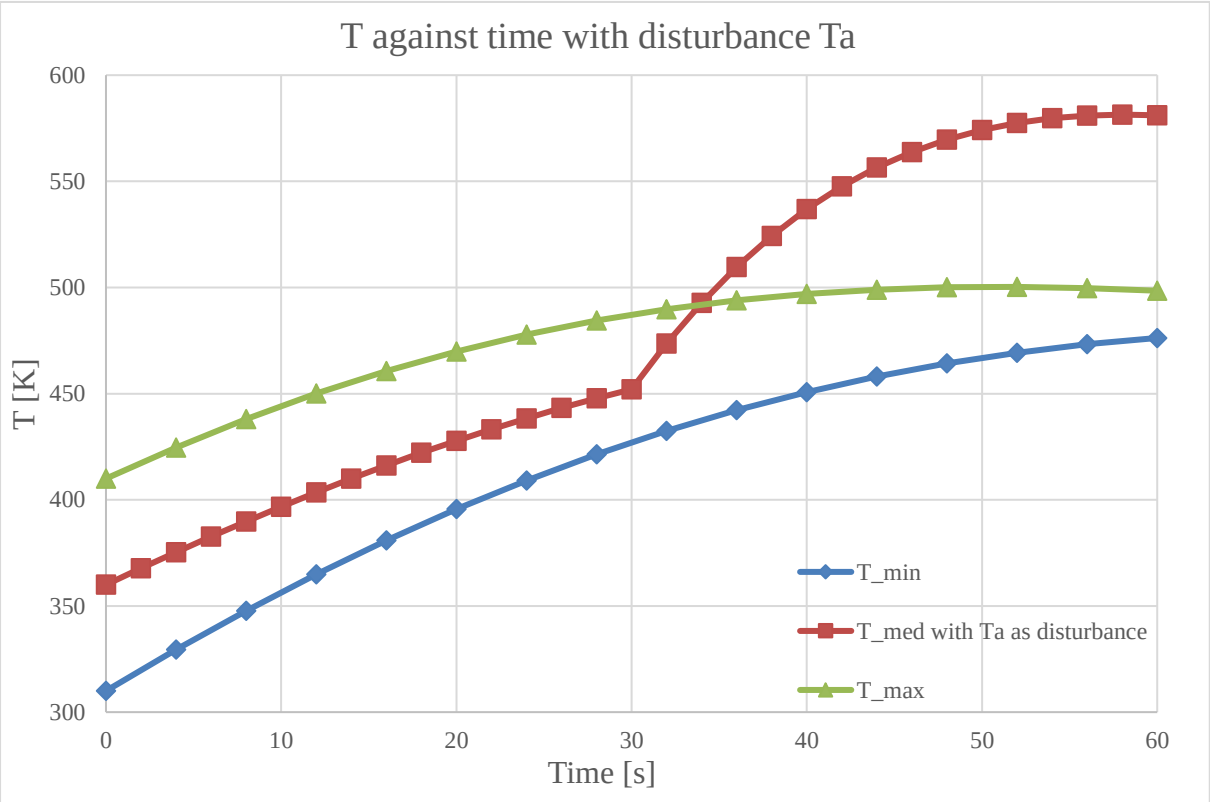
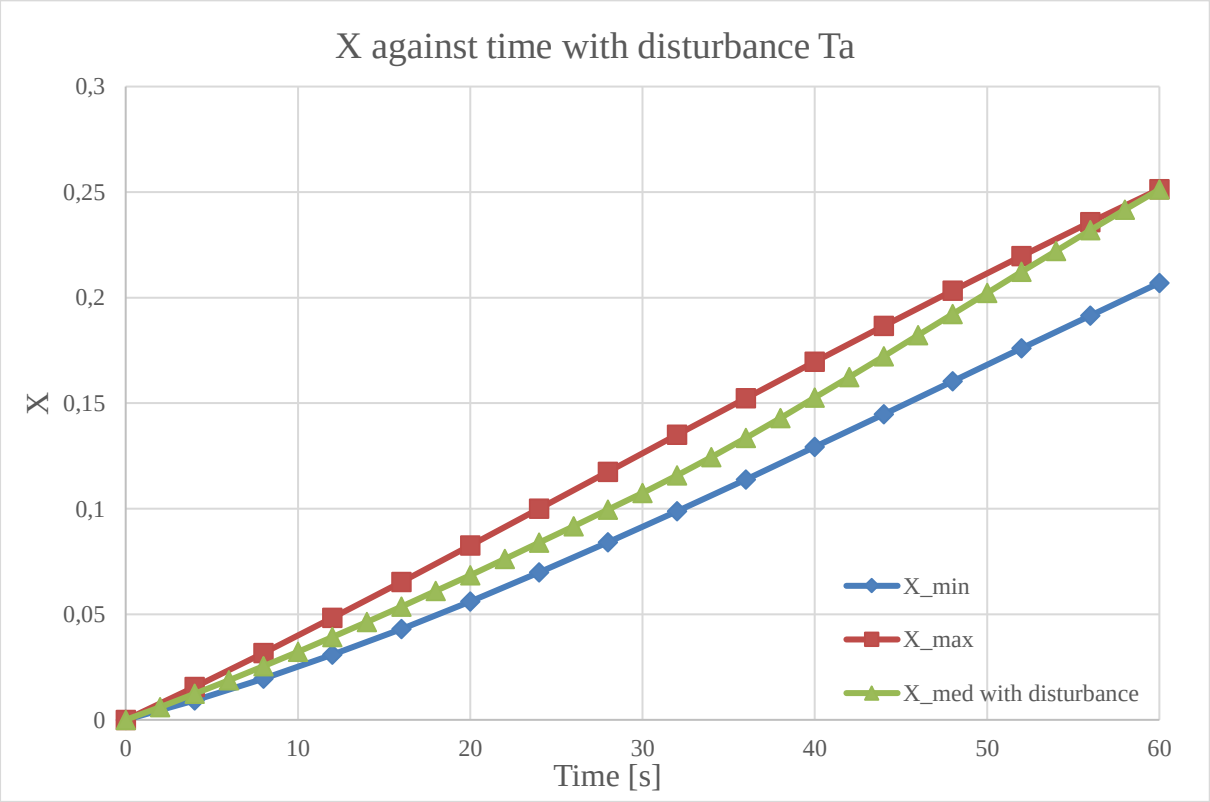


Figure 4.10: A disturbance acts on T_a profile

What is expected is that the profile of the exercise fluid temperature goes suddenly outside the upper limit when there is the variation. The reactor temperature increases in correspondence of the variation in the value of the initial cooling/heating fluid temperature and overcomes the upper limit:



(a)



(b)

Figure 4.11: Effect of the T_a disturbance on temperature (a) and conversion (b) profile

The profile of the reactor temperature changes its behaviour in correspondence of the disturbance and goes outside the bounds. The conversion, instead, remains inside the limits until 60 seconds where it reaches the upper bound.

It’s needed a controller in order to avoid the spillage of the reactor temperature trajectory from the safety region.

5. RESULTS

For all the case studies, a Proportional-Integral (PI) Controller has been used, in which there is the need to define the manipulated parameter and the state variable. It is represented by: $C_{PI}(t) = K_p * e(t) + T_i * \int e(t)\,dt$ in which K_p is the proportional gain, T_i is the integral time and $e(t)$ is the error that is function of time.

TABLE 5: PARAMETERS USED FOR THE PI CONTROLLER FOR EACH CASE STUDIED

CASE STUDIES	DISTURBANCE	CONTROLLED VARIABLE	TUNING PARAMETERS
1. First Order Irreversible Series Reaction	${C_A}^0\ (0.2\frac{kmol}{m^3})$	C_A	$K_p = 0.4$ $T_i = 0.1$
2. Exothermic Batch Reactor (case 1)	$T^{feed}(430\ K)$	T	$K_p = 0.5$ $T_i = 0.5$
3. Exothermic Batch Reactor (case 2)	$T^{feed}_{exercise\ fluid}(500\ K)$	T	$K_p = 0.6$ $T_i = 0.2$ $2^{nd} example$: $K_p = 0.1$ $T_i = 0.08$
4. Exothermic Batch Reactor with balance on the jacket (case 3)	$T^{feed}_{exercise\ fluid}(350\ K)$	$T_{exercise\ fluid}$	$K_p = 0.3$ $T_i = 0.00001$

5.1.First Order Irreversible Series Reaction

For the First Order Irreversible Series Reaction scheme, the concentration of A has been changed therefore this latter one will be the disturbance. The system is relatively simple, so C_A^0 could be used as the disturbance and C_A as the variable to control and manipulate. The error depends on the concentration of component A and is defined as the difference between the desired concentration of A and its measurement: $e(t) = C_{A,des}(t) - C_{A,measured}(t)$. The ODE system is constituted of the previous equations and also by the error function.

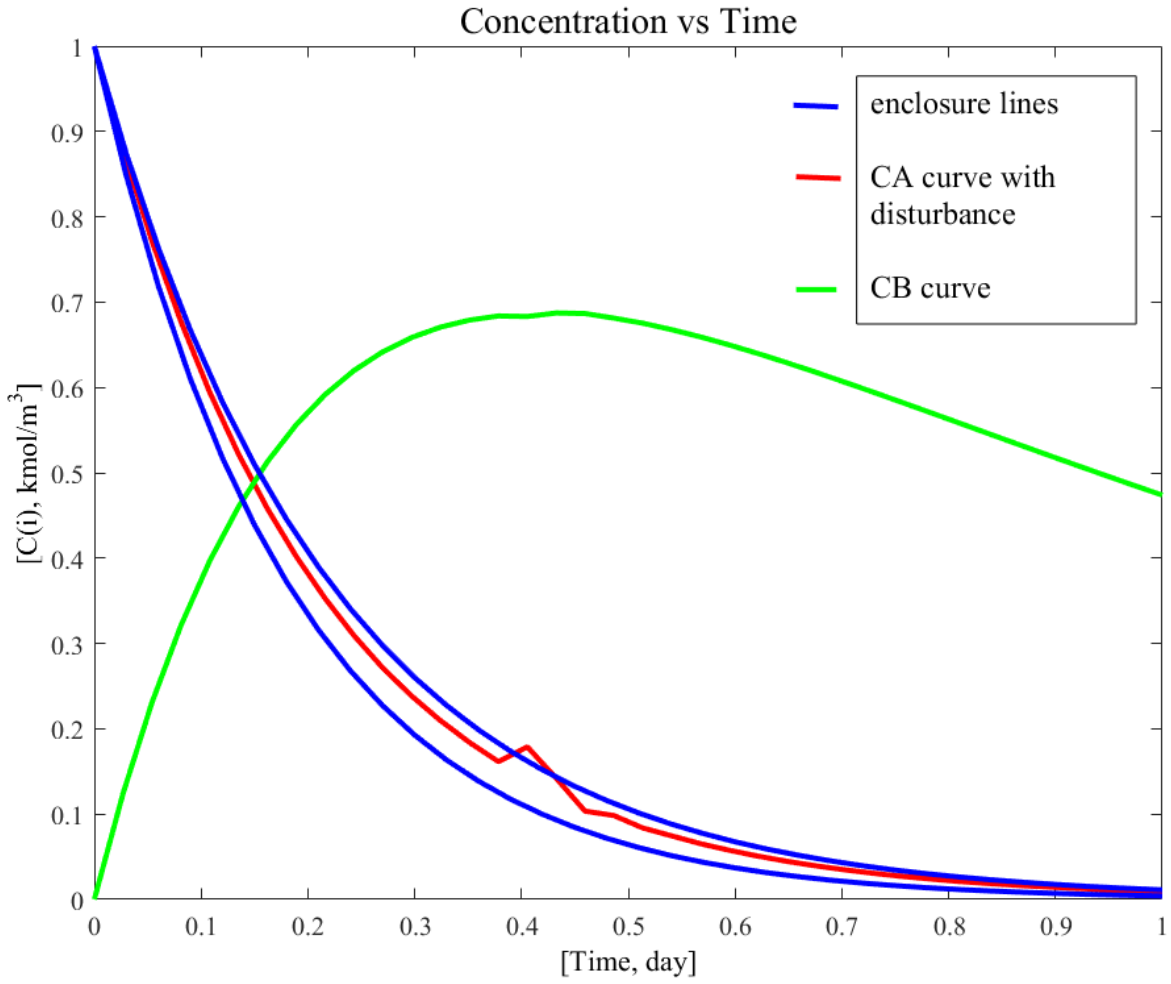


Figure 5.1: Effect of the PI controller on the concentration profile in the presence of a disturbance

The graph shows the profile of the concentration of A: at the beginning, it has an intermediate behaviour. Then, at time 0.4, there is a disturbance and the concentration goes outside the limit, thus reaching the value 0.2. Finally, thanks to the controller actions, it goes back inside the limit and never leaves the enclosure again. In the trajectory of C_B, instead, there is a little variation at the time equal to 0.4.

There are a lot of values that can be used for the integral time and the proportional gain, but it's important to maintain the proportional gain below 0.6 and the integral time below 0.1 in order to have a good control quality. For the same reason, by increasing K_p the value of T_i must decrease. For the PI controller, the following values have been used: $K_p = 0.4$ and $T_i = 0.1$ (37 as number of steps).

5.2.Exothermic Batch Reactor

5.2.1. Case 1) T^{feed} used as disturbance and T used as controlled variable

The feed temperature is used as disturbance and the reactor temperature as manipulated variable. The error is defined as the difference between the desired reactor temperature and that measured in real time: $e(t) = T_{des}(t) - T_{measured}(t)$. The ODE system is constituted of the aforementioned equations and also of the error function.

Also in this case, a PI controller has been used but the integral time and the proportional gain don't affect too much the behaviour of the system, thus they can be maintained below 1: in

particular the following values have been selected: $K_p = 0.5$ and $T_i = 0.5$ (25 as number of steps).

