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On the selection of control structures using process operability analysis

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ABSTRACT

This work aims to develop a generalizable framework for control structure selection using process operability analysis. Current approaches for selecting controlled variables in chemical processes are limited to assessing system attributes individually, focusing on controller performance or the economic impact based on a constant setpoint policy. However, the competitive industrial manufacturing market requires a holistic approach for control structure selection in large-scale plants that takes into account multiple factors. In particular, process operability can help to enable a generalizable approach that is able to select control structures that are operable considering economic and performance factors simultaneously. To achieve this goal, a framework that uses the Operability Index (OI) as a metric for ranking the achievability of the control objectives for the selected control structures is developed. To test the framework, a depropanizer distillation column is investigated as a case study associated with large-scale energy systems. This work thus introduces novel formulations and algorithms for the control structure selection problem, enhancing the design, operations, and synthesis of existing and future industrial systems.

1. Introduction

In process systems engineering (PSE), the selection of a control structure in an industrial process is essential. It determines how effectively industrial processes can be managed with respect to setpoint changes due to market demands or operational changes, as well as disturbance rejection. Although there are classical methods of selecting control structures based on controllability analysis for example, there is currently a lack of a methodology that encapsulates more than one overall objective in a large-scale process, such as economic profitability, controller performance, market regulations and/or constraints. In PSE, a method that could assist in this choice is process operability analysis (Gazzaneo, Carrasco, Vinson, & Lima, 2020; Lima & Georgakis, 2010; Vinson & Georgakis, 2000). In particular, process operability has been developed as a systematic approach to quantifying simultaneous design and control objectives of a chemical/industrial process early in the conceptual phase. This potentially enables designing a process that when operated in reality, has a higher chance to be operable (i.e., capable of performing the overall objectives that were conceptualized initially). To analyze the operability of any given process model, operability tools perform mapping tasks either in the forward or inverse directions, to obtain regions in the Cartesian system that will give insights into the feasibility and operability of the system studied. However, chemical process models of industrial scale are typically mathematically described as systems of nonlinear equations with nonlinear constraints. Furthermore, there can be input/output multiplicities and/or combinatorial explosions associated with the obtained solutions due to the nature of the problem studied. To address such complexities, the formalization of a method to map the possible control structures of a process in a generalized fashion can be invaluable. Therefore, systematic approaches for the efficient control structure selection employing process operability tools present themselves as an alternative to provide a comprehensive analysis to tackle the control structure selection challenges.

This work aims to propose a new research direction that employs process operability tools in the control structure selection of industrial, large-scale processes. The expectation is that a generalizable and systematic framework is developed, avoiding the use of ad-hoc solutions that are typically employed. To achieve this goal, the formalization of a control structure selection framework employing operability analysis is performed, by introducing a new operability set. The proposed approach should be able to rank control structures based on their operability characteristics, quantified by the operability index, opening a new scientific venue for analysis of industrial processes.

This work is structured as follows: Section 2 outlines prior work and preliminary concepts to situate the reader. Section 3 describes the proposed approach including the formalization of a new operability set, namely the *Setpoint Interval Set* (SIS). Section 4 presents a case study, namely a depropanizer distillation column that has been extensively studied in plantwide control literature (Alves, Lima, Silva,

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& Araujo, 2018; Lima, Alves, & de Araujo, 2020; Skogestad, 2000), and the control structures obtained from an operability perspective are compared against the ones obtained using the Self-Optimizing Control approach (Skogestad, 2000). Lastly, Section 5 gives conclusions and future recommendations.

2. Prior work and preliminary concepts

2.1. Prior work

The control structure selection problem deals with the selection of a subset from a large available set of candidate controlled variables (CVs) to consume degrees of freedom as manipulated variables (MVs) (Umar, Hu, Cao, & Kariwala, 2012). This problem has been studied extensively for example in self-optimizing control research (Araújo & Skogestad, 2008; Cao, Rossiter, & Owens, 1998; Cao & Saha, 2005; de Araújo, Govatsmark, & Skogestad, 2007; Kariwala & Cao, 2009; Kariwala, Cao, & Janardhanan, 2008; Saha & Cao, 2003; Skogestad, 2000). However, in the process operability literature, there is no work on trying to deal with or at least formalize a framework to tackle the inherent combinatorics of the control structure selection problem. There are only works that limit themselves to proof the independence of the operability index (OI) concerning the inventory control layer in plantwide systems (Vinson & Georgakis, 2002) and formalizing operability sets to reduce the dimensionality of plantwide processes (Subramanian & Georgakis, 2005). Therefore, there is an opportunity for employing process operability analysis and characteristics in the optimal selection of controlled variables.

