Robust state feedback predictive controller project for concentration and level control of a continuous stirred tank reactor (CSTR)

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***Summary* - The article discusses the concentration and level control of a continuous stirred-tank reactor, CSTR (acronym in English for *continuous stirred-tank reactor*). As they are equipment widely used in the chemical industry, they need to operate under specific production conditions, given that the safety of these processes depends on the balance and stability of the chemical reactions that occur inside them. In this context, in addition to the explanation of theoretical aspects related to the robust predictive control techniques used to design the controller for some CSTR variables, the linearization stage, which precedes the control itself, was also described, as well as the specifications required for the project. in question. Furthermore, some expressions used in the project development stages were highlighted and, finally, some discussions were raised about the results obtained.**

***Keywords* - CSTR, linearization, robust control, fluid, level, concentration**

I. INTRODUCTION

With the growing demand for products for the most varied applications, from the cleaning and sanitizing sector to the production of medicines, the chemical industry has been standing out for the increase in its production scale and number of active factories. The transformation of raw materials into products and by-products goes through several stages in a chemical industrial plant, and this involves a series of processes and chain reactions under specific conditions and under strict control and monitoring.

A. Chemical reactors

In this context, a group of equipment present in industrial plants stands out, the reactors, which are the places where these reactions actually occur. These structures are large containers duly designed to contain reactions and provide typical conditions for them to occur in an escalated manner. However, as it is a dangerous activity with many associated risks, it is necessary to have a monitoring and process control infrastructure compatible with the complexities of these reactions, in order to guarantee the efficiency of the production process and the mitigation of possible negative effects.

A common example of these large containers used in the chemical industry are continuous stirred tank reactors, or CSTR, whose representation model can be seen in Figure 1. These reactors have a striking feature, which is the presence of agitators responsible for homogenizing the mixtures of reagents involved in the chemical reaction.

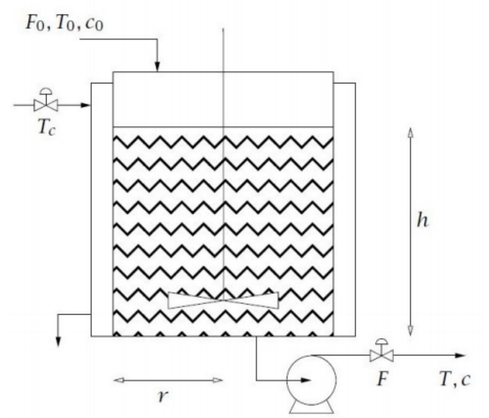

Figure 1. Continuous stirred tank reactor (CSTR). Source: Rawlings, Mayne and Diehl

However, it is worth highlighting that there are a series of variables involved in a chemical reaction on a scale, which necessarily need to be considered for the correct functioning of the plant, such as temperature, concentration of reactants in the mixture, level, among others. Thus, this article brings some aspects related to the control of some of these chemical reaction variables, highlighting everything from the mathematical modeling of their operation to the particularities involved in the control of these variables, complying with pre-established requirements.

B. Work objectives

As the main objective, in this article the steps involved in the design of a robust predictive controller for level and concentration control in a CSTR of a given industrial chemical plant were described.

Chapter II brings some theoretical concepts that guided the construction of the project, highlighting the equations of interest and related themes. In addition, the technical specifications required for the project are exposed.

Chapters III and IV present, respectively, the development and discussions about the progress of the project, where the theoretical foundations presented are applied and the simulations carried out in the software environment *Matlab* are highlighted. Finally, chapter V discusses the conclusions regarding the control work developed, concluding the reasoning on this topic.

II. THEORETICAL FOUNDATION

The first step in making it possible to carry out any type of control in a system is to describe its behavior through mathematical models that come as close as possible to reality. In this context, some techniques used before the control itself facilitate the mathematical description of the system, such as linearization, used to simplify the mathematical representation and allow the use of known control models, in this case, robust predictive control.

A. Linearization and Discretization of the mathematical model

As discussed previously, the CSTR is a reactor where chemical reactions occur until the final product is obtained. Several variables are involved in this process, which interfere in different ways in the reactions. Therefore, the fact that the reactor is a complex system naturally makes its mathematical representation far-fetched, which initially makes it difficult to implement techniques to control it.