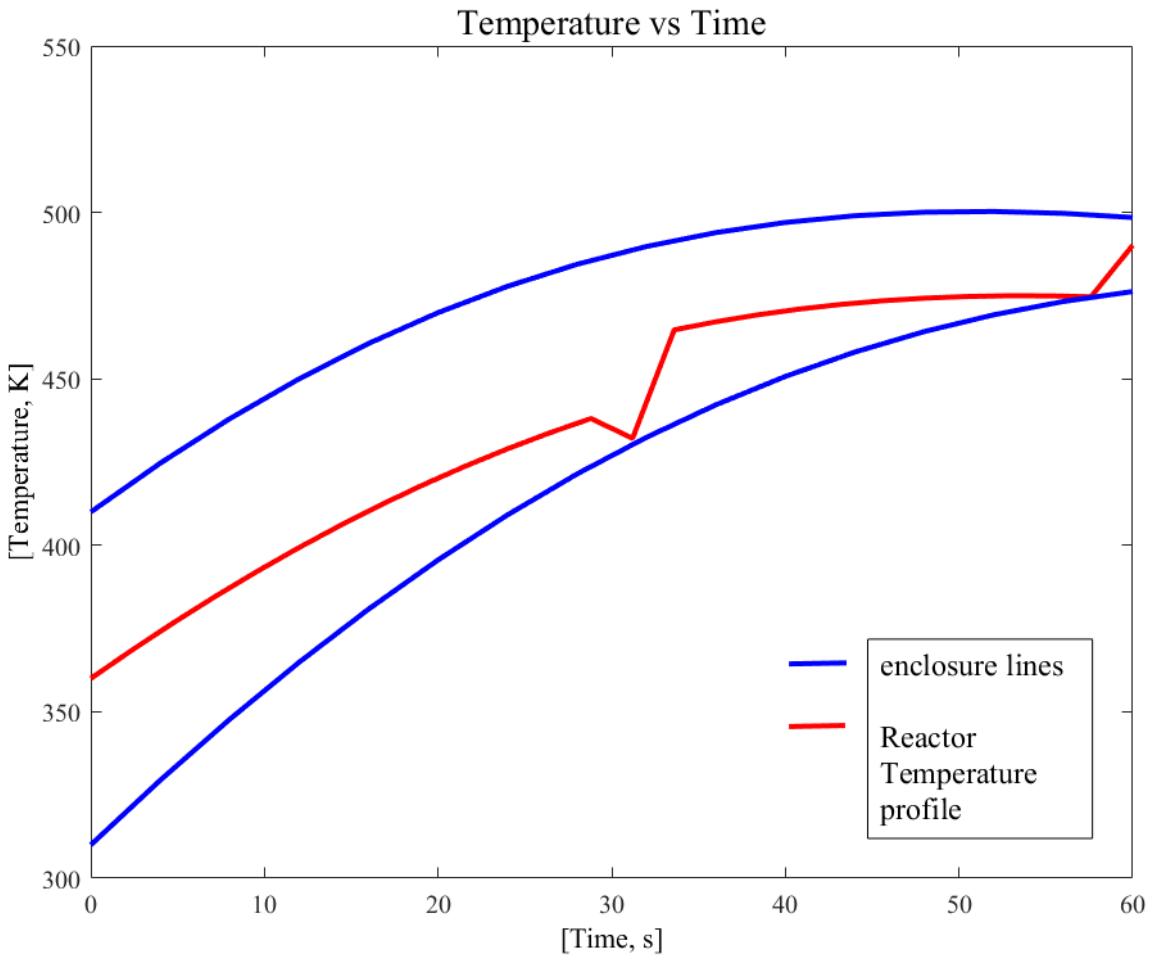


Figure 5.2: Effect of the PI controller on the T profile in the presence of a disturbance in T^{feed}

As the reactor temperature profile is approaching the lower limit, it is kept inside the enclosure thanks to the PI controller, and then the temperature continues behaving like before and reaches again the lower limit so the PI controller must act a second time.

5.2.2. Case 2) T_a^{feed} used as disturbance and T used as controlled variable

In this case, by focusing the attention on the reactor temperature, it is needed to find a controller able to keep the curve inside the limit, despite the presence of a disturbance.

In the Proportional-Integral (PI) Controller the manipulated variable and the controlled variable are defined: the feed temperature of the cooling/heating fluid is used as the disturbance and *T* has been selected as the manipulated variable because the interest is based in keeping its curve inside the limit, especially for safety reasons.

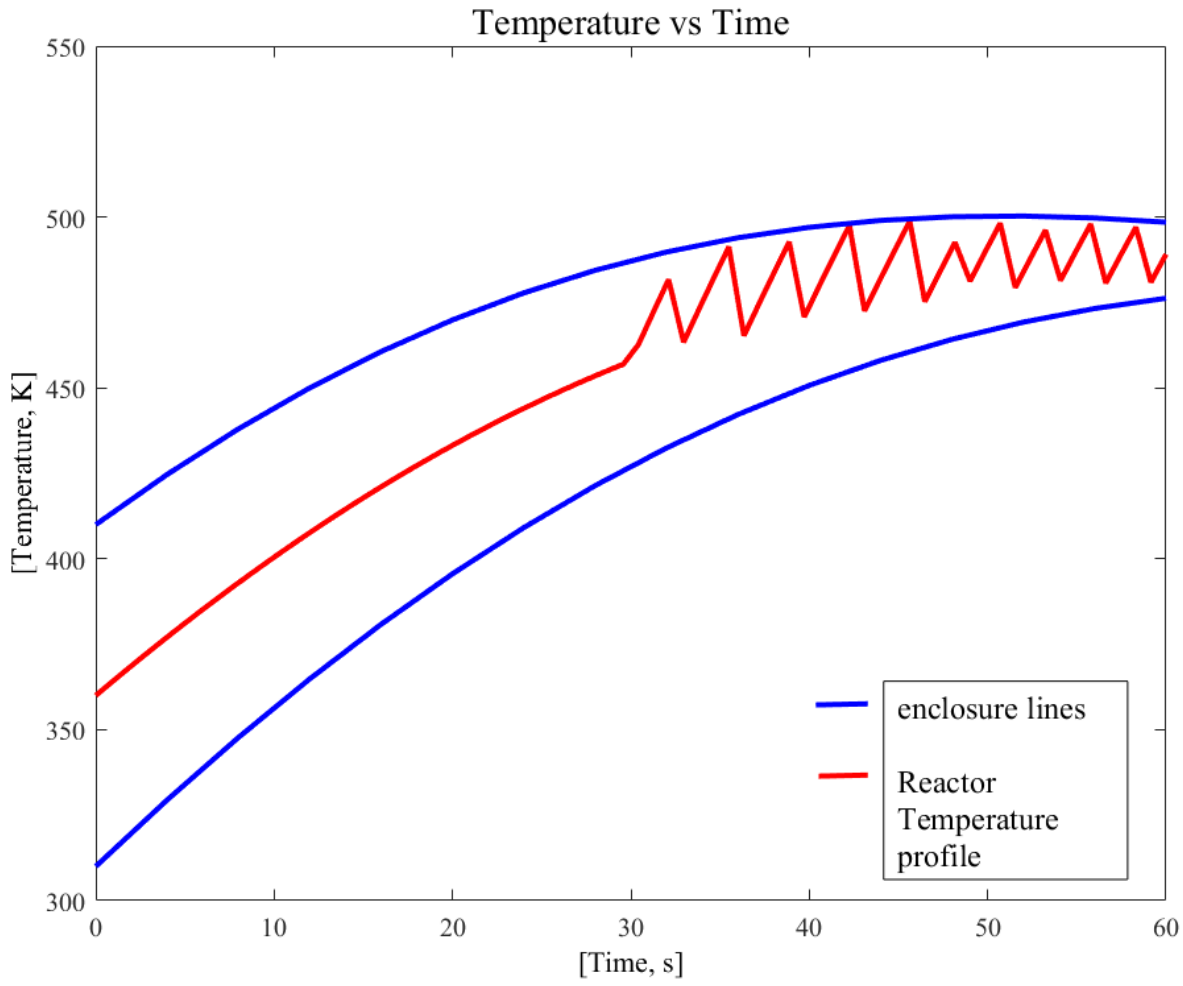


Figure 5.3: Effect of the PI controller on T profile in the presence of a disturbance in T_a^{feed}

The graph shows the behaviour of the reactor temperature over the time: at the beginning, it has an intermediate behaviour; at 30 seconds, there is a disturbance generated by a change in the value of the cooling/heating fluid temperature and the reactor temperature starts to increase. Then, thanks to the controller, it remains inside the limit. The result is an oscillating trajectory with some points reaching the upper bound. For the PI controller, the following values have been used: $K_p = 0.6$ and $T_i = 0.2$ (71 as number of steps).

There is the possibility to use also other values of proportional gain and integral time but the important aspect is to find a compromise between these two values in order to have a satisfactory temperature trend (for example: Ns=41, $K_p = 0.3$ and $T_i = 0.2$; if it is used a very low value for the number of steps, it is needed to consider larger values of K_p and T_i). By decreasing K_p and T_i the oscillations induced by the controller become smaller. The following graph shows the behaviour of the reactor temperature, if the parameters are: $T_i = 0.08$, $K_p = 0.1$ and $N_s = 21$.

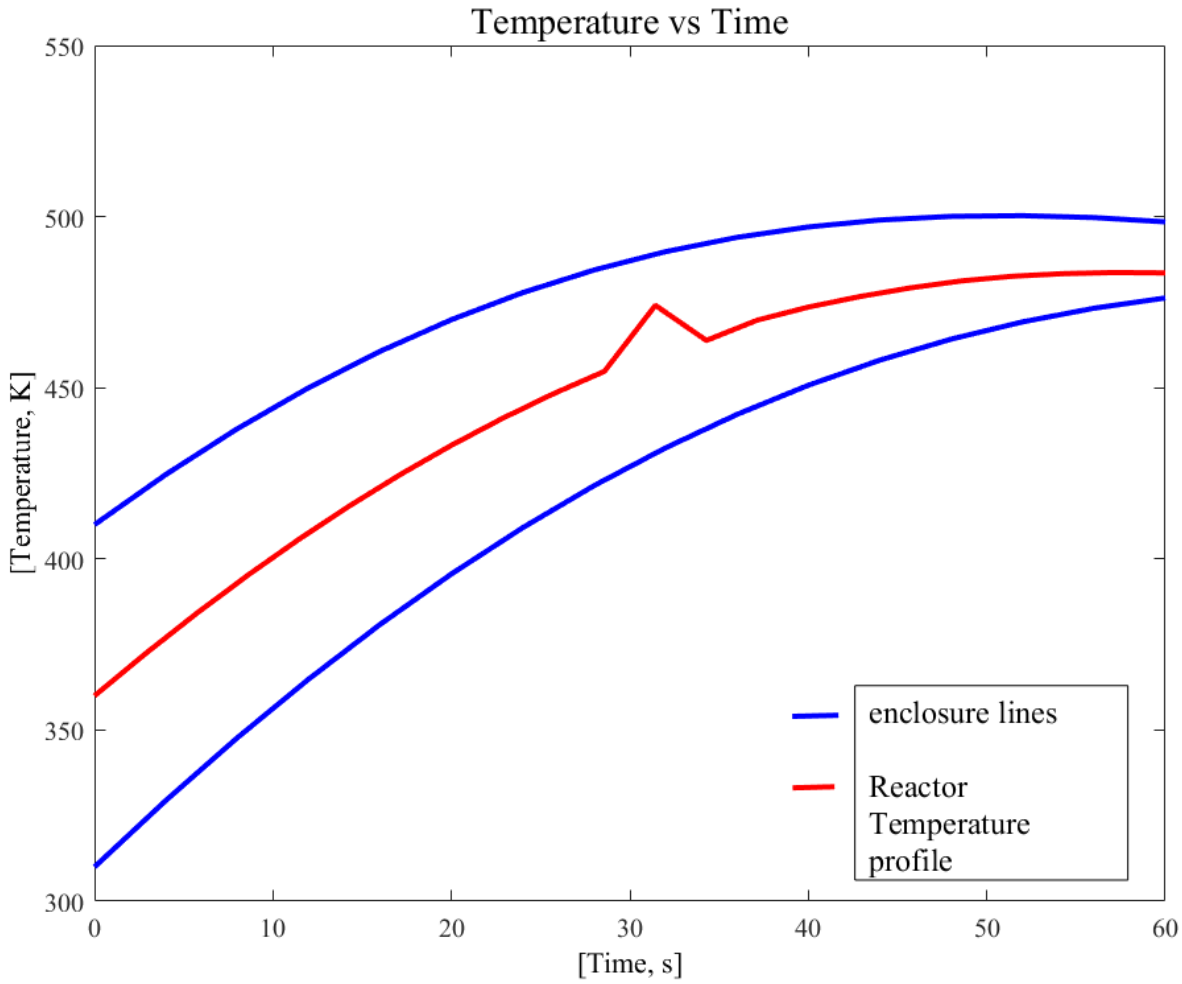
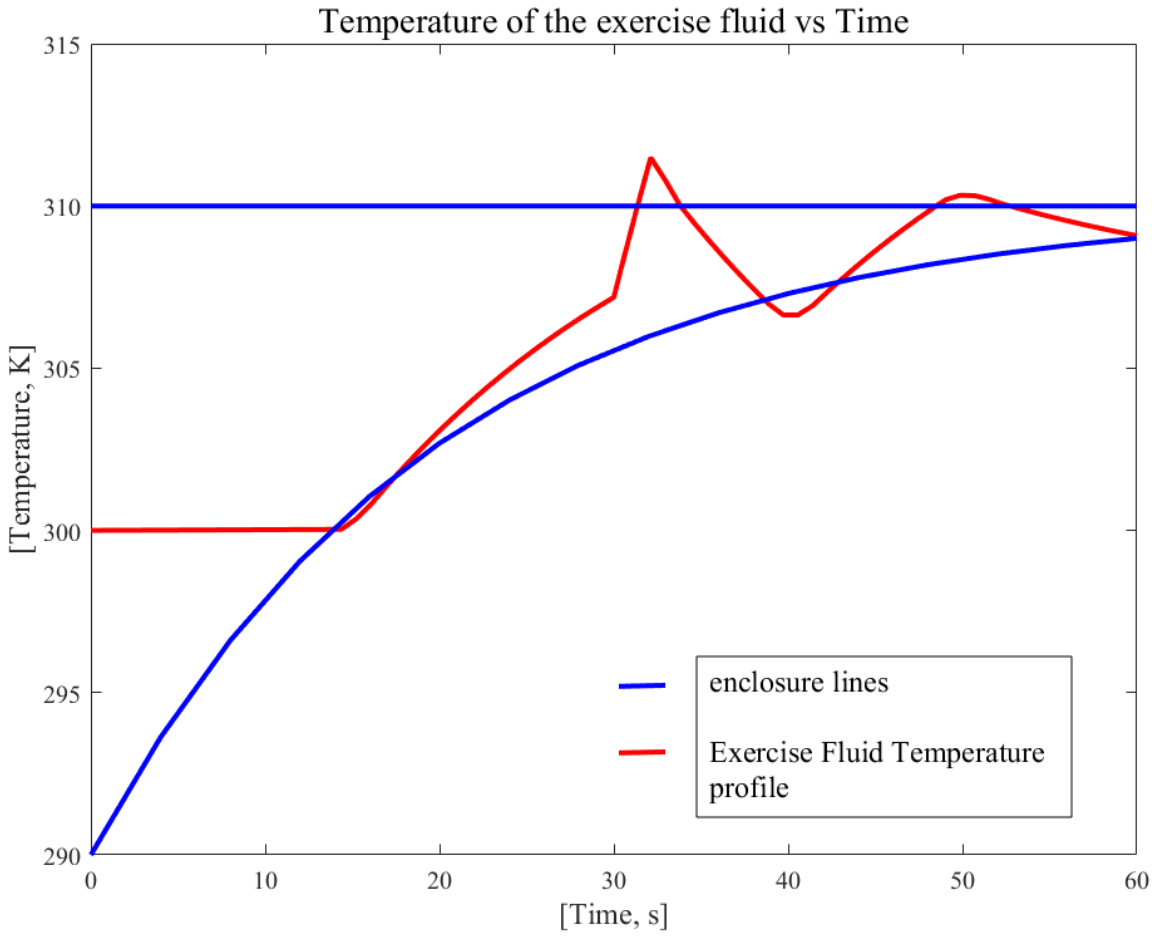


