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A plantwide control proposal for ethylbenzene production

Proposta de estrutura de controle plantwide para uma planta de produção de etilbenzeno

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Resumo
No presente artigo, propõem-se uma estrutura de controle plantwide para o processo de alquilação do benzeno. O modelo matemático utilizado nas simulações desenvolvidas no software livre Scilab, versão 6.1, foi baseado em estudos anteriores. Inicialmente, as restrições operacionais foram avaliadas e as possíveis variáveis controladas foram escolhidas com base nos objetivos operacionais e testadas realizando perturbações degrau para validação dos critérios. A escolha dos melhores pares foi realizada através da matriz de ganho relativo RGA (Relative Gain Array). As decisões estruturais adotadas e os resultados obtidos através da simulação computacional indicaram que apesar de haver interações entre os loops de controle os possíveis pares, T_1-F_{R2} e T_4-Q_4, minimizam as interações do sistema. Os parâmetros ajustados do controlador se mostraram eficazes quanto ao controle da perturbação apresentando pouco ou nenhum overshoot com satisfatórios tempos de subida e resposta. A estrutura de controle adotada com o controlador PID é apenas um dos passos fundamentais dentro da metodologia de controle plantwide e mostra a capacidade do controlador em atender aos objetivos estruturais propostos.
Palavras-chave: Plantwide. PID. Controle.

Abstract
In the present article, a plantwide control structure is proposed for the benzene alkylation process. The mathematical model used in the simulations developed in scilab free software, version 6.1, was based on previous studies. Initially, operational restrictions were evaluated and possible controlled variables were chosen based on operational objectives and tested by performing step disorders to validate the criteria. The choice of the best pairs was made through the RGA (Relative Gain Array) relative gain matrix. The structural decisions adopted and the results obtained through computational simulation indicated that although there are interactions between the control loops, the possible pairs, T_1-F_{R2} and T_4-Q_4, minimize the system interactions. The adjusted parameters of the controller were effective in controlling the disturbance, presenting little or no overshoot with satisfactory ascent and response times. The control structure adopted with the PID controller is just one of the fundamental steps within the plantwide control methodology and shows the controller's ability to meet the proposed structural objectives.
Keywords: Plantwide. PID. Control.

1. Introduction

Ethylbenzene production process, based on the alkylation of benzene with ethylene, is routinely used in the petrochemical industry. Dehydration of the product produces styrene, an intermediate monomer used as a raw material in the production of plastics, such as polystyrene, synthetic rubbers and other copolymers. The process consists of a system of four CSTR's and a separation flash tank operating at high pressure, as schematized in Figure 1.

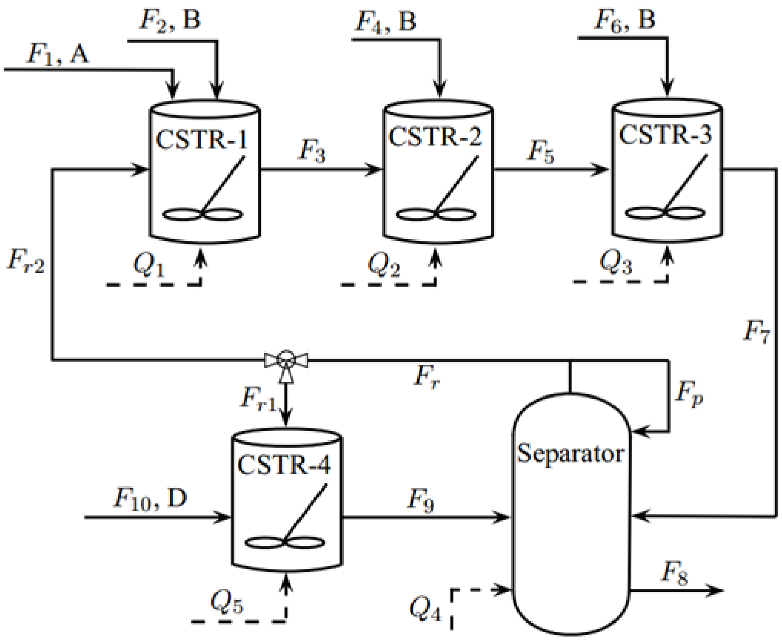

Figure 1: Process flowchart for the production of ethylbenzene proposed by Chen (2012).

