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SCUOLA POLITECNICA E DELLE SCIENZE DI BASE
DIPARTIMENTO DI INGEGNERIA ELETTRICA E TECNOLOGIE DELL’INFORMAZIONE

NONLINEAR DYNAMICS AND CONTROL
Continuous Stirred Tank Reactor

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CAPITOLO 1. CONTEXT

Continuous Stirred Tank Reactor (CSTR) is a type of chemical reactor widely used in industry to carry out chemical reactions under continuous flow conditions.
The CSTR is used to perform chemical reactions in a controlled and continuous manner, while maintaining adequate mixing of the reactants. Reagents enter the reactor continuously.
Inside, an agitation system keeps the contents well mixed, ensuring uniform temperature and concentration distribution. Reaction products are continuously drawn from the reactor.

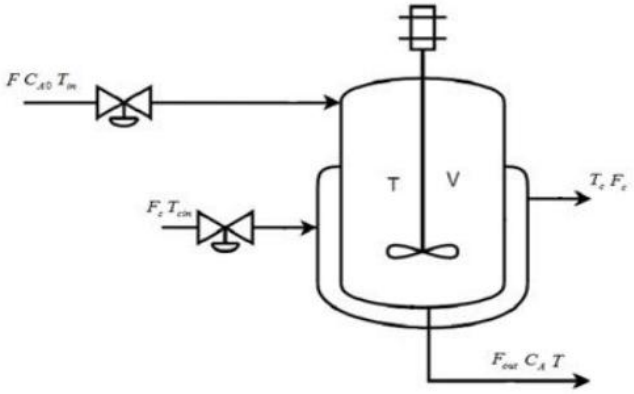

Fig. 1. Continuous Stirred Tank Reactor

The mathematical model of the CSTR is based on mass and energy balances. The system is described by non-linear differential equations representing the dynamic behaviour of the reactor.

Total Mass Balance:

$$\frac{dV}{dt} = F_{in} - F_{out}$$

- V is the reactor volume (constant).
- Fin is the inlet flow rate.
- Fout is the output flow rate.

Mass Balance of Component A:
The equation describes how the concentration of A inside the reactor varies over time, taking into account three main factors: inlet flow, outlet flow and chemical reaction

$$\frac{dCa}{dt} = \frac{V}{F}(C_{a0}) - \frac{V}{F}(C_a) - K_0 C_a e^{-\frac{E}{RT}}$$

where:

- C_A is the concentration of component A in the reactor. (equal to the output concentration)

- C_{A0} is the concentration of component A at the input
- k_0 is the pre-exponential factor.
- E is the activation energy.
- R is the gas constant.
- T is the reactor temperature.

Reactor Energy Balance:
The temperature variation within the reactor is influenced by three main factors. The first is the heat carried by the input fluid, whose temperature can contribute to heating or cooling the system. The second is the heat generated or absorbed by the chemical reaction, which can be exothermic, releasing heat, or endothermic, subtracting it (this depends on the value of Hr, which in the case analysed is less than zero, so the reaction releases heat, exothermic).
Finally, the third factor is the heat exchange with the environment and the cooling fluid, which is a control element for controlling the system.

$$\frac{dT}{dt} = \frac{V}{F}(T_{in} - T) - \frac{K_0 C_a}{\rho C_p}(H_r)e^{-\frac{E}{RT}} - \frac{UA}{\rho C_p V}(T - Tamb - u)$$

where:

- T_{in} is the temperature of A at the input.
- H_r is the heat of reaction.
- ρ is the density.
- C_p is the heat capacity.
- UA s the heat transfer coefficient.
- T_{amb} is the ambient temperature. (20°C =293K)
- u is the difference between the ambient temperature and the refrigerant in the jacket.

Variable	Description	Nominal operating Values
V	Reactor volume (l)	50
F_{in}	Inlet volumetric flow rate to the reactor (l/min)	50
F_{out}	Outlet volumetric flow rate from the reactor (l/min)	50
C_A	Concentration of component A in outlet stream (mole/l)	-
C_{A0}	Feed concentration of component A (mole/l)	1
K_0	Pre-exponential factor (l/min)	$7.8^{*}10^{10}$
E	Activation energy in the Arrhenius equation (Cal/mole)	E/R=8567
R	Universal gas constant (Cal/mole. K)	
ρ	Density of the inlet and outlet stream (g/l)	900
C_p	Heat capacity of inlet and outlet stream (Cal/g.K)	0.329
T	Temperature of the reactants in the reactor (K)	-
T_{in}	Inlet stream temperature (K)	350
H_r	Heat of reaction (Cal/mole)	$-5^{*}10^{4}$
UA	Heat transfer term (Cal/min. K)	$5^{*}10^{4}$
T_c	Temperature of the coolant water in the jacket (K)	-
ρ_c	Density of the coolant water in the jacket (g/l)	1000

Tab. 1. Variables and nominal CSTR parameter values

The refrigerant temperature relative to the ambient temperature(20°C) is the control input of the system. When the control input u is positive, the refrigerant is heated, while when u is negative, the refrigerant is cooled.

An increase in temperature within the reactor accelerates the speed of the chemical reaction, thus reducing the concentration of the Ca component in the reactor and, consequently, also in the output flow.

Through temperature control, our goal is to regulate the amount of A leaving the system, ensuring that the process operates under the desired conditions.

$$\dot{x}_1 = \frac{V}{F}(C_{a0}) - \frac{V}{F}(x_1) - K_0 x_1 e^{-\frac{E}{Rx_2}}$$

$$\dot{x}_2 = \frac{V}{F}(T_{in} - x_2) - \frac{K_0 x_1}{\rho C_p}(H_r)e^{-\frac{E}{Rx_2}} - \frac{UA}{\rho C_p V}(x_2 - Tamb - u)$$

Hypothesis:

The strongest assumption is that the temperature of the coolant can be controlled quickly, without considering the heat exchange of energy from the reactor to the refrigerant.

Considering that thermal time constants are notoriously high, the model adopts minutes as the unit of time, rather than seconds. As far as the graphical representation is concerned, the following units will be used:

Temperature: measured in kelvin (K).
Concentration of component A (Ca): measured in millimoles per litre (mmol/L) to ensure better visualisation and interpretation of results.
This choice allows a clearer appreciation of the trend of variables over time and facilitates system analysis.
Acceptable temperature values within the CSTR (Continuous Stirred Tank Reactor) must be maintained in a range between 300 K and 400 K. i.e. 27-127 degrees Celsius (°C)

Concentration values of A (Ca):

- Acceptable range: 0.15 mol/L - 0.7151 mol/L
- Lower region (Lower): 0.15 mol/L (high transformation rate)
- Middle region: 0. 554 mol/L
- Upper region (Higher): 0.7151 mol/L (low transformation rate)

Numerical Substitution

$$\dot{x}_1 = 1 - x_1 - 7.8 * 10^{10} x_1 e^{-\frac{8567}{x_2}}$$

$$\dot{x}_2 = (1339.49) + 1{,}317 * 10^{13} * x_1 * e^{-\frac{8567}{x_2}} - 4{,}377 x_2 + 3{,}37\mathbf{7}u$$

CAPITOLO 2. OPEN-LOOP ANALYSIS

2.1 Equilibrium- point

To analyze the equilibrium points, one must set the derived terms to zero. Under the given hypothesis:

$$0 = \frac{V}{F}(C_{a0}) - \frac{V}{F}(x_1) - K_0 x_1 e^{-\frac{E}{Rx_2}}$$

$$0 = \frac{V}{F}(T_{in} - x_2) - \frac{K_0 x_1}{\rho C_p}(H_r)e^{-\frac{E}{Rx_2}} + \frac{UA}{\rho C_p V}(x_2 - Tamb)$$

$$x_1 = (C_{a0})/(1 - \frac{F}{V}K_0 e^{-\frac{E}{Rx_2}})$$

$$0 = \frac{V}{F}(T_{in} - x_2) - \frac{K_0(C_{a0})}{\rho C_p(1 - \frac{F}{V}K_0 e^{-\frac{E}{Rx_2}})}(H_r)e^{-\frac{E}{Rx_2}} + \frac{UA}{\rho C_p V}(x_2 - Tamb)$$

The eqaution system has been solved graphically and the only Equilibrium point is x*= [0.9366, 308.46] i.e. stability is achieved in open loop at about 35°C and chemical reactions affect less than 7% of the component A introduced in the static state.

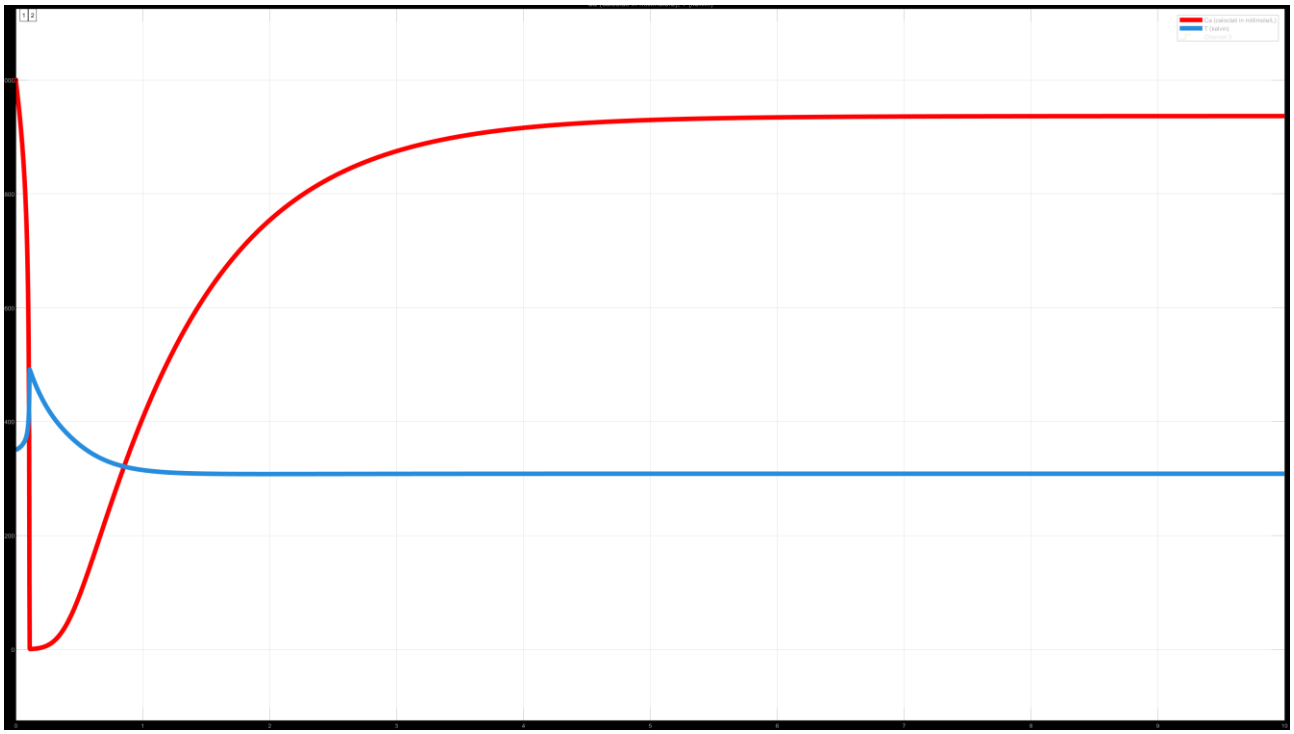

Fig. 2. Open-loop simulation with temperature T(Kelvin) and CA (the concentration of component A in the reactor measured in millimoles/l)