As one of the most necessary characteristics for this type of system is precisely the ease of controlling the process (aiming to prevent unwanted failures during reactions), it is necessary to use devices that bring a more simplified version (mathematically) of the mathematical representations and , consequently, a facilitation of the methods for the project to control the variables of interest to the CSTR.

In this context, the artifice of linearization stands out, which is nothing more than an approximation in a linear model of the system's behavior around a specific operating point, in which approximate linear curves are defined around it. Using this technique, it is possible to more easily predict the behavior of the system in the vicinity of this operating point, which does not allow the prediction of the behavior of the system as a whole, but greatly simplifies the design of the associated controller.

The method chosen to linearize the system for the operating points provided was using the concepts of Hessian matrix, in which we use partial derivatives to find the state space matrices. Below you can see how the terms of the Hessian matrix are defined.

$$
H\left[f(x_1,x_2,x_3,\ldots,x_n)\right] = \begin{bmatrix} \dfrac{\partial^2 f}{\partial {x_1}^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial {x_2}^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}
$$

Figure 2. Hessian matrix for linearization

Due to the control method discussed, there is a need to transform the linear model in continuous time to discrete time, that is, to generate system samples with a predetermined period. For this discretization, the zero-order insurer was used, which generates samples of the input signals considering their constant values during the sampling period.

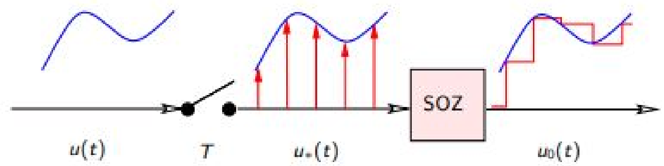

Figure 3. Exemplification of the zero-order insurer (SoZ)

B. Robust Predictive Control

Robust predictive control is a procedure that encompasses several control methodologies, which allows the prediction of future system outputs, based on samples generated periodically from the system, providing a reduction in the cost function.

In addition to being used when it is necessary to deal with uncertainties due to the variation of the parameters of the dynamic system, the procedure allows the determination of the controller's gains with a view to minimizing the performance index $J_p(k)$ over the forecast horizon P.

The process of optimization and determination of the gain K for the system is done through the use of LMIs, whose resolutions allow finding 3 optimization values: γ, W1 matrix and W2 matrix. The γ is the value that minimizes the system's robust performance index. Minimizing this value allows the system to be asymptotically stable according to Lyapunov and for disturbances to have minimal impact on the controller's performance. The W_2 and W_1 matrices are optimal matrices that allow the controller gains to be calculated using the equation:

$$K = W_2 W_1^{-1}$$

Since W_2 and W_1 are obtained by solving the following convex optimization problem:

$$\min_{\gamma, W_1, W_2} \quad \gamma,$$

sujeito a

$$\begin{bmatrix} 1 & x(k|k)^T \\ x(k|k) & W_1 \end{bmatrix} \succeq 0,$$

$$\begin{bmatrix} W_1 & W_1 A_j^T + W_2^T B_{2j}^T & W_1 Q^{1/2} & W_2^T R^{1/2} \\ A_j W_1 + B_{2j} W_1 & W_1 & 0 & 0 \\ Q^{1/2} W_1 & 0 & \gamma I & 0 \\ R^{1/2} W_2 & 0 & 0 & \gamma I \end{bmatrix} \succeq 0,$$

$$j = 1, 2, \ldots, L.$$

Since A_j and B_{2j} are discretized matrices of the linearized model of the system at operating points 1 and 2, which are vertices of the uncertainty polytope.

C. Basic job requirements

For the development of the work, two operating points were given with their respective linearization points, as seen in Table I below.

Table I
PREDEFINED OPERATING CONDITIONS

	Operação 1	Operação 2	Nominal
x_1^s $[k\ mol/m^3]$	$0,791$	$0,966$	$0,878$
x_2^s $[K]$	$332,399$	$308,755$	$324,5$
x_3^s $[m]$	$0,659$	$0,659$	$0,659$
u_1^s $[K]$	$302,79$	$285,556$	300
u_2^s $[m^3/min]$	$0,1$	$0,1$	$0,1$

Furthermore, in this same table a nominal point is given, with its linearization values, which will be the system reference to be followed. Therefore, the system will start from the initial condition given below and must follow the reference, which in this case will be the nominal point.

$$\begin{bmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \end{bmatrix} = \begin{bmatrix} 0.96 \\ 300 \\ 0.659 \end{bmatrix}$$

Finally, the sampling time must be equal to 1 minute and the weighting matrices for the control being $Q = C_2^T C_2$ and $R = 100000 I_2$.