Figure 5.4: Effect of the PI controller on T profile in the presence of a disturbance in T_a^{feed} with change in the tuning parameters

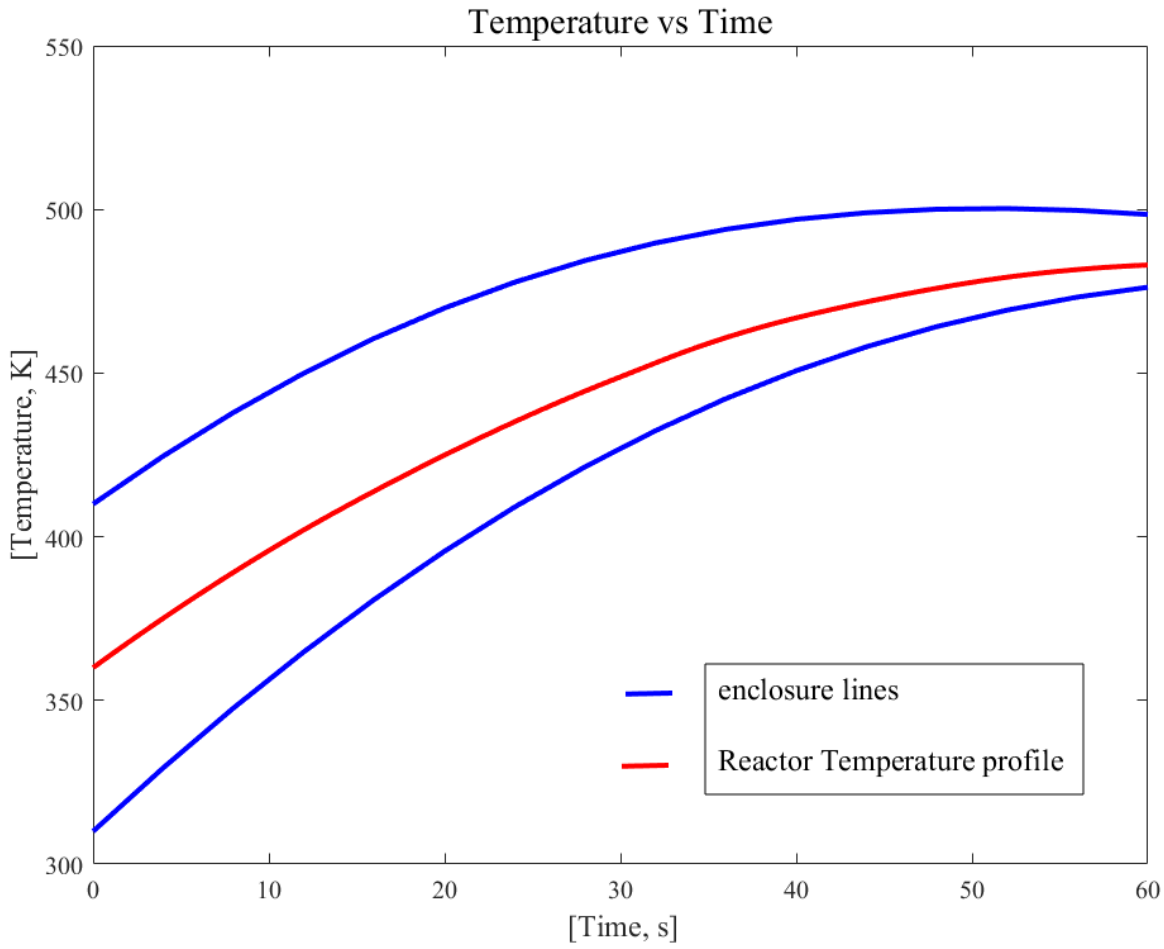
As shown, by decreasing the two tuning parameters a better stability can be achieved.

5.2.3. Case 3) T_a^{feed} used as disturbance and T_a used as controlled variable

With the PI controller, the objective is to manage the value of the temperature of the cooling/heating fluid in order to control the temperature of the reactor.



(a)



(b)

Figure 5.5: Effect of the PI controller on T_a (a) and T (b) profile with T_a^{feed} as disturbance

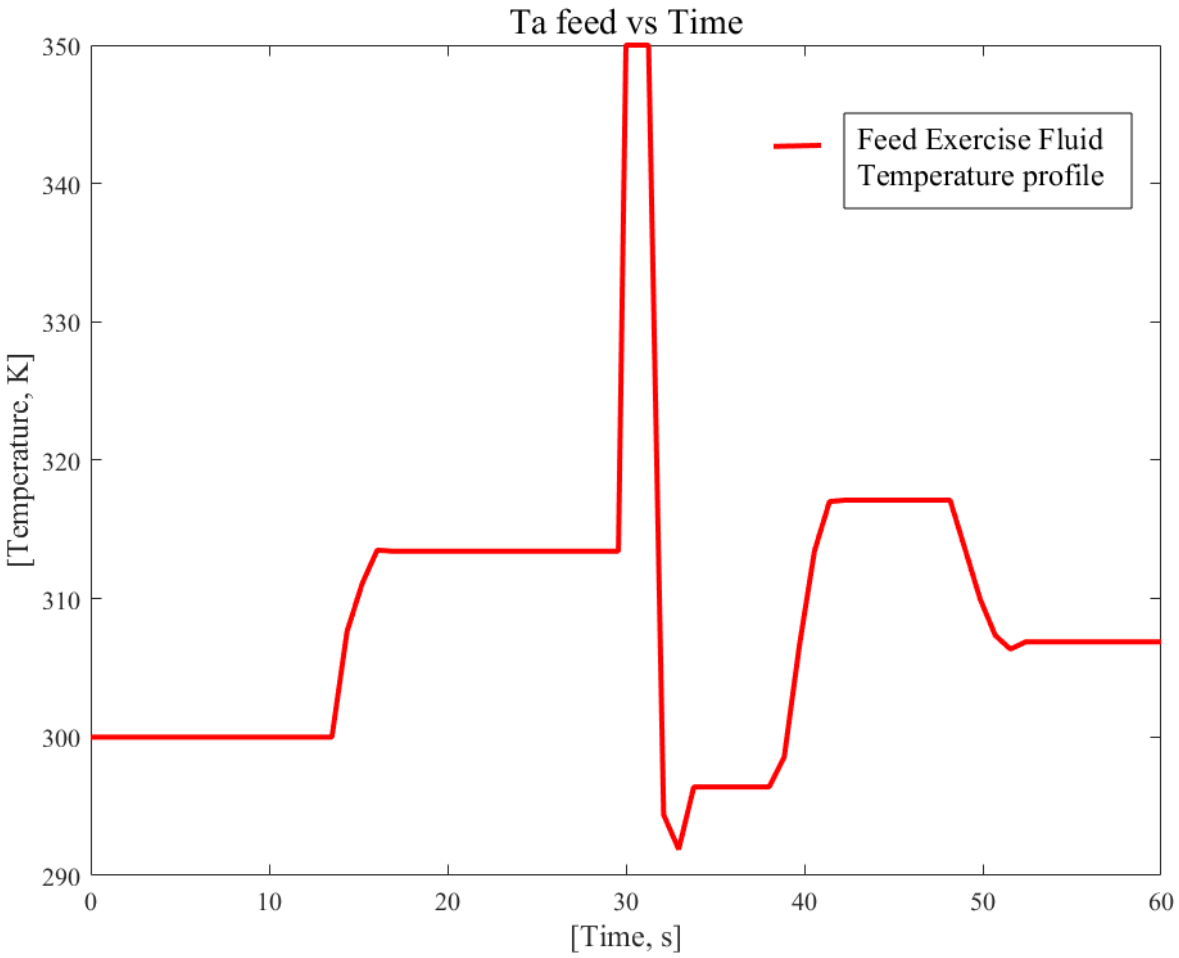


Figure 5.6: Profile of T_a^{feed} against time

As shown in the graphs, by applying the proposed improvement to the model:

- the profile of the exercise fluid's temperature goes outside both the limits, then there are oscillations due to the high disturbance and after is reported inside thanks to the PI controller;
- the profile of the reactor temperature is affected by a slight variation because of the sudden increase of T_a^{feed} but, since T_a can be immediately controlled and manipulated by the PI controller, the reactor temperature has no time to reach and overcome its limits; the only variation consists in the approaching to the lower limit.

So, by changing the model and using a controller to manipulate the exercise fluid temperature, it is possible to control the reactor temperature easily and more efficiently.

5.2.4. Optimal Profile

TABLE 6: INITIAL TEMPERATURE, DISTURBANCES AND TUNING PARAMETERS USED FOR EACH CASE STUDIED

CASE STUDIES	INITIAL TEMPERATURE VALUE	DISTURBANCE	TUNING PARAMETERS
1. Exothermic Batch Reactor (case 1)	$T^{feed} = 400\ K$	$T^{feed}(430\ K)$	$K_p = 0.5$ $T_i = 0.5$
2. Exothermic Batch Reactor (case 2)	$T^{feed} = 400\ K$	$T^{feed}_{exercise\ fluid}(600\ K)$	$K_p = 0.1$ $T_i = 0.08$
3. Exothermic Batch Reactor with balance on the jacket (case 3)	$T^{feed} = 409\ K$	$T^{feed}_{exercise\ fluid}(350\ K)$	$K_p = 0.3$ $T_i = 0.00001$