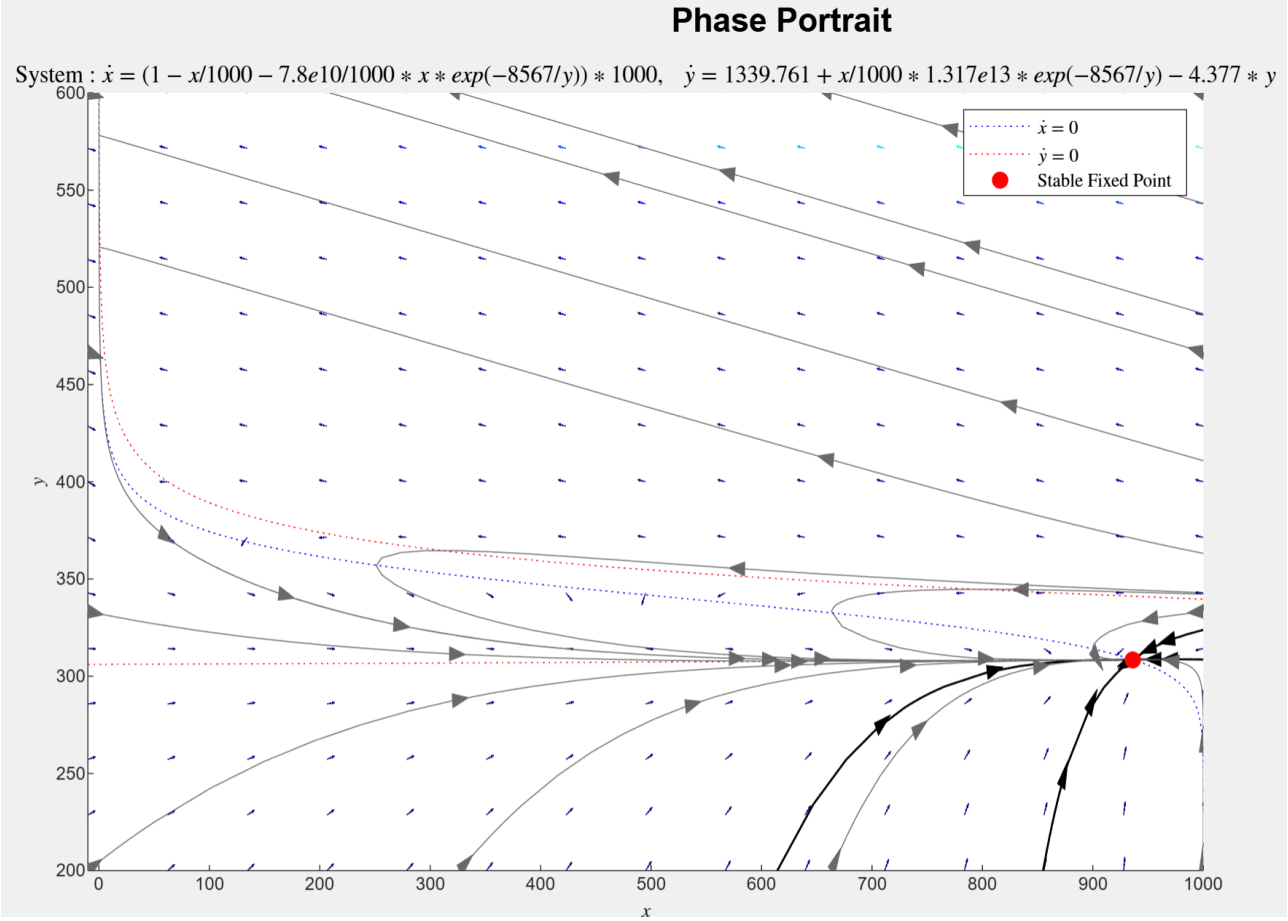

Fig. 3. Open-loop phase portrait

Although the graph emphasises the stability of the system, the values obtained during transients are unacceptable, reaching a peak of 500 kelvin degrees and a reaction rate at steady state that is too low. an appropriate control will be necessary.

2.2 Linearization in open loop

Let's analyse the behaviour of the system in the neighbourhood of X*= [0.9366, 308.46]
From the equations we calculate the Jacobian

$$J = \begin{bmatrix} -\left(\frac{F}{V}\right) - K_0 e^{-E/(RT)} & -K_0 C_A e^{-E/(RT)} \frac{E}{RT^2} \\ -\frac{K_0 H_r}{\rho C_p} e^{-E/(RT)} & -\left(\frac{F}{V}\right) + \frac{K_0 C_A H_r}{\rho C_p} e^{-E/(RT)} \frac{E}{RT^2} - \frac{UA}{\rho V C_p} \end{bmatrix}$$

Evaluated in x*

$$J(0.9366,308.46)=\begin{bmatrix} -1{,}067 & 0.0057 \\ 11{,}42 & -5.34 \end{bmatrix}$$

The matrix trace τ=-6.4082
Determined of the matrix =5.6366
It can be deduced that the equilibrium point is stable and being τ^2- 4Δ>0 it's a node

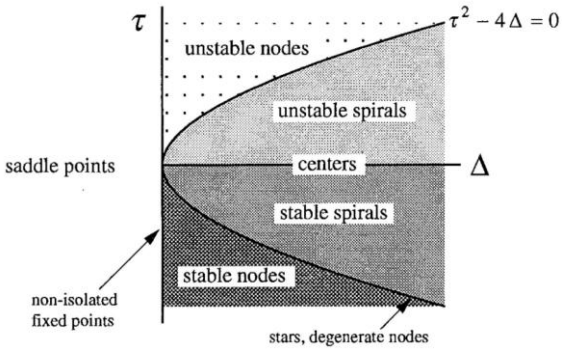

Fig. 4. Stability Diagram of Fixed Points

From the above analysis, it can be concluded that the system is locally stable, so that there exists a metrix P>0 that is such that:

$$A^T P + PA = -Q < 0$$

2.3 Dulac Criterion

Let D $\underline{C}$ R^2 be a simple connected region where:

$$\text{div f}(x) = \frac{\partial f1}{x1} + \frac{\partial f2}{x2}$$

is not identically null and does not change sign. Then, D does not contain any closed orbit.
Considering the region D (x1>=0 and x2>=0) a physically obvious assumption.

$$\text{div f}(x) = -\frac{V}{F} - K_0 e^{-\frac{E}{Rx_2}} - \frac{V}{F} + \frac{EK_0x_1}{R\rho C_p}(H_r)e^{-\frac{E}{Rx_2}}\frac{E}{Rx_2{}^2} - \frac{UA}{\rho C_p V}$$

It can be deduced that div f$(x) < 0 \ \forall x \in D$.
In fact, all parameters are positive except for Hr (the heat of reaction) which makes its term negative.
It can be concluded that within D $\underline{C}$ R^2 there are no limit circles.

2.4 Lyapunov stability

Local asymptotic stability of the origin can be proven through the Lyapunov stability theorem. The first step is to find a Lyapunov candidate function. the easiest choice is:

$$V(x) = (x - x*)^T P(x - x*)$$

Since we already know that there is a matrix P that locally repeats the formula:

$$A^T P + PA = -Q < 0$$

Choosing Q equal to the unit matrix, we solve the lyapunov equation with Matlab
Then it can be shown that:

1. V : Ω → R is continuosly differentiable;
2. V (x*) = 0;
3. V (x) > 0, ∀(x) ∈ Ω, (x) ≠ (x*)

In order for x*= [0.9366, 308.46] to be locally asymptotically stable, the following condition must hold true:

4. $\dot{V}(x1, x2) < 0, \forall (x1, x2) \in \Omega, (x) \neq (x^*)$

$$\dot{V}(x) = (x\text{-}x^*)\ P\ \dot{x}$$

The derivative of the Lyapunov function can be calculated numerically as shown in figure 5.
a set Ω where the function $\dot{V}$ (x) is always negative is Ω={0≤x1≤1 , 200≤x1≤350}

