

**Estrutura de controle plantwide simplificada para a planta de Williams-Otto:
otimização descentralizada coordenada com IBMF**

**A simplified plantwide control structure for William-Otto plant: IBMF
coordinated decentralized optimization**

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optimización descentralizada coordinada con IBMF**

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Resumo

Os sistemas de controle de plantas inteiras, também conhecido como controle plantwide, podem ter centenas de variáveis e isso resulta em um complexo problema de otimização, exigindo técnicas eficazes para resolver problemas de grande escala. Este artigo investiga a aplicação de uma abordagem descentralizada coordenada pelo Método do Balanceamento de Interações (IBMF) para a camada de otimização de sistemas de controle hierárquico. Essa camada é baseada na decomposição do problema matemático original em problemas menores de otimização local. A camada de coordenação tem a tarefa de garantir que as soluções do problema de otimização local também atendam às restrições dos demais subsistemas. Essa técnica é aplicada a planta de Williams-Otto com a coordenação IBMF. Os resultados são satisfatórios e apresentam uma solução razoável para o problema de otimização, obtendo o valor da função objetivo em torno de 95-105% daquele para obtido para o mesmo problema quando resolvido pela abordagem centralizada. Há uma redução de até 30% nas alterações das variáveis manipuladas na presença de uma perturbação no processo.

Palavras-chave: Descentralização; Otimização coordenada; Controle hierárquico; Sistemas em larga escala.

Abstract

Plantwide control systems may have hundreds of variables and this results in a complex optimization problem, requiring effective techniques to solve large scale problems. This paper investigates the application of an IBMF coordinated decentralized approach to the optimization layer of hierarchical control systems. This layer is based on a decomposition of the original mathematical problem into smaller local optimization problems. The coordination has the task of ensuring that the solutions to the local optimization problems also satisfy the constraints of the other subsystems. This technique is applied to a Williams--Otto plant with IBMF (Interaction Balance Method with Feedback) coordination. The results are satisfactory and produce a reasonable solution to the optimization problem, obtaining a value of the objective function around 95-105% of that for the same problem when solved with a centralized optimization. There is a reduction of up to 30% in the required changes of the variables manipulated in the presence of a process disturbance.

Keywords: Decentralization; Coordinated optimization; Hierarchical control; Large scale systems.

Resumen

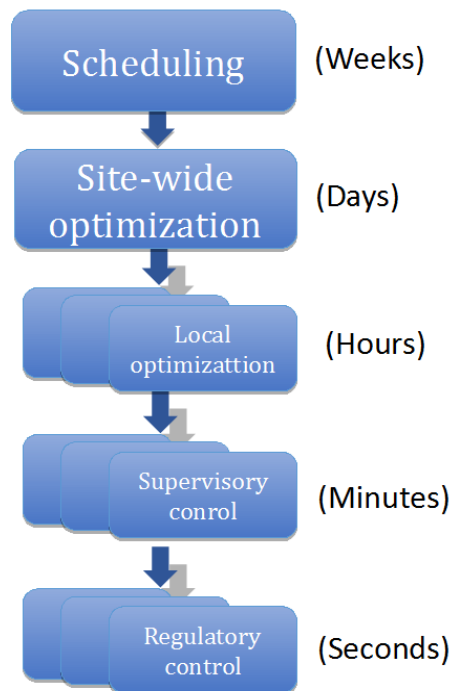
Los sistemas de control de plantas enteras, también conocidos como control plantwide, pueden tener cientos de variables y esto resulta en un complejo problema de optimización, que requiere técnicas efectivas para resolver problemas a gran escala. Este artículo investiga la aplicación de un enfoque descentralizado coordinado por el Método de Equilibrio de Interacción (IBMF) para la capa de optimización de los sistemas de control jerárquico. Esta capa se basa en la descomposición del problema matemático original en problemas más pequeños de optimización local. La capa de coordinación tiene la tarea de garantizar que las soluciones del problema de optimización local también cumplan las restricciones de los otros subsistemas. Esta técnica se aplica a la planta Williams-Otto con coordinación de IBMF. Los resultados son satisfactorios y presentan una solución razonable al problema de optimización, obteniendo el valor de la función objetivo alrededor del 95-105% del obtenido para el mismo problema cuando se resuelve mediante el enfoque centralizado. Hay una reducción de hasta un 30% en las alteraciones de las variables manipuladas en presencia de una perturbación en el proceso.

Palabras clave: Descentralización; Optimización coordinada; Control jerárquico; Sistemas en gran escala.

1. Introduction

Plantwide control systems are hierarchical multilevel structures composed of several layers. These can be defined based on the task runtime of each level. Considering that the decisions of each layer depend on information from the other, it is important to ensure that each task is performed effectively. Figure 1 presents this hierarchical structure, defined by Larsson and Skogestad (2000).

Figure 1: Plantwide hierarchical control systems.



Source: Adapted by Skogestad (2004).

Optimization and regulatory control layers are some examples of levels of the hierarchical control and the resolution of these tasks can become a complex problem in large scale systems because they have hundreds of variables to be determined and the integration of the several operating units that compose them is complicated. Traditional techniques of modeling, analyzing, controlling, and optimizing them do not constitute a reasonable solution for this kind of system. In engineering, optimization is applied to the design of a process and equipment, the definition of the operational conditions, as well as the planning of production

and control processes, resulting in more effective, profitable and secure systems. In plantwide control systems, an optimization layer is an important part of the plantwide control structure and aims to determine the optimal point of operation to be used as a reference for the control layer (Ebrahiimpour et al., 2014).

Decomposing large-scale systems optimization problem into smaller problems and without interactions between them is an approach used in the 1960s and 1970s decades to solve complex optimization problems (Himmelblau, 1966; Yang, Zhao, & Cai, 2012). However, the use of decentralized structures for the optimization and control of complex systems with integration requires a mechanism that ensures that the local control and optimization tasks reach the global objectives of the plant. The coordination stage aims to ensure that, given the local objectives of each minor problem that makes up the plant, the overall objective of the process is also guaranteed (Inalhan, Stipanović, & Tomlin, 2002). Most control of large scale systems was based in decentralization of control structure, most of the time, exclusively, in the control layer. However, this alternative ignores possible interactions between subsystems.