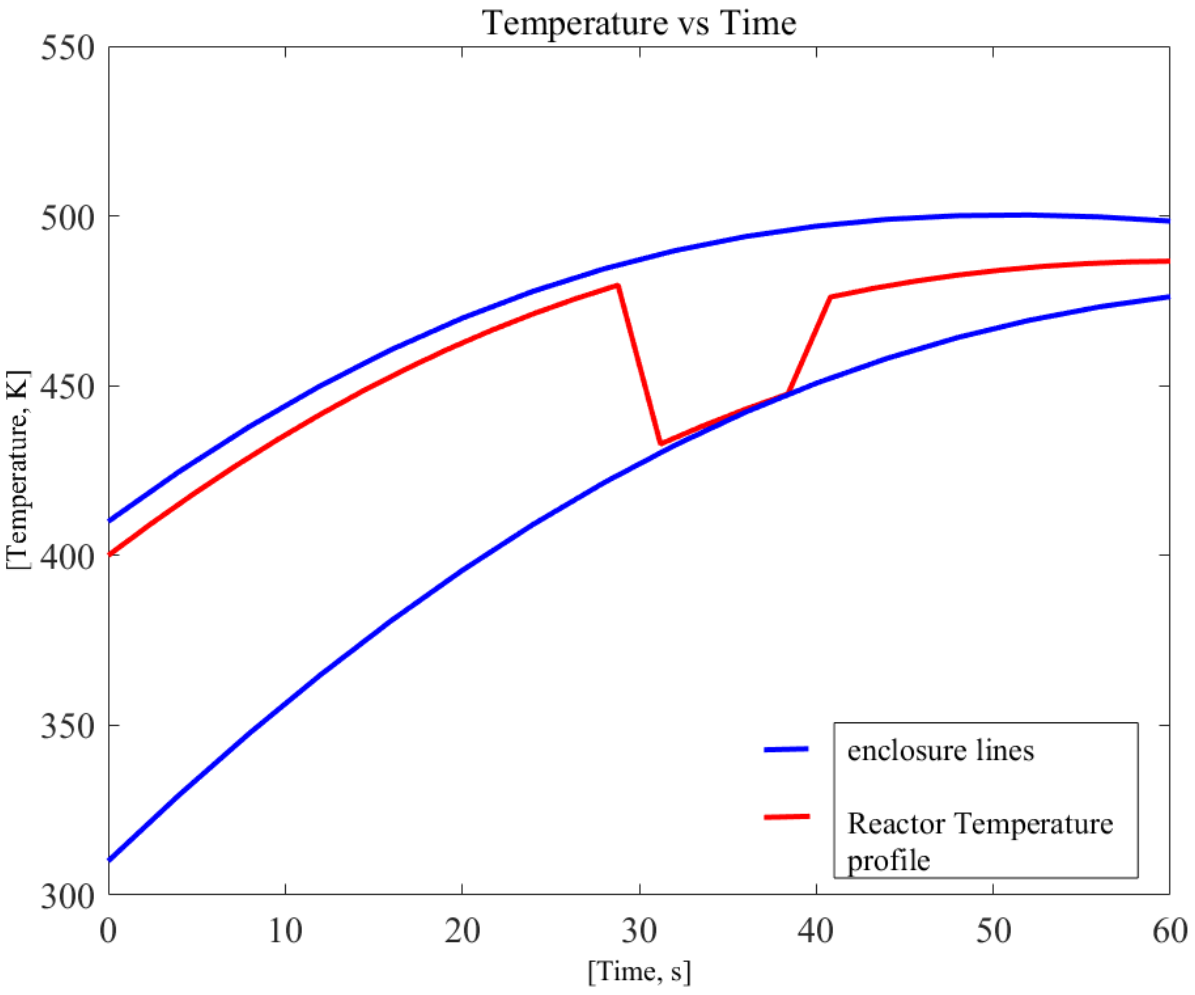
The optimal profile is now investigated. It is represented by the temperature profile able to maximize the yield. The yield is given by the product between the selectivity and the conversion, so in order to increase the yield there is the need to increase the conversion: the optimal temperature profile is the one able to maximize the conversion.

$$\frac{d\chi}{dt} = (1-\chi)k_0 exp\left(-\frac{E_{att}}{RT}\right)$$

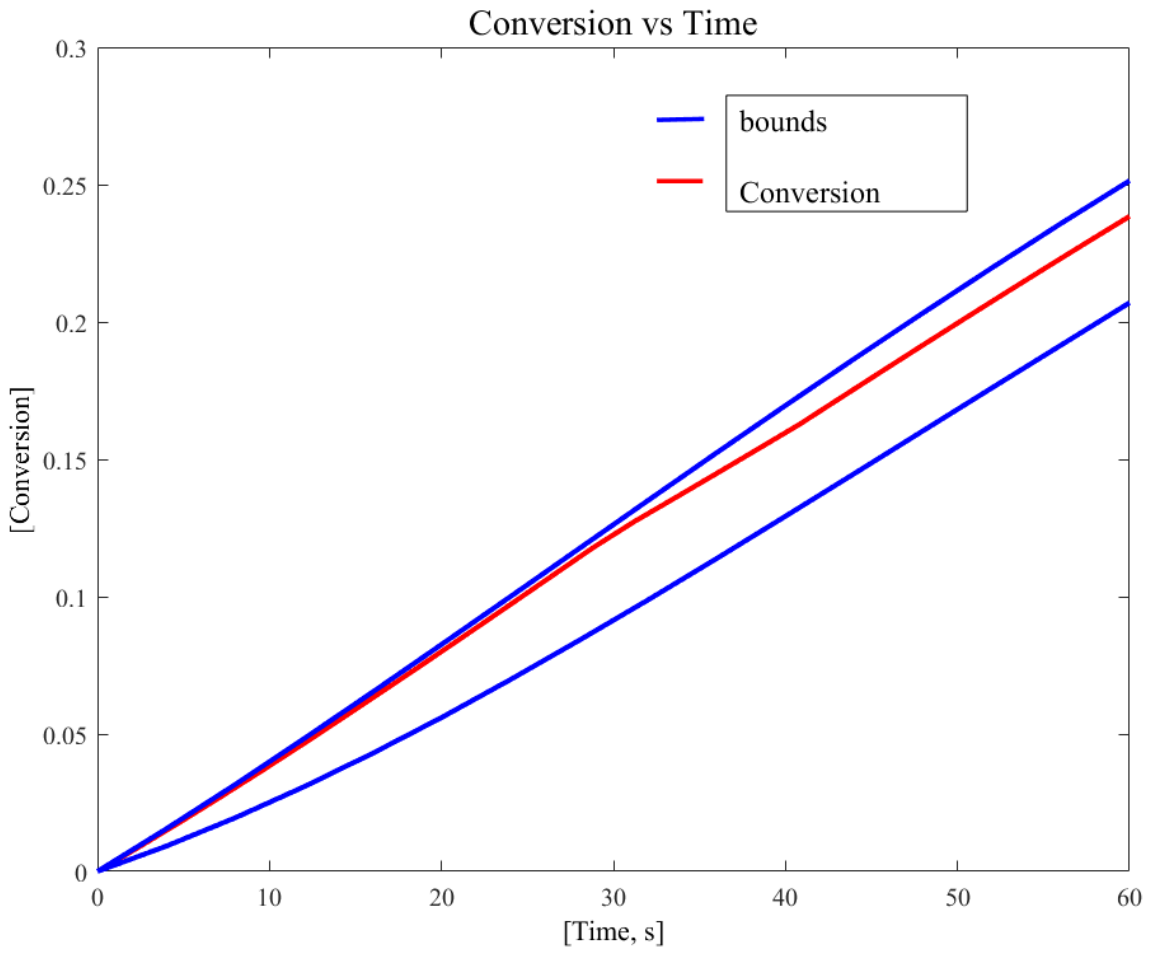
The aforementioned equation, used previously in the ODE system, represents the behaviour of the conversion against time: in order to increase the conversion, we need to increase the temperature. This principle is used to analyse the three previous cases for the exothermic batch reactor. The optimal profile was found manually by manipulating, especially by increasing, the initial value of the temperature.

5.2.4.1. Case 1) T^{feed} used as disturbance and T used as controlled variable

For the first case in which T^{feed} was defined as disturbance and T as controlled variable, the initial value of temperature has been set to $400\ K$: it is inside the initial interval $[310, 410]$ and it is high enough to obtain a good value for the conversion. In order to see what happens if there is a disturbance, the value of T has been changed to $430\ K$ at $t = 30s$.



(a)



(b)

Figure 5.7: Optimal temperature (a) and conversion (b) profile with a disturbance on T^{feed} subjected to the effect of the PI controller

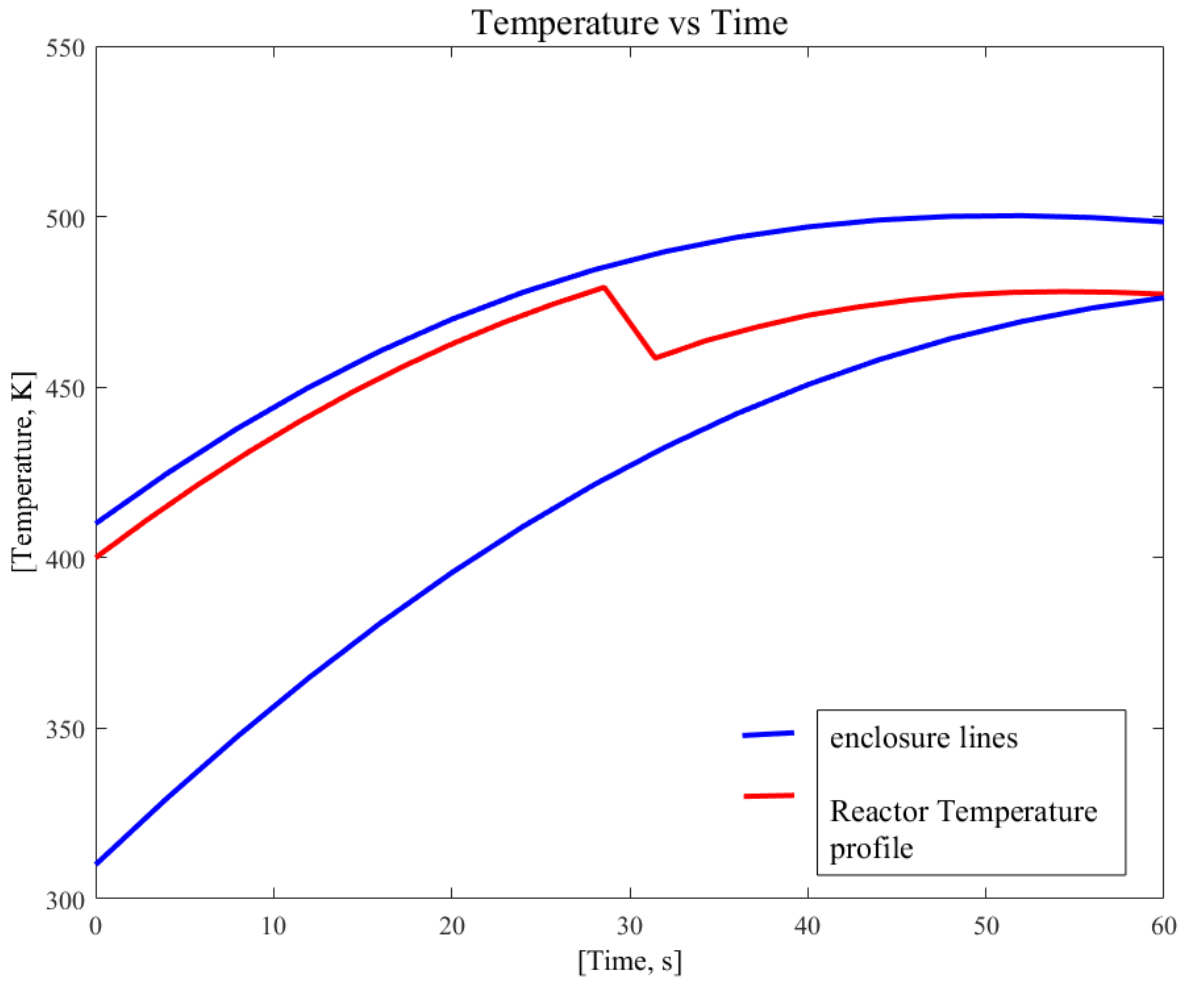
The temperature profile at the beginning is quite close to the upper bound, then follows the instruction and goes to $430\ K$ at 30 seconds; after the presence of the disturbance, it continues behaving like before until it reaches the lower bound where the controller acts in order to avoid that the temperature profile overshoot the limit. It is kept inside the limit for all the time.

As shown, the conversion profile at the beginning is very close to the upper bound: the highest conversion is obtained. Then, due to the disturbance, it becomes more distant from the upper bound but it still keeps high values. The upper and lower bounds of the conversion are obtained by using the aforementioned equation and exploiting the maximum and the minimum values of temperature respectively.

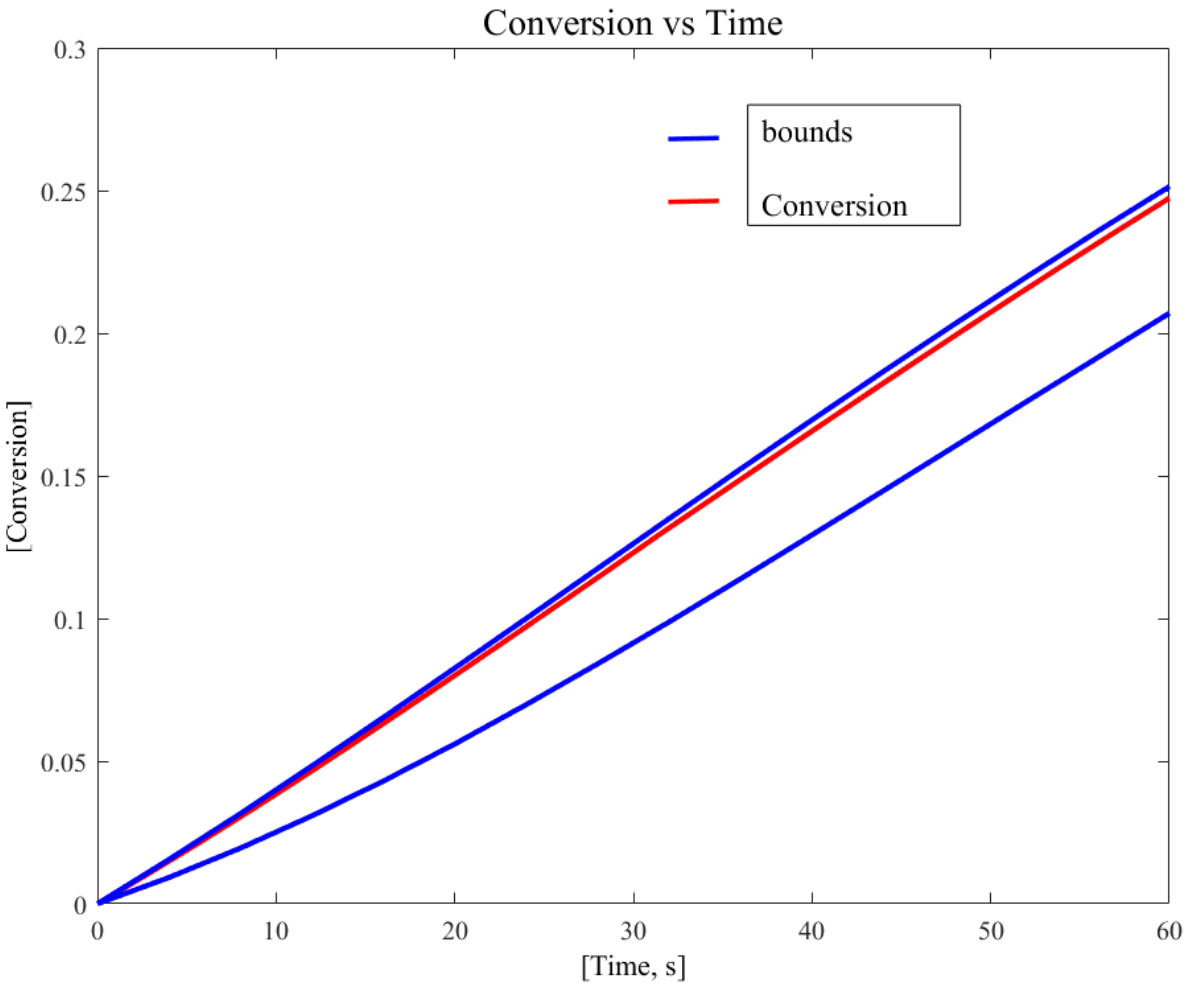
The goals of the optimal temperature behaviour and of the non-violation of the bounds are achieved.

