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Controllability evaluation of the separation zones of a carbon-hydrogen-oxygen symbiosis network through the SVD technique: Conventional and intensified options

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ABSTRACT

It has previously been reported how the introduction of intensified processes in the design of Carbon-Hydrogen-Oxygen symbiosis networks (CHOSYNs) generally leads to improved sustainability indicators. However, since these networks are macrosystems with a high level of integration and now adding intensified processes, it is important to investigate how intensification affects the controllability of the network to ensure that the design remains feasible. Addressing this concern, this study aims to investigate the theoretical control of CHOSYNs to compare whether the intensification performed in specific feasible areas of a network improves or worsens its controllability. A case study is proposed: a CHOSYN configuration with two distillation sequences as areas for intensification. The analysis was implemented under different scenarios with different intensification options for both sequences. The singular value decomposition technique was employed to assess the theoretical controllability of the different scenarios. The results indicate that some scenarios with intensification are as controllable as the conventional network. This means better sustainability characteristics: better economic performance, lower environmental impact, energy savings, and, with the present study, assurance that the control of the network is not complicated by the intensification of the network.

1. Introduction

The modern framework of consumption-production has surpassed the ratio of resource consumption to resource generation. This situation has demonstrated the unsustainability of traditional production processes, paving the way for schemes that specifically aim to optimize resource utilization. These new processing schemes are encouraged by the current policies of sustainable development under the agenda 2030. In this context, the design of these new schemes must be innovative and efficient to increase productivity but not at the cost of overexploitation of the environment and resources. This primarily addresses objectives 12 and 13, but also promotes energy efficiency, as it is proposed in objective 7. The Carbon-Hydrogen-Oxygen symbiosis networks, or CHOSYNs, have emerged as an alternative to traditional individualistic processing systems and may provide a tool to meet these objectives in the hydrocarbon-processing sector. These schemes belong to the eco-

industrial park processing schemes [1], where the main objective is to efficiently utilize available resources in a set of processing plants. This objective is achieved by sharing resources among the set of involved participants in the park, in a kind of symbiosis in an industrial ecosystem that minimizes the use of energy and mass resources throughout the entire system [2–4]. For a plant to be considered part of the CHOSYN, it must process carbon-hydrogen-oxygen compounds. The CHOSYNs processing schemes are of particular interest, mainly because of the lower environmental impacts and better economic performance than the individual processing schemes, typically the two most mentioned targets of sustainability. Since the introduction of the concept of CHOSYN, numerous research works have been published addressing the design and final configuration of these networks using different approaches, all with the goal of achieving efficient mass and energy resource utilization plants [5–8]. Integration between plants through mass exchange networks (MENs) and heat exchange networks (HENs) has been the primary

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means of achieving this efficiency [9].

Numerous research works have addressed the task of upgrading the sustainability of eco-industrial parks [10–13], some papers place special emphasis on safety objectives [14], CO₂ footprint reduction [15], while others primarily aim to increasing the economic performance of the network through the revaluation of some products produced by the network [16–17]. In the case of the CHOSYNs, it is important to note that while the design of the multi-plant system aims for optimal resource integration to maximize overall efficiency, due to the nature of the processes involved in the network, there are also opportunities to enhance the efficiency of individual processes as better energy efficiency, to reduce equipment and operating costs, and even reduce the environmental impact which implies a general improvement of the network.

In the last few decades, the application of intensified processes has gained more popularity due to the advantages that these new technologies offer to make the processes more competitive and thanks to the advances that have been presented in this field [18–21]. In this sense, process intensification techniques are useful tools that can be used to further improve the efficiency and design of the CHOSYNs, thus improving the sustainability aspects of the network beyond those achieved with plant-to-plant integration. Intensification techniques have been widely used to improve processing systems. According to Staniewicz & Moulin, process intensification is the development of equipment or techniques that allow for decreasing equipment-size/production-capacity ratio, energy consumption, and waste production resulting in cheaper, safer, and cleaner technologies [22]. Some authors have discussed the relationship between process integration and intensification, Ponce-Ortega et al. [23] identified that process intensification is wider than process integration, and Baldea [24] proposed that process intensification is the limit case of tight integration. Although most of the reported papers on process intensification deal with the advantages of using intensified processes, they have only partially penetrated the industry. Keil [25] discussed many of the important ideas and developments proposed in the area of process intensification and highlighted distillation technology, micro-engineering, and membrane separation as the technologies that have penetrated the industry the most.

Juarez-Garcia et al. [26] emphasized the advantages of incorporating intensification techniques into CHOSYN design; the results indicate significant energy savings, reduced equipment and operating costs, and lower environmental footprint, making these networks even more attractive as sustainable processing schemes. This previous work identified two distillation sequences as areas of opportunity for the implementation of intensification, which meant the aforementioned improvements since distillation units are well known for their significant contribution to total process costs and their low thermal efficiencies [26].

Although, as the literature indicates, the intensification of processes would improve the overall efficiency of the network, with the investigation of process intensification techniques for industrial application, the concern about the controllability of intensified processes has arisen. This is mainly because some intensified processes such as distillation columns turn out to be more complex than their non-intensified counterparts. Etchells [27] highlighted the benefits of using PI for process safety and operability, but also pointed out the disadvantages and noted that intensified processes are not always the better choice over the conventional process, pointing out mainly two aspects: that the system may be more complex or may need a more complex control system, and that as equipment and residence time are minimized, the system becomes more susceptible to changes in process conditions. Harmsen [28] pointed out lower costs, lower energy, and lower safety risks as the main drivers for PI technologies to be successfully implemented in the industry in addition to the other technical aspects. Several research works address the concern of integrating the design and the control in intensified processes and highlight the complex problem this represents [29,

30], Pistikopoulos et al. [31] discuss the need to integrate operability and control analysis at the conceptual PI design stage, they studied the role played by the loss of degrees of freedom and the process constraints on the operability and control characteristics of the intensified vs conventional process. Also some strategies have been presented to deal with this concern, Medina-Herrera et al. [32] proposed a useful toolbox to integrate the design and control of reactive distillation systems due to the concern of operability of these intensified units, Iftakher et al. [33] developed a control scheme that combines suitable process design and control in multiproduct reactive distillation which allows smooth product transitions while keeping product specifications, Iftakher et al. [34] presented an integrated design-control framework to improve the controllability of reactive distillation systems based on the driving force concept, they highlighted that for these intensified systems designed at the maximum driving force would be the easiest to operate. Liñan and Ricardez-Sandoval [35] proposed the first deterministic framework for the optimal design of a catalytic distillation system considering the multitasking and the dynamic behavior of the system, Toffolo et al. [36] proposed a strategy based on nonlinear model predictive control to reduce the costs for implementation of a feedback control of packed bed chemical-looping combustion process. Kiss and Bildea [37] presented an overview of the available control strategies for divided wall columns, they highlighted that DWC are not difficult to control with an appropriate control structure, Alcántara-Ávila et al. [38] made an analysis for thermodynamically equivalent structures for four component mixture distillation concluding that the dynamic responses for the equivalents are different from their corresponding original thermally coupled configuration, Segovia-Hernández et al. [39] presented a case of a separation of a five-component mixture in different thermally coupled distillation sequences, they found that for some sequences the dynamics is equal or better than for the conventional sequence. Thus there is evident the need to consider the control criteria in addition to all the inherent characteristics of intensification (smaller, cheaper, and cleaner).

