Theoretical Control Properties Assessment for a Carbon-Hydrogen-Oxygen Symbiosis Network with Intensified Processes

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Abstract

The introduction of intensified processes in the design of Carbon-Hydrogen-Oxygen Symbiosis Networks (CHOSYNs) leads to improve the general sustainability performance of the network; this mainly means lower costs and lower environmental impact. Due the complex nature of these networks, where several plants are interacting through integration lines and recycles, with the inclusion of intensified processes these networks result in even more complex systems where the control properties are well worth to investigate. In this context, this study aims to determine the theoretical control properties of a set of design solutions for a CHOSYN, including conventional processes and intensification performed in specific feasible zones of the network. The objective is to assess whether the intensification improves or worsens the controllability of the network, and in the latter case to identify a solution that balances the benefits of intensification with this possible drawback. The proposed case study is a CHOSYN configuration with two distillation sequences as areas for intensification. Twelve solutions or scenarios were generated for the network through combinations of conventional and different intensified options for these two sequences. The analysis of the control properties for the different scenarios was carried out using the condition number and the singular value decomposition (SVD). The results show that in some scenarios including intensified processes the control properties remain the same as in the conventional case, indicating that for these solutions the sustainability performance can be maintained without affecting the control of the network.

**Keywords**: process intensification, process integration, process control.

* 1. Introduction

The Carbon-Hydrogen-Oxygen symbiosis networks aims to enhance resource efficiency by integrating processing plants that handle mainly carbon, hydrogen and oxygen compounds (Noureldin & El‐Halwagi, 2015). This inter-plant integration allows minimizing the overall requirements of raw materials and minimizing the waste generation, which leads to lower costs and sustainability of the process. However, improving individual processes within the network through other techniques such as process intensification enhances the overall efficiency of the network. Previously, it was reported that incorporating intensified processes in the design of the CHOSYNs, particularly distillation processes, improves the sustainability performance of the network (cost and environmental impact reduction) beyond what is allowed by integration due the intensive energy use and the inefficiency presented in these units (Júarez-Garcia et al. 2022).

However, another key aspect of the sustainability is the controllability of the process, and the inherent safety associated with it (Jiménez-González et al. 2012). The design of the CHOSYNs implies the allocation of multiple integration lines throughout the network and recycles from one plant to another, which implies that they are already complex systems with a high level of interaction between plants. Through the inclusion of intensified processes in the design, this complexity is likely to increase. This concern arises because intensified processes often result in more complex designs than their conventional counterparts such as distillation sequences. Therefore, it is worthwhile to analyze how the inclusion of these intensified processes in a complex processes such as CHOSYNs affects their control properties, whether it improves or worsens them, and in the case that control is negatively affected, analyze what level of intensification tradeoffs this effect with the benefits in the other sustainability indicators. This paper presents the analysis of the control properties of a case study, a previous CHOSYN design where the intensification is focused in two distillation columns. To assess the control properties it is proposed to use the condition number and the technique of Singular Value Decomposition (SVD), which has been used extensively in this context because it provides meaningful insights about controllability.

* 1. Proposed Approach
     1. SVD technique

The Singular Value Decomposition method allows to measure in a qualitative way the control properties of a processing system. This technique is a matrix factorization method, and it decomposes a matrix (G) into three factors as shown in Eq. (1):

|  |  |
| --- | --- |
|  | (1) |

Where Σ contains all the non-zero singular values of G. The ratio of the maximum singular value () to the minimum () is the condition number of G:

|  |  |
| --- | --- |
|  | (2) |

The condition number of a matrix is an indicator of how “well-conditioned” or sensitive is the matrix; it gives a measure of how much the output variables of the system change when the input variables experience a perturbation. In control context, the matrix G is the steady state gain matrix, which relates the control and manipulated variables of the system. Large condition numbers indicate that small disturbances in the system result in large changes in the control variables or that the system is more sensitive, conversely small condition numbers indicates a system less sensitive.

* + 1. Case study

Juarez-Garcia et al. (2022) presented a CHOSYN configuration of nine processing plants with several shared streams: (P1) the auto thermal reforming of natural gas section of a gas to liquid process which shares residual streams containing H2, CO2 and CO with methanol production plants (P6 and P7). The ethylene plant and propane dehydrogenation process share waste streams containing CH4 with the steam methane reforming process (P9) and H2 streams with the methanol plants, which in turn feed the methanol to propylene process (P4) and acetic acid plant (P8). The acetic acid is sent to vinyl acetate monomer production plant (P5). In Figure 1, it is shown a schematic representation of this case study; the product streams (network outlets) are also displayed.

|  |
| --- |
|  |
| Figure 1. Schematic representation of the case study |

The distillation sequences from ethylene process for ethylene purification and propylene purification from PDH plant were intensified. There were proposed thermally coupled sequences (see Figure 2 and 3), these processes compared to the conventional reported better economic performance, energy savings and CO2 emissions reduction.