5.2.4.2. Case 2) T_a^{feed} used as disturbance and T as controlled variable

In the second case, the reactor temperature is the controlled variable and the initial cooling/heating fluid temperature is the disturbance variable. Also in this scenario, the initial value of T is set to $400\ K$. In order to see what happens if there is a disturbance the initial value of T_a has been change from $310\ K$ to $600\ K$ at t=30s.



(a)



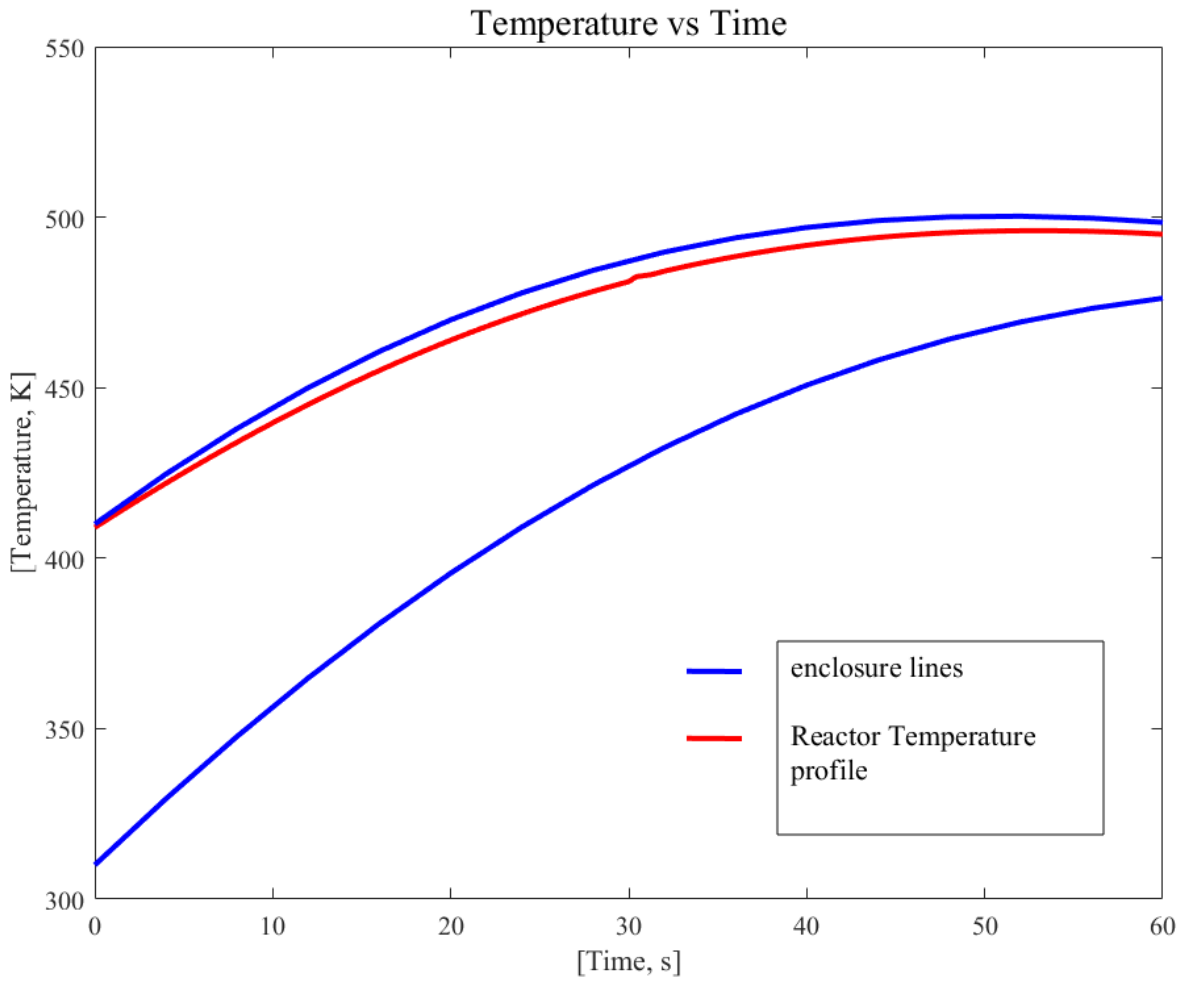
(b)

Figure 5.8: Optimal temperature (a) and conversion (b) profile with a disturbance on T_a^{feed} subjected to the effect of the PI controller

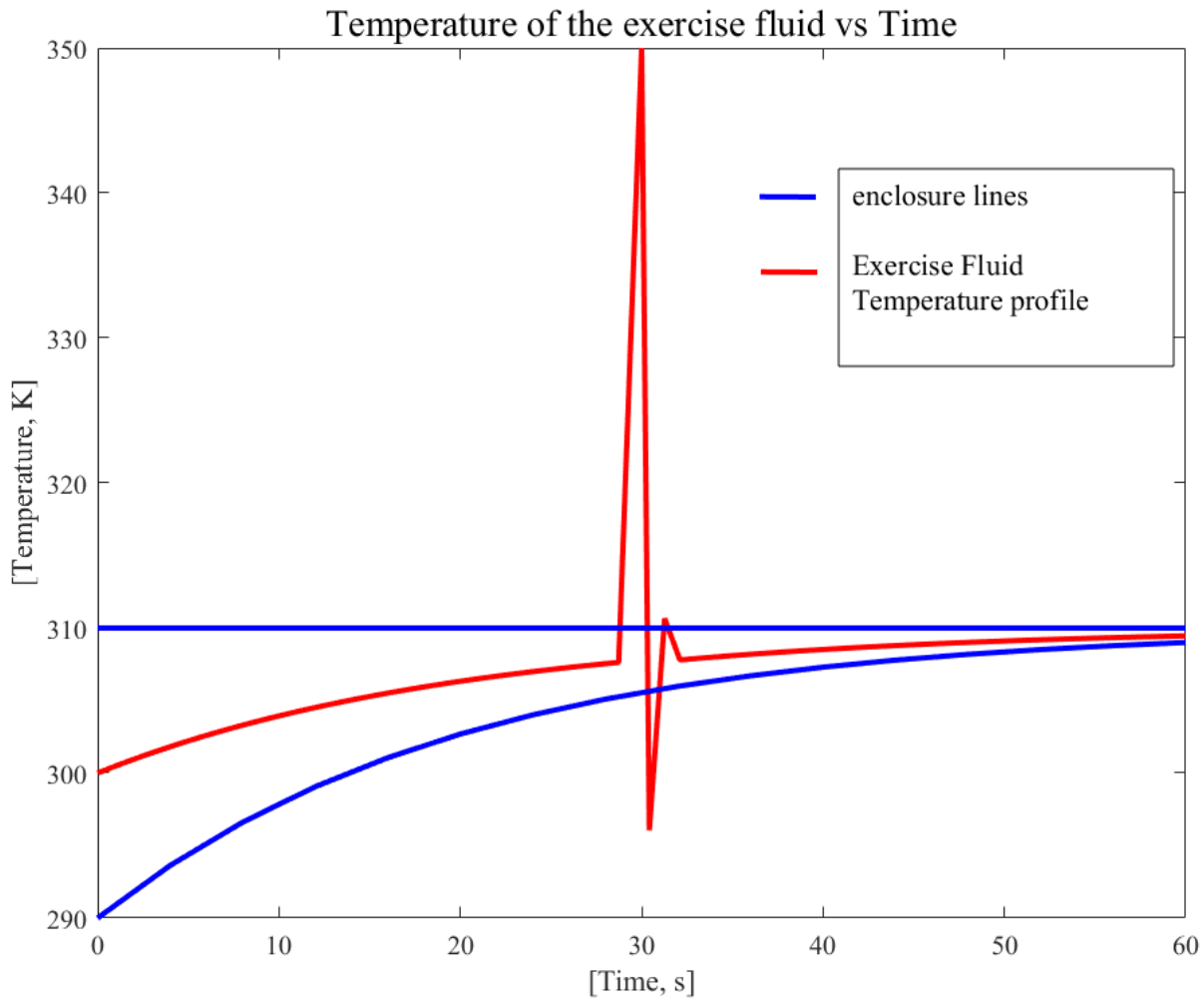
As shown in the first graph, the temperature profile is very close to the upper bound until the disturbance takes over; then the trajectory decreases until 60 seconds where it reaches the lower bound without overcome it. The conversion is very close to the upper bound along the entire profile, so it is not affected by the disturbance.

5.2.4.3. *Case 3) T_a^{feed} used as disturbance and T_a used as controlled variable*

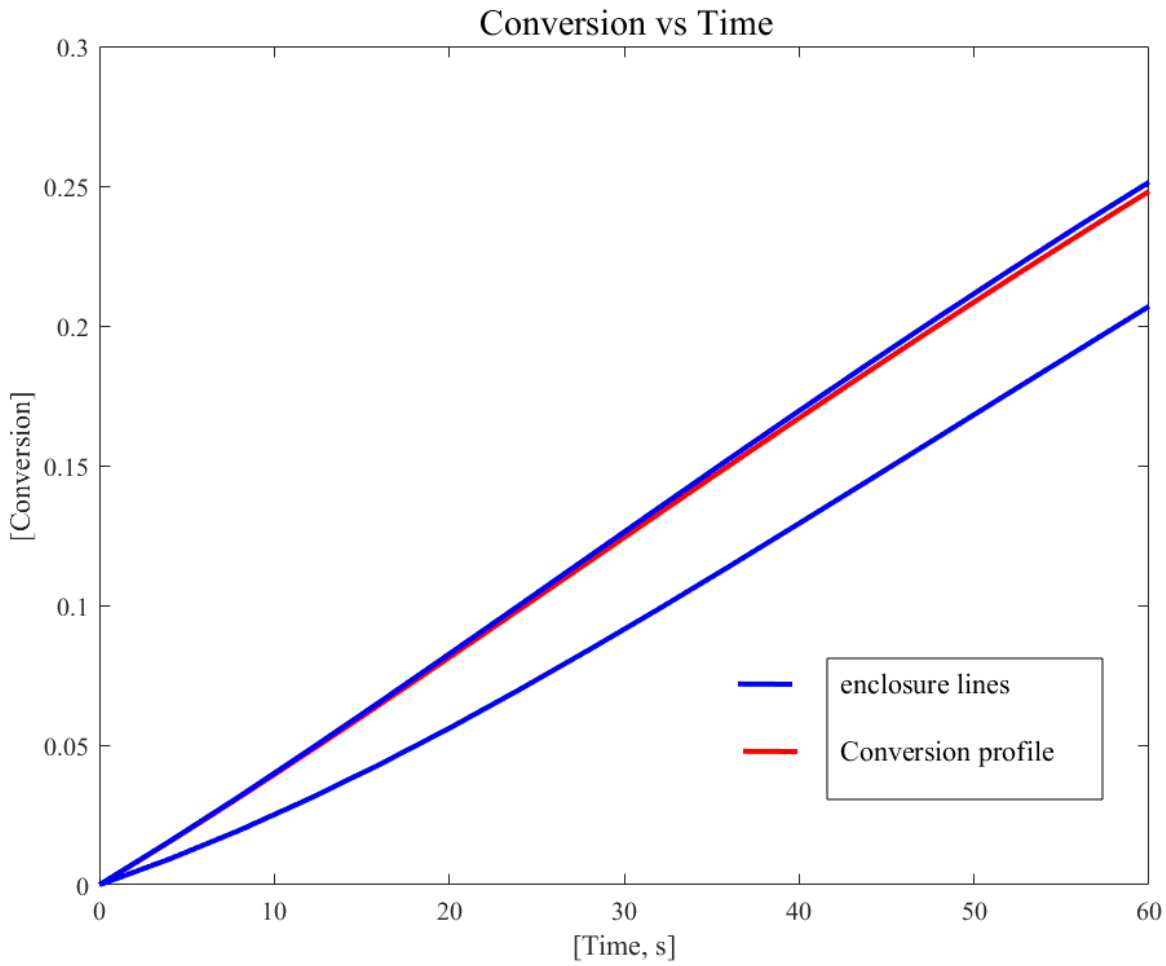
In the third case, the initial temperature of the cooling/heating fluid is defined as the disturbance and T_a as the controlled variable. The initial value of T is set to $409\ K$, very close to the maximum value; while the initial value of T_a is set to $300\ K$. The value of T_a^{feed} has been changed to $350\ K$ at 30 seconds and these are the results in terms of cooling/heating fluid temperature, reactor temperature and conversion:



(a)


Temperature of the exercise fluid vs Time
350
340
330
320
310
300
290
[Temperature, K]
0
10
20
30
40
50
60
[Time, s]
enclosure lines
Exercise Fluid
Temperature profile

(b)



(c)

Figure 5.9: Optimal profile of the reactor temperature (a), cooling/heating fluid (b) temperature and conversion (c) with a disturbance on T_a^{feed} subjected to the effect of the PI controller

The cooling/heating fluid is submitted to a sudden change in its trajectory due to the disturbance and then is kept inside the limits thanks to the PI controller. The reactor temperature profile is very close to the upper bound at the beginning and then there is a little variation due to the presence of the disturbance that brings the trajectory closer to the upper limit. The conversion profile overlaps the upper bound so in this case we obtain the highest values of conversion along the entire trajectory. The goals of the optimal temperature behaviour, of the non-violation of the bounds and of the control of T through T_a are achieved.