Several approaches are investigated to design control structure for large-scale systems with interactions (Liu, Zhang, Xiao, & Sun, 2019; Luyben, 2019; Moraru & Bildea, 2017; Thakur, Ojasvi, Kumar, & Nitin, 2017). Liu et al. (2019) transformed large scale interconnected systems to several nominal isolated subsystems and using tracking control problem and a new discounted performance cost concerning the tracking error energies and the whole control input consumption. However, extending this decentralized approach to optimization may be an alternative to the design of a more robust and stable control system when coupled with well-established heuristics for plantwide control (Xie, Xie, Ying, Jiang, & Gui, 2019; Zotică, Nord, Kovács, & Skogestad, 2020).

This work presents a design of plantwide control of Williams-Otto Plant, a large-scale system with interactions, handle optimization of complex chemical plants with integration through coordinated decentralized method using a multi-branch decomposition and compares the results obtained with those from a centralized optimization approach. For this, a hierarchical control structure is developed, its optimization layer being composed of two steps: a coordination layer that uses online plant measures variables to ensure that the bottom layer in which the optimization problem of the plant is decomposed into problems smaller find a result that meets the overall system goals.

2. Decentralized Coordinated Optimization

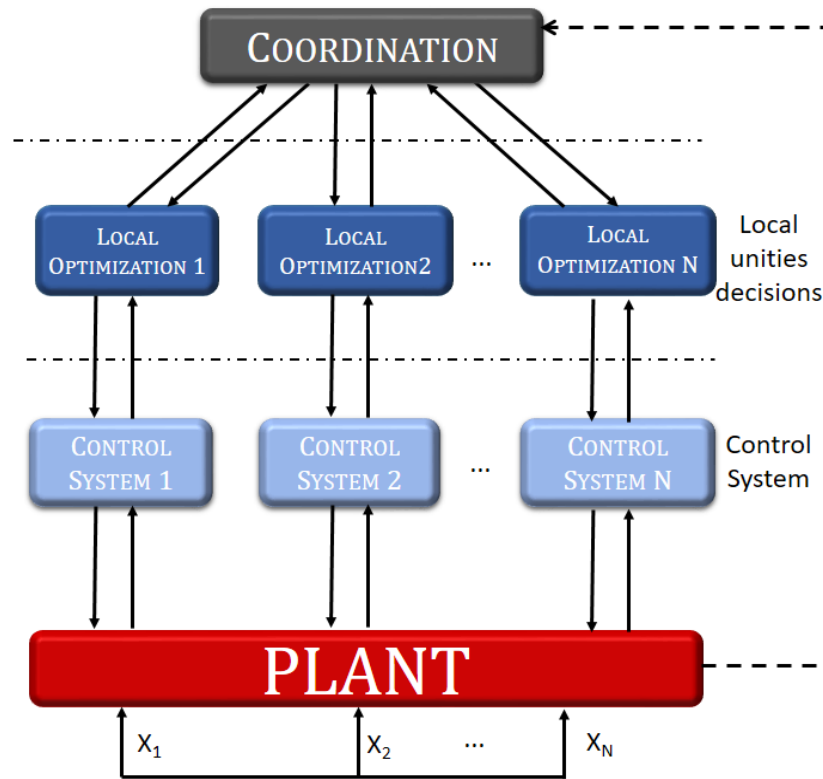
Chemical processes are large scale systems and require attention in selection of methods to choose the setpoints of the controlled variable which correspond to economically optimal steady states operations of industrial process, mainly when the system is subject to unexpected disturbances. Chai, Qin and Wang (2014), aware that an effective control system must not only keep the process at the chosen setpoint, but operate at economically optimal points (Ebrahiimpour et al., 2014), proposed a optimal operational control to a shaft furnace system, combine operational control with optimization with feedback, operational index prediction with self-tuning and self-recovering control from fault operations conditions. The proposed method presented great results, solving the optimal operational control for complex plants.

Plantwide control systems have been designed with a decentralized structure, decomposing the system into smaller problems that are simpler and easier to handle (Zhao, Cai, Ding, & Chang, 2013). However, it is necessary to guarantee that the decisions of each subsystem also meet aims of the others local systems and of the global plant. Skogestad (2004) approaches self-optimizing control as a methodology for designing structures that lead to simplicity. In it some setpoints are set and the system operates indirectly in optimum conditions reaching an acceptable loss.

Hori (2005) proposed a decentralized coordinated quadratic programming solution of dynamic matrix control (QDMC) to guarantee that the interactions between the subsystems that compose control systems are considered. Decentralized QDMC presents similar performance to the centralized alternative. Though coordination can be effective at the supervisory level, it does not guarantee that the optimization problem can reach the global objectives of the plant and the local aims, simultaneously.

The same approach used by Hori (2005) and Skogestad (2004) is applied to the optimization layer, but now it is defined by two levels. At the lower level are the local optimization problems for each subsystem that makes up the plant. The upper level addressed the coordination problems that whose main objective is to certify that the solution of each local optimization problem meets the global demands, considering the interactions between them. Figure 2 presents the decentralized coordinated optimization structure.

Figure 2: Plantwide hierarchical control systems with decentralized coordinated optimization layer.



Source: adapted by Findeisen et al. (1980) and Kwong (1992).

Consider the chemical process described by Equations (1)-(2):

$$\dot{\mathbf{x}} = f(\mathbf{x}, \mathbf{u}, \mathbf{d}) \quad (1)$$

$$\mathbf{y} = h(\mathbf{x}, \mathbf{u}, \mathbf{d}) \quad (2)$$

in which $\mathbf{x} \in \mathfrak{R}^{n_x}$, $\mathbf{m} \in \mathfrak{R}^{n_m}$, $\mathbf{d} \in \mathfrak{R}^{n_d}$ and $\mathbf{y} \in \mathfrak{R}^{n_y}$ are states, manipulated, disturbances and controlled variables of the systems. The global optimization goal is to find \mathbf{m} manipulated variables solutions for the solutions of the problem described in Equation (3).

$$\min_{\mathbf{u}} \int_0^T \Phi(\mathbf{y}, \mathbf{u}, \mathbf{d}) dt \quad (3)$$

subject to $\dot{\mathbf{x}} = f(\mathbf{x}, \mathbf{u}, \mathbf{d})$, $\mathbf{y} = h(\mathbf{x}, \mathbf{u}, \mathbf{d})$ and $g(\mathbf{x}, \mathbf{u}, \mathbf{d}) \leq 0$.