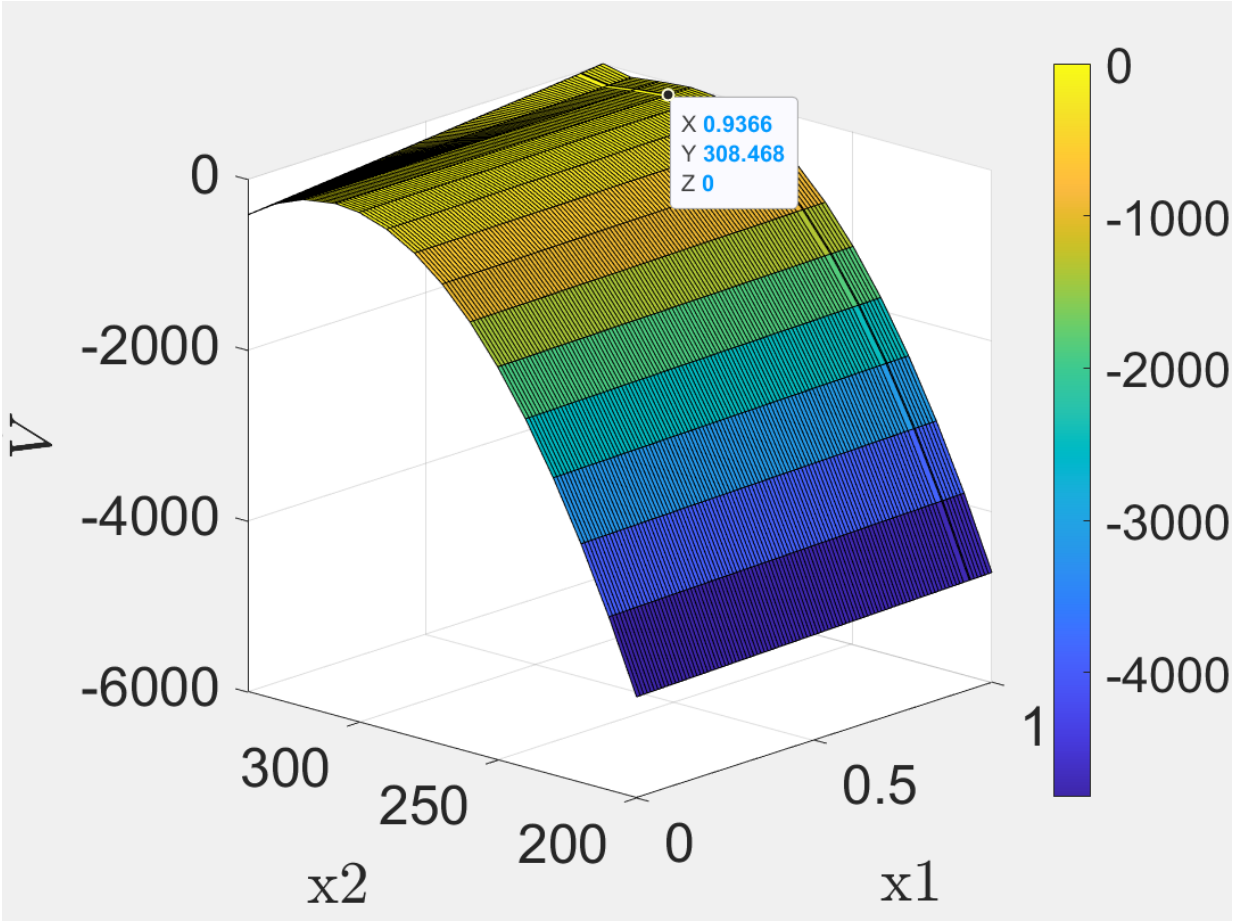

Fig. 5. The derivative of the Lyapunov with respect to time in the set Ω

CAPITOLO 3. SYNTHESIS: REACTOR START-UP

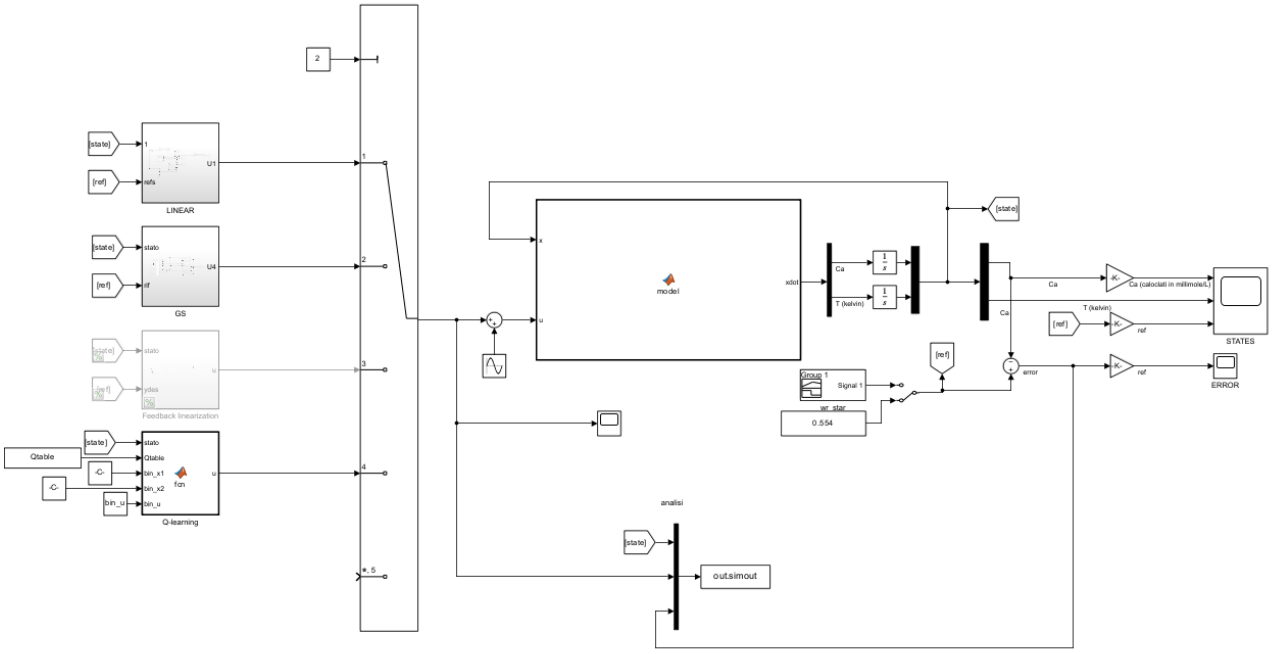

Fig. 6. Full SIMULINK scheme with control selection

3.1 Clear formulation of the control problem.

Goal 1: the objective of the control is to succeed in initiating the reaction in the CSTR and stabilise the A (Ca) concentration values in the value of 0.554 mol/L (middle region) ensuring that the reactor temperature is always between 300 K and 400 K. i.e. 27-127 degrees Celsius (°C).
The initial conditions from which the system starts are 1000 moles/L at the initial temperature of 350K as reported in the article [1].

3.2 Synthesis of a linear control strategy

For the linearisation of control, the point f(x*,u*)=0 where x*=[0.554 ,338.89] and u*=20 was chosen:

$$\partial x = x - x*$$
$$\partial u = u - u*$$

$$\dot{\partial x}=J(x*,u*)\,\partial x+\ \partial f/\partial u(x*,u*)\ *\ \partial u$$

$$J(x*,u*)=\begin{bmatrix}-1.8190 & 0.0336\\ 138.3057 & -10.0516\end{bmatrix}$$

$$\partial f/\partial u(x*,u*)=\begin{bmatrix}0\\ 3{,}377\end{bmatrix}$$

it is possible to prove that the system is completely controllable, since it is full rank:

$$\text{Wc= (B AB)=}\begin{bmatrix}0 & 0.011\\ 3.377 & -33.77\end{bmatrix}$$

A proportional integral (PI) controller was implemented on the concentation error to control the system. Using a Trial and Error procedure, Kp=-9 and Ki=-4 values were chosen to stabilise the system.

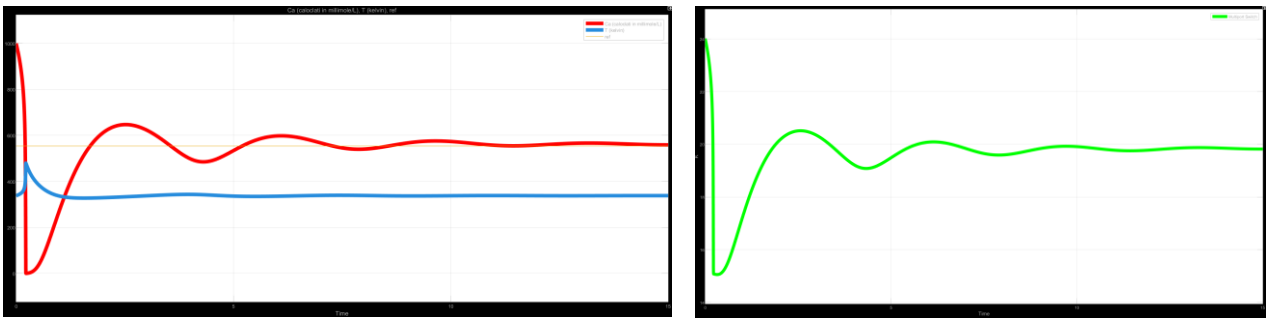

Fig. 7. evolution of the state and control input over time, on the non-linear system with initial condition 1000 mmol/l and 350K

As in the case of free evolution during the transient, the system reaches unacceptable regions of operation (460K). Furthermore, with a linear control of this type, it is impossible to follow a reference, in fact the neighbourhood in which the linear system is equal to the non-linear system is too small.

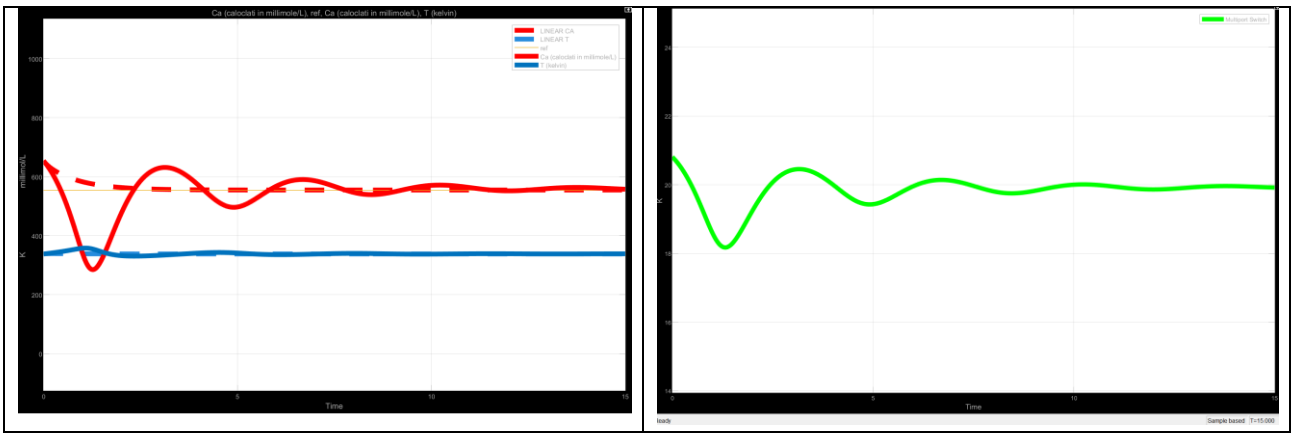

Fig. 8. evolution of the state and control input over time, on the non-linear system with initial condition 654 mmol/l and 338K

By choosing initial conditions closer to the equilibrium point, the behaviour of the system became admissible with zero steady-state error. The PI control applied to the non-linear system also managed

to achieve good behaviour when tracking a signal around the origin, mainly due to the integral action.