CSTR-1 to CSTR-3 is arranged in series correspond to the process steps in which benzene is alkylated with ethylbenzene. Pure benzene (A) is fed into the current F1 and pure ethylene (B) is fed into the currents F2, F4 and F6, obtaining ethylbenzene (C) and 1,3 diethyl benzene (D) as a byproduct. Effluent in CSTR-3, including products and unconverted feed, is fed to the separation tank flash. Benzene is separated by vaporization and condensation and recycled back to the plant, while the product ethylbenzene (C) is withdrawn in the background current. Top stream is separated into Fr and FP, which is recycled to the separator to increase the benzene separation efficiency. A f recycled fraction, FR2, is fed into CSTR-1 while FR1 feed CSTR-4 with an additional current F10 which contains 1,3 ethylbenzene. Reactions involved in the process are shown in Equation. 1, Equation 2 and Equation 3.

$$C_6H_6 + C_2H_4 \rightarrow C_8H_{10} \quad (1)$$

$$C_8H_{10} + C_2H_4 \rightarrow C_{10}H_{18} \quad (2)$$

$$C_{10}H_{18} + C_6H_6 \rightarrow C_8H_{10} \quad (3)$$

Chen, McAvoy, & Zafiriou (2004), defines that a design of the control system consists of two fundamental parts: i) the determination of the interaction between the processes and ii) given the interactions, how to systematize an effective control structure. Muñoz (2019) defines that the central problem to be solved is based on the set of structural decisions that must be adopted to form effective control meshes, which is defined as control plantwide. In line with these ideas, Foss (1973) raises some essential questions that need to be addressed in control system design: Which variables should be measured? Which inputs should be handled? What are the control loops and what connections existing between them?

The first task in defining a plantwide control structure is to identify the controlled variables, followed by establishing control settings and choosing appropriate controllers. Skogestad (2000) has developed a comprehensive methodology consisting of two main stages: top-down and bottom-up, further divided into 8 tasks covering various aspects from planning and optimization to regulatory control.

During the top-down phase, operational objectives are defined, and decisions are made about the controlled and manipulated variables, as well as operational restrictions. This stage is critical in setting the foundation for the control system. Chen, McAvoy, & Zafiriou (2004) suggest that process information can be extracted from previously developed models using steady-state data obtained through computer simulations.

Once steady-state definitions are in place, the bottom-up step focuses on evaluating potential pairs of manipulated and controlled variables and testing diverse control strategies, emphasizing the dynamic aspects of the system. Key decisions are highlighted for each step: for the top-down step, the critical choice is selecting economic controlled variables, while for the bottom-up step, the focus is on choosing stabilizing controlled variables Jahanshahi et al. (2020).

The objective of this work is to propose a plantwide control structure for the benzene alkylation process, utilizing methodologies from control system design, conducting simulations to evaluate the proposed system's effectiveness for process control.

2. Methodology

The methodology used in this article is adapted from the studies and observations proposed by Skogestad (2000), Chen, McAvoy, & Zafiriou (2004) and Muñoz (2019). For mathematical simulations, the Free Scilab software version 6.1 was employed, utilizing the model developed by Chen (2012). Skogestad (2000) outlines the fundamental tasks involved in determining the control structure as follows:

The mathematical model used in the simulations developed in software Free Scilab, version 6.1, builds on Chen (2012). Skogestad (2000) lists the basic tasks of the procedure to be carried out for the determination of the control structure as:

1. Selection of controlled variables:
    i. The ideal value of the controlled variable should be insensitive to disturbances, resulting in small setpoint errors.
    ii. The controlled variable should be easy to measure and control with precision.
    iii. The controlled variable's value should be sensitive to changes in the manipulated variable.
    iv. In cases with multiple controlled variables, the selected variables should not have strong correlations.
2. Selection of manipulated variables.
3. Selection of measurements, which are variables that assist in stabilizing the system.
4. Selection of control configurations.
5. Selection of the controller.