In a multilayer structure, the control task of the first layer - $\mathbf{y}(\mathbf{x}, \mathbf{m}, \mathbf{d}) = \mathbf{y}_{SP}$ - is the keep the controlled variables at their respective setpoints.

In decentralized coordinated optimization, the chemical plant is decomposed into subsystems, defined according to their structure and the separability of the constraints and the objective function of the problem. The system can be decomposed into N subsystems described by Equation (4)-(6).

$$\dot{\mathbf{x}}_i = f_i(\mathbf{x}_i, \mathbf{u}_i, \mathbf{d}_i) \quad (4)$$

$$\mathbf{y}_i = h_i(\mathbf{x}_i, \mathbf{u}_i, \mathbf{d}_i) \quad (5)$$

$$g_i(\mathbf{x}_i, \mathbf{u}_i, \mathbf{d}_i) \leq 0 \quad (6)$$

Coordination methods were discussed in the last four decades in order to determine the most appropriate technique for optimizing large systems. Bakalis and Ellis (1992) tested the Direct Method, the Interaction Balance Method (IBM) and the Method of Integrating System Optimization and Parameter Estimation (ISOPE) in a steady-state vaporization plant. They demonstrate that the first and second methods are ineffective when there are significant differences between the plant and the model.

Findeisen et al.(1980) presents a study of the coordination in optimization problems with four different methods. Strategies with plant feedback tend to be more effective than versions that do not use measured variables in the coordinating step, besides being indifferent to disturbances in the controlled variables. Therefore, the coordination method chosen for the present paper is the IBMF. This method considers the interactions between the subsystems to be constraints for local optimization problems. At the coordination level, the price vector λ takes into account the difference between the model and the plant and defined to satisfy Equation (7).

$$\mathbf{u}_i - \mathbf{u}_i^* = 0 \quad (7)$$

in which the \mathbf{u}_i are the interconnection variables of the subsystems calculated by the problems of local optimization and \mathbf{u}_i^* are the measurements of these variables from the real plant.

Simultaneously, local optimizations problems minimize φ_i (Equation 8), sharing their results with the coordination level, which then selects new values for λ_i

$$\begin{aligned}\Phi(\mathbf{x}, \mathbf{u}, \mathbf{d}, \boldsymbol{\lambda}) &= \sum_{i=1}^N \Phi_i + \sum_{i=1}^N \lambda_i^T \left(-\mathbf{u}_i + \sum_{j=1}^N \mathbf{H}_{ij} \mathbf{y}_j \right) \\ \Phi(\mathbf{x}, \mathbf{u}, \mathbf{d}, \boldsymbol{\lambda}) &= \sum_{i=1}^N \Phi_i - \sum_{i=1}^N \lambda_i^T \mathbf{u}_i + \sum_{i=1}^N \lambda_i^T \sum_{j=1}^N \mathbf{H}_{ij} \mathbf{y}_j \\ \Phi(\mathbf{x}, \mathbf{u}, \mathbf{d}, \boldsymbol{\lambda}) &= \sum_{i=1}^N \Phi_i - \lambda_i^T \mathbf{u}_i + \sum_{j=1}^N \lambda_j^T \mathbf{H}_{ij} \mathbf{y}_j \\ \Phi(\mathbf{x}, \mathbf{u}, \mathbf{d}, \boldsymbol{\lambda}) &= \sum_{i=1}^N \varphi_i(\mathbf{x}_i, \mathbf{u}_i, \mathbf{d}_i, \boldsymbol{\lambda}_i)\end{aligned}\tag{8}$$

The application of IBMF is conditioned on the availability of measurements of the interconnection variables in the subsystems.

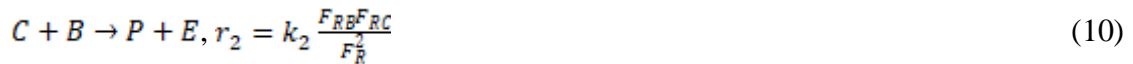
3. Methodology

This work has a theoretical-computational nature and uses Matlab® (*fmincon* function for constrained nonlinear multivariable optimization present in Matlab Optimization Toolbox), using Sequential Quadratic Programming (SQP) algorithm, to perform the simulations of the optimization problem and control systems proposed.

3.1. Williams–Otto Plant

The Williams–Otto plant (Jung, Miroshi, & Ray, 1971) has been the focus of several studies due to their complexity. Such a system has been decomposed into two subsystems according to its structure and the separability of the objective function as well as the constraints of the optimization problems.

A reactor is fed with species A and B feed to produce P. The reactions involved in the process and their rates are presented in Equations (9)–(11).



The reactions are exothermic and their coefficients are given by the Arrhenius equation $k_i = A_i e^{\frac{-B_i}{T_R}}$, for $i = 1, 2, 3$. T_R is the reactor temperature, F_R and F_{Ri} are the total flow and the flow of i th specie flow, respectively, in lb/h. C and E are intermediates and/or by-products and have no sales value as chemical products but can be disposed as fuels. It is a waste material, resulting in an extra cost for the process.

The model for the optimization problem considers an isothermal reactor with constant volume and a pseudo-stationary system; the subsystem reaction dynamics is slower than the separation system dynamics. Thus, the last one can be in a stationary state. The dynamic behavior of the plant differs from the model because it includes the temperature variation over time through the energy balance. A complete description of the system is in Appendix A.