3.3 The choice of non-linear controllers

For the selection of a non-linear control strategy, three proposals were analyzed, evaluating the advantages and disadvantages of each approach.

Non-linear control	**Pro**	**Con**
Q-learning	It can adapt to changes in the environment Does not require a deep knowledge of the model	Critical choice of cost function Long training time Critical choice of variable discretisation
Gain-scheduling	Simple transient adjustment	Many trim points are required to reach all equilibrium points. Away from the trim points the system behaviour is not good
Input-output FBL	in our model there are no internal dynamics	the denominator Lg(Lf(h)) must not be zero

Tab. 2. Comparison of possible control strategies

3.4 Synthesis of Q-learning controller

Q-learning is a reinforcement learning algorithm used to train agents to make optimal decisions in complex environments. The goal of Q-learning is to find the best action-selection policy that maximizes the cumulative reward over time.

Q-learning (off-policy TD control) for estimating $\pi \approx \pi_*$

Algorithm parameters: step size $\alpha \in (0, 1]$, small $\varepsilon > 0$
Initialize $Q(s, a)$, for all $s \in \mathcal{S}^+, a \in \mathcal{A}(s)$, arbitrarily except that $Q(terminal, \cdot) = 0$

Loop for each episode:
  Initialize S
  Loop for each step of episode:
    Choose A from S using policy derived from Q (e.g., ε-greedy)
    Take action A, observe R, S'
    $Q(S, A) \leftarrow Q(S, A) + \alpha\big[R + \gamma \max_a Q(S', a) - Q(S, A)\big]$
    $S \leftarrow S'$
  until S is terminal

Fig. 9. Q-learning pseudocode

The main problem to be addressed is discretization; empirical tests have shown that at least 100 samples per minute are required.
The discretization of the 2 states was done at a constant interval with numbers of nStates = [8 11]
In addition, the desired steady-state value of Concentration of component A Ca = 0.554 was forced.
The number of possible control inputs are 11, varying continuously over the interval [+50 to -50],
The control input is the temperature of the refrigerant in relation to the ambient temperature.

```
%% parameters
Nsteps = 500;% (I look ahead up to 5 min) Maximum number of steps per episode
gamma = 0.99;  % Discount rate 0.9
alpha = 0.1;  % Learning rate 0.1
Nep = 5000;     % Maximum number of episodes in training
%%EPSILON
epsilon_start = 0.4;
epsilon_end = 0.05;
epsilon_decay = (log(epsilon_end) - log(epsilon_start)) / (Nep - 1);
epsilon = epsilon_start * exp(epsilon_decay * (0:Nep-1));
```

Nsteps
Maximum number of steps per single episode (corresponding to 5 minutes of simulation).
gamma
discount rate
γ=1The agent fully considers future rewards.
γ<1Future rewards have less weight than immediate rewards.
alpha
alpha is the learning rate, it controls how much new data overwrites existing values in the Q-table.
High values Fast but unstable learning.
Low values Slow but more stable learning.
epsilon
manages trade-offs between exploration and exploitation
The agent explores a lot at the beginning (high values of ϵ) and progressively explores less (low values of ϵ). It ensures a transition from exploration to exploitation as the training progresses.

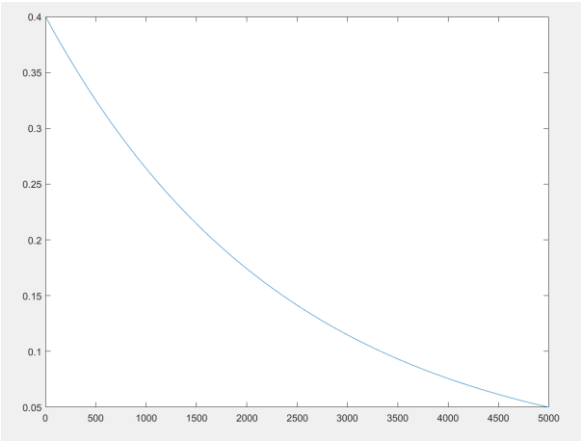

Fig. 10. Epsilon value varying the number of episodes

The cost function was defined after numerous experimental tests. As the units of the variables involved are very different from each other, a normalisation of the data was initially carried out. Subsequently, greater weight was given to the state to be controlled, Ca, than to temperature, which naturally tends to remain within acceptable limits and therefore did not require a significant penalty. From the simulations carried out, it was observed that, in the absence of a constraint on the input, the system reached the desired regime, but presented a marked phenomenon of chattering around the mean value of the input , figure 13. To mitigate this effect and ensure greater consistency with the physical laws of the system - considering that the coolant temperature cannot vary instantaneously - the previous input was introduced into the cost function in the next step. This arrangement resulted in a more stable and realistic control of the system.

In the remainder of this study, Q4 will refer to the Q-learning approach incorporating a function that mitigates chattering, while Q5 will denote the Q-learning approach with a lower weighting on chattering suppression in the control input.

Chatter in the control input could be mitigated by the use of a Simple Moving Average (SMA) filter, which should be appropriately sized.

$$\text{Cost function (Q4)} = 50\frac{|Ca - Ca*|}{Ca_{max} - Ca_{min}} + 1\frac{|T - T*|}{T_{max} - T_{min}} + 30\frac{|U - U_{old}|}{U_{max} - U_{min}}$$

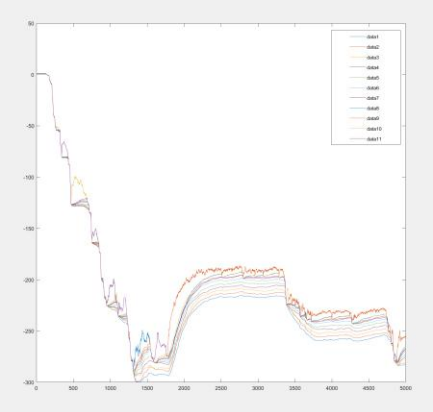

Fig. 11. Convergence of the 11 values of the possible Q-table inputs in the steady state (data 8= 20K)

```
Progress: 99.98%
Progress: 100.00%
Tempo di assestamento: 4.920000e+00 min
```

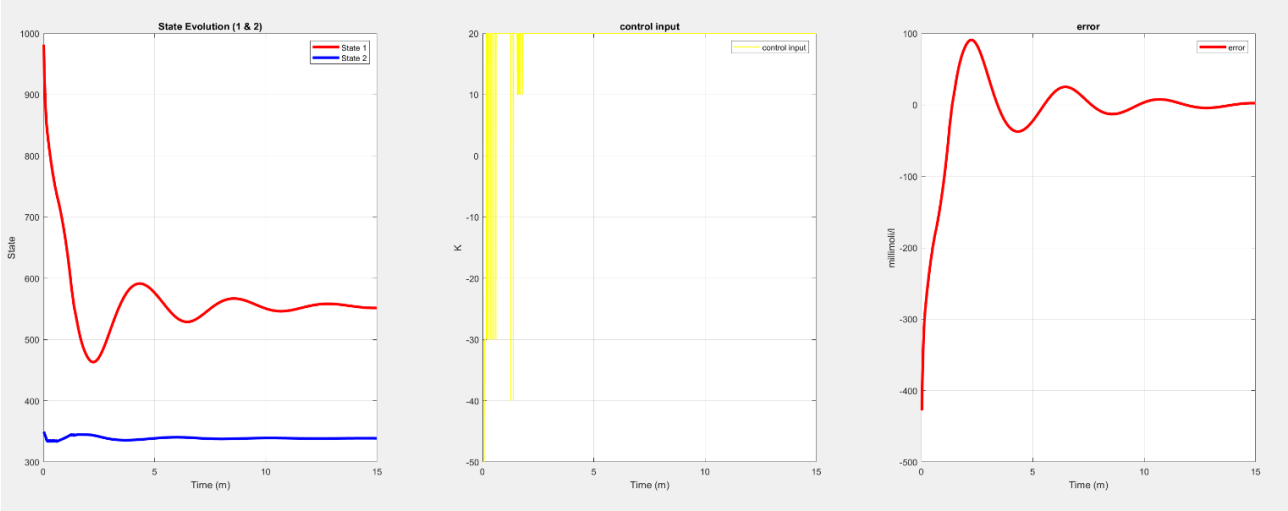

Fig. 12. Q4 Simulation result (settling time 5% 4.9 min)

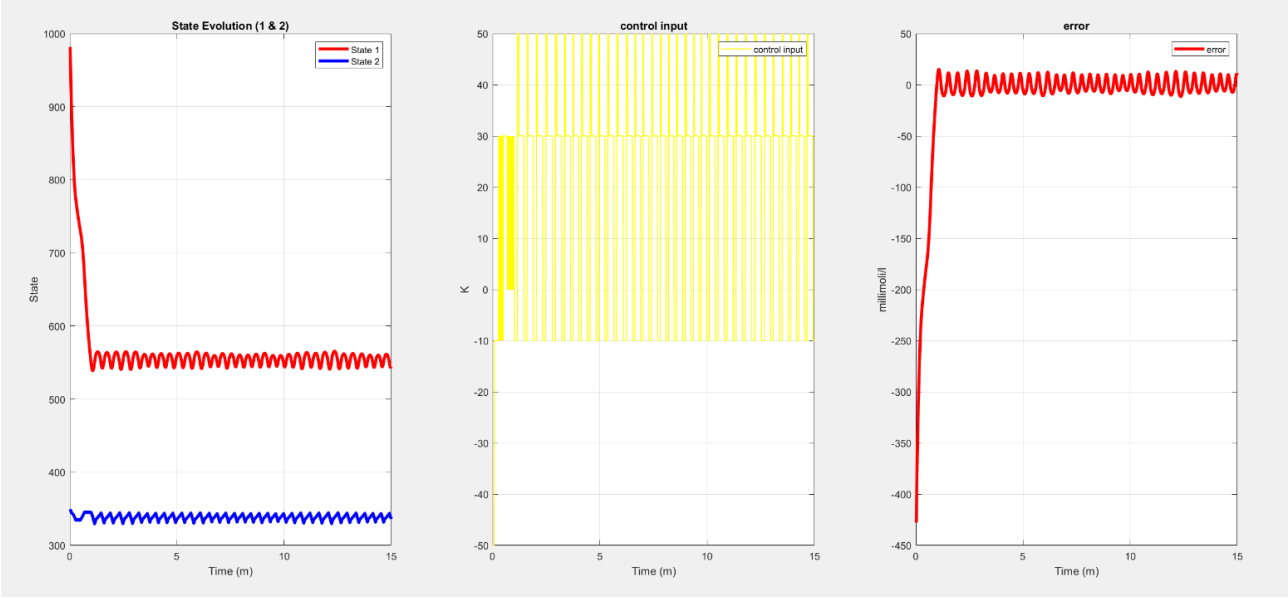

Fig. 13. Q5 Simulation result (settling time at 5% 0.9 min)