6. COMPARISON between MPC and PI

6.1.Model Predictive Control

Model Predictive Control is a control scheme which uses a process model. The main tasks are to explicitly predict the behaviour of future plants and to compute an appropriate corrective control action that is required to drive the predicted output as close as possible to the desired target value.

This type of model is able to handle time delays and inverse response, to compensate for the effect of measurable and unmeasurable disturbances, to handle process interactions with ease. In fact, it is particularly easy to use for multivariable systems and it utilizes a process model without a particular rigid model form. Since it is posed as an optimization problem, it is capable of meeting the control objectives by optimizing control effort and, at the same time, it's able to handle constraints of all kinds.

MPC can be best suited to processes with any combination of the following characteristic:

- Multiple input and output variables with significant interactions between SISO (Single Input Single Output) loops
- Either equal or unequal number of inputs and outputs
- Complex and unusually problematic dynamics
- Constraints in input and/or output variables

It takes a substantial amount of time for the full effect of each single control action to be completely manifested in the observable process output. That's why chemical processes often have slow dynamics. In order to decide which control action is the best to take at the current time instant, it can be useful to consider how the process output will behave in the future if no

further control action is taken and to target control action towards rectifying what remains to be corrected after the full effects of the previously implemented control action have been completely manifested. These are the fundamental motivation behind MPC as a controller design methodology.

Four elements characterize the framework of MPC and they are shared in common by all such schemes:

1. Reference trajectory specification: the definition of a desired target trajectory for the process output, $y*(k)$, is the first element of Model Predictive Control. This can be a desired reference trajectory that is less abrupt than a step or simply a step to the new set-point value.
2. Process output prediction: in order to predict the process output over a predetermined, extended time horizon in the absence of further control action, some appropriate model, M, is used. Therefore, this is equivalent, for discrete-time models, to predict $\hat{y}(k+1), \hat{y}(k+2), \dots \hat{y}(k+i)$ for i sample times into the future based o9n all actual past control inputs $u(k), u(k-1), \dots u(k-j)$.
3. Control action sequence computation: in order to calculate a sequence of control moves, the same model, M, is used. It must satisfy some specified optimization objective, namely: minimizing the predicted deviation of the process output from target over the prediction horizon, and minimizing the expenditure of control effort in driving the process output to target. In this way, it means construct and utilize a suitable model inverse, M*, which is able to predict the control input sequence $u(k), \dots u(k+n-1)$ required for achieving the prespecified output behaviour "p" times step into the future.

4. Error prediction update: plant measurement, $y_m(k)$, is compared with the model prediction, $\hat{y}(k)$, and the prediction error, $\hat{\varepsilon}(k) = y_m(k) - \hat{y}(k)$, thus obtained is used to update future predictions.

The most popular forms for conventional Model Predictive Control schemes are the linear, discrete versions of:

- Finite convolution models: it consists of an impulse-response model form

$$y(k) = \sum_{i=0}^{k} g(i)u(k-i) \tag{6.1}$$

And a step-response model form

$$y(k) = \sum_{i=0}^{k} \beta(i)\Delta u(k-i) \tag{6.2}$$

In which $g(i)$ is the process impulse response function, $\beta(i)$ is the step-response function and $\Delta u = u(k) - u(k-1)$

The system obtained is

$$\begin{cases} g(i) = \beta(i) - \beta(i-1) \\ \beta(i) = \sum_{j=1}^{i} g(j) \end{cases} \tag{6.3}$$

All realistic discrete-time systems exhibit the mandatory one-step delay; in fact, for all real, causal systems both $g(0)$ and $\beta(0)$ are equal to zero. The impulse coefficients are typically obtained either directly from plant data or they are deduced from other so-called parametric model forms.

- Discrete state-space models: they can be represented by the following equation

$$y(k) = \sum_{i=0}^{k} a(i)y(k-i) + \sum_{i=0}^{k} b(i)u(k-i-m) \tag{6.4}$$

In which m is the delay and $a(i), b(i)$ are the coefficients. They are obtained by fitting the model to plant data.

- Discrete transfer function models: they can be represented by the following equation

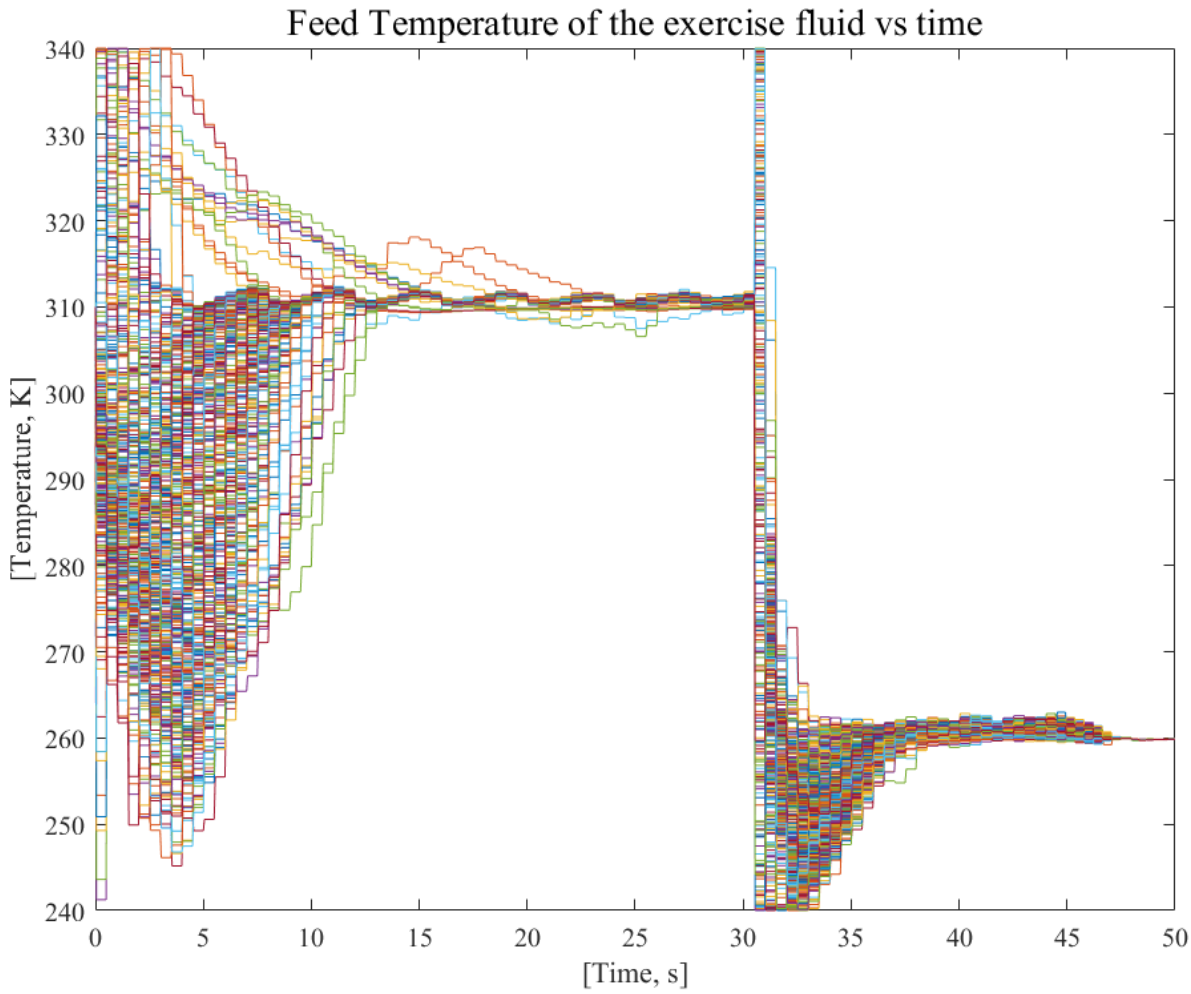
$$y(z) = \frac{z^{-m}B(z^{-1})}{A(z^{-1})}u(z) \tag{6.5}$$

6.2. Comparison between MPC and PI

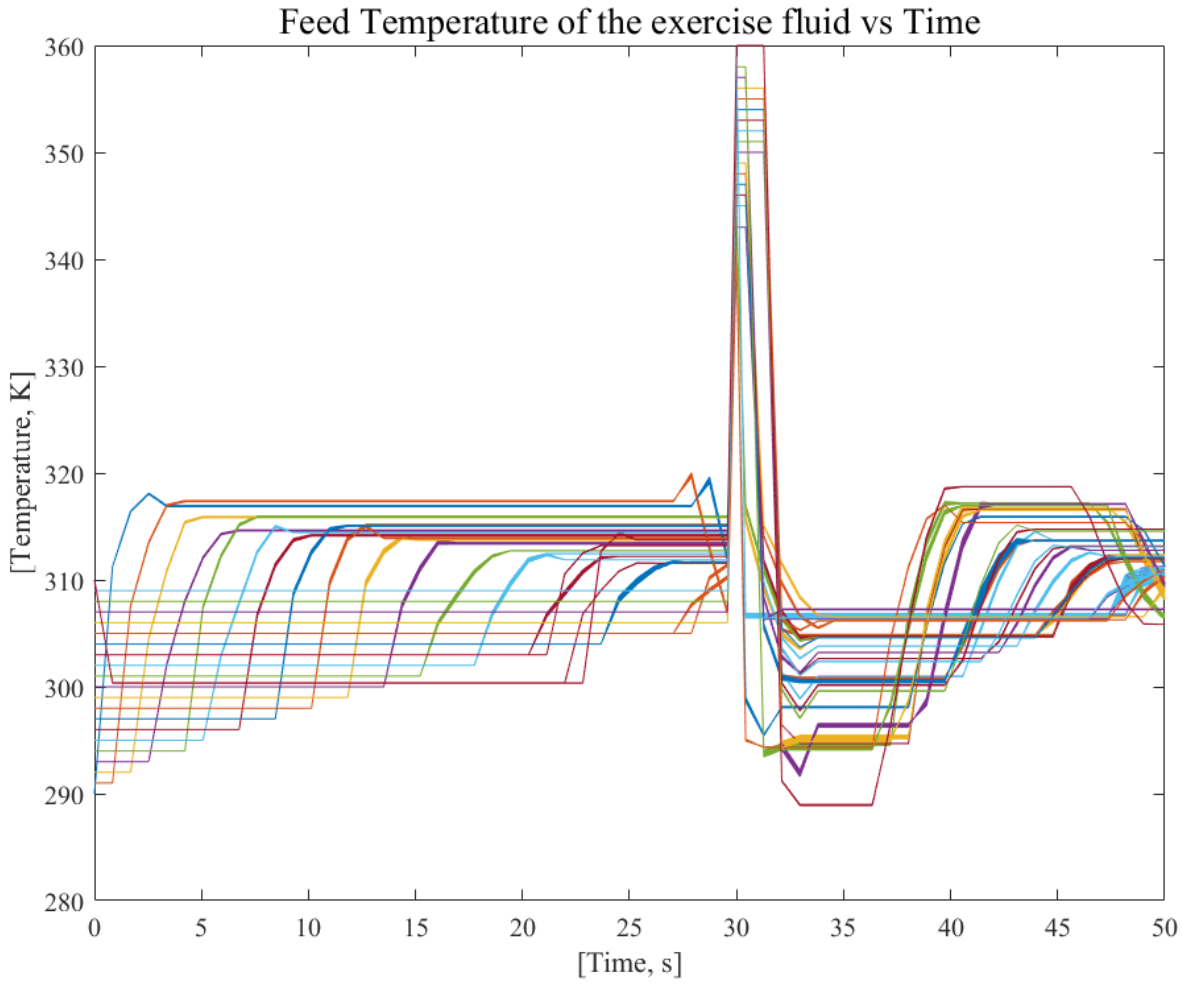
Now we consider the Exothermic Batch Reactor in which T_a^{feed} is used as disturbance and manipulated variable. As represented before, the main aim is to avoid the leak of the fluid exercise temperature from its enclosure: therefore, T_a is the controlled variable.

The simulations have been carried out in MATLAB. We used different values for the feed temperature of the reactor and for the feed temperature of the exercise fluid, both included in the bounds (T^{feed} between 310 and 410 K, T_a^{feed} between 290 and 310 K). The intervals are constant for both the temperatures. In the simulations, all the possible combinations between the values are considered and, since the number of values in both cases consists of 21, the number of simulations carried out is 441.

In the following graphs are reported the behaviours of the feed temperature of the exercise fluid, the temperature of the exercise fluid and the reactor temperature for both cases, namely: the first one in which the Model Predictive Control is applied, the second one in which the Proportional Integral Control is exploited.