* + - 1. Intensified option for the case study

The sequence of the purification of ethylene is a three-column sequence, the intensified option is a retrofit design with two vapor/liquid couplings between columns; one replaces the reboiler of C-201 column, the other one replaces the condenser of C-202. The purification sequence of the propylene consists of two columns, this purifies a stream rich in propylene, and for this sequence, it is proposed a main column with a side stripper arrangement. For this sequence, unlike ethylene, a physical rearrangement of the sequence sections is implemented (Hernández & Jiménez, 1996).

|  |  |
| --- | --- |
|  |  |
| 1. Conventional sequence | 1. Thermally coupled option |
| Figure 2. Ethylene purification sequence. | |

|  |  |
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|  |  |
| 1. Conventional sequence | 1. Thermally coupled option |
| Figure 3. Propylene purification sequence. | |

From these two intensified option and the conventional solution four scenarios can be analysed, the scenario A is the conventional configuration shown in Figure 1, scenarios B and C are combinations of conventional and intensified processes, and Scenario D both intensified options replaced the conventional sequences.

Table 1. Proposed scenarios.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Scenario A | Scenario B | Scenario C | Scenario D |
| Ethylene sequence P2 | Conventional | Conventional | Intensified | Intensified |
| Propylene sequence P4 | Conventional | Intensified | Conventional | Intensified |

* + 1. Methodology

The proposed methodology consists in two main tasks: setting the gain matrix and then determine the condition number through SVD technique.

To build the gain matrix, the first step is to define the control variables of interest for the analysis; in general, these variables should be the outlet streams of the network. However, being the objective to determine the influence of intensification over the network controllability and for the specific case study where the intensified zones coincide with network outlets, only control variables of these specific areas are used. This allows reducing the size of the matrix while guaranteeing the significance of the results. Table 2 summarizes the control variables (*y*i), the molar purity of the distillate and bottoms of the two sequences, and the corresponding manipulated variable (*ui*), the reflux ratio (RR) and reboiler duty (RD) of each column.

Table 2. Control variables-Manipulated variables pairing.

|  |  |  |  |
| --- | --- | --- | --- |
| *ui* | | *yi* | |
| *u1* | RR1 / C-201 | *y1* | / Distillate C-201 |
| *u2* | RD2 / C-202 | *y2* | / Bottoms C-202 |
| *u3* | RR3 / C-203 | *y3* | / Distillate C-203 |
| *u4* | RD3 / C-203 | *y4* | / Bottoms C-203 |
| *u5* | RD1 / C-401 | *y7* | / Bottoms C-401 |
| *u6* | RR2 / C-402 | *y8* | / Distillate C-402 |
| *u7* | RD2 / C-402 | *y9* | / Bottoms C-402 |

The next step consists is to generate a perturbation in each of the manipulated variables and measure the response in the control variables. For this, a perturbation of 0.5 % of the nominal value of the variable was used. The coefficients of the gain matrix are the difference between the molar purity of the component *n* after disturbance in the *m* manipulated variable () and the molar purity of the *n* component in the nominal state () as it is shown in Eq. (3). These coefficients were determined using steady-state simulations in Aspen Plus.

|  |  |
| --- | --- |
|  | (3) |

* 1. Results and discussion.

Four 7x7 matrices were obtained, one for each scenario, the decomposition into singular values and the calculation of the condition number was computed in Matlab. The results are shown in Table 3.

Table 3. Condition number for each scenario.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Scenario A | Scenario B | Scenario C | Scenario D |
| Condition number (γ) | 376.6 | 376.6 | 893.1 | 893.1 |

As mentioned above, the condition number is an indicator of the control properties of a system; in this case, the conventional scenario A is the reference to compare the controllability of the scenarios B, C and D that include intensification. From the conventional scenario A to scenario B the condition number do not vary and it can be assumed that the control properties remain the same, therefore the topological difference between the conventional scenario and scenario B has no influence on the controllability of the network. For scenario C the number of conditions increases significantly, but is the same for scenario D, so the control properties for these two scenarios are the same. The scenario B and D use the intensified arrangement of the main column and the side stripper for the propylene purification sequence, consequently, using this intensified option does not alter the control of the network but maintains the benefits of energy savings, cost and emission reductions. On the other hand, the topological difference between scenarios A and B with scenarios C and D is the thermally coupled arrangement for ethylene purification, which in this case is the sequence that complicates the controllability of the system. In summary, the network configuration that includes the intensified sequence with a physical rearrangement (main column with side stripper) has as good control as its conventional equivalent, while the configuration with the retrofit sequence makes the network more sensitive to disturbances. To understand why this happens, see Figure 2, the coupling between C-201 and C-202 replaces the reboiler of C-201, as the whole design is fixed, then the steam flow generated in C-202 must supply both columns so a much higher steam flow than in the conventional sequence is expected. And a perturbation of Q2 would generate a backward perturbation affecting the composition of the C-201 distillate (something that does not happen with the conventional sequence), but in turn also affects the C-203 products forward. Something similar happens when looking at the coupling between C-203 and C-202, which replaces the C-202 condenser, and a variation in both, RR3 and Q3, affects both the purity of the C-203 products, as well as the purity of the C-202 and C-201 products. Then in the latter system, the variables have more interactions with each other, mathematically making the gain matrix more ill-conditioned.

* 1. Conclusions

This work presented a study of the control properties of intensified CHOSYNs complementing previous studies that allow advancing in the industrial implementation of CHOSYNs as schemes with responsible production aiming to reduce the environmental impact generated during the processing of carbon, hydrogen, and oxygen compounds. For the case study presented here, intensification was focused on the distillation units, the study findings demonstrate that the control properties of the intensified options are influenced by the specific structures and configurations of the thermodynamic equivalents. Therefore, with the results shown in this study, it is recommended for the case study to use the intensified option for propylene purification, for ethylene purification, other options should be explored.

References

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