III. DEVELOPMENT

The development of the work was guided along three main axes: linearization, control design via LMI of the linearized model and closed-loop simulation with the non-linearized model. The project stages were described below, as well as the results obtained in each of them:

A. Linearization and Discretization

The equations that represent the behavior of the dynamic system, the CSTR, are quite complex, including variables in the exponents, as can be seen below:

$$\begin{cases} \frac{dc(t)}{dt} = \frac{F_0(c_0 - c(t))}{\pi r^2 h(t)} - k_0 c(t) e^{-\frac{E}{RT(t)}}, \\ \frac{dT(t)}{dt} = \frac{F_0(T_0 - T(t))}{\pi r^2 h(t)} - \frac{\Delta H}{\rho C_p} k_0 c(t) e^{-\frac{E}{RT(t)}} + 2\frac{U}{r\rho C_p}(T_c(t) - T(t)). \\ \frac{dh(t)}{dt} = \frac{F_0 - F(t)}{\pi r^2}, \end{cases}$$

Figure 4. Nonlinear mass and energy balance model

where K_0 is the reaction rate constant, E/R is the activation energy, C_p is the specific heat, is the density of the substance, H is the heat of reaction, U is the coefficient of heat transfer and r is the radius of the tank. Using x_1, x_2 and x_3, respectively, for c(t), T(t), h(t) - concentration, temperature and level - as well as u_1 and u_2 for T_c (t) F(t) - temperature of the cooling liquid and exit flow - it was possible to rewrite the equations as follows

$$\begin{cases} \frac{dx_1(t)}{dt} = \frac{F_0(c_0 - x_1(t))}{\pi r^2 x_3(t)} - k_0 x_1(t) e^{-\frac{E}{Rx_2(t)}}, \\ \frac{dx_2(t)}{dt} = \frac{F_0(T_0 - x_2(t))}{\pi r^2 x_3(t)} - \frac{\Delta H}{\rho C_p} k_0 x_1(t) e^{-\frac{E}{Rx_2(t)}} + 2\frac{U}{r\rho C_p}(u_1(t) - x_2(t)) \\ \frac{dx_3(t)}{dt} = \frac{F_0 - u_2(t)}{\pi r^2}. \end{cases}$$

Figure 5. Model rewritten based on state variables

Applying the concept of the Hessian matrix to perform linearization, the elements of the state matrices were defined for each of the vertices of the polytope, that is, the pre-defined operating points.

To define the state matrix A, expressions were derived with respect to the state variables x_1, x_2 and x_3; and operating conditions applied; To define the state matrix B_2, expressions were derived with respect to the signals u_1 and u_2. After the calculation, it was realized that the values depended only on parameters associated with the tank, having no relationship with the operating conditions. Therefore, the B_2 matrix was the same for both conditions; Matrices C and D were defined so that their dimensions were compatible with the variables with which they relate, matrix C to define the concentration (State x1 of the system) as output y1 and the level (State x2 of the system) as output y2. And the matrix D is a zero with dimensions compatible with the system.

From this, using the Matlab tool it was possible to discretize these two state spaces (from operating point 1 and 2) through the function *c2d()*, with a sampling time of 1 minute and the method applied being the zero-order insurer.

B. Controller design

The controller project can be divided into four distinct parts: The definition of the polytopes, the creation of a repetition loop that implements the sliding horizon strategy in the code, the declaration and resolution of the LMIs and finally the resolution of the nonlinear system with the control signal of the present sample.

The first part of the process is the creation of the uncertainty polytope vertices in the code. The differences between the two models are between matrices A, due to the linearization points, and matrix B_2, due to the discretization process that modified it into two: B_{21} and B_{22} . To declare the LMIs, it is necessary to know the dimensions of the polytope, which were determined using the *size()* function.