Process operability has been developed in the last twenty years as a framework that allows the qualitative and quantitative assessment of design and control objectives of industrial processes simultaneously, whenever these are subject to disturbances and constraints. It has been employed to steady-state systems and later extended to dynamic processes as well (Gazzaneo et al., 2020; Lima & Georgakis, 2010). Since the introduction of process operability concepts (Georgakis, Uztürk, Subramanian, & Vinson, 2003; Vinson & Georgakis, 2000), numerous advancements have addressed challenges such as high-dimensionality, nonlinearity, and input–output multiplicity in chemical processes. Examples can be mentioned such as response surface modeling (RSM) to reduce model complexity (Georgakis & Li, 2010), as well as nonlinear programming (NLP)-based methods to evaluate feasible outputs and their corresponding inputs (Carrasco & Lima, 2015, 2017a, 2017b). Operability concepts were further refined for plantwide systems, focusing on key variables such as product purity and production rate (Subramanian & Georgakis, 2005). Recently, NLP-based approaches were expanded to encapsulate modularization and process intensification targets, towards modular manufacturing goals. Additionally, mixed-integer linear programming (MILP) formulations for operability analysis were formalized (Gazzaneo et al., 2020; Gazzaneo & Lima, 2019), taking advantage of computational geometry principles to delineate operability regions for process design and control. Moreover, supervised machine learning was used in terms of Gaussian process regression (GPR) to evaluate the operability sets with reduced computational time while maintaining accuracy (Alves, Gazzaneo, & Lima, 2022). Lastly, these algorithms were consolidated into both an open-source MATLAB Operability App (Gazzaneo et al., 2020) and a Python package (Alves et al., 2024), facilitating broader dissemination in academia and industry.

2.2. Control structure selection

Control structure selection is a vast field of study in PSE that encompasses the task of selecting controlled variables (CVs) and manipulated variables (MVs), as well as the pairings between such variables (Umar et al., 2012). When dealing with a chemical process, a considerable amount of output measurements are available, each being a potential CV to be used in a control loop with a respective MV. This task has combinatorial properties based on the number of CVs and MVs as discussed in the literature (Araújo & Skogestad, 2008; Skogestad, 2000). Studies in the 1980s and 1990s have been reviewed in van de Wal and de Jager (2001) based on controllability and achievable performance that lead to CVs that are easy to control, but do not necessarily guarantee the overall objectives of the plant (Umar et al., 2012). In plantwide control and self-optimizing control (Alves et al., 2018; Skogestad, 2000) this problem is well-studied, using the economic loss generated by a feedback control policy as a metric for selecting the CVs. This yields to the analysis of using the economic loss exclusively as a metric for ranking candidate controlled variables among a large subset. Several examples and applications have been tested using this approach such as hydrodealkylation (HDA) (de Araújo et al., 2007) and ammonia synthesis processes (Araújo & Skogestad, 2008) to name a few. A detailed review of applications that take advantage of self-optimizing control concepts to deal with the control structure selection problem is available in Vasudevan and Rangaiah (2012). As an illustrative example, Ref. de Araújo et al. (2007) shows that for the HDA process, with 13 degrees of freedom (MVs) and 70 measurements (CV candidates), there are $\binom{70}{13} = 70!/13!57! = 4.7466 \times 10^{13}$ control structures, excluding alternative inventory control strategies that are also available. Clearly, this can be considered as an NP-hard problem due to its combinatorial properties, drawing the attention of researchers in trying to tailor algorithms to quickly assess the overall subset of CVs and rank them accordingly using for example minimum singular value criterion, Hankel singular values or the self-optimizing control loss as measures (Cao & Kariwala, 2008; Cao et al., 1998; Cao & Saha, 2005; Jones, Bhattacharyya, Turton, & Zitney, 2014; Kariwala & Cao, 2009; Kariwala et al., 2008; Saha & Cao, 2003). In addition, Real-Time Optimization (RTO) strategies have been developed in the literature as an approach to evaluate optimal values for control structures. However, they present challenges related to the cost of model development, in addition to difficulties in quantifying uncertainty and numerical robustness. Conflicts also often arise with the planning layer of decisions in industrial processes, and there are human-related aspects to consider, as RTO requires constant maintenance and monitoring (Krishnamoorthy & Skogestad, 2022). Therefore, despite the promises as being an effective way of determining control structures and its optimal values, RTO is not as widely used in practice as expected (Krishnamoorthy & Skogestad, 2022).