Feed Temperature of the exercise fluid vs time
[Temperature, K]
[Time, s]
340
330
320
310
300
290
280
270
260
250
240
0
5
10
15
20
25
30
35
40
45
50

(a)

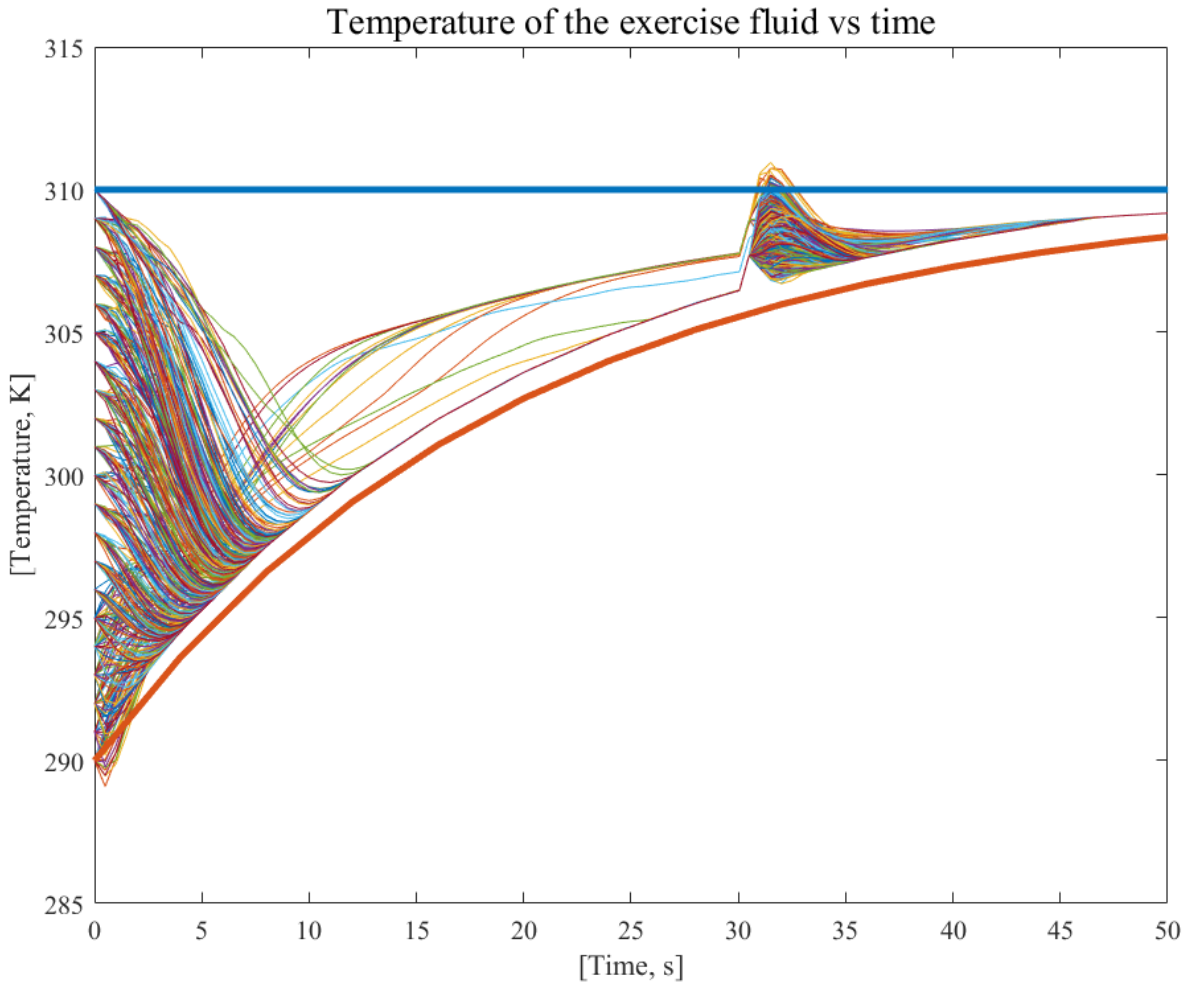


(b)

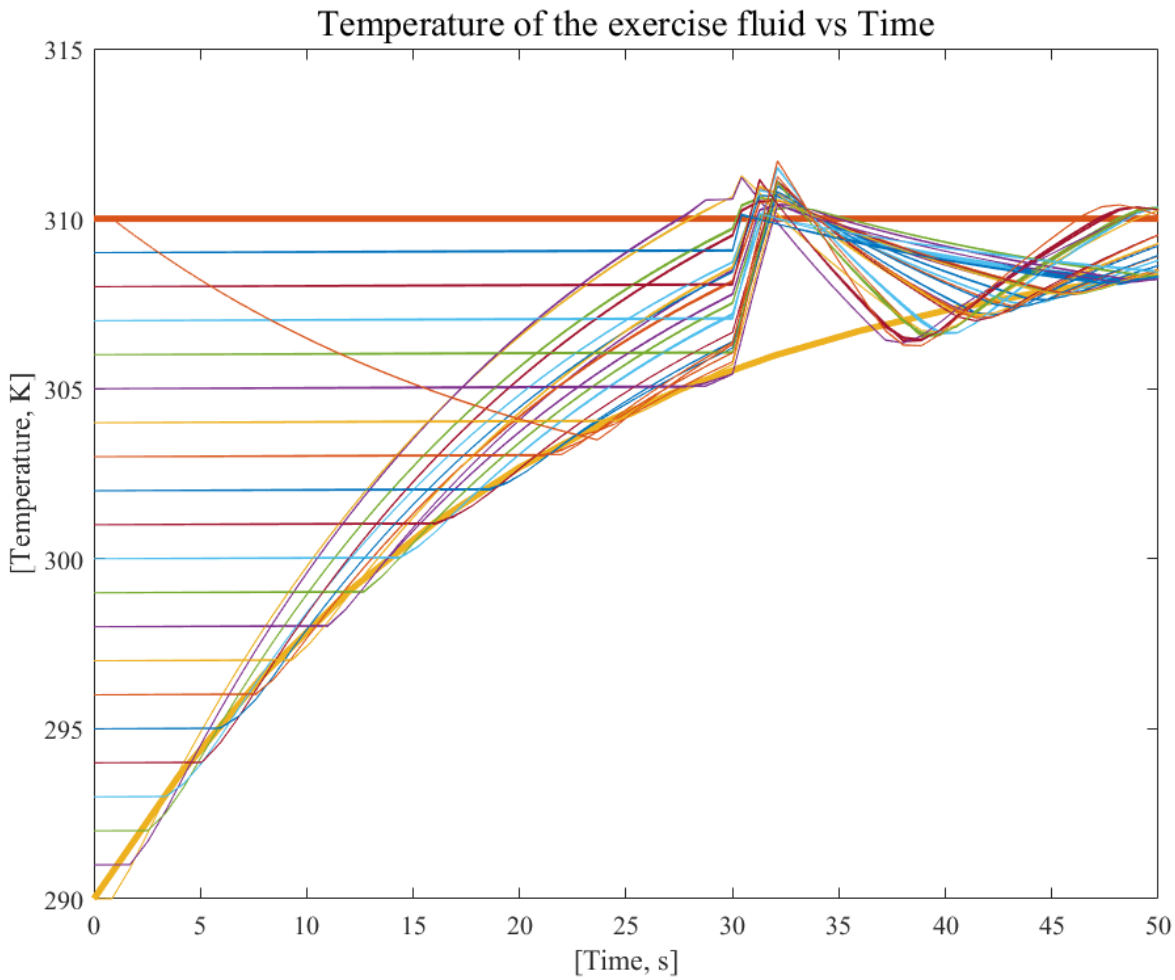
Figure 6.1: Profile of the feed temperature of the exercise fluid with the application of the MPC (a) and of the PI control (b)

In the figures above, the profiles of the feed temperature are reported. At 30 seconds, it is affected by a disturbance of the entity of 50 K; at this point, the profiles are subjected to an abrupt increase. In the case where the Proportional Integral Control is used, the values reached by the profile are more or less between 340 and 360 K; instead, when the Model Predictive Control is exploited, the maximum value reached consist of 340 K, less than in the previous case.

At the end, thanks to the controller's action, the behaviours of the temperatures have been reported to the values taken initially, in the PI scenario, and to lower values compared with the initials, in the MPC scenario.



(a)



(b)

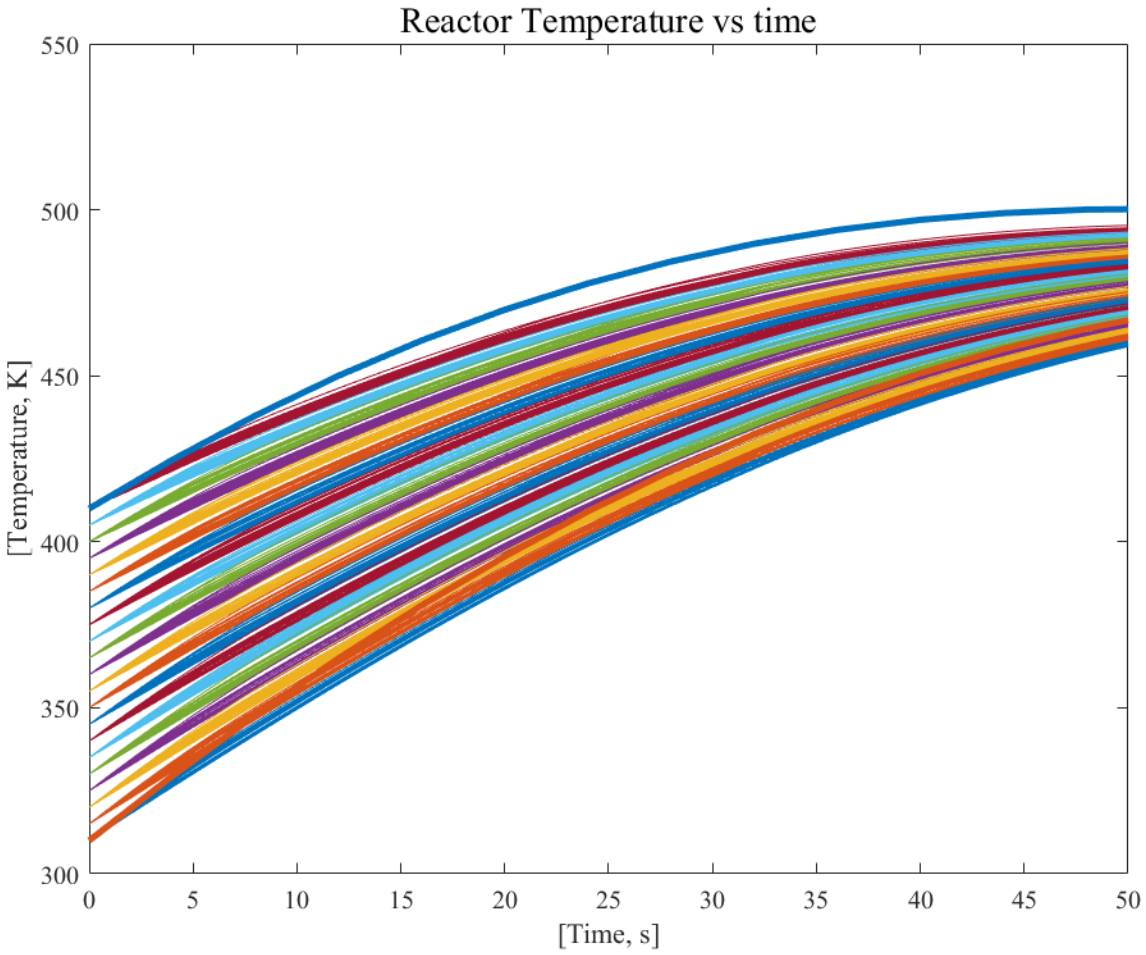
Figure 6.2: Profile of the temperature of the exercise fluid with the application of the MPC (a) and of the PI control (b)

It's very interesting to analyse and comment the different behaviour of the exercise fluid's temperature in the two cases. At 30 seconds, when the variation of 50K is applied on the feed temperature of the exercise fluid, the temperature of the exercise fluid starts to increase. In both cases it overcomes the upper limit and then, thanks to the controller's action, it is reported inside the bounds.