Considering the major importance attached to separation processes, especially distillation trains, within chemical plants, their relevance is emphasized by the significant energy outlay and operational costs associated with these complex systems. It is necessary to study the controllability characteristics of distillation trains, given their direct implications on system efficiency and overall plant performance. An analysis of controllability within distillation trains makes it possible to discern the responsiveness of the system to external disturbances and fluctuations in operating conditions. This understanding is the basis for devising and implementing sophisticated control strategies aimed at enhancing the stability and robustness of distillation processes [40]. Such enhancements, in turn, generate improvements in the reliability and efficiency of the entire chemical plant. As each section of the plant contributes synergistically to the overall process, and the distillation trains play a key role in plant performance a thoughtful investigation of the inherent control properties of distillation trains provides a holistic appreciation of the controllability landscape of the plant.

This holistic standpoint is indispensable for plant engineers and operators, enabling them to make judicious decisions, implement targeted optimizations, and refine overarching control strategies governing the entire chemical facility. In essence, the examination of control properties within distillation trains transcends mere isolation, representing a strategic initiative to attain a comprehensive and integrated understanding of the operational intricacies characterizing the chemical plant.

2. Proposed approach

This paper proposes to study the controllability of a CHOSYN, and then to compare this property when the network is integrated with only conventional processes and when the network includes intensified processes. For this, a previously reported CHOSYN design with

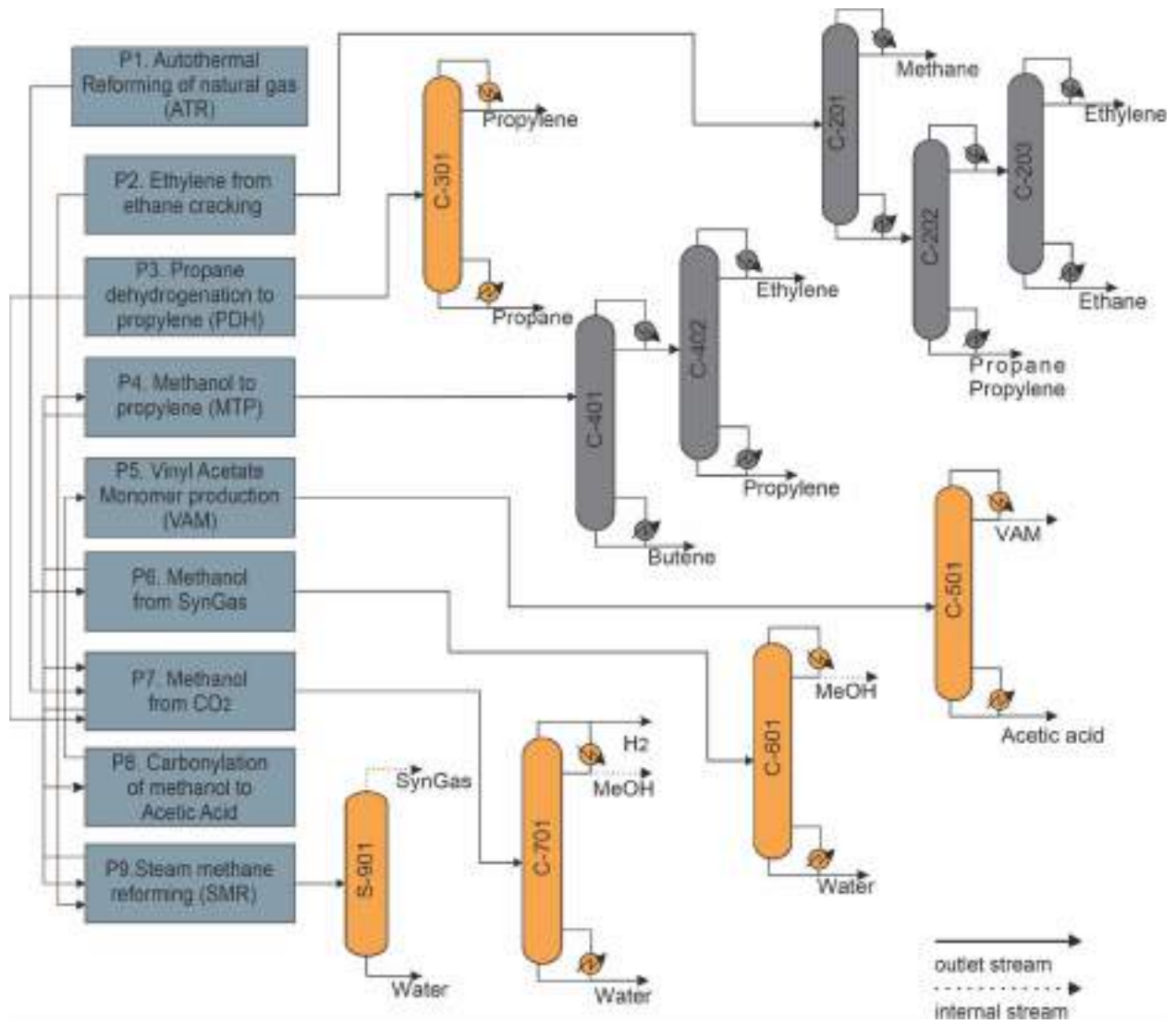


Fig. 1. Representation of the case study.

intensification in the separation zones is proposed as the case study, several scenarios were derived from the original reported configuration of the CHOSYN, and these include different intensified alternatives. This analysis is expected to determine whether process intensification interferes with the controllability of the network offsetting the economic and environmental benefits that intensification offers, or whether the network control is not degraded or improved by intensification, in addition to the other sustainability goals. For the control analysis, the technique of singular value decomposition (SVD) of the gain matrix is used, in a summarized way it consists of the following steps:

- (1) To determine the control variables (of interest) in the network and the manipulated variables.
- (2) To generate the gain matrix from the set of control and manipulated variables for each scenario.
- (3) To determine the singular value matrix and calculate the condition number of the matrix for each scenario.