Regarding process operability, the only works that try to link this field with the problem of control structure selection are when proving the independence of the OI from the inventory (regulatory) control layer (Vinson & Georgakis, 2002) and the definition of operability sets for key variables in plantwide control processes (Subramanian & Georgakis, 2005), with none of them mentioning how to address the challenges in the control structure selection in large-scale systems. This leaves a gap in the literature since the control structure selection problem can benefit from a more comprehensive metric that assesses process controllability and achievability in terms of the plant's overall objectives, such as the operability index (OI).

2.3. Process operability concepts

Process operability has been developed as a framework that integrates both design and control objectives simultaneously early in the conceptual phase of industrial processes (Gazzaneo et al., 2020; Lima & Georgakis, 2010), as opposed to the typical sequential design and control assessment that is followed in chemical engineering applications. The process operability approach thus provides guidelines for designing a process that has a higher chance of operating as expected in terms of its overall objectives, as its operability capabilities are not hindered (Alves et al., 2024). In order to perform a process operability analysis, concepts were defined in geometrical terms to quantify the achievability of any given process based on their available inputs, respective achievable outputs and the expected disturbances that might impact a process, as discussed thoroughly in the literature (Gazzaneo et al., 2020; Georgakis et al., 2003; Lima, Jia, Ierapetritou, & Georgakis, 2010; Vinson & Georgakis, 2000).

In mathematical terms, a process model (either derived from first-principles or data-driven) is needed to perform an operability analysis. This model should be able to describe the relationships between the input (manipulated and/or disturbance) and output variables (Georgakis et al., 2003). Strictly speaking, a process model M with m inputs, p outputs, q disturbances and n states, is defined in Eq. (1).

$$M = \begin{cases} \dot{x}_s = f\left(x_s, u, d\right) \\ y = g\left(x_s, u, d\right) \\ h_1\left(\dot{x}_s, x_s, y, \dot{u}, u, d\right) = 0 \\ h_2\left(\dot{x}_s, x_s, y, \dot{u}, u, d\right) \geq 0 \end{cases} \tag{1}$$

In which $u \in \mathbb{R}^m$ are the input variables, $y \in \mathbb{R}^p$ correspond to the process outputs, $d \in \mathbb{R}^q$ are disturbance variables and $x_s \in \mathbb{R}^n$ are state variables. In addition, f and g are nonlinear maps and h_1 and h_2 correspond to equality and inequality process constraints, respectively, if present.

Based on the process model M and the aforementioned variables, operating spaces named as operability sets were formalized to allow the operability calculations and quantification of a metric defined as the operability index (OI) (Georgakis et al., 2003). These sets are briefly summarized below, based on literature (Alves et al., 2022).

Available Input Set (AIS): Manipulated inputs ($u \in \mathbb{R}^m$) based on the design of the process that is limited by the process constraints (Vinson & Georgakis, 2000). These are typically manipulated variables and/or design variables.

$$\text{AIS} = \left\{u \mid u_i^{\min} \leq u_i \leq u_i^{\max}; 1 \leq i \leq m\right\} \tag{2}$$

Expected Disturbance Set (EDS): Disturbance variables ($d \in \mathbb{R}^q$) that can represent process uncertainties and variabilities. Disturbances of endogenous or exogenous nature are common in process control applications. Examples of these can be cited as parametric uncertainty due to parameters of the model (e.g., kinetic parameters, activation energy constants, heat/mass transfer coefficients; Dinh & Lima, 2023) or process conditions that are not controllable, such as the ones coming from upstream processes (inlet feed temperatures, inconsistent feed streams, etc.). The characterization of such disturbances are described below as bounds of the expected disturbance range (Dinh & Lima, 2023) as in Eq. (3). An alternative EDS formulation can also be found in the literature (de Araujo, Lima, & Bispo, 2021; Dinh & Lima, 2023) as being an ellipsoid that represents correlated data as described in Eq. (4).