The goal of the optimization problem is defined set points for the controlled variables that maximize the investment return per hour. The objective function is defined in Equation (12).

$$\Phi(\%) = 100 \frac{M - \text{SARE} - U - \text{FCP}}{\text{PIN}} \quad (12)$$

in which there are defined

- gross return per hour: $M = 8400(P_P F_P + P_D F_D - P_A F_A - P_B F_B - P_G F_G)$
- Fixed charges (depreciation, labor and others) $\text{FCP} = 60V_R \rho_R$
- Initial investments: $\text{PIN} = 600V_R \rho_R$
- Sales, administration, research and engineering:

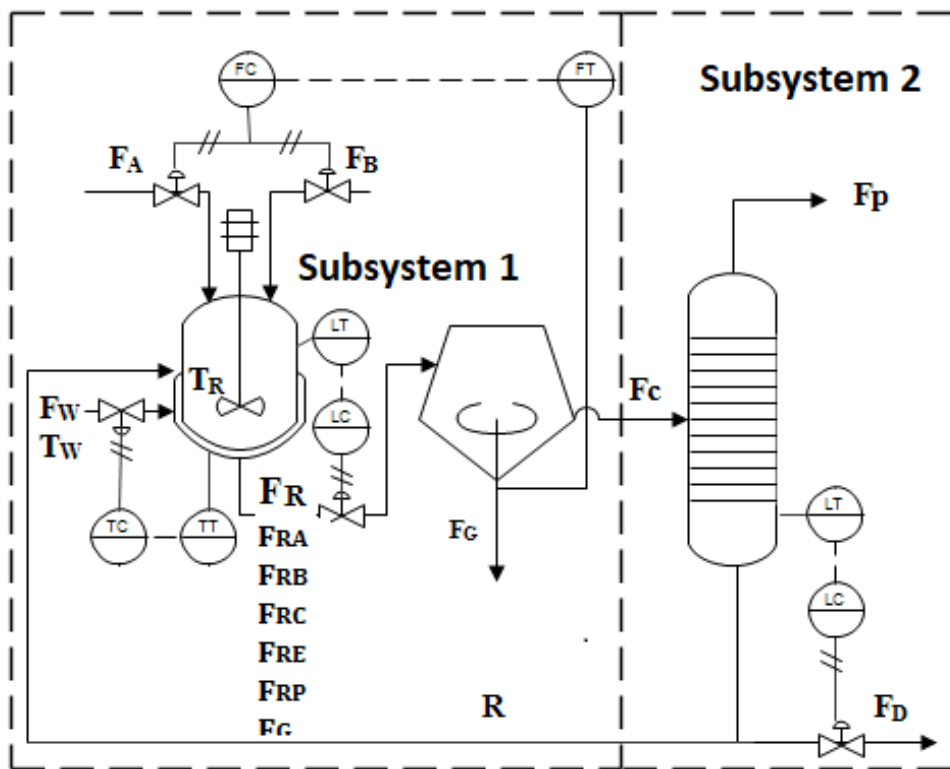
$$\text{SARE} = (0.124)(8400)(P_P F_P + P_D F_D)$$

- Utility Costs: $U = 8400(C_1 R^{1.5} + C_2 F_C^{1.5})$

F_i e P_i are flow rates and unit prices of each flow. The availability of raw materials is limited, $12400 \text{ lb/h} \leq F_A \leq 16600 \text{ lb/h}$ and $F_B \leq 56000 \text{ lb/h}$. To avoid decomposition of product $580^\circ\text{R} \leq T_R \leq 680^\circ\text{R}$. That the model be a steady stationary model completes the set of system constraints.

In the present paper, the decomposition of the process is based on the separability of the constraints and the objective function. This decomposition ensures that the number of interconnection variables is as small as possible, since the flows of each component, leaving the reactor F_{Ri} will compose Subsystem 1. The top product of the column is pure P. The other products will come out completely in the bottom product of the column. The interconnections variables for this scenario are F_C and R . Figure 3 present the proposed control system.

Figure 3: Williams-Otto Plant Control System.



Source: Authors.

Subsystem 1 has 10 restrictions, including the overall mass balance, mass balance for the subsystem and decanter, besides the definition of F_R . Subsystem 2 contains only the overall mass balance of the subsystem as a restriction.

The value of F_P was fixed at its optimal value, equal to 4763 lb/h. $P_P = \$0.3(\text{lb/h})^{-1}$, $P_A = \$0.02(\text{lb/h})^{-1}$, $P_B = \$0.03(\text{lb/h})^{-1}$, $P_G = \$0.01(\text{lb/h})^{-1}$ e $P_D = \$0.0068(\text{lb/h})^{-1}$ have been adopted.

In the coordination layer with the IBMF, the optimization problem determines $\lambda = [\lambda_1 \lambda_2]^T$ that satisfies Equation 13.

$$\begin{bmatrix} F_C \\ R \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{F}_C \\ \hat{R} \end{bmatrix} \quad (13)$$

Some aspects of the plant-wide control theory were adopted to formulate the hierarchical control structure for the Williams–Otto Plant: equipment inventories should be kept constant. Thus, F_R will be manipulated to control the reactor level and the bottom flow of column must be determined to guarantee the specification of the desired product at the top; reagents should be fed in stoichiometric proportions so, F_A will be manipulated to control F_G and F_B will be adjusted to guarantee this and F_W will be manipulated to control T_R .

The proposed control structure was applied to the Williams–Otto plant, using the coordination technique that considers the difference between the model and the plant, IBMF. The optimum point found by the centralized optimization using the complete model, with all the mass and energy balances, was also used for the centralized control structure in order to obtain a reference to verify the performance of the proposed system.

4. Results and discussion

To analyze the performance of the control systems, simulation scenario has two disturbances in time:

- **Slow disturbances:** these disturbances characterize the need to perform new steady state prediction. For this analysis, there was initially defined $F_{P,ss1} = 3334.1$ lb/h and the desired amount of product is changed at $t = 25$ h, to $F_{P,ss2} = 4763$ lb/h.
- **Rapid disturbances:** rapid disturbances are introduced in the variables T_B (in $t = 12.5$ h a step disturbance of 5%, keeping this until $t = 13$ h) and R (in $t = 37.5$ h a step disturbance of 5%, keep this until $t = 38$ h) to verify that, even in the presence of this type of disturbance and without the determination of a new steady state, the proposed system achieves

control objectives.

The setpoints defined to this simulation scenario with the centralized method and the IBMF are presented in Table 1. These values are selected after performing arbitrary test for the optimization problem in centralized and decentralized way in order to allow an adequate analysis of the control system.

When $F_{P,ss1} = 3334.1$ lb/h, there is a slightly lower result than the centralized simplified model. For this method, we find $\lambda = [1.9 \times 10^{-7} \ 1.528 \times 10^{-5}]$.