The following sections explain the methodology and its fundamentals in more detail as it is implemented.

3. Case study

The case study presented by Juárez-García et al. [26] is a CHOSYN configuration including nine processing plants; two of these processes have separation trains with opportunity for intensification. Four different scenarios were identified using the intensified option with the higher energy saving and lowest total annual cost. In this work, from the set of four solutions, it is used the solution that presents the best total annual cost of the whole network as the case study. This work presents a wider range of intensified options for the two intensified zones; the

Table 1
Composition of the stream products.

| | Methane | Ethane | Ethylene | Propane | Propylene |
|------|---------|--------|----------|---------|-----------|
| Feed | 0.2385 | 0.0461 | 0.6905 | 0.0061 | 0.0180 |
| D1 | 0.9936 | 0 | 0.0063 | 0 | 0 |
| B2 | 0 | 0.0535 | 0.0022 | 0.2354 | 0.6879 |
| D3 | 0.0005 | 0.0003 | 0.9990 | 0 | 0 |
| B3 | 0 | 0.9996 | 0.0003 | 0 | 0 |

Table 2
Parameters and characteristics of ethylene purification sequence.

| | C-201 | C-202 | C-203 |
|--------------------|----------|---------|----------|
| Reflux ratio | 6.11 | 0.59 | 3.68 |
| Feed stage | 8 | 20 | 47 |
| Total stage | 26 | 42 | 86 |
| Reboiler duty (kW) | 877.12 | 622.2 | 1303.3 |
| Light key | Methane | Ethane | Ethylene |
| Heavy key | Ethylene | Propane | Ethane |

objective is to analyze the controllability for the largest number of scenarios of the CHOSYN configuration.

This CHOSYN configuration consists of nine processing plants (see Fig. 1): Auto thermal Reforming of Natural Gas Process (ATR), Ethylene production from ethane cracking, Propane dehydrogenation to propylene Process (PDH), Methanol to propylene process (MTP), Vinyl Acetate Monomer production (VAM), Methanol production from syngas, Methanol production from CO₂/H₂, Carbonylation of methanol to produce Acetic acid and Steam methane reforming. Material streams from the individual processes are recirculated to the interception network to be used in other plants, which means from internal sources and to internal

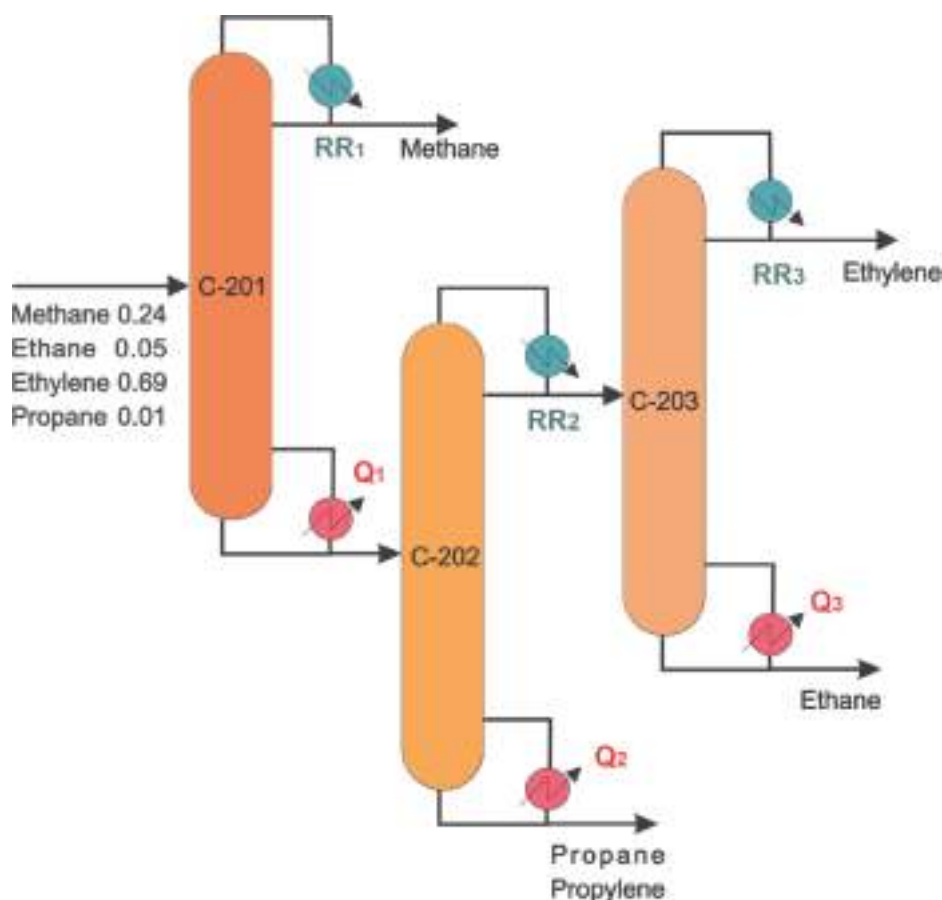


Fig. 2. Conventional sequence for ethylene purification.

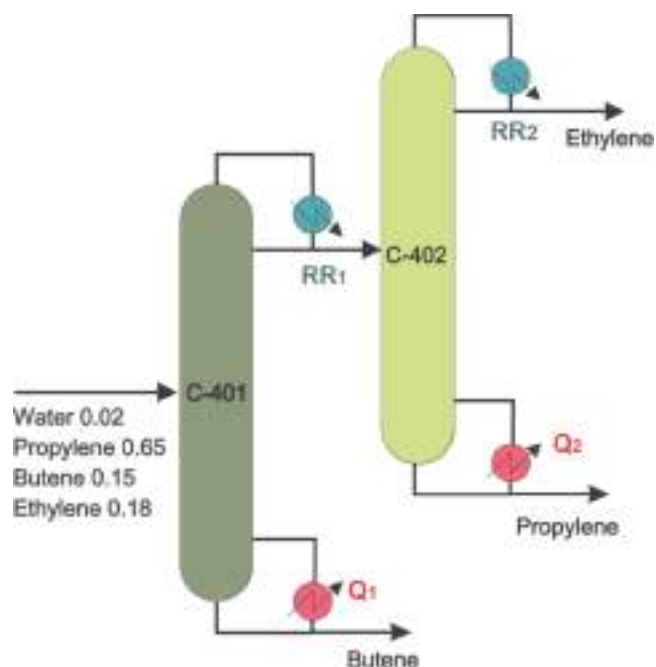


Fig. 3. Conventional sequence of propylene purification.