Based on Chen (2012), the objective function of the problem is to increase the reaction rates represented by Equation 1 and Equation 3, while suppressing the reaction rate represented by Equation 2 due to the generation of by-products. Optimization problem's constraints require that the sum of ethylene distributed through the flow F2, F4 by F6 must be equal to FMAX= 0.0026091 mol/sec.

The system’s initial states are considered stable at (X0, t = 0) represented by steady-state inputs u = [Q1, Q2, Q3, Q4, Q5, F2, F4, F6, Fr2, FR, F7, F9] where Qi=1,2,3,4,5 is the heat in J/sec in each equipment. Steps 3, 4 and 5 were jointly developed following the criteria proposed by Skogestad (2000). The selection of possible controlled variables was based on the operational objectives and tested by performing step perturbations to validate the criteria. The initially chosen manipulated variables were adapted from Chen's model (2012).

Once the controlled variables were selected, a step perturbation was applied to each possible pair of manipulated and controlled variables. Ziegler-Nichols first method was utilized to obtain the potential gains for each of these pairs. Best pairs were selected using the Relative Gain Array (RGA). Subsequently, for each selected pair of variables, a PID controller was implemented with initial parameters determined based on the Ziegler-Nichols method applied to the open-loop system response to a step perturbation. In this study, a 10% variation in the initial steady state was considered as setpoint for implementing the controllers. In light of to the control plantwide assumptions the levels in each reactor depicted in Figure 1 must remain constant. Therefore, mass balance calculations were performed, and source code was developed to adjust the flow rates to meet this requirement. Once the simulation models were developed, simulations were run, and the tuning of the controllers was performed.

3. Results

3.1 Control Structure Selection

To enhance selectivity and reaction yield, the reactors are set up in series with ethylbenzene being slowly introduced into each reactor through the flows F_2, F_4 and F_6. Keeping low concentrations of ethylene (C_B) helps minimize the production of 1,3 diethyl benzene, which reduces the reaction rate represented by Equation 2, fulfilling one of the operational objectives. Consequently, controlling C_B involves regulating the temperature in reactor 1 (T_1) and controlling the concentration of C in reactor 4 (C_{C4}) which in turn implies controlling T_4 since reaction rates are temperature functions. The RGA results for the best arrangements are presented in Table 1 where λ_{ij} represents the relative gain between the controlled and manipulated variables.

Table 1 – Relative Gain Array.

Pair	Controlled Variable	Manipulated Variable	Element λ_{ij}	Element $1-\lambda_{ij}$	Element $1-\lambda_{ij}$	Element λ_{ij}
1	T_1	Q_1	0,048609	0,951391	0,951391	0,048609
	T_4	F_{R2}				
2	T_1	Q_2	0,017785	0,982215	0,982215	0,017785
	T_4	F_{R2}				
3	T_1	Q_3	0,017784	0,982216	0,982216	0,017784
	T_4	F_{R2}				
4	T_1	Q_4	0,017755	0,982245	0,982245	0,017755
	T_4	F_{R2}				
5	T_1	Q_5	0,017759	0,982241	0,982241	0,017759
	T_4	F_{R2}				
6	T_1	F_4	0,017744	0,982256	0,982256	0,017744
	T_4	F_{R2}				
7	T_1	F_6	0,017748	0,982252	0,982252	0,017748
	T_4	F_{R2}				
8	T_1	F_{10}	0,017813	0,982187	0,982187	0,017813
	T_4	F_{R2}				

The results of the RGA indicated that there is iteration between the control loops. Nevertheless, this may be the preferred pairing to minimize interactions. Among all the simulations performed, only the simulation for array 4 achieved satisfactory results, meeting the proposed criteria and reflecting real simulation values. As a result, the pair of variables in array 4 was selected as the plantwide control variables for the methodology. The process diagram, including the defined control loops and the loops for maintaining constant levels, is illustrated in Figure 2.