3.5 Synthesis of Input-output FBL

Input-Output Feedback Linearisation (FBL) is a nonlinear control technique that transforms a nonlinear dynamic system into a linearised form by means of appropriate state feedback. The main objective is to design a control law that can compensate for the inherent nonlinearities of the

system, allowing the application of linear control techniques.

$$u = \frac{1}{L_g L_f^{r-1} h(x)} \left(v - L_f^r h(x)\right)$$

In our case, we choose to observe the first state (Ca), defining the output as:

$$y = h(x) = x1$$

Since the relative degree is always less than or equal to the total number of states in the system, and since the Lie derivative of the output with respect to g(x) is zero, i.e. Lg(h)=0 , the system has a degree r=2.

The calculation of Lg(Lf(h)) showed a dependence of the value on both state and input. However, a numerical analysis showed that the input u does not affect the value of the considered variable. As shown in Figure 14

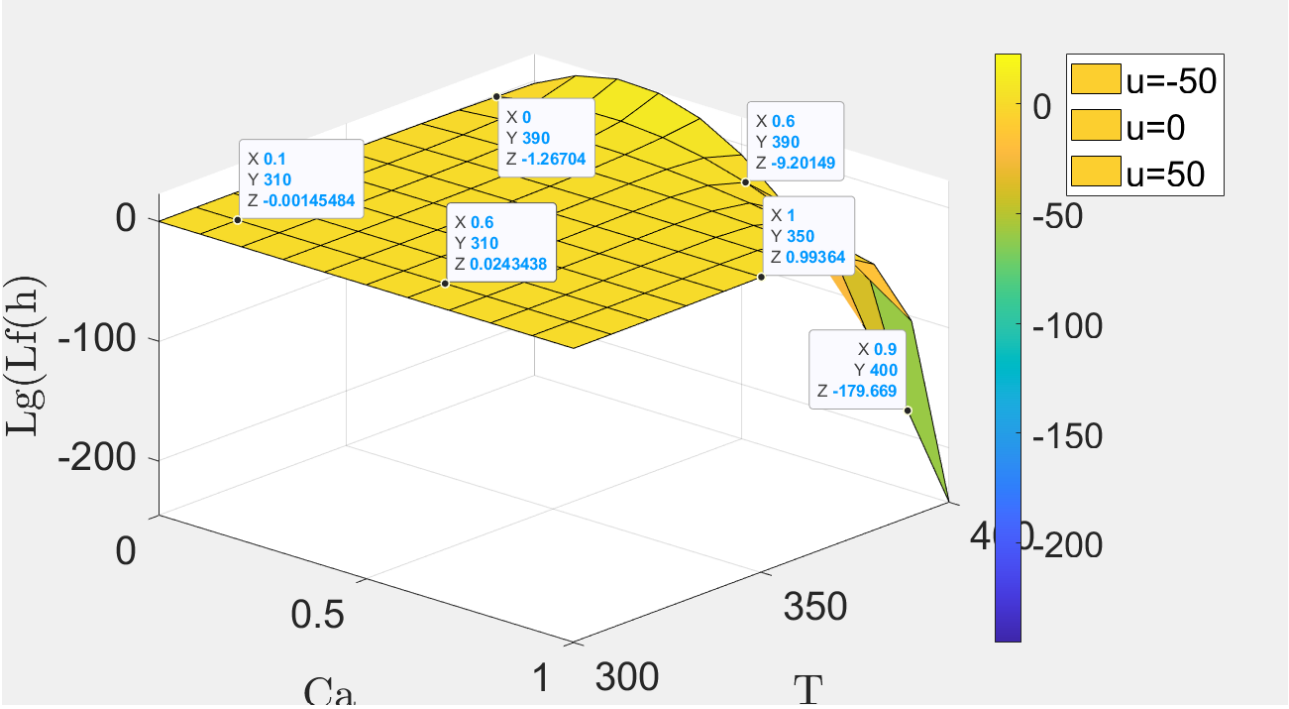

Fig. 14. Value of Lg(Lf(h)) as the state varies and as the inputs (these are 3 different surfaces, athough no differences can be seen)

The analysis of images 14 and 15 shows that it is not possible to apply this control technique since in both the initial state and the equilibrium point, Lg(Lf(h)) acquires too low values, which could easily lead to an instability of the control.
The point highlighted in image 15 is the initial state of the system, which is in a neighbouring area to where the scalar function is zero. For these reasons, it was not possible to apply this type of control to the system

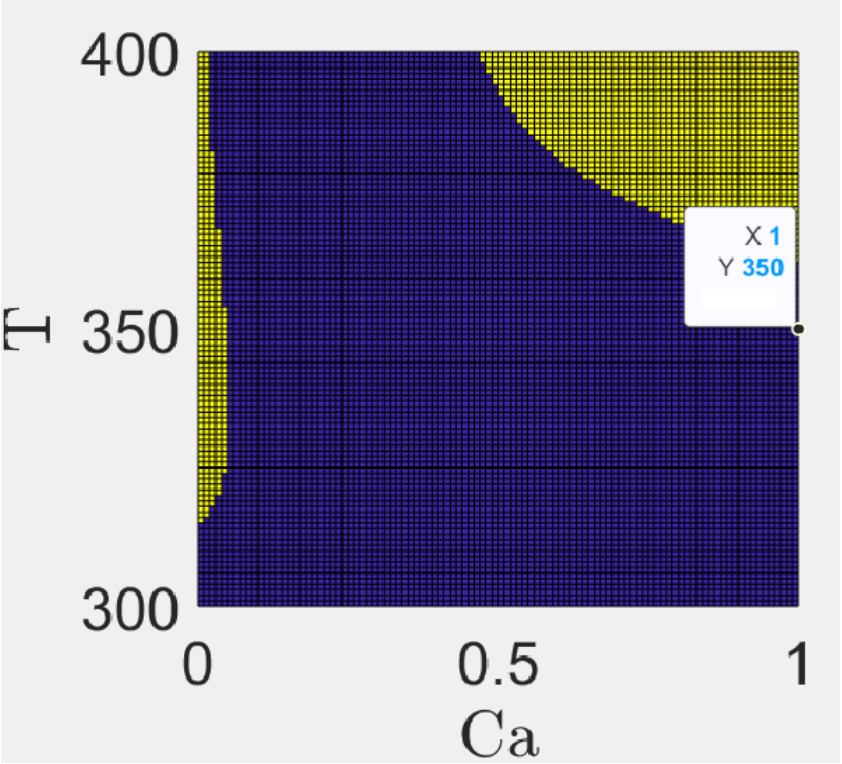

Fig. 15. Mappa degli stati in cui è possibile controllare il sistema con questo metodo (i punti nella la zona viola ha un valore di $Lg(Lf(h)) > -0.1$

3.6 Synthesis of Gain-scheduling

Gain Scheduling is a control technique in which the controller gains are dynamically updated based on the operating conditions of the system.

The synthesis of a Gain Scheduling (GS) controller follows these steps:

1. Identification of equilibrium points (trim points).
2. Linearization of the nonlinear system around each equilibrium point.
3. Design of a family of linear controllers for the linearized system at each trim point.
4. Interpolation of the linear controllers to obtain a nonlinear GS controller.
5. Local and global validation of the GS controller through simulations.

To determine the trim points, a process has been automated using a MATLAB script. For each selected value of u∗, the corresponding unique equilibrium point was computed, allowing the definition of a set of operating conditions for the system.

By choosing the parameters ωn and ζ, the controller gains K and Kr were calculated..

$$\partial u = -K * \partial x + Kr * r$$

$$[\dot{\partial x}]=\begin{bmatrix} a_{11} & a_{12} \\ a_{21}-bK_1 & a_{22}-bK_2 \end{bmatrix}$$

$$K_1 = \frac{\omega_n^2 + a_{12}a_{21} + a_{11}bK_2 - a_{11}a_{22}}{ba_{12}}$$

$$K_2 = \frac{a_{11} + a_{22} + 2\zeta\omega_n}{b}$$

$$K_r = \frac{1}{C(A-BK)^{-1}B}$$

The number of equilibrium points calculated is greater than those reported in the table to improve control accuracy. This was necessary since Gain Scheduling without integral action may exhibit non-optimal performance away from the equilibrium points.

A Simulink scheme was created to interpolate the gains, ensuring smoother transitions between equilibrium points.

The operating condition is a function that takes as input the concentration values of A (Ca) and the reference value and outputs the control to be used.

During the transient phase, the system uses the control associated with the trim point closest to the reference direction relative to the current position.

If the system is already at the trim point closest to the reference, the control maintains the current trim point without updates.