$$\text{EDS} = \left\{d \mid d_i^{\min} \leq d \leq d_i^{\max}; 1 \leq i \leq q\right\} \tag{3}$$

or

$$\text{EDS} = \left\{d \mid (d - \bar{d})^{\mathrm{T}} \Sigma^{-1} (d - \bar{d}) \leqslant l^2; \quad l^2 = \text{Inv}_{\chi^2}\left(99\%; n_d\right)\right\} \tag{4}$$

In which $\bar{d}$ is the mean of the disturbances and Σ the covariance matrix that represents the correlated disturbance variables. Also, l^2 corresponds to the inverse cumulative distribution function of the chi-squared statistics with n_d degrees of freedom (Dinh & Lima, 2023). The 99% or $\approx \pm 6\sigma$ is chosen as a bounding factor of the originally unbounded distribution (Dinh & Lima, 2023) as most of the statistics tend to the Gaussian at this level of confidence.

Achievable Output Set (AOS): Range of the outputs ($y \in \mathbb{R}^n$) that can be achieved using the inputs inside the AIS for a given disturbance d from the EDS. This set is obtained through the forward mapping of the process model.

$$\text{AOS}(d) = \{y \mid y = M(u, d); u \in \text{AIS}, d \text{ is fixed}\} \tag{5}$$

Desired Output Set (DOS): Corresponds to production/target/efficiency requirements for the outputs that do not necessarily meet

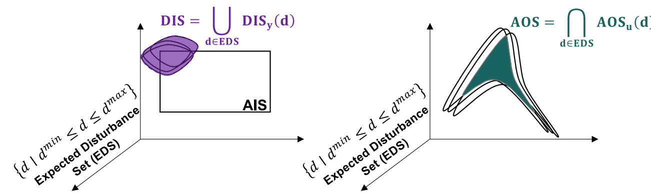

Fig. 1. The effect of the Expected Disturbance Set (EDS) on the AOS and DIS.

the ranges of the AOS. Typically, the definition of the DOS ranges is made in an ad-hoc fashion by the researcher/practitioner, based on market demands, process knowledge and/or product specifications for a specific plant operation.

$$\text{DOS} = \left\{y \mid y_i^{\min} \leq y_i \leq y_i^{\max}; 1 \leq i \leq n\right\} \tag{6}$$

Although the AIS and DOS are commonly represented as box-constraints, this is not a hard requirement and can be written as intervals (Lima et al., 2010) or constrained spaces by nonlinear equations.

Desired Input Set (DIS): Set of inputs required to reach the entire DOS, given a disturbance vector d. In order to obtain the DIS, an inverse mapping technique is required, either based on nonlinear programming (NLP) (Carrasco & Lima, 2015, 2017a, 2017b, 2018) or via differentiable programming (Alves, Kitchin, & Lima, 2023).

$$\text{DIS}(d) = \left\{u \mid u = M^{-1}(y, d); y \in \text{DOS}, d \text{ is fixed}\right\} \tag{7}$$

An additional remark that is worth making here regards to the effect of the EDS in the operability sets. The effect of the EDS on the AOS and DIS calculations is to shift them throughout the specified disturbance range, as depicted in Fig. 1.

Hence, both the AOS and the DIS would need to be rewritten in the output space and input space respectively, in order to reflect this shift. For the AOS, it will be represented as the intersection of each AOS for each disturbance realization, $\text{AOS}_\text{u}(\text{d})$:

$$\text{AOS} = \bigcap_{d \in \text{EDS}} \text{AOS}_u(d) \tag{8}$$

And as the union of each DIS in the input space ($\text{DIS}_\text{y}(\text{d})$) for each disturbance realization:

$$\text{DIS} = \bigcup_{\mathbf{d} \in \text{EDS}} \text{DIS}_y(d) \tag{9}$$

Lastly, Fig. 2 illustrates the connection among the main process operability sets based on the definitions described in this section. In the first part (A), the bounds for the manipulated and/or design variables define the AIS. The evaluation of the AIS through the process model (M) yields the AOS (B). A desired operating region from the outputs' perspective defines the DOS with its intersection with the AOS shown in red (C). Lastly, the DIS is obtained via an inverse mapping (M^{-1}), and its intersection with the AIS is illustrated in red as well (D).