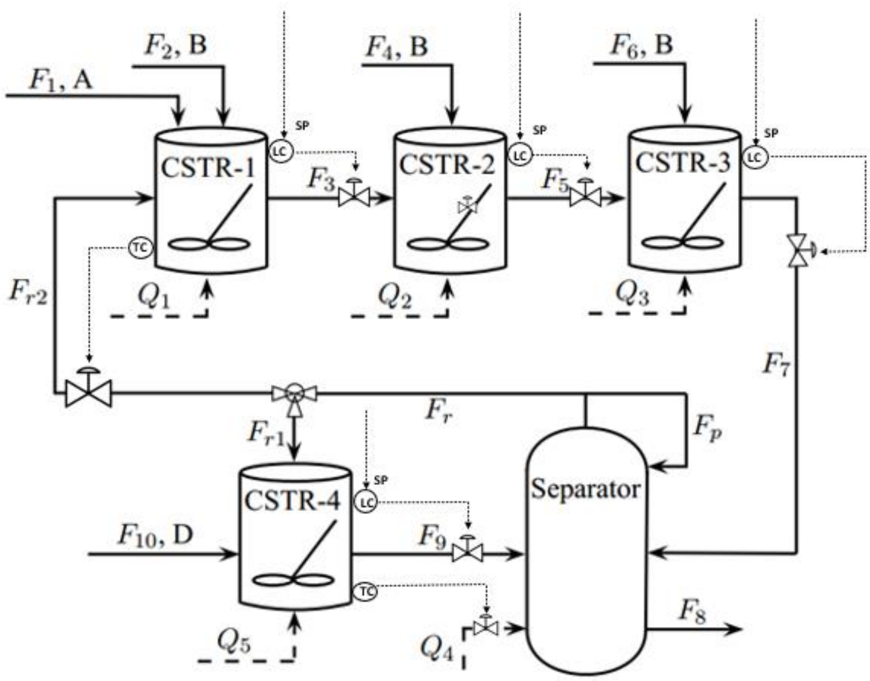

Figure 2: Control loops. Adapted from Chen (2012).

The controllers were tuned using Ziegler-Nichols method as the initial step, and the fine adjustments subsequently made to minimize the response time and setpoint overshoot. Table 2 displays the parameters of the implemented PID controller where: K represents the gain, τ_I and τ_D represents integral and derivative spacetime, respectively.

Table 2 - PID controller parameters.

Pair	K	τ_I	τ_D
T_1-F_{R2}	546,874260	605,600000	0,003785
T_4-Q_4	-25,742502	-0,5357000	-0,1339250

In Figure 3, the simulation result illustrates the effect of the PID controller for the pair T1-FR2. Upon analysis, it is evident that the system response to the applied perturbation is non-oscillatory, reaching the final value without overshoot. he designed controller effectively regulates the system, gradually bringing it to a new steady state. The system achieves a rise time of approximately 82 minutes after the step disturbance.

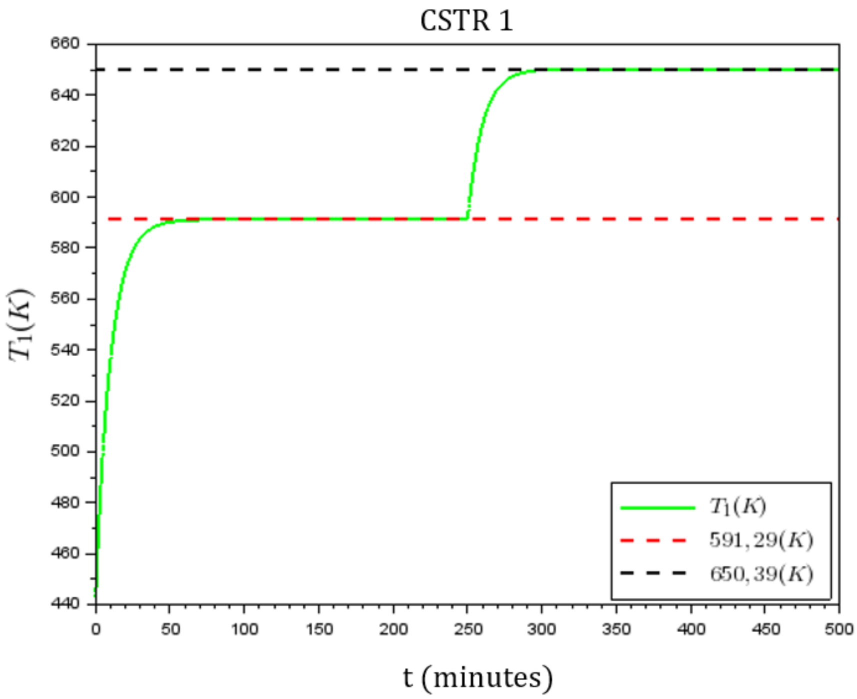

Figure 3: Temporal response of the PID controller to a step disturbance in the temperature of Reactor 1, T1.