U*	**X1***	**X2***	**K1**	**K2**	**Kr**
-20	0.98728	291.08	504.76	-0.83131	920.82
-15	0.98097	295.18	346.82	-0.86246	633.18
-10	0.97164	299.4	239.33	-0.90737	436.95
-5	0.95771	303.8	165.63	-0.97256	301.71
0	0.9366	308.47	114.94	-1.0687	207.5
5	0.90366	313.6	80.35	-1.2144	141.14
10	0.84939	319.55	57.834	-1.4475	93.737
15	0.75045	327.22	46.951	-1.86	59.325
20	0.55406	338.66	59.838	-2.6672	35.558
25	0.34377	350.63	123.41	-3.6151	25.902
30	0.2301	358.87	229.28	-4.3149	23.128
35	0.16447	365.26	386.18	-4.9504	22.077
40	0.12208	370.75	620.21	-5.6286	21.648
45	0.092838	375.74	972.02	-6.4093	21.517
50	0.071802	380.41	1503.1	-7.3389	21.555

Tab. 3. Tabella dei trim point con i valori dei parametri K calcolati ipotizzando ωn =2 and ζ=0.7

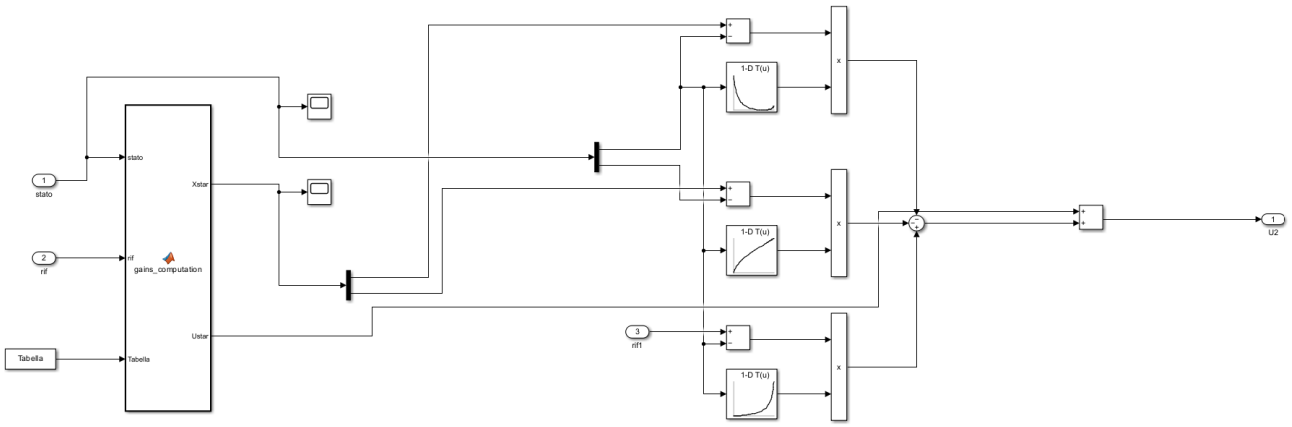

Fig. 16. control scheme of Gain-scheduling

simulations at the variation of the parameter ωn in figure 17,18 and 19 will now be shown, more information on the graphs will be given later in the table 7 comparing the controls.

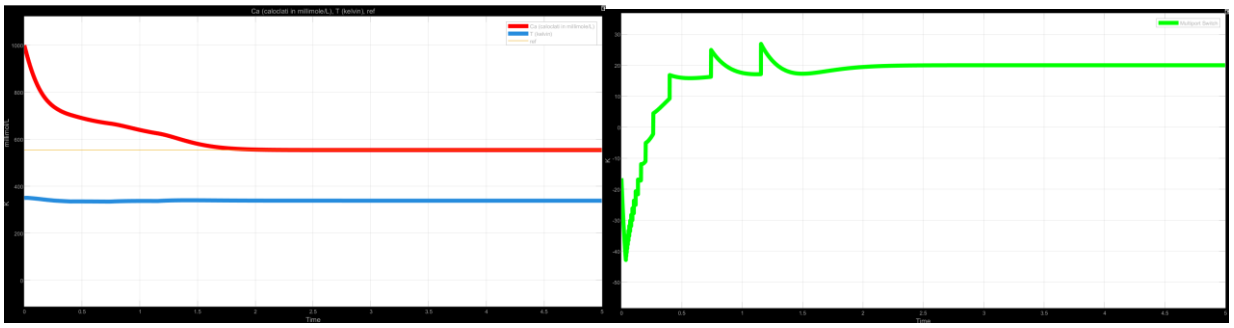

Fig. 17. simulation result (ωn =2 and ζ=0.7)

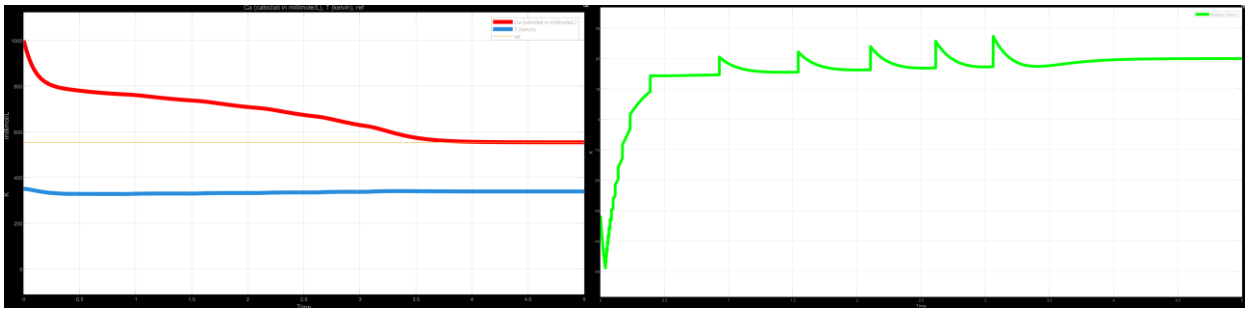

Fig. 18. simulation result (ωn =1.5 and ζ=0.7)

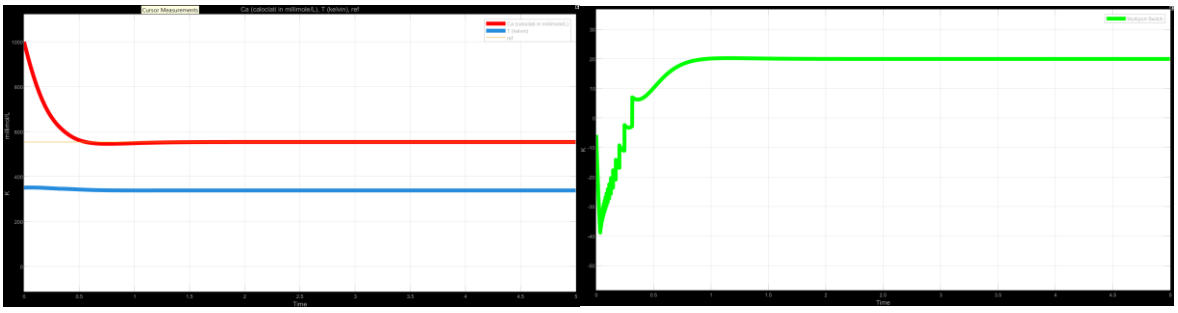

Fig. 19. simulation result (ωn =2.3 and ζ=0.7)

CAPITOLO 4. SYNTHESIS 2: TRACKING

In this short chapter, we check whether the designed controllers are able to effectively regulate the operation of the reactor, ensuring compliance with the specifications on maximum and minimum temperature values.
In the CSTR (Continuous Stirred Tank Reactor), the temperature must remain within an acceptable range between 300 K and 400 K (i.e. 27°C - 127°C).The operator must be able to choose the Concentration values of A (Ca):

- Lower region (Lower): 0.15 mol/L (high transformation rate)
- Middle region: 0. 554 mol/L
- Upper region (Higher): 0.7151 mol/L (low transformation rate)

The aim is to follow a reference signal that allows all three regions of operation of the reactor to be explored, thus assessing the ability of the controllers to adapt to different operating conditions.

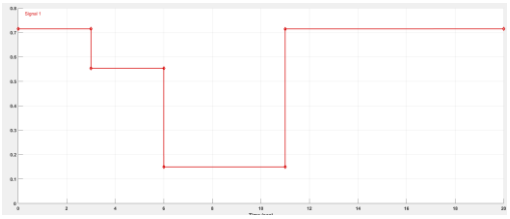

Fig. 20. reference that varies between operating conditions evaluated in moles/l

Among the controllers tested, the Gain-Scheduling controller proved to be the only one capable of adapting effectively to varying conditions, ensuring not only excellent settling times but also significantly reduced steady-state errors. In contrast, the PI controller struggled to track a reference that varied so drastically across the different operating zones. Similarly, the Q-learning controller, when using pre-trained Q-tables, was unable to follow a dynamic reference. To track such references, the model would need to be retrained, as the current implementation does not account for reference inputs.
Retraining the Q-learning model would involve increasing the size of the Q-table, which in turn would extend training times. Additionally, the discretization of states would need to be adjusted to ensure higher precision in the regions where the system's output (Ca) is desired to converge. Although this would increase the model's complexity, it is reasonable to think that such adjustments can be made, leading to an improvement of the system while also increasing its robustness

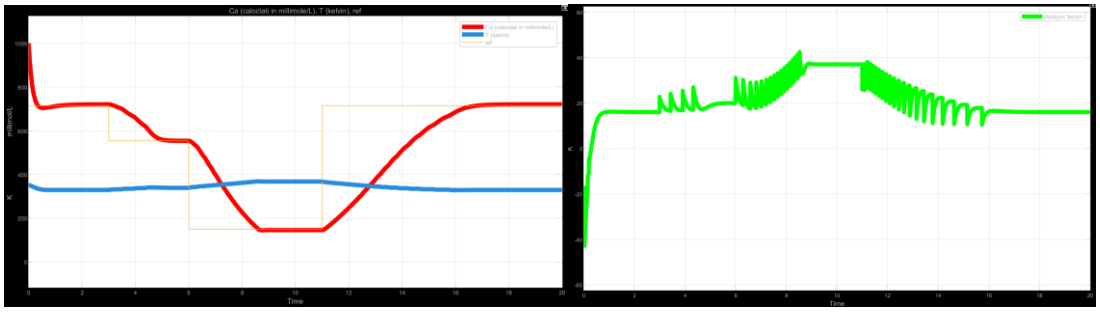

Fig. 21. Gain-scheduling ωn =2

CAPITOLO 5. ROBUSTNESS ANALYSIS OF CONTROLLERS IN THE PRESENCE OF DISTURBANCES AND PARAMETRIC UNCERTAINTIES

4.1 Controllers in the presence of disturbance

For the disturbance analysis, we assume the presence of an additive sinusoidal disturbance in the second equation of state, which represents the derivative of the temperature in the reactor. From a physical point of view, this phenomenon could describe either an oscillation proportional to the temperature of the coolant or an oscillation of the temperature of component A at the reactor inlet (T_{in}).

$$\dot{x}_1 = \frac{V}{F}(C_{a0}) - \frac{V}{F}(x_1) - K_0 x_1 e^{-\frac{E}{Rx_2}}$$

$$\dot{x}_2 = \frac{V}{F}(T_{in} - x_2) - \frac{K_0 x_1}{\rho C_p}(H_r)e^{-\frac{E}{Rx_2}} - \frac{UA}{\rho C_p V}(x_2 - Tamb - u) + \mathbf{d(t)}$$

It is assumed that this input disturbance varies with a peak-to-peak amplitude of 10 degrees, and with a frequency of 10 rad/min.(please note that all variables are expressed in minutes and not in seconds.)