Table 3
Composition of the stream products.

| | Ethylene | Propylene | Butylene | Water |
|------|----------|-----------|----------|--------|
| Feed | 0.1806 | 0.6520 | 0.1485 | 0.0188 |
| B1 | 0 | 0.0375 | 0.8500 | 0.1123 |
| D1 | 0.9999 | 0 | 0 | 0 |
| B2 | 0 | 0.9904 | 0.0095 | 0 |

Table 4
Parameters and characteristics of propylene purification sequence.

| | C-401 | C-402 |
|--------------------|-----------|-----------|
| Reflux ratio | 1.68 | 15.15 |
| Feed stage | 26 | 18 |
| Total stage | 50 | 33 |
| Reboiler duty (kW) | 5164 | 9005.1 |
| Light key | Propylene | Ethylene |
| Heavy key | Butylene | Propylene |

sinks. Fig. 1 shows the set of 15 outlet flow streams of the network, (i.e. the flows that will no longer be used as internal sources for other plants), which are the streams that contain the products of interest of the network; therefore, they are the streams that are to be controlled and therefore where the control study will be performed.

The different intensified options for the considered scenarios were obtained as described below.

3.1. Ethylene recovery sequence

The ethane steam cracking process to produce ethylene consists of three sections: cracking and quenching (reaction zone), compression and cooling, and recovery. This recovery section involves three distillation columns (see Fig. 2), the effluent from the cooling zone is a stream rich in ethylene (0.69 mole fraction) and methane (0.25 mole fraction), along with traces of ethane, propane, and propylene. In the first column, C-201, methane is separated as the overhead product. The bottoms of the second column, C-202, contain traces of propane and propylene. Finally, in the third column, C-203, ethylene is separated in the

distillate, while ethane is obtained at the bottom of the column, Table 1 shows the composition of the different streams of the sequence and Table 2 shows some parameters of the columns.

3.2. Propylene recovery sequence

The first step of this process consists of two reaction steps: the conversion of methanol into dimethyl ether (DME) in an adiabatic reactor, and then the main reaction where ethylene, propylene, and butenes are produced and then sent to the distillation zone. This sequence involves two columns (see Fig. 3). The feed to the first column, C-401, consists of propylene (0.65 mole fraction), butene (0.15 mole fraction), and ethylene (0.18 mole fraction), along with traces of water. In the first column, the butenes and heavier components are separated at the bottom, while in the second column, C-402, propylene is separated as the bottom product, and ethylene is obtained from the dome. The composition of the streams are shown in Table 3 and the column parameters in Table 4.

3.3. Intensified alternatives to conventional distillation sequences

There have been proposed several methods for the design of thermally coupled distillation sequences, the most common is using analytical and graphical techniques or a combination of both, and, although there is no systematic and formal method for designing thermally coupled distillation sequences with the aid of simulation software, many authors choose to use these techniques. This work opts for the use of Aspen Plus for the design of the different intensified options for the two distillation sequences of the case study. The method used can be described as follows:

- (1) A first simulation for an initial approximation of the design parameters by shortcut methods, for the given mixture and based on the flowsheet of the conventional process.
- (2) A rigorous simulation of the conventional sequence, from this simulation it is possible to describe the architecture of the sequence and determine the number of trays contained in each section.
- (3) A rigorous simulation of the thermally coupled sequences options, in this work some of the alternatives of the search space were selected a priori.
- (4) Determine the liquid and/or vapor flow rates that represent the minimum heat duty of the sequence through a sensitivity analysis, some authors also call this step optimization.

As it was mentioned above, the alternatives were selected a priori, three thermally coupled distillation sequences for the ethylene purification sequences, and two thermally equivalent alternatives for the propylene purification sequence proposed using the dynamic method proposed by Hernandez and Jiménez [41], resulting in the intensified options described below.

3.3.1. Intensified ethylene recovery sequence

For this sequence are presented three alternatives obtained through thermal couplings (see Fig. 4), the first option R-I is a partially thermally coupled configuration, it is obtained by a thermal coupling between a vapor stream from the second column C-202 to the first column C-201 and a liquid stream from C-201 to C-202. The second option R-II is another partially thermally coupled configuration, this is obtained in a similar way by a thermal coupling between a vapor stream from the second column C-202 to the third column C-203 and a liquid stream from C-203 to C-202. The third option R-III is a fully thermally coupled arrangement with both two thermal couplings between C-201 and C-202, and between C-202 and C-203. Table 5 shows the parameters describing the thermally coupled sequences for ethylene purification.