In Figure 4 the temporal response of the manipulated variable FR2 is depicted. It is observed that the new steady state results in an increase of approximately 35% in the recycle flow F_{R2} compared to the initial steady state. This increase is in accordance with the imposed flow restrictions presented at the beginning of the section, demonstrating that the control system effectively manages the process within the specified constraints.

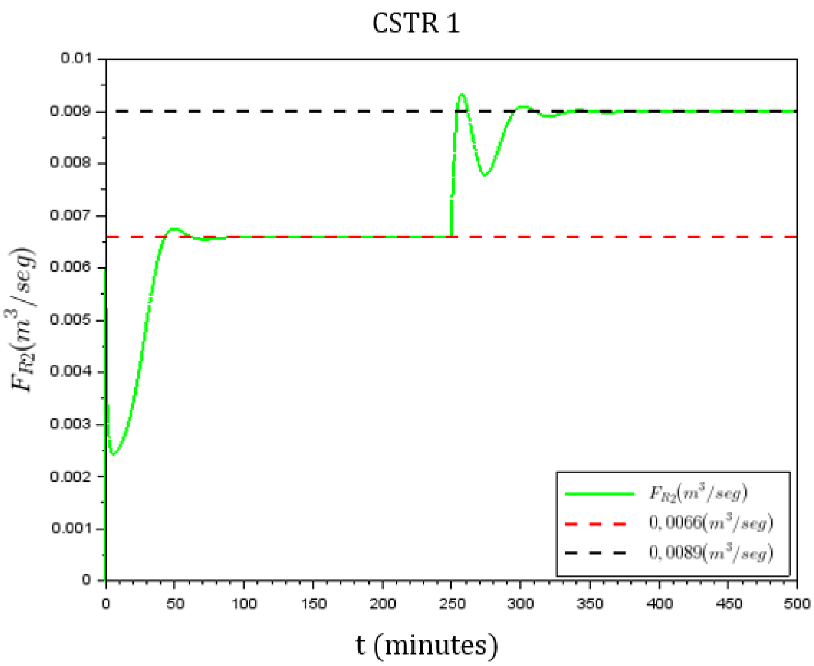

Figure 4: Temporal response manipulated variable F_{R2}.

In Figure 5, the simulation result shows the effect of the PID controller for the pair T4-Q4 In Figure 6 the behavior of the manipulated variable Q4 is presented.