The second part of this controller is to implement a *looping* in the code that represents the sliding horizon strategy, that is, the technique of calculating a new control signal as the system works over time. This was carried out with a repetition loop *for()* varying Kt from zero to a determined time in minutes, where Kt is the discrete variable that will represent each sampling instant and *time*, is precisely the code simulation time. Furthermore, it was necessary to subtract the nominal linearization point from the state vector when leaving the resolution of the nonlinear model and add this nominal linearization point to the control signal vector before entering the resolution of the nonlinear model. This procedure was necessary precisely because of the implementation of a control based on a linear model.

Regarding the issue of matrix inequalities, through the function *setlmis([])*, we declare the variables and LMIs - mentioned in the Robust Predictive Control section in the Theoretical Foundation - which will be used as a mathematical basis to ensure that control will make the system asymptotically stable by Lyapunov. The matrices found in the discrete model enter the LMIs as the constants described in them, and γ and the optimization matrices W_2 and W_1 enter as variables to be determined in the optimization with the function *mincx()*. Furthermore, the LMIs that concern the guarantee that γ and W_1 will be positive definite are declared.

When determining the gain K for each iteration, a control signal *u(k)* is generated given by:

$$u(k) = Kx(k) + \begin{bmatrix} u_1^s \\ u_2^s \end{bmatrix}$$

Where this will enter the equations given in Figure 5 and will be solved using the Matlab function *ode45()* with a new initial condition vector for the states calculated at each iteration.

C. Simulations and Results

Once the control system was designed, simulations were carried out in Matlab. The objective of the simulation is to take the system from the initial condition (x1(0) = 0.96, x2(0) = 300 and x3(0) = 0.659) to the nominal operating point (x1(0) = 0.878, x2(0) = 324.5 and x3(0) = 0.659), whose points correspond respectively to concentration, temperature and tank level.

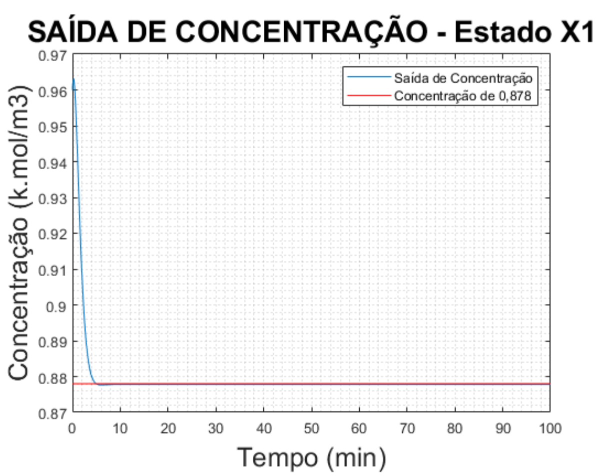

Figure 6. Concentration curve in the tank and expected nominal value

The behavior of the concentration curve in the tank is as expected. The output signal leaves the initial value and goes to the nominal reference value and stabilizes at this value. The system took around 5 minutes to achieve this result. There is a small overshoot, but it is not significantly high and settles quickly.

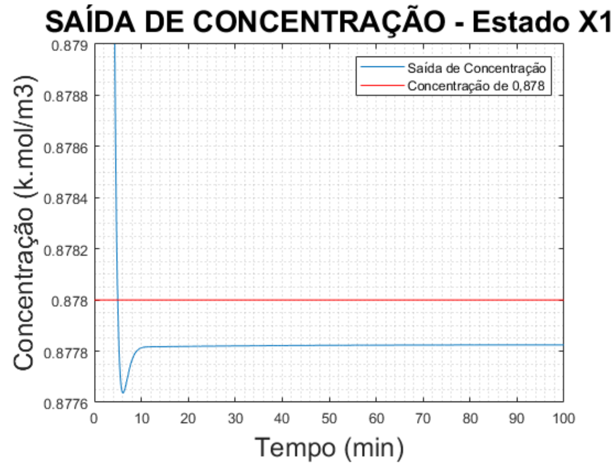

Figure 7. Focus on the nominal value of the concentration curve

To improve visualization of the results, we can see the figure above that explains the results around the nominal operating point for the concentration value. It is notable that the system does not settle exactly at the nominal value, but at 0.02% of the nominal value, which is a negligible error.