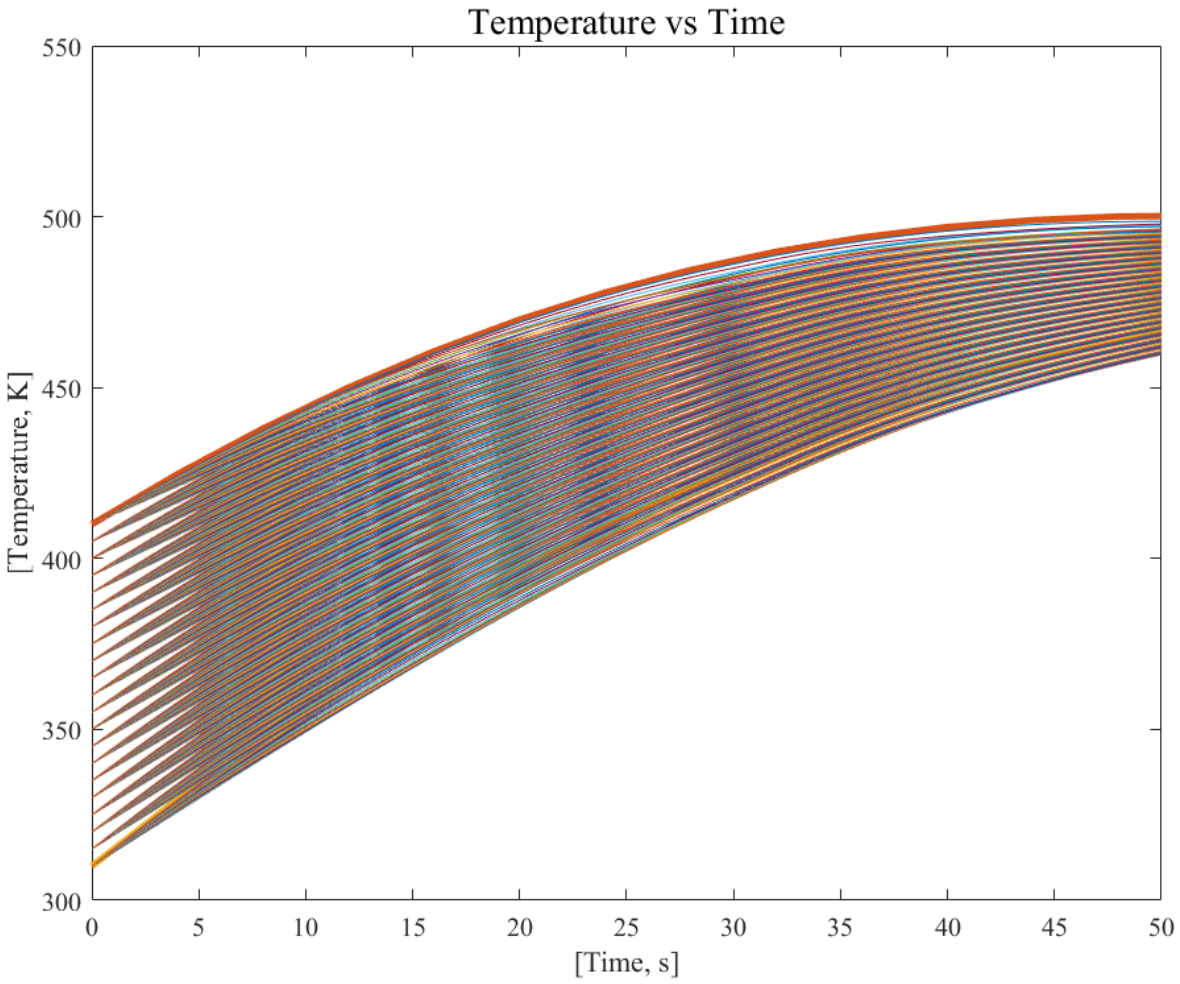
Despite the overall behaviour is similar in the both cases, they differ for the following characteristics:

- In the PI scenario, the profile goes out from the bounds several times, before the disturbance acts, and each time it is reported inside the limit thanks to the controller; instead the Model Predictive Control is able to predict the behaviour of the system in the future and, therefore, tries to prevent the overcome of the limits;
- When the disturbance acts, the profile overcomes the upper limit in all the simulations with the PI controller; instead only few cases, in the MPC, go out from the upper bound;
- After the disturbance has acted, there is a continuous oscillation of the temperature profile that lead to overcome again the bounds, in the PI scenario; in the MPC case instead, the temperature profile in all simulations is kept inside the enclosure and, at the end (from 45 seconds) all the lines converge to only one.

This means that, thanks to the ability to predict future behaviours, the MPC controller is able to prevent the overcome of the limits and to guarantee a better stability than the PI controller.


Reactor Temperature vs time
[Temperature, K]
[Time, s]
550
500
450
400
350
300
0
5
10
15
20
25
30
35
40
45
50

(a)



(b)

Figure 6.3: Profile of the reactor temperature with the application of the MPC (a) and of the PI control (b)

The graphs above show the profile of the reactor temperature in the scenarios where PI and MPC controller act on the exercise fluid's temperature. After the disturbance on the feed temperature of the exercise fluid acts, the behaviour of the reactor temperature departs from the upper limit, but it never overcomes the bounds. The lines of the enclosure are underlined in order to see that they are respected along the entire length of the process. The temperature is not too much affected by a variation in the exercise fluid temperature because the exercise fluid's flow rate is quite small compared to the fluid's flow rate.

7. DISCUSSION

The comparisons between the different models indicate that it is important to work with stable system when the trajectories are subjected to tight bounds. Since the enclosure is as tight as possible, maintaining the profile inside the limits can be difficult. The process cannot be carried out, if the performance of the variable of interest is too close to the upper or lower limit, because it could be dangerous: the profile could easily overcome the safety bounds. Therefore, we have to be sure that the trajectories are quite far from their limits and also that we are working with stable system in order to don't incur in dangerous conditions that could lead the entire process to explode. For each case studied is necessary to find a good compromise between the proportional gain and the integral time in order to be able to fix with the controller the error create by the disturbance.

The first case studied is easy to manage and control: it is composed by a first order irreversible series reaction in which the variable of interest, namely the concentration of component A, has been identified as the controlled variable and its initial value as the disturbance. In order to operate in the safety region, it's enough to put a PI controller that keeps the parameter inside the bounds, despite the presence of a disturbance variable.

For the exothermic batch reactor, we obtain different results depending on which variables are defined as controlled and disturbance. In the case 1 the reactor temperature was identified as the controlled variable and T^{feed} as the disturbance: we are able to control it directly and immediately when the disturbance occurs. The trajectory is kept inside the safety limits thanks to the PI controller. In the case 2 the reactor temperature is kept controlled and the initial cooling/ heating fluid temperature is the disturbance: the first one is kept inside the limit by the controller, but the system is not very stable. It's important, in fact, to find a compromise

between the parameters on which the controller is based: by changing the values of the proportional gain and the integral time a better stability can be achieved. In the case 3, the cooling/heating fluid temperature is defined as the controlled variable and its initial value as the disturbance: it's very interesting because we are able to maintain the reactor temperature in the safety region by controlling and managing the temperature of the cooling/heating fluid. The system is very stable because, even if there is a big disturbance, the reactor temperature shows a little variation in its profile. This case is the most important: we can control a parameter by manipulating a different one. In the last case, we can find the optimal reactor temperature profile, which is the one able to ensure the highest conversion and, thanks to the PI controller, we are able also to guarantee that the profile of the variable of interest does not violate the safety limits. This means that we are able to find a compromise between the proportional gain and the integral time so that the optimal temperature trajectory approaches only the upper or the lower limit without overshooting them never (in the period of time that we consider). It's important to underline that working in these conditions could be dangerous, because the reactor temperature profile is very close to the upper limit and also a small disturbance can lead to overshoot the limit and to work in unsafe conditions. Maintain the trajectories inside the enclosure is very difficult, so we must be sure that the system is stable.

From the comparison between the MPC and the PI control, what arise is that in the first scenario the controller is capable to predict the future behaviour of the variables of the system and, therefore, it knows in advance when and where the profile will overcome the limits: thanks to this ability, it can prevent the effects of the disturbance and it tries to take care of the constraints. On the other hand, this type of controller is difficult to use from an industrial point of view. In fact, it calculates the optimal input by using the predictions and this step can take a lot of time. In the PI scenario instead, the controller is not able to predict the future profile of the variable

of interest and, therefore, it acts only when there is a violation of the upper or lower limit. It operates in a way to get the profile again inside the enclosure and then it will act only when there is another violation. A better stability can be achieved with the MPC controller because it is capable to avoid oscillation; it satisfies the safety conditions for almost the entire duration of the process. We can say that the entity and the periodicity of the violation from the enclosure is less when the Model Predictive Control is used.

8. CONCLUSIONS

The problem of finding an enclosure and of remaining inside the bounds during the entire length of the reaction/process was considered. In particular, the aim is to work with very tight enclosure and to explore the ability to determine dynamic optimal performance within the aforementioned strict bounds.

The enclosures inside which the profiles of the variables of interest should lie have been defined by using a simulator: the results are the upper and the lower limits along time. The enclosure allows to define the space inside which the behaviour of the parameters can act: since it must be as tight as possible, the margin of error that can be assumed in the presence of a disturbance cannot be high.

In order to remain inside the bounds, the possible presence of a disturbance variable that could lead the parameter of interest to go outside the safety region was investigated. It's necessary, in fact, to don't work in dangerous conditions: the profile of the variable studied, since the beginning, must not lie too close to the upper limit or to the lower one; it must be enough away from them so that, if there are disturbances, it remains inside the enclosure defined before without problems.

Toward this end, it is needed to define the general structure of the PI Controller which can be used for the different cases considered. The controller should be able to act in the proper way: for this reason, it is needed to arrange the values of the proportional gain and the integral time. The controller, in fact, should be able to maintain the profile inside the enclosure if it is not too affected by the disturbance, to bring it back inside the bounds if it presents a big error, to avoid an oscillating behaviour that results in an unstable system. From this condition, several

experiments have been presented which differ for the variables that are considered as disturbance or as controlled.

The controller has been tested upon the different experiments: a lot of simulations have been carried out by changing the tuning parameters, namely the proportional gain and the integral time. This was done in order to find out the PI controller's best structure. In fact, it is required to satisfy two key conditions: remaining inside the safety bounds and achieving the best stability. The results can be different: the profile could reach the upper/lower bound once and in this case the controller will act by maintaining it inside the enclosure; the profile could oscillate inside or outside the limits and in this case the controller can act but maybe not in the proper way (if the system continues oscillating). It depends a lot from the variables that can act as a disturbance. So, there is the need to find a compromise between the two parameters and to evaluate if it is possible to satisfy both conditions of the enclosure and of the stability.

The experiments demonstrated that with the PI controller the system is able to manage and to maintain inside the enclosure different ODE systems, despite the presence of a disturbance.

The results of the PI controller can be compared with those of the MPC controller: the main difference is that, in the first scenario, the controller operates only when the disturbance acts; in the second case, the controller tries to control a system by creating predictions about the future using a model while taking care of the constraints. The overall behaviour of the profile along time is similar, but there are several differences in the way the controller acts, namely: in the PI scenario, the limits are exceeded a lot of times and, only when this happens, the controller starts to operate; in the presence of a disturbance, it's impossible to avoid the violation of the enclosure; keeping the profile inside the bounds can lead to its oscillation, that is equivalent to have a not good stability. While, thanks to the ability to predict future, MPC is able to: avoid the violation of the enclosure (in the case where there is no disturbance); to

reduce the variation, in the presence of the disturbance, and, in some cases, to keep the profile inside the bounds; to achieve a very good stability once the profile has been reported inside the limits. This means that, thanks to the ability to predict future behaviours, the MPC controller is able to prevent the overcome of the limits and to guarantee a better stability than the PI controller.

REFERENCES

Babatunde A Ogunnaike, W. Harmon Ray 1994. Process Dynamics, Modeling, and Control.

Chachuat, B. and Latifi, M.A., 2004. A new approach in deterministic global optimisation of problems with ordinary differential equations. In Frontiers in global optimization (pp. 83-108). Springer, Boston, MA.

Chachuat, B., Singer, A.B. and Barton, P.I., 2006. Global methods for dynamic optimization and mixed-integer dynamic optimization. Industrial & Engineering Chemistry Research, 45(25), pp.8373-8392.

Esposito, W.R. and Floudas, C.A., 2000. Deterministic global optimization in nonlinear optimal control problems. Journal of global optimization, 17(1), pp.97-126.

Esposito, W.R. and Floudas, C.A., 2000. Global optimization for the parameter estimation of differential-algebraic systems. Industrial & Engineering Chemistry Research, 39(5), pp.1291-1310.

Kearfott, R.B., 2011. Interval computations, rigour and non-rigour in deterministic continuous global optimization. Optimization Methods & Software, 26(2), pp.259-279.

Limon, D., Bravo, J.M., Alamo, T. and Camacho, E.F., 2005. Robust MPC of constrained nonlinear systems based on interval arithmetic. IEE Proceedings-Control Theory and Applications, 152(3), pp.325-332.

Lin, Y. and Stadtherr, M.A., 2006. Deterministic global optimization for parameter estimation of dynamic systems. Industrial & engineering chemistry research, 45(25), pp.8438-8448.

Lin, Y. and Stadtherr, M.A., 2007. Deterministic global optimization of nonlinear dynamic systems. AIChE Journal, 53(4), pp.866-875.

Lin, Y. and Stadtherr, M.A., 2008. Fault detection in nonlinear continuous-time systems with uncertain parameters. AIChE journal, 54(9), pp.2335-2345.

Lygeros, J., Tomlin, C. and Sastry, S., 1999. Controllers for reachability specifications for hybrid systems. Automatica, 35(3), pp.349-370.

Papamichail, I. and Adjiman, C.S., 2002. A rigorous global optimization algorithm for problems with ordinary differential equations. Journal of Global Optimization, 24(1), pp.1-33.

Papamichail, I. and Adjiman, C.S., 2004. Global optimization of dynamic systems. Computers & chemical engineering, 28(3), pp.403-415.

Perez-Galvan, C. and Bogle, I. D. L., 2017. Global Optimisation for Dynamic Systems using Novel Overestimation Reduction Techniques. Dissertation, University College London.

Scott, J.K. and Barton, P.I., 2010. Tight, efficient bounds on the solutions of chemical kinetics models. Computers & Chemical Engineering, 34(5), pp.717-731.

Scott, J.K. and Barton, P.I., 2013. Bounds on the reachable sets of nonlinear control systems. Automatica, 49(1), pp.93-100.

Singer, A.B. and Barton, P.I., 2006. Global optimization with nonlinear ordinary differential equations. Journal of Global Optimization, 34(2), pp.159-190.

Singer, A.B., Taylor, J.W., Barton, P.I. and Green, W.H., 2006. Global dynamic optimization for parameter estimation in chemical kinetics. The Journal of Physical Chemistry A, 110(3), pp.971-976.

Zhao, Y. and Stadtherr, M.A., 2011. Rigorous global optimization for dynamic systems subject to inequality path constraints. Industrial & Engineering Chemistry Research, 50(22), pp.12678-12693.