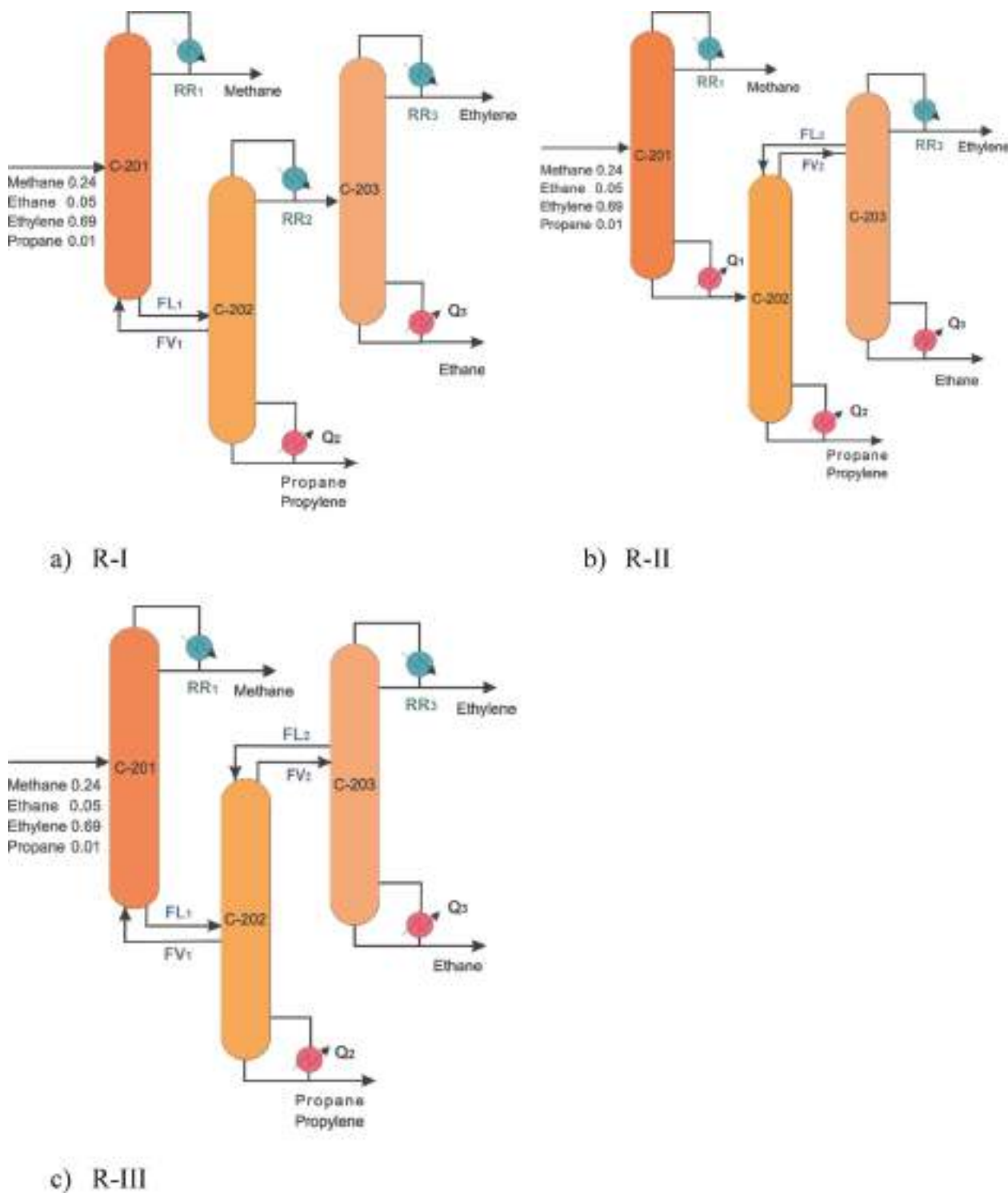


Fig. 4. Thermally coupled configurations for ethylene recovery sequence.

3.3.2. Intensified propylene recovery sequence

For this sequence there were analyzed two options, the first alternative is the fully thermally distillation column also known as Petlyuk column (see Fig. 5). This arrangement allows replacing the reboiler and the condenser of the first column (pre-fractionator) with vapor/liquid links with the second column, the second option is a partially thermally coupled distillation arrangement, one column, and a side stripper. Table 6 shows the parameters describing the thermal equivalents for the purification of propylene.

4. Theoretical controllability assessment

To assess the evaluation of the theoretical controllability of the CHOSYN, in this work it is used the concept of condition number and the technique of Singular Value Decomposition (SVD). This technique was performed at frequency zero (steady state). In the field of process control, the SVD provides meaningful insights about controllability, sensor location and controller pairing, also can be used directly as a decoupling control strategy [42]. Taking into account the purpose and scope of this analysis, this technique is selected due to its widespread use for

Table 5

Description of the thermally coupled distillation sequences.

| | R-I | R-II | R-III |
|--------------------------|--------|--------|---------|
| RR ₁ | 6.2 | 6.11 | 6.52 |
| RR ₂ | 0.54 | – | – |
| RR ₃ | 3.68 | 3.78 | 3.81 |
| Q ₁ (kW) | – | 877.12 | – |
| Q ₂ (kW) | 1497.1 | 632.8 | 1525.05 |
| Q ₃ (kW) | 1303.3 | 1100 | 1129.1 |
| FL ₁ (kmol/h) | 596.7 | – | 605.7 |
| FL ₂ (kmol/h) | – | 110 | 100 |
| FV ₁ (kmol/h) | 411 | – | 420 |
| FV ₂ (kmol/h) | – | 289.3 | 279.3 |

evaluating the controllability features of intensified distillation systems. Multiple studies have demonstrated its use and reliability in ranking systems as a function of their controllability. It is worth mentioning that there are other techniques such as Relative Gain Array (RGA) employed to obtain information about the dependence of composition on more than one manipulated variable [43–45].

The SVD technique is used to decompose a matrix into a set of factors, this is why this technique is also called factorization. A matrix $G \in \mathbb{R}^{m \times n}$ can be represented by three factors:

$$G = U\Sigma V^T \tag{E1}$$

Where $U = [u_1 u_2 \dots u_3] \in \mathbb{R}^{m \times n}$ is an orthogonal matrix containing the “left singular vectors” of G , and $V = [v_1 v_2 \dots v_3] \in \mathbb{R}^{m \times n}$ is an orthogonal matrix containing the “right singular vectors” of G , whereas Σ is a $m \times n$ diagonal matrix containing all the non-zero “singular values” of G ordered from highest to lowest ($\sigma_1 > \sigma_2 > \dots > \sigma_n > 0$):

$$\Sigma = \begin{bmatrix} \sigma_1 & \dots & \emptyset \\ \vdots & \ddots & \vdots \\ \emptyset & \dots & \sigma_n \end{bmatrix} \tag{E2}$$

The condition number (γ) of the matrix G is the ratio between the maximum singular value (σ^*) and the minimum (σ_*):

$$\gamma = \frac{\sigma^*}{\sigma_*} \tag{E3}$$

The condition number of a matrix indicates how “well-conditioned” or sensitive the matrix is. The higher the condition number, the more sensitive or ill-conditioned the matrix is, this means that small changes in its coefficients result in a large change in the solution, conversely, for

a well-conditioned matrix, with low condition numbers, small changes in its coefficients are unlikely to yield considerable changes in the solution. In the case of the gain matrix in control process analysis, the condition number gives us a measure of how sensitive is the process to perturbations in the manipulated variables (input data). A small condition number indicates that the process is more robust to changes in operating conditions, and a large condition number indicates a more sensitive process [46,47]. Even without a scale indicating the extent of smallness or largeness, the condition number provides a means to discriminate or compare between a variety of options. In this work, it was used a relative steady-state gain matrix, which takes into account the multivariable interactions of the system. The matrix coefficients are generated by introducing a small disturbance in the manipulated variables and measuring the variation in the control variables. One of the drawbacks of the SVD is the fact that the singular values depend on the system of units used, and the application of the SVD to transfer functions with units lacks validity, since matrix transformations will include the effect of such units. This has given rise to the need to find a scaling method that eliminates that dependency and provides reliability in the results and also a physical meaning. Morari et al. [48] point out that a scaling method should be used to minimize the condition number. However, the implementation of this idea is not so clear, practically any scaling method achieves the above, even if it lacks physical bases, moreover, the normalization criterion minimizes the number of condition changes in each case. Johnston and Barton [49] presented a physically based method, which considers the actual operation of the system, in which the manipulated variables and measurements are scaled differently. They proposed that outputs be scaled in such a way that a change of a given magnitude has the same meaning for all outputs, from a controllability point of view. Each variable has a different influence on the process, the same scaling factor cannot be used for all variables.