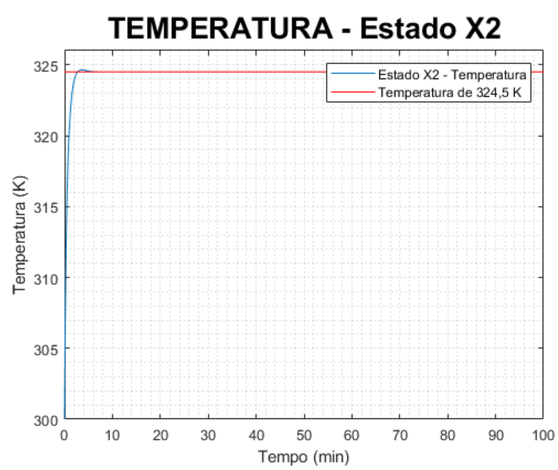

Figure 8. Temperature curve and expected nominal value

The behavior of the temperature curve in the tank is as expected. The output signal leaves the initial value and goes to the nominal reference value and stabilizes at this value. The system took around 5 minutes to achieve this result. There is a small overshoot, but it is not significantly high and settles quickly.

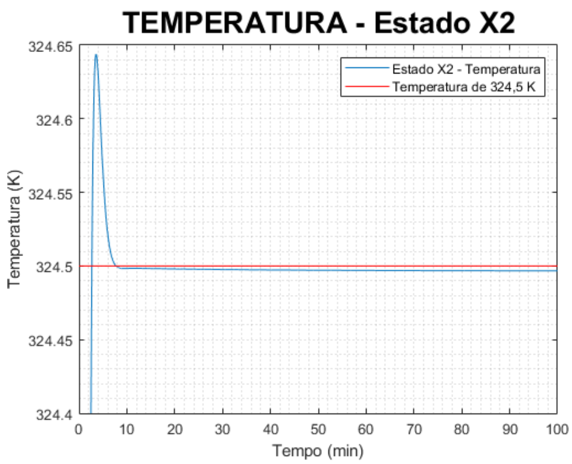

Figure 9. Focus on the nominal value of the temperature curve

To improve visualization of the results, we can see the figure above that explains the results around the nominal operating point for the temperature value. It is notable that the system does not exactly accommodate the nominal value, but the difference is less than 0.003%, which is negligible, as is the overshoot.

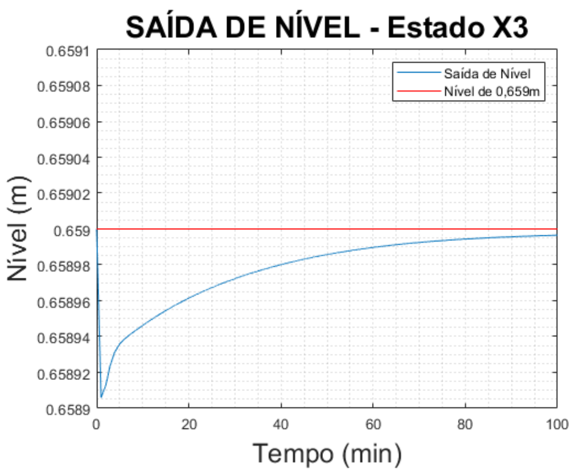

Figure 10. Level curve in the tank and expected nominal value

The behavior of the level curve, despite the shape of the curve being different, is also as expected. There is a small variation (in absolute and percentage terms) in the value due to an overshoot caused by the system transient, but which then settles down . The apparent delay in reaching the exact nominal value is due to the fact that the system is less than 0.001 from the nominal value, which makes the response slower. Similarly, this small variation also occurs in the other two signals, with the value it reaches during the simulation time not being exactly the nominal one, but very close.

IV. CONCLUSIONS

We can therefore conclude that the predictive control carried out for the CSTR tank was satisfactory. The three variables reached nominal values, or values very close to them, in a short time relative to the simulation time. It is evident that the robust predictive method is capable of guiding the system to the nominal operating point by predicting subsequent states and, despite requiring greater processing power from the plant, it performs closed-loop system control for the non-linear system . with great precision. It is a reliable and flexible robust control technique that allows controlling highly complex systems with operational parameters appropriate for the chemical industry, which involves slower systems, therefore making it possible to use predictive control without using large computational power.

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