After the definition of the operability sets, the operability index (OI) is formalized as shown in Eqs. (10)–(11) from the input and output perspectives, respectively. A process is said to be fully operable when the OI is 1 (there is total intersection between desired and achievable operations) and if it is less than 1, some regions of the DOS are not achievable (Lima & Georgakis, 2010) (with partial intersection between desired and achievable operations).

$$\text{OI} = \frac{\mu(\text{AOS} \cap \text{DOS})}{\mu(\text{DOS})} \tag{10}$$

$$\text{OI} = \frac{\mu(\text{AIS} \cap \text{DIS})}{\mu(\text{DIS})} \tag{11}$$

In which μ indicates the measure of regions. The definition of this measure varies depending on the dimensionality of the considered sets.

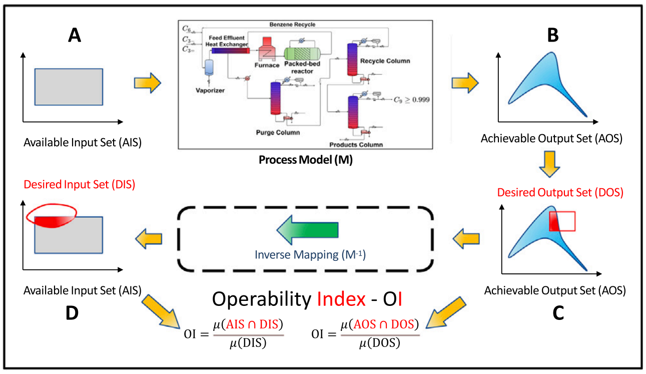

Fig. 2. Visual exploration of main process operability sets and definitions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

For a 1D system, this would be a length measure, for 2D systems an area, for 3D systems a volume, and hypervolumes for systems of higher dimensionality (Gazzaneo et al., 2020).

The evaluation of the OI from either perspective depends on the objective of the operability analysis and opens the possibility of choice for the researcher/practitioner as well. Additionally, the numerical value of the OI is the same from the inputs and outputs perspective exclusively when analyzing a linear model (Georgakis et al., 2003). When dealing with nonlinear systems and models, the evaluation of the OI from the input and output perspectives yields different values and the choice of evaluating from an input or output perspective depends on the overall objective of the study. For the inverse mapping problem that naturally arises when obtaining optimal and modular design regions (Carrasco & Lima, 2015, 2017a, 2017b, 2018), the analysis of the OI from the inputs perspective should be the choice. When investigating the output operability characteristics of systems given a certain set of inputs, the evaluation of the OI from the outputs perspective would be selected. This flexibility in choosing in which domain the operability analysis will take place greatly helps researchers when investigating the capabilities of a given process. In this work, as the objective is to use the OI to rank competing control structures, the outputs perspective is chosen to analyze the overall objectives of a given process with given set points regions.

Irrespective of the perspective employed, the following features of the OI makes it an attractive metric for a PSE application:

1. Inherently nonlinear metric (Vinson & Georgakis, 2000). This was one of the original motivations for formalizing process operability analysis. The original idea was to have a nonlinear measure of output controllability that is generalizable and that could serve as a counterpart to measures of controllability that are usually available in the literature from linear control systems theory.
2. Independence of the type of controller used (Vinson & Georgakis, 2002). This is one of the most important properties of the OI. It allows the analysis of the system's operability characteristics regardless of the controller type that will be implemented (e.g., decentralized PIDs, Model Predictive Control - MPC, etc.), in terms of setpoint tracking and disturbance rejection capabilities. This is particularly important when analyzing competing control structures, which is the scope of this paper.
3. Disturbances' evaluations under "worst-case" scenario situations. Since the OI is independent of the controller type and it can be interpreted as a fundamental characteristic of the system studied, it will give the best (or worst) possible performance in terms of disturbance rejection. Once again, another feature that is of paramount importance when synthesizing a control structure.