Controller	Ampiezza T	Ampiezza Ca	Ampiezza del controllo
Linear (initial condition 654 mmol/l and 338K)	3.5 K	14 mmoles/l	0.1 K
Q-learning (Q4)	3.5 K	13 mmoles/l	0 K
Q-learning (Q5)	14 K	15 mmoles/l	60 K
Gain-scheduling	3.5 K	9 mmoles/l	10 K

Tab. 4. Summary of relevant parameters in the presence of a disturbance

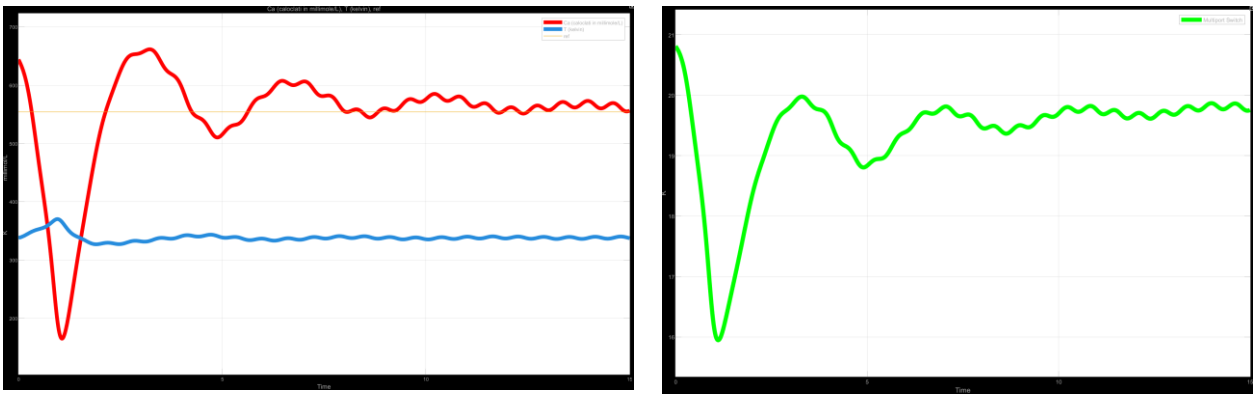

Fig. 22. evolution of the state and control input over time, on the non-linear system with initial condition 654 mmol/l and 338K in the presence of a disturbance

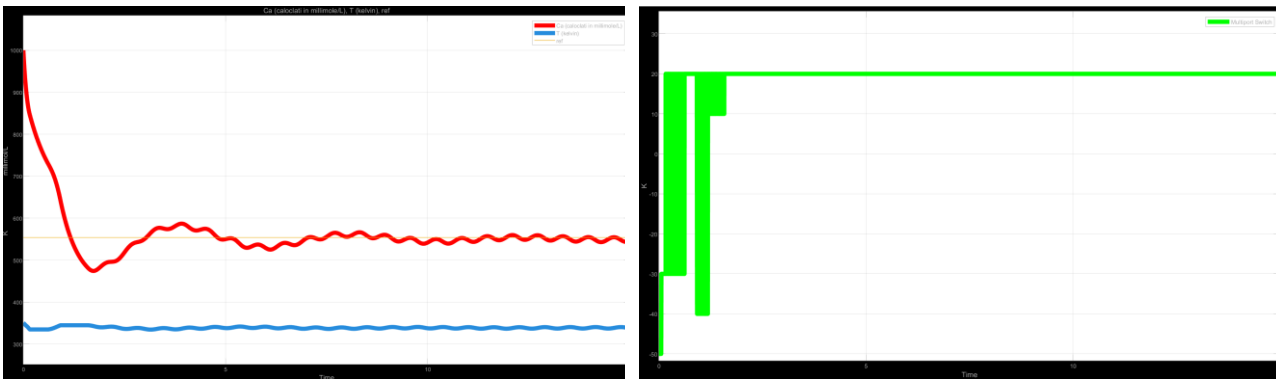

Fig. 23. evolution of the state and control input over time, with Q-learning (Q4) control in the presence of a disturbance

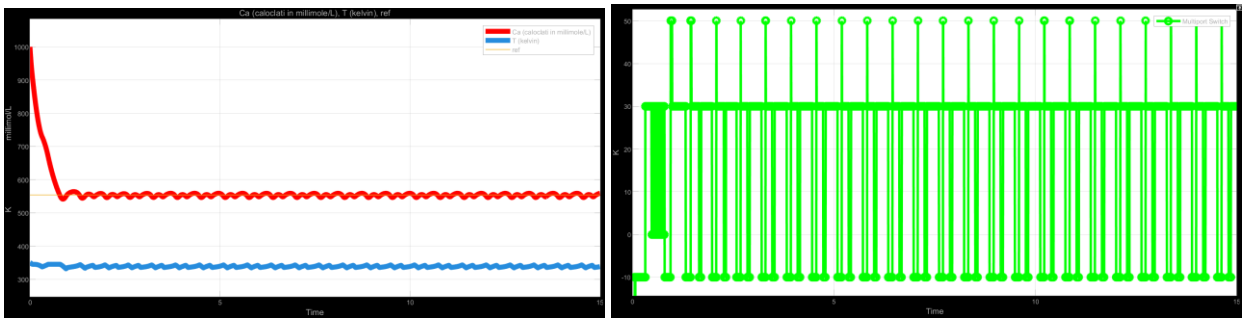

Fig. 24. evolution of the state and control input over time, with Q-learning (Q4) control in the presence of a disturbance

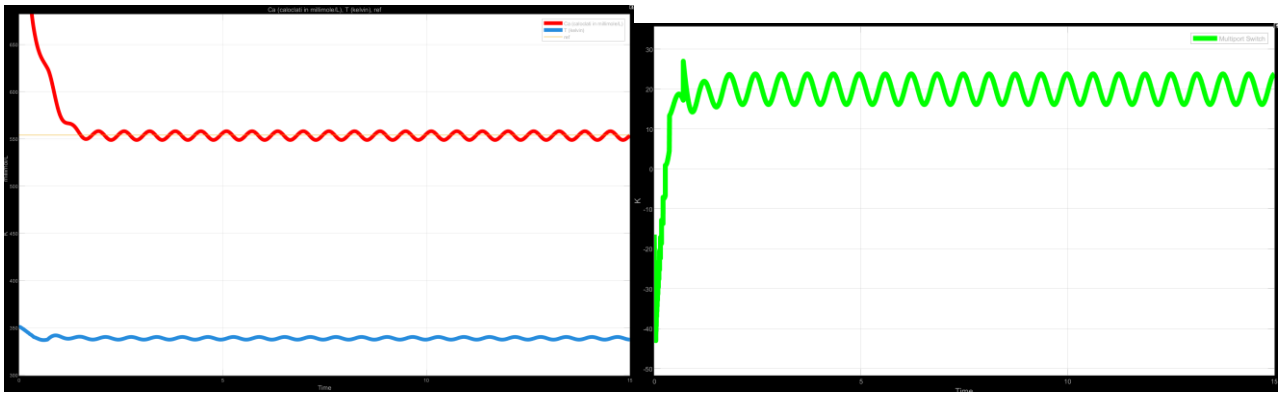

Fig. 25. evolution of the state and control input over time, with gain-scheduling in the presence of a disturbance

The analysis of the responses of the three controllers to the disturbance revealed significant differences in their performance.

The Q-learning controller (Q4) did not react to the disturbance, a behavior attributed to the constraint imposed during the training phase to prevent chattering in the control. As a result, the system maintained a stable response but lacked the ability to adapt to perturbations.

In contrast, the Q5-based table controller demonstrated better adaptability in the presence of

disturbances, successfully controlling the Ca output within an acceptable range. However, it amplified the temperature disturbance by 40%, introducing an undesirable variation in the system.
The Gain-Scheduling controller proved to be the most effective at attenuating the oscillations in the Ca concentration, ensuring a more stable response and an acceptable impact on the control signal.
On the other hand, the PI controller applied to the linear model showed some limitations: the system's settling time increased by 25%, while the control input variation was negligible. This indicates lower adaptability compared to the Gain-Scheduling controller.
Finally, simulations conducted at higher frequencies confirmed the system's low-pass behavior, naturally attenuating the high-frequency components of the disturbance as expected.

4.2 Controllers in the presence of parametric uncertainties

$$\dot{x}_1 = \frac{V}{F}(C_{a0}) - \frac{V}{F}(x_1) - K_0 x_1 e^{-\frac{E}{Rx_2}}$$

$$\dot{x}_2 = \frac{V}{F}(T_{in} - x_2) - \frac{K_0 x_1}{\boldsymbol{\rho C_p}}(H_r)e^{-\frac{E}{Rx_2}} - \frac{UA}{\boldsymbol{\rho C_p} V}(x_2 - Tamb - u)$$

So far, all analyses have been conducted using a generic component A, with values chosen for the simulation based on the scientific article [1]. It is now assumed that component A is replaced by another material, keeping some fundamental chemical-physical parameters such as activation energy (E), heat of reaction (H_r) and pre-exponential factor (K_0), constant, while introducing a change in the product between density ρ and heat capacity Cp of the reactant fluid.
Since in the energy balances analysed, the terms ρ and Cp lways appear multiplied by each other, the system will be affected not by the individual variations of each of these quantities, but by their combination. In particular, suppose we choose a new component A such that the product ρCp increases by 40% from its original value.

ρ	Density of the inlet and outlet stream (g/l)	900
C_p	Heat capacity of inlet and outlet stream (Cal/g.K)	0.329

Tab. 5. Variables and nominal CSTR parameter values before the change

From a physical and mathematical perspective, this implies that the thermal capacity of the system, i.e., its ability to absorb and release heat, will increase proportionally.
As a result, the thermal response of the reactor will become slower, since an increase in ρCp requires a greater amount of energy to achieve the same temperature variation, extending thermal transients.
Moreover, the system's thermal inertia will grow, making the reactor's response slower to temperature changes imposed by the environment or control, complicating any rapid regulation.
Finally, a reduction in thermal oscillations can be observed, as the fluid, with a greater capacity to absorb energy variations without rapidly changing its temperature, will be less sensitive to sudden disturbances.