The IBMF defines the optimal point to be close to those defined by centralized optimization with the simplified model with $F_{P,ss2} = 4763$ lb/h, finding $\lambda = [-1.496 \times 10^{-4} \ 1.526 \times 10^{-4}]$ and an error of $|e| = 0.0075$ between the model and the plant, which can be considered negligible due to the magnitude of the interconnection variables. Again, the use of the alternative was decentralized with a reduction of less than 1 % compared to the centralized alternatives similarly to the results presented by Findeisen, Pulaczewski and Manitius (1970) and Kwong (1992).

Table 1: Setpoints defined in the optimization layer in the hierarchical control systems for the Williams-Otto Plant.

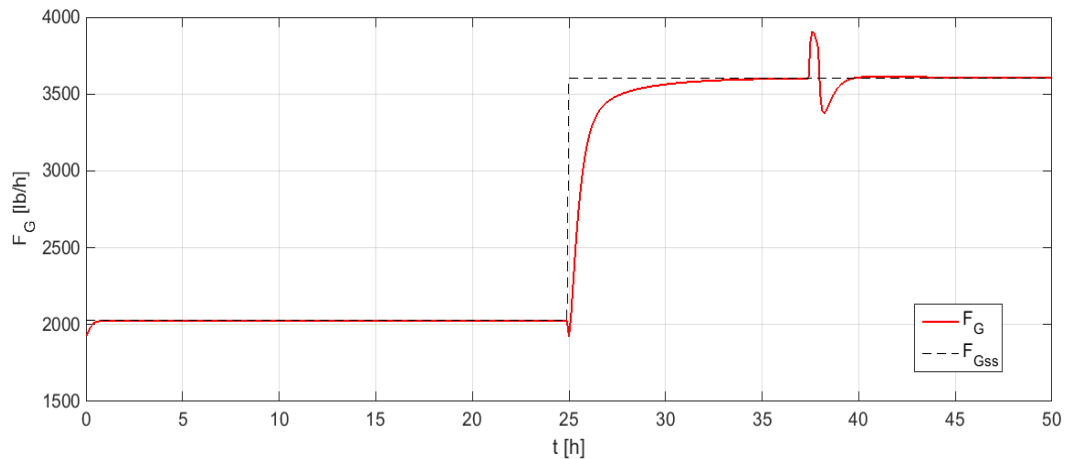
Method	IBMF	Centralized
$F_{G,ss1}$ (lb/h)	2025.635	3069.187
$T_{R,ss1}$ (°R)	630.099	641.040
Φ_1 (%)	71.613	71.249
$F_{G,ss2}$ (lb/h)	3608.810	3586.056
$T_{R,ss2}$ (°R)	655.893	655.600
Φ_2 (%)	88.822	88.333

Source: Authors.

For simulation to analyze the performance of the control, all the variables were first set to 95% of the steady states values defined for the optimization, except $T_R(0) = 0.99T_{R,ss}$. Figure 4 and Figure 5 presents the dynamic behavior of the controlled variables with the IBMF coordinated decentralized control systems.

At $t=12.5$ h, when the disturbance in T_B was applied, it is possible to verify that the control system minimizes the effects of this in T_R , while F_G does not present any changes at this instant. When the disturbance in R occurs, the decentralized coordinated control with IBMF takes the system to the expected steady states, obtaining an overshoot of 1.31% in reactor temperature.

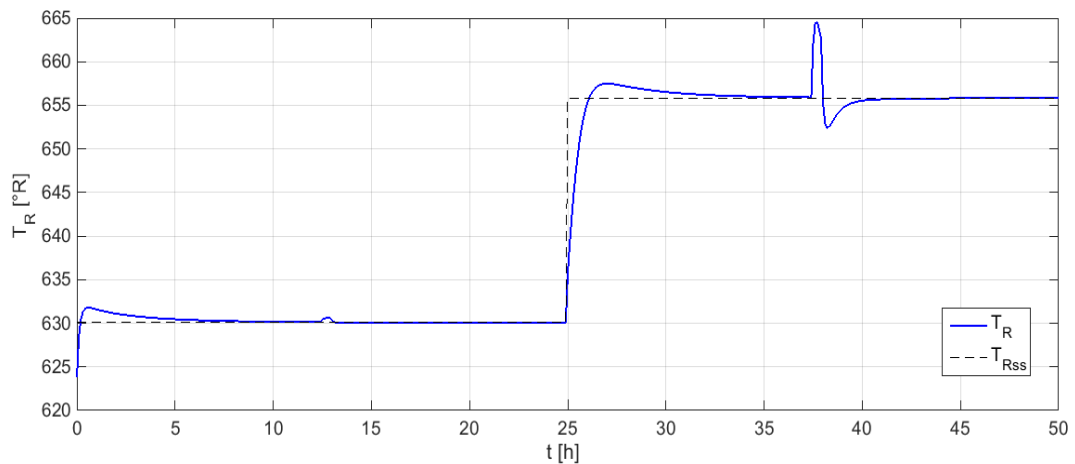
Figure 4: Dynamic behavior of F_G with the IBMF coordinated decentralized control.



Source: Authors.

The Williams–Otto plant is subjected to a setpoint change in $t=37.5$ h. So that F_G will reach the new value set of steady states, the control actions produce an oscillatory behavior of the variable. First, there is an increase of 300.19 lb/h followed by a decrease of 236.81 lb/h, less than 10% variation in relation to the steady states for this instant. Figure 6 and Figure 7 presents the control actions for F_A , F_W , F_B and F_D .