Table 6

Description of the thermodynamically equivalents for propylene purification.

| | Petlyuk column | | Side stripper arrangement | |
|-------------------------|----------------|--------|---------------------------|--------|
| | C-401' | C-402' | C-401' | C-402' |
| Total stage | 17 | 84 | 68 | 15 |
| Feed stage | 3 | – | 44 | – |
| Side product draw stage | – | 32 | – | – |
| Feed stage of liquid | 1 | 60 | – | 1 |
| Feed stage of vapor | 17 | 28 | 19 | – |

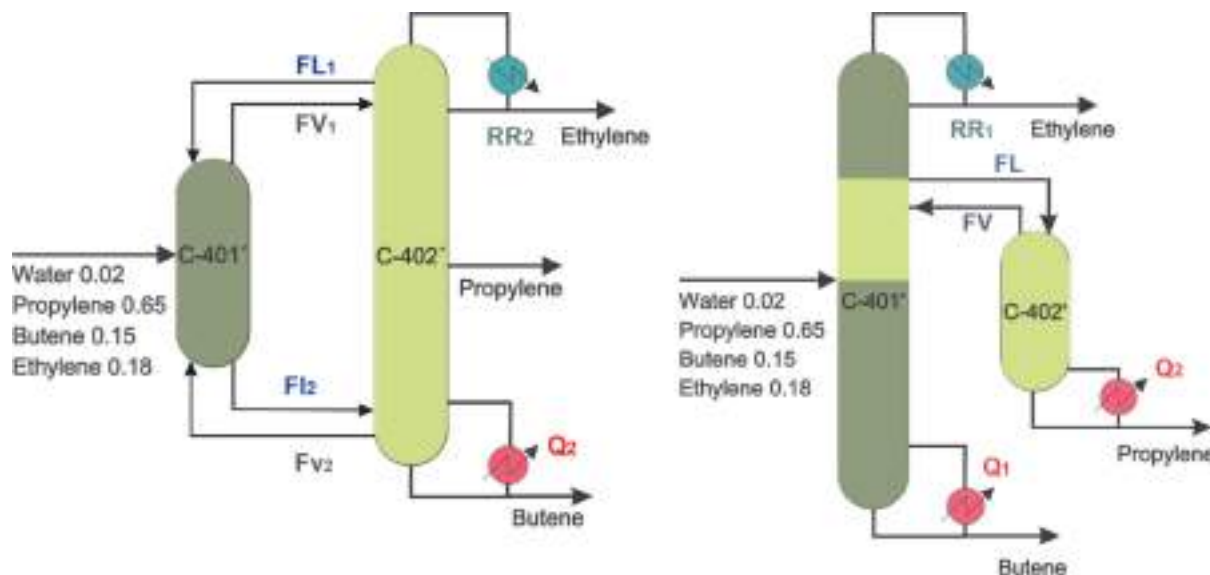


Fig. 5. Thermodynamically equivalents for propylene purification.

According to this, the variables had to be scaled so that, a given magnitude change would represent an equivalent amount of control action for all variables. Based on this work, for the distillation sequences to be studied there are important variables to control, such variables are the mole fractions of each of the components of the corresponding mixture, and they are bounded between 0 and 1. They are used to manipulate variables that are reflux ratio or reboiler duty, which have units and are not naturally bounded. To eliminate this drawback, it is proposed to limit the range change of the manipulated variables considering that the maximum opening that the control valves can reach is twice the nominal value of the stable state, therefore, in principle the valves are open at 50 %. This implies that to obtain the gain matrix, the step change implemented in the manipulated variable must be divided by two times the stable state in order to have the same range of variation in both the closing and opening operation of the control valves. This allows a physical interpretation of the way the manipulated variables are scaled, by linking the magnitude of change of the manipulated variables with the magnitude of change of the stem position of the corresponding valves, which can only vary between 0 and 100 % opening (0 and 1). With this form of scaling, the normalization and dimensionalization of the manipulated variables are simultaneously achieved.

In this work, a typical I-V control is used. This scheme involves the composition of the top of the column being altered using the liquid of the reflux rate, whereas the compositions at the top of the column are adjusted by modifying the reboiler duty (vapor used in the reboiler) this structure was used to select the manipulate and control variables of the distillation column [50]. This control arrangement is one of the most used to evaluate the controllability aspect of distillations columns [51, 52]. The molar purities of the stream were considered as control variables to perform the SVD analysis. It is important to note that there are other variables, such as the boiling temperature at 95 % evaporation, known as the TD86 standard, which can be used as a control variable to avoid the use of chromatographs connected inline [52]. This TD86 temperature is widely employed as control variable for hydrocarbon mixtures. However, this variable requires experimental determination and inferential control strategies for studying controllability, which increase the complexity of the study. However, for the case of preliminary control studies, or to evaluate the stability of different control systems, compositions are one of the most widely used variables, as they can be easily calculated from liquid-vapor equilibrium data. Additionally, they have proven to be good reference variables for verifying the controllability of different distillation schemes [52–54]. The reflux ratio (RR) and the reboiler duty (RD) in each column were selected as manipulated variables according to I-V arrangement. Thus, the coefficients of the gain matrix are the difference between the molar purity of the component n after disturbance in the m manipulated variable (x_n^{sp}) and the molar purity of the n component in the set point or nominal state (x_n^{sp}).