Controller	Error at steady state	settling time 5%
Linear (initial condition 654 mmol/l and 338K)	0	2.45 min
Q-learning (Q4)	51.42 mmoli/L	3.14 min
Q-learning (Q5)	4 mmoli/L	1.18 min
Gain-scheduling	5.86 mmoli/L	0.87 min

Tab. 6. Summary of relevant parameters in the presence of a disturbance

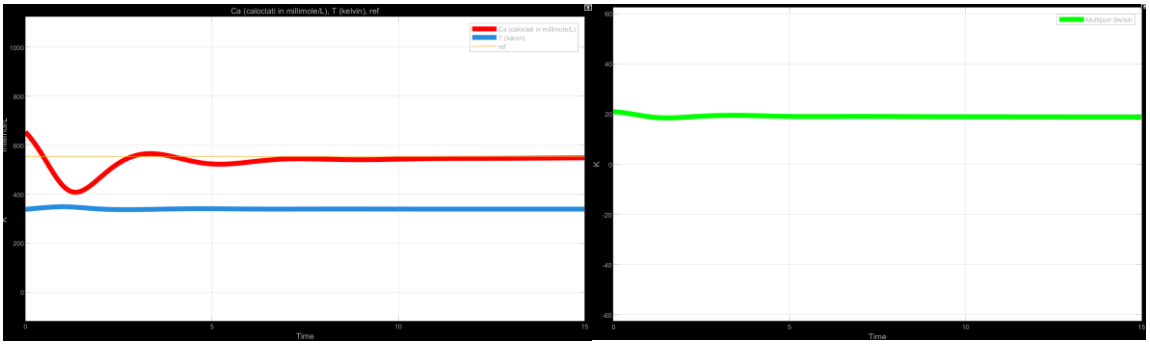

Fig. 26. evolution of the state and control input over time, on the non-linear system with initial condition 654 mmol/l and 338K in the presence of parametric uncertainties

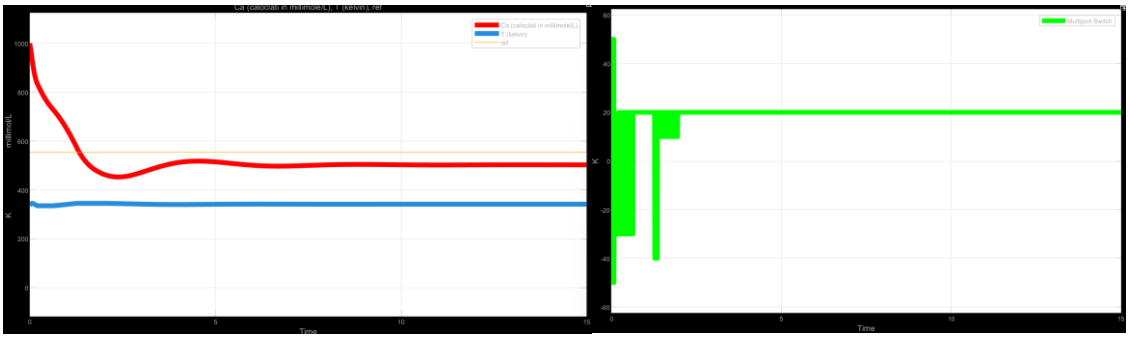

Fig. 27. evolution of the state and control input over time, with Q-learning (Q4) control in the presence of parametric uncertainties

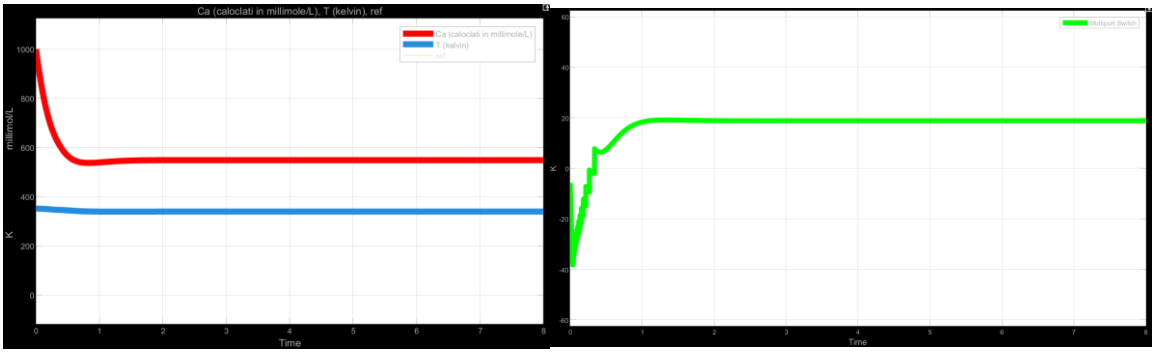

Fig. 28. evolution of the state and control input over time, with gain-scheduling in the presence of parametric uncertainties

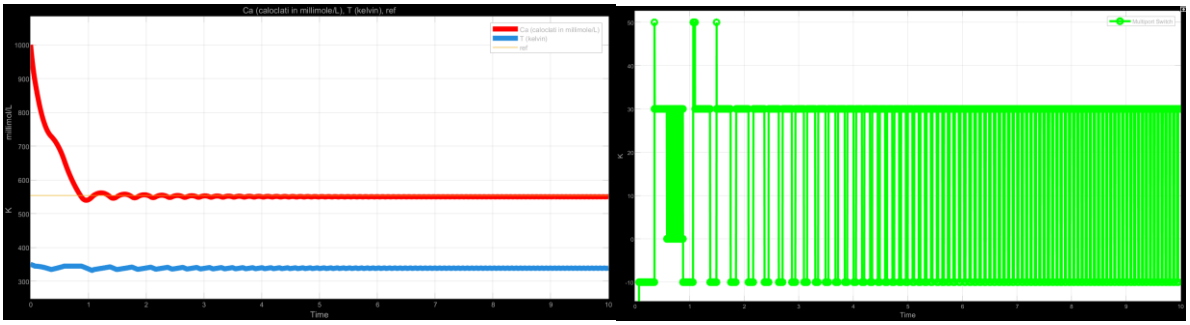

Fig. 29. evolution of the state and control input over time, with Q-learning (Q5) control in the presence of parametric uncertainties

The variation of parameters was effectively managed by the linear control, which demonstrated zero steady-state error due to its integral action and achieved a good settling time. However, it is important to note that the initial conditions for the linear control were not identical to those of the other controllers: it started from a state closer to the equilibrium point, which may have favored its performance.

As far as the Q-learning controller (Q4) is concerned, it was unable to reach the reference, showing a difficulty in compensating for parameter variations. In contrast, the Q5 controller achieved a much lower settling time than the others, but also ensured a small steady-state error.

The gain-scheduling controller, also provided excellent settling time and an acceptable steady-state error that could be further reduced by increasing the number of trim points.

This analysis highlighted that a percentage variation in the fluid's density or thermal capacity does not compromise the system's stability, confirming the robustness of the adopted control strategy.

CAPITOLO 6. QUANTITATIVE COMPARISON BETWEEN THE PERFORMANCES OF THE LINEAR AND NONLINEAR CONTROLLERS

Now we compare all the implemented controllers, also analyzing their performance under varying parameters. The data analysis was conducted using a MATLAB script.

In addition to standard evaluation criteria such as settling time, maximum and minimum values of states and control input, undershoot, and steady-state error, other key aspects were considered to assess the quality of the controllers. Specifically, the ability to track a reference and to operate effectively from any initial condition was analyzed. Another important evaluation criterion is the control input behavior, which should avoid chattering to ensure smooth and stable system regulation

Controllers	ST5%	Tmax	Tmin	Umax	Umin	S%	Err∞	tracking	initial conditions	chattering
Linear (initial condition 1000 mmol/l and 350K)	7.05 min	503.71K	326.29K	24.01 K	14.71 K	56.03 %	-4.78 mmoli/L is theoretically zero	✗	✗	✗
Linear (initial condition 654 mmol/l and 338K)	7.41 min	358.84K	329.47K	20.90 K	17.04 K	28.5%	-2.25 mmoli/L is theoretically zero	✗	✗	✗
Q-learning (Q4)	4.86 min	345.02K	334.98K	50.00 K	-50.00K	9.2 %	2.10 mmoli/L	✗	✓	✗
Q-learning (Q5)	54sec	345.01K	324.98K	50.00 K	-40.00K	0.8%	3.34 mmoli/L	✗	✓	✓
Gain-scheduling ωn =1.5	2.57 min	350.02K	327.61K	27.33 K	-48.88K	0 %	-0.06 mmoli/L	✓	✓	✗
Gain-scheduling ωn =2.0	1.12 min	350.66K	334.74K	26.90 K	-42.86K	0 %	-0.06 mmoli/L	✓	✓	✗
Gain-scheduling ωn =*2.3*	20sec	351.56K	338.46K	20.27 K	-38.84K	0.8%	-0.06 mmoli/L	✓	✓	✗

Note: the steady state error was calculated after 15 min

Tab. 7. Quantitative comparison between the performances of controllers

As shown previously, the linear control was not able to start the reactor correctly. Furthermore, its performance in terms of settling time and overshoot was significantly lower than that of the non-linear controllers.

Gain Scheduling proved to be the best solution by far, allowing it not only to reach the reference faster than other controllers, but also to adapt to different reference values. Furthermore, it ensured superior performance even in the presence of disturbances and parametric variations, ensuring both that the desired concentration of component A was maintained and that the reactor temperature remained within the correct band.

Gain Scheduling (Q4) was also able to start the reactor well, but did not prove robust against parametric variations. In contrast, Gain Scheduling (Q5) was able to handle such variations, but without preventing chattering.

For future developments of this project, the inclusion of a moving average filter on the control input calculated by Gain Scheduling (Q5) could be considered, as well as retraining the model to consider reference tracking.

CAPITOLO 7. BIBLIOGRAPHY

[1] S. Anbu and M. Senthilkumar, "Modelling and Analysis of Continuous Stirred Tank Reactor through Simulation," *Asian Journal of Engineering and Applied Technology*, vol. 7, no. 1, pp. 78-83, 2018.

[2] Artificial intelligence was used to revise the English text and properly format the layout of the mathematical formulas.