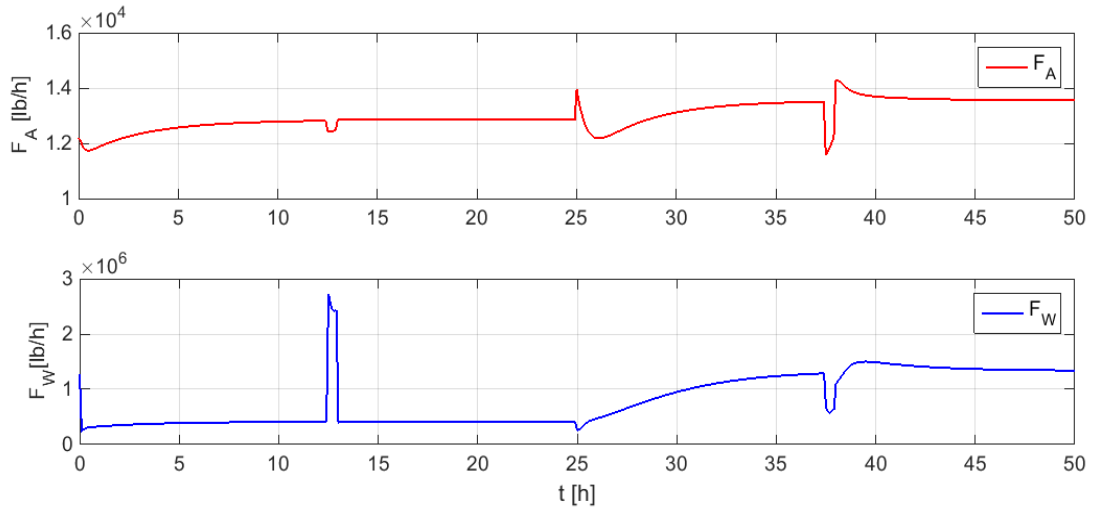
Figure 5: Dynamic behavior of T_R with the IBMF coordinated decentralized control.



Source: Authors.

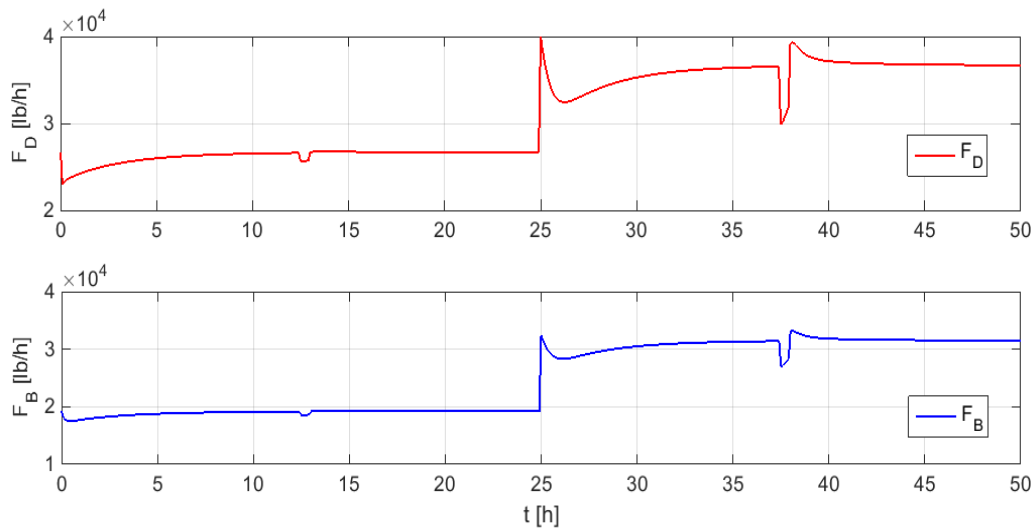
According to results, a disturbance in T_B requires six times as much of a change in F_W , while it realizes smoother changes in the other manipulated variables. Even with this increase, the system quickly returns to where it was. At the instant of the system optimization and steady state change, the reagent flows are driven more abruptly while the heat exchange fluid flow is smoothly adjusted to the new reference value.

Figure 6: Control actions for F_A and F_W with coordinated decentralized control systems.



Source: Authors.

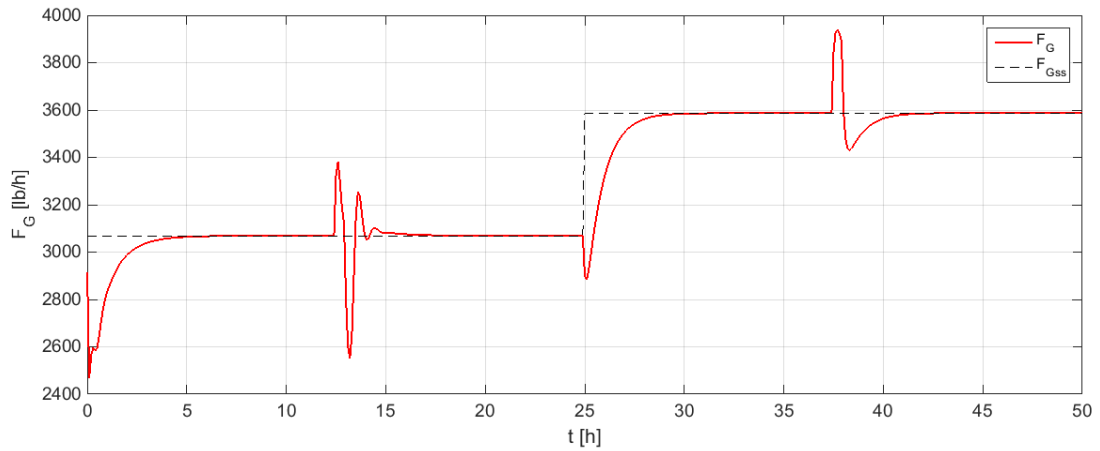
Figure 7: Control actions for F_D and F_B with coordinated decentralized control systems



Source: Authors.

A similar scenario was simulated with a hierarchical control system with centralized optimization. Figure 8 and Figure 9 presents the resulting dynamic behavior of this approach.