The disturbance is a step change (p) and for the present analysis is 0.5 % of the nominal value of the variable. This magnitude aligns with the minimum recommended value by Luyben, particularly in the context of complex systems [55]. This chosen disturbance magnitude enables the assumption of a first-order system for the purposes of the present analysis [56]. Table 8 shows the list of manipulated variables and control

Table 7
Parameters for the thermodynamically equivalents for propylene purification.

| | Petlyuk column | Side stripper arrangement |
|--------------------------|----------------|---------------------------|
| RR ₁ | – | 22.8 |
| RR ₂ | 19 | – |
| Q ₁ (kW) | – | 5221.4 |
| Q ₂ (kW) | 12,713 | 6269.4 |
| FL ₁ (kmol/h) | 3650 | 3690 |
| FV ₁ (kmol/h) | 4394.3 | 2234.4 |
| FL ₂ (kmol/h) | 2788.7 | – |
| FV ₂ (kmol/h) | 1300 | – |

Table 8
Input/output variables for the relative gain matrix.

| u_i | | y_i | |
|----------|-------------------------|----------|------------------------------------|
| u_1 | RR ₁ / C-201 | y_1 | $x_{methane}$ / Distillate C-201 |
| u_2 | RD ₂ / C-202 | y_2 | $x_{propylene}$ / Bottoms C-202 |
| u_3 | RR ₃ / C-203 | y_3 | $x_{ethylene}$ / Distillate C-203 |
| u_4 | RD ₃ / C-203 | y_4 | x_{ethane} / Bottoms C-203 |
| u_5 | RR / C-301 | y_5 | $x_{propylene}$ / Distillate C-301 |
| u_6 | RD / C-301 | y_6 | $x_{propane}$ / Bottoms C-301 |
| u_7 | RD ₁ / C-401 | y_7 | x_{butene} / Bottoms C-401 |
| u_8 | RR ₂ / C-402 | y_8 | $x_{ethylene}$ / Distillate C-402 |
| u_9 | RD ₂ / C-402 | y_9 | $x_{propylene}$ / Bottoms C-402 |
| u_{10} | RR / C-501 | y_{10} | x_{VAM} / Distillate C-501 |
| u_{11} | RD / C-501 | y_{11} | x_{HAc} / Bottoms C-501 |
| u_{12} | RD / C-601 | y_{12} | x_{water} / Bottoms C-601 |
| u_{13} | RR / C-701 | y_{13} | x_{lights} / Distillate C-701 |
| u_{14} | RD / C-701 | y_{14} | x_{water} / Bottoms C-701 |
| u_{15} | Temperature / S-901 | y_{15} | x_{water} / Bottoms S-901 |

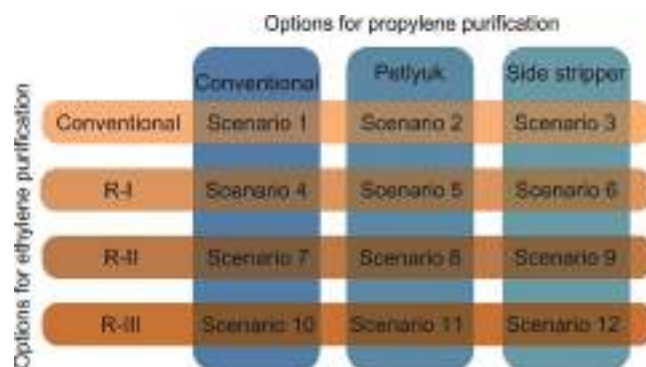


Fig. 6. Different scenarios for the case study.

variables for the case study, the relative gain matrices generated are 15×15 through E4 form.

$$\begin{bmatrix} G_{11} & \dots & G_{1n} \\ \vdots & \ddots & \vdots \\ G_{m1} & \dots & G_{mn} \end{bmatrix} = \begin{matrix} u_1 \\ \vdots \\ u_m \end{matrix} \begin{bmatrix} \frac{x_1^{y_1} - x_1^{sp}}{0.5p} & \dots & \frac{x_n^{y_1} - x_n^{sp}}{0.5p} \\ \vdots & \ddots & \vdots \\ \frac{x_1^{y_m} - x_1^{sp}}{0.5p} & \dots & \frac{x_n^{y_m} - x_n^{sp}}{0.5p} \end{bmatrix} \quad (E4)$$

In the case of the Petlyuk column (see Fig. 5), the side stream flow is added as a manipulated variable and its composition as a control variable to complete the matrix.

Fig. 6 shows the different scenarios that were analyzed and the condition number was calculated for each one. Twelve different scenarios were generated; the scenario 1 is the network that includes the two conventional sequences (conventional/conventional). The following scenarios are the networks which present combinations between conventional and intensified options, scenarios 2 and 3 are the combination of conventional sequence for ethylene purification with the Petlyuk column and with the side stripper arrangement respectively for the propylene sequence. Scenarios 4, 5 and 6 are the same combinations replacing the conventional sequence for ethylene purification by R-I option (see Fig. 4). The rest of the scenarios are proposed in the same way, thus scenario 12 is the network with R-III option for ethylene purification and the side stripper arrangement for propylene purification.

5. Results and discussion

The relative gain matrix was generated for each scenario (see Fig. 6

and Eq. (4)). Illustratively, the matrices for scenarios 1 and 12 are shown below, G^1 in E5, which is the conventional/conventional scenario, and G^{12} in E6, which is the scenario with R-III and side stripper options, it can be seen how the interactions between manipulated and control variables increase.

The condition numbers for each of the twelve scenarios are shown in Table 9, in the rows are the ethylene purification sequence options, and in the columns are the propylene purification sequence options, so for the scenario where the conventional ethylene sequence and the con-

$$G^{\text{scenario}1} = \begin{bmatrix} -0.0800 & 0.4142 & -0.0227 & 0.0167 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -29.548 & 0.1097 & -4157 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1.3388 & 0.08754 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.1061 & -21.6437 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2.3781 & 0.345 & 0.0301 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.0004 & -0.2974 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.2821 & 0.0302 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.5243 & 1.2021 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.6827 & -4.1258 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -17.7002 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.9 \times 10^{-13} & 0.145 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 72.3083 & -0.0036 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.17 \times 10^{-6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.0061 & 1.1323 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.0025 & -1.1942 \end{bmatrix} \tag{E5}$$

$$G^{\text{scenario}12} = \begin{bmatrix} -0.0691 & -9.9693 & -0.0919 & 0.0451 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.04275 & -55.5915 & 0.0991 & -21.1396 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.0210 & -32.9050 & -1.5764 & 0.0967 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -0.0242 & 16.0653 & 0.0942 & -21.8055 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -4.1142 & 0.7796 & -0.3029 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2.4084 & 0.0345 & 0.0012 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8.0519 & -8.6803 & 0.0012 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.5243 & 1.2021 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.6827 & -4.1258 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -17.7002 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.9 \times 10^{-13} & 0.145 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 72.3083 & -0.0036 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.17 \times 10^{-6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.0061 & 1.1323 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.0025 & -1.1942 \end{bmatrix} \tag{E6}$$

Table 9
Condition number values for the different scenarios of the case study.

| | Conventional | Petlyuk | Side stripper |
|--------------|--------------|---------|---------------|
| Conventional | 376.6 | 376.6 | 376.6 |
| R-I | 734.1 | 734.1 | 734.1 |
| R-II | 641.5 | 641.5 | 641.5 |
| R-III | 893.1 | 893.1 | 893.1 |

ventional propylene sequence are used, the calculated condition number is 376.6.