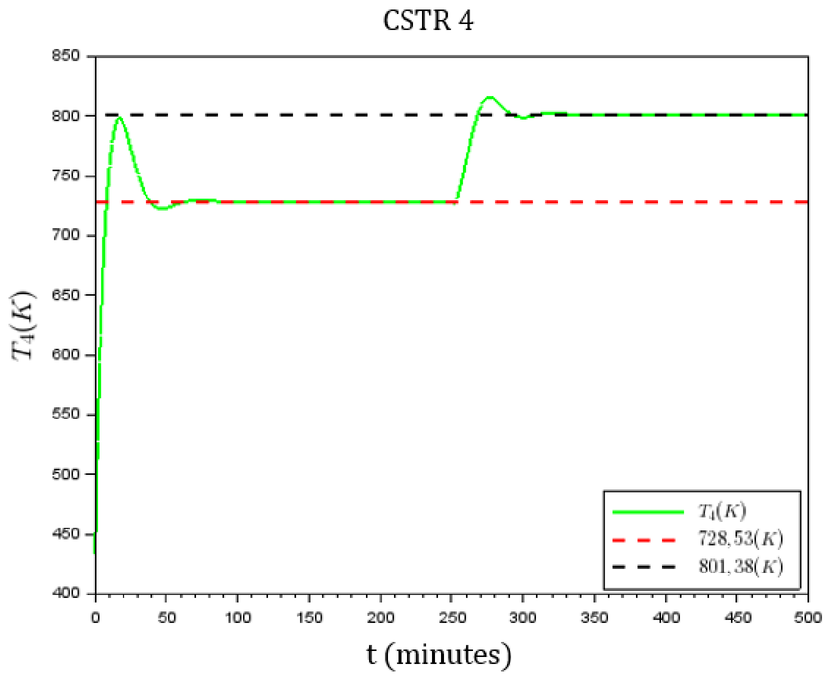

Figure 5: Temporal response of the PID controller to a step disturbance in the temperature of Reactor 4, T4.

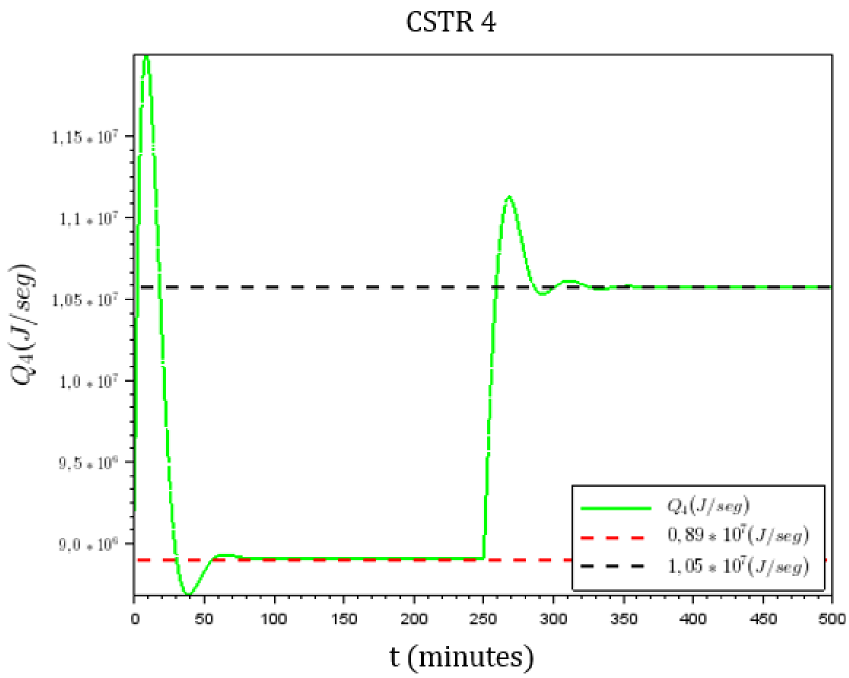

Figure 6: Temporal response manipulated variable Q_4.

The response of variable T4 for the adopted control structure it is critically damped, with a small overshoot of 1.74%. The peak and rise time are approximately 27 and 19 minutes, respectively, in relation to the new steady state. For control of a variable T4 results in a variation of about 18% in Q4 when compared to the initial steady state.

Regarding the concentrations CB1 (ethylene concentration in reactor 1) and CC4 (concentration of ethylbenzene in reactor 4) the control structure proves to be effective as both concentrations show a small variation in regard to the initial steady state. For CB1, the percentage change is approximately -7% while CC4 presents a variation of 1.38%.

4. Conclusion

In this work, a plantwide control linked to a PID controller was proposed for an ethylbenzene production plant. The adopted structural decisions and the results obtained through the computational simulation indicated that although there were interactions between the control loops, the possible pairs T1-FR2 It is T4-Q4, minimize system interactions. The adjusted parameters of the controller proved to be effective in controlling the disturbance, resulting in a small or no overshoot with satisfactory rise and response times. While controlling T1 requires a 36% variation in FR2, controlling T4 necessitates an 18% variation in Q4.

The control structure adopted with the PID controller is just one step within the plantwide control methodology, yet it is fundamental and demonstrates the controller's ability to achieve the proposed structural objectives, given the multivariable nature of the process and the presence of model restrictions. The implemented structure easily allows for further in-depth future studies, including the use of predictive controllers with different control structures.

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