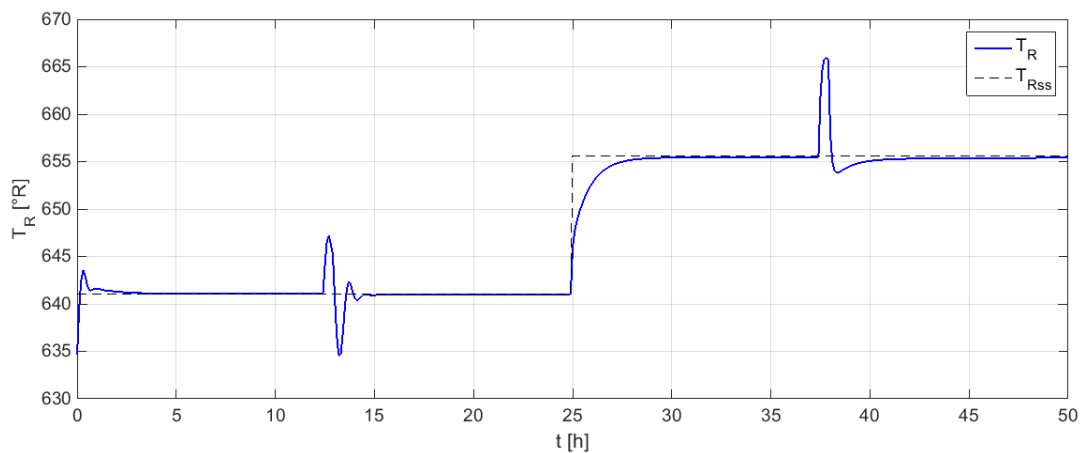
Figure 8: Dynamic behavior of F_G with hierarchical control systems with centralized optimization.



Source: Authors.

For this case, it is possible to verify that, unlike the strategy that used co-ordinated decentralized optimization, the control system cannot neutralize the influence of the disturbance in T_B . Both controlled variables present oscillatory behavior in $t=12.5$ h.

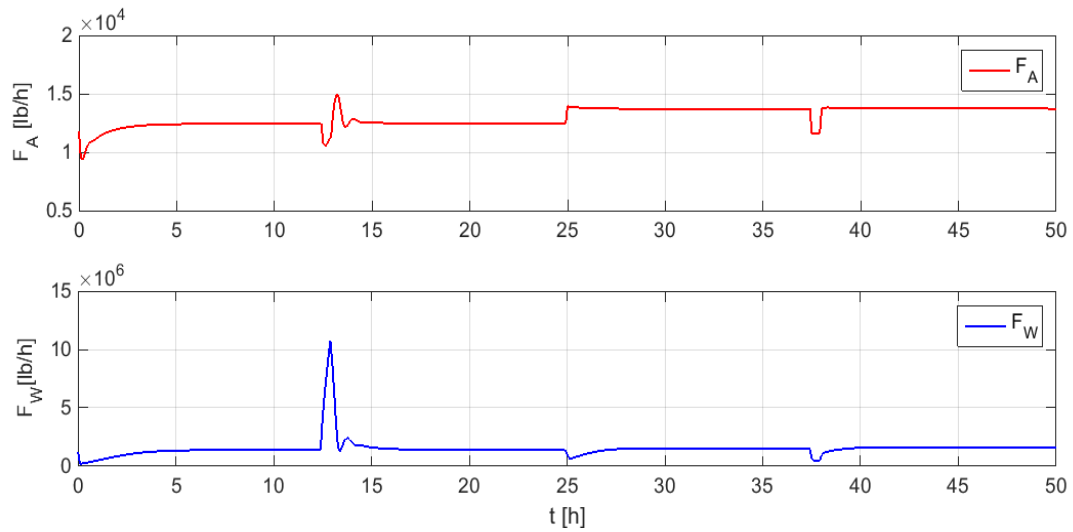
Figure 9: Dynamic behavior of T_R with hierarchical control systems with centralized optimization.



Source: Authors.

In this time, T_R reaches a maximum value of 647.2°R , falling to 634.7°R and then returning to $T_{R,ss1} = 641.040^\circ\text{R}$. Following the same trend, there is an oscillation in F_G , which reaches values corresponding to a decrease of about 15% from the setpoint. Figure 10 and Figure 11 present the control actions to F_A , F_W , F_B and F_D .

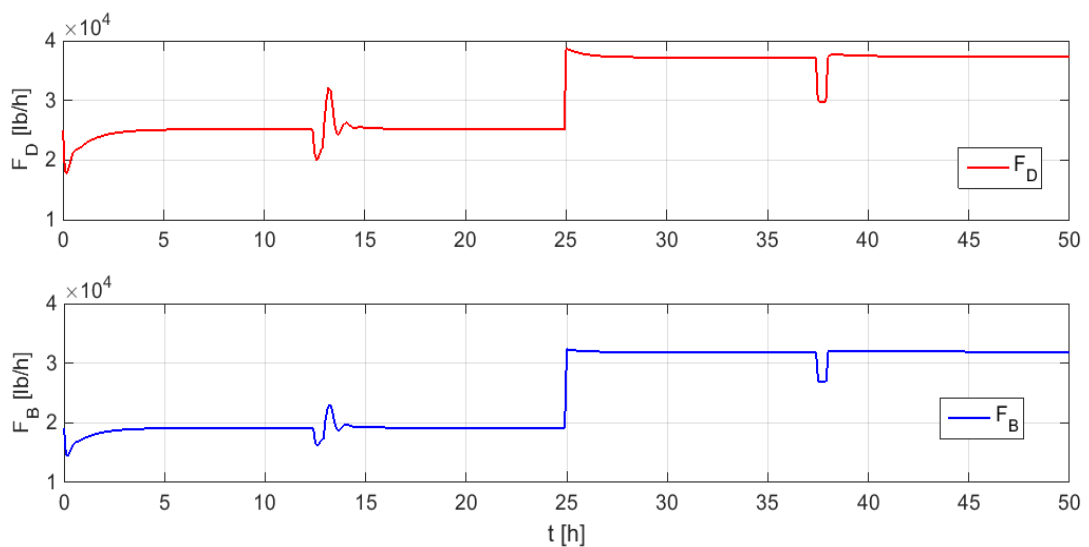
Figure 10: Control actions for F_A and F_W with hierarchical control systems with centralized optimization.



Source: Authors.

In the behavior of the manipulated variables presented by this control strategy, what stands out most is the requirement of the controller in the presence of the rapid perturbations of the system in relation to the manipulated variables. In $t = 12.5$ h, the control system requires a 20% increase in the feed flows F_A and F_B , while for the decentralized alternative this change, be it increase or decrease, is no more than 4%.

Figure 11: Control actions for F_D and F_B with hierarchical control systems with centralized optimization.



Source: Authors.