Comparing this value along the first row, it is observed that it remains constant for the scenarios with the conventional ethylene sequence and the intensified options: petlyuk and side stripper option. The same is true for each row, which means that the controllability remain the same as in the conventional scenario for any intensified option of the propylene sequence. If we analyze Tables 5 and 7, we can see the advantages of using the intensified options such as energy

savings, the side stripper arrangement represents 81 % of the energy expended in the original sequence, while the Petlyuk column represents 89.7 %. So for these three scenarios, it is possible to have energy savings while ensuring that the control of the network is at least as good as that of the conventional network.

Meanwhile the columns show the different ethylene purification sequence options, first the conventional one, then the sequence with a recycle from the second column to the first one (R-I), then with a recycle from the third column to the second one (R-II), and the sequence that has both recycles (R-III), it is noticeable how the condition number increases its value from the conventional option scenarios, this indicates that using an of these intensified options worsens the controllability of the network in comparison to the scenarios where the conventional option is used for this sequence. Being R-II the option that degrades the control the least, followed by R-I, and R-III is the one that worsens it the most.

This can be explained by understanding the interaction between the three pairs of variables (control and manipulated) and the way in which a disturbance in some manipulated variable of the system propagates through the system, and how the position of the recycle or recycles affect this propagation. In the conventional option, with no recycles a perturbation in the manipulated variables in the first column affects the control variables of the three downstream columns, which does not occur upstream, i.e. a change in the input variable of the second column does not affect the first column, and a change in the input variable of the third column does not affect either the second or the first column. These low interactions between the three pairs of variables result in a better-conditioned gain matrix.

For the intensified options with recycles, the effect of the propagation of the perturbation in both directions of the sequence must be understood. This implies that the pairs of variables have more interactions between them and the condition number of the matrix is greater. When there is a recycle between the first two columns (R-I), a disturbance in the first or second column will affect the three columns due to the effect of the recycle itself, which carries this disturbance from the second to the first and then from the first to the second and so on until the system assimilates the disturbance and returns to the set point of the control variables. Something similar happens when there are two recycles (R-III), in this case, a disturbance in any column will affect the values of the control variables in the three columns, and this disturbance will go downstream and countercurrent through the two recycles and three columns until the system returns to its original state, the scenarios which include this intensified option are those with the worst control characteristics. In the case of the scenarios with the R-II option, the recycle is located between columns two and three, therefore a disturbance in any of these two columns does not extend to the first one, and the system absorbs this disturbance better or faster, and there are less control variables affected.

Generally it is expected that large flowrates favor the controllability of a systems as it helps to eliminate dead times and decreases the response time of the system. Although it should be considered that this relationship between the flowrate and dead times depends on the nature of the system, for this case the flowrates of liquid and vapor of the second recycle are lightly greater for R-II (see Table 5), which may also explain why this option presents a lower condition number than the other intensified options.

Then, the thermal equivalents options for propylene purification involving restructuring the condition number does not vary from the conventional case, and in the retrofitting options for ethylene sequences the condition number changes from the conventional case and in each option. This is due precisely to the restructuring of the sequences. In the case of ethylene options, the fact that there is no restructuring makes it possible to physically use the same equipment by replacing the condenser and reboiler, and the heat duty is minimized as a function of the liquid/vapor flows of the interconnections. In the case of the proposed sequences for the purification of propylene, there is a restructuring of the sequence sections, i.e. a design with a different

architecture, and in this case, in the design of the sequence other parameters can be optimized such as the number of trays in addition to the interconnection flows. The optimized design to minimize the heat duty should, at the same time, reduce the number of stages. For this work, the minimization of the heat duty was carried out in function of the interconnection flows, but not the number of stages, and the same number of total stages as in the conventional sequence were used as indicated by the method proposed by Hernández and Jiménez [41]. Therefore, it seems that these designs present an over-specification in the number of stages, which can allow mitigating disturbances, whether it be in the reflux ratio or reboiler heat duty, keeping product compositions almost invariable. It is important to note that this oversizing does not imply that the design is erroneous, only that the optimization was carry out in terms of the interconnection liquid/vapor flows only, as in the ethylene sequence.

Juárez-García et al. [26] determined that CHOSYNs with intensified processes involved presented a slightly higher risk index compared to the CHOSYNs with all conventional processes. The safety of a process is related to inventory, flowrates, operating conditions and equipment size and according to the green chemistry principle #11 (real-time analysis for pollution prevention) a real-time analysis and control of the process is important to prevent waste generation, by identifying excursions as they occur and avoid poor quality products and safety issues [57,58], which would be more feasible in a stable system. In this sense, scenarios 2 and 3 could present the same advantage of the conventional network, however, a simultaneous quantitative control and safety study would be necessary to verify this [46].

While the investigation has primarily focused on the dynamics of distillation trains within the separation zone, there is recognition of the need to broaden the analysis to encompass the overall dynamics inherent in industrial eco-parks. Given the varied timescales associated with individual equipment and the overarching eco-park timescales, there is a proposal for extending the study to include detailed modeling of interconnections and their dynamics. This extension aims to provide a better understanding of the interactions within the entire chemical plant network, attempting to provide a more accurate representation of how perturbations in individual units, such as distillation trains, may impact the performance of the interconnected eco-park. This work offers a nuanced perspective of the chemical plant controllability landscape, lays the groundwork for understanding broader control strategies and their potential plant-wide implications by providing valuable insights that can be extended beyond the specific boundaries of the distillation zone.

CRediT authorship contribution statement

Maricruz Juárez-García: Investigation, Methodology, Writing – original draft, Writing – review & editing. **Juan Gabriel Segovia-Hernández:** Conceptualization, Methodology, Supervision, Validation. **José María Ponce-Ortega:** Conceptualization, Investigation, Software. **Gabriel Contreras-Zarazúa:** Conceptualization, Investigation, Methodology.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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