For F_D , this increase is 27.5%. For F_W , an increase by a factor of 7.7 times is required, emphasizing that this was already much higher than the value defined by the decentralized coordinated control systems with IBMF. The results demonstrate that this strategy achieves a more optimal overall plant operation when compared with centralized alternative similarly work develop by Xie et al. (2019), making the goal of control system easier to achieve.

5. Conclusions

Plantwide control assigns a global view to the concept of control of chemical plants, with strategies that use local controllers, decomposing the plant into smaller problems, easier to handle. Coordinated decentralized optimization seeks to ensure that the solution of the local problems defined by the plant decomposition meets the global demands and those of the other subsystems. These techniques seek to reduce the differences between the solutions of the interconnection variables defined by the local problems or even those with the measures sent from the plant to the coordinator in order to guarantee the result.

The performance of the IBMF strategy for the problems developed was always very close to that obtained with centralized optimization, always being around 1% to 5% of the value of the objective function. Using plant-wide control concepts and coordinated decentralized optimization results in a robust control system capable of dealing with disturbances in a smoother way in terms of the behavior resulting from the controlled variable, with minimum oscillations during disturbances. Also observed a reduction of up to 30 % in the required changes of the variables manipulated in the face of a process disturbance, when compared with the centralized approach.

However, the application of coordinated decentralized optimization only, does not guarantees the efficiency of the control system of a chemical plant. The application of plantwide control heuristic allied with this approach proved to be a good alternative to minimize the effects of disturbances. It is suggested to apply techniques such as data reconciliation and parameters actualization to update the model periodically in order to ensure that the objectives of the optimization layer are in line with the objectives of the real systems.

A1. Complete model for Williams-Otto Plant

Equations A.1-A.10 presents mass and energy balances for Williams-Otto Plants and parameters of model are in Table A.1 (Jung et al., 1971).

Table A.1: Parameters of Williams-Otto Plant's model (Jung et al., 1971).

Parameters of Model	
$A_1 = 5.9755 \times 10^9 \text{ h}^{-1}$	$B_1 = 12000^\circ\text{R}(\text{based in A ou B})$
$A_2 = 2.5962 \times 10^{12} \text{ h}^{-1}$	$B_2 = 15000^\circ\text{R}(\text{based in B})$
$A_3 = 9.6283 \times 10^{15} \text{ h}^{-1}$	$B_3 = 20000^\circ\text{R}(\text{based in C})$
$H_1 = -125 \text{ Btu. (lb C)}^{-1}$	$H_2 = -50 \text{ Btu. (lb E+P)}^{-1}$
$H_3 = -143 \text{ Btu. (lb G)}^{-1}$	$V_R = 60 \text{ ft}^3$
$\rho_R = 50 \text{ lb.ft}^{-3}$	$C_{pR} = 0.3 \text{ Btu.h}^{-1}\text{ }^\circ\text{R}^{-1}$
$W_w = 428.68 \text{ lb}$	$U_w = 50 \text{ Btu.ft}^{-2}\text{h}^{-1}\text{ }^\circ\text{R}^{-1}$
$C_{pw} = 0.4 \text{ Btu.h}^{-1}\text{ }^\circ\text{R}^{-1}$	$C_{pA} = 0.3 \text{ Btu.h}^{-1}\text{ }^\circ\text{R}^{-1}$
$C_{pB} = 0.3 \text{ Btu.h}^{-1}\text{ }^\circ\text{R}^{-1}$	$C_{pL} = 0.3 \text{ Btu.h}^{-1}\text{ }^\circ\text{R}^{-1}$
$T_A = 527.7^\circ\text{R}$	$T_B = 527.7^\circ\text{R}$
$T_{w,in} = 519.67^\circ\text{R}$	$A_w = 328.2 \text{ ft}^2$
$F_w = 1335785 \text{ lb.h}^{-1}$	

Source: Authors.

$$\frac{V_R \rho_R}{F_R} \frac{dF_{RA}}{dt} = F_A + R \left(\frac{F_{RA}}{F_R - F_G - F_P} \right) - F_{RA} - r_1 V_R \rho_R \quad (\text{A.1})$$

$$\frac{V_R \rho_R}{F_R} \frac{dF_{RB}}{dt} = F_B + R \left(\frac{F_{RB}}{F_R - F_G - F_P} \right) - F_{RB} - r_1 V_R \rho_R - r_2 V_R \rho_R \quad (\text{A.2})$$

$$\frac{V_R \rho_R}{F_R} \frac{dF_{RC}}{dt} = R \left(\frac{F_{RC}}{F_R - F_G - F_P} \right) - F_{RC} + 2r_1 V_R \rho_R - 2r_2 V_R \rho_R - r_3 V_R \rho_R \quad (\text{A.3})$$

$$\frac{V_R \rho_R}{F_R} \frac{dF_{\mathcal{R}l}}{dt} = R \left(\frac{F_{\mathcal{R}l}}{F_R - F_G - F_P} \right) - F_{\mathcal{R}l} + 2r_2 V_R \rho_R \quad (\text{A.4})$$

$$\frac{V_R \rho_R}{F_R} \frac{dF_{RC}}{dt} = R \left(\frac{F_{RP} - F_P}{F_R - F_G - F_P} \right) - F_{RP} + r_2 V_R \rho_R - 0.5 r_3 V_R \rho_R \quad (\text{A.5})$$

$$\frac{V_R \rho_R}{F_R} \frac{dF_G}{dt} = -F_G - 1.5 r_3 V_R \rho_R \quad (\text{A.6})$$

$$\rho_R V_R C_{pR} \frac{dT_R}{dt} = R C_{pL} T_L + F_A C_{pA} T_A + F_B C_{pB} T_B - F_R C_{pR} T_R - 2 r_1 \rho_R V_R H_1 - 3 r_2 \rho_R V_R H_2 - 1.5 r_3 \rho_R V_R H_3 - A_w U_w (T_R - T_w) \quad (\text{A.7})$$

$$W_w C_{pw} \frac{dT_w}{dt} = F_w C_{pw} (T_{w,in} - T_w) + A_w U_w (T_R - T_w) \quad (\text{A.8})$$

$$F_C = F_R - F_G \quad (\text{A.9})$$

$$F_C = F_D + F_P + \hat{R} \quad (\text{A.10})$$

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