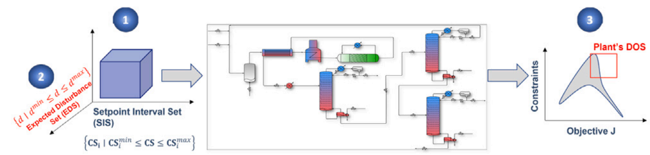

Fig. 3. Steps 1–3: Defining one SIS for each control structure, the respective EDS for the overall process, and the plant overall objectives in the AOS/DOS. This allows the evaluation of several control structures contained within each SIS in the next steps.

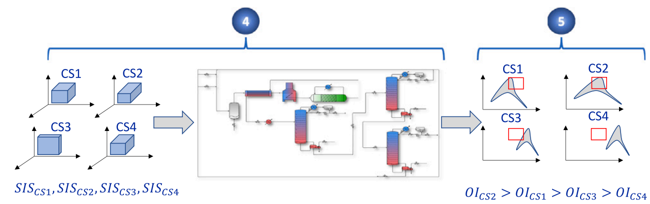

Fig. 4. Steps 4–5: The process model is run for each SIS at all discretized setpoint values, and for each disturbance scenario in the EDS. With each AOS obtained for each SIS, the OI can be evaluated for each control structure and ranked in descending order.

3. Proposed approach

The control structure selection framework employing process operability analysis for plantwide systems is presented in this section and the results in the next section show that process operability metrics can be used as a tool to rank control structures. The fundamental idea of using operability analysis to help solving the control structure selection problem is to use the operability index (OI) as a measure of achievability of control structures, being able to rank them from more operable to less operable. This way, the CVs can be chosen at the conceptual design phase using a steady-state model of the process, guaranteeing that the CVs held constant would maximize the operability of a given system. The main assumptions of the conceptualized framework are:

1. There is integral action on the yet-to-be-implemented control structure: This assumption is needed since integral action guarantees no offset and the desired steady states can be fully reached.
2. The analyzed process is governed by steady-state operation: Since a steady-state process model is used, it is implicitly assumed that its operation is governed by fixed set points instead of a trajectory (e.g., in batch operations).

The proposition is that the use of process operability analysis, with the inherent OI measure as a metric to assess control structures, would yield more comprehensive control structures. Essentially, instead of analyzing exclusively economic profitability or controller performance, the multidimensional characteristic of the operability sets allows for the synthesis of AOS/DOS regions that encapsulates several objectives of a given process simultaneously. In addition, the operability sets are generalizable, as the researcher/practitioner is the one who selects what variables will constitute each dimension of such sets. Lastly, this approach potentially bridges a gap between process operability theory and industrial implementation as the control structure selection problem is relevant for industrial systems.

The main steps of the proposed method are depicted and numbered accordingly in Figs. 3–4 and discussed step-by-step in this section.

The main steps of the proposed method are:

1. **Employ a newly defined operability set, the Setpoint Interval Set (SIS) to quantify the achievability of the analyzed control structures:** In this step, the ith control structures, CS_i, are listed, and the ranges for each candidate controlled variable

are defined. This way, each control structure will have one SIS composed of not necessarily the same variables.

2. **Define the EDS for study:** In this step, the EDS variables and their respective ranges are selected. This step will ensure that the proposed approach will evaluate the operability index (OI) for each control structure taking into consideration the effect of disturbances. This way, the control structures with the highest OIs are promising as they have better disturbance rejection capabilities. On the other hand, control structures with low values of the OI ($OI \approx 0\%$) are unable to reject the selected disturbances and need to be discarded.
3. **Define the AOS/DOS considering the plant's overall objectives:** The goal in this step is to incorporate the main objectives of the plant (e.g., related to product specifications, pollutant emissions and/or sustainability metrics; Li, Ruiz-Mercado, & Lima, 2020) into the dimensions of the AOS/DOS. The limits of the DOS are defined according to process knowledge, market demands and/or product specifications. For example, possible dimensions of the DOS can be the plant's economic objective function and the main product purity, such as in distillation columns, or even the conversion in a chemical reactor.
4. **Evaluate process model for each SIS and each disturbance in the EDS:** For each SIS and EDS defined in previous steps, the process model is evaluated. The AOS is then obtained, encompassing the overall plant's objectives and compared against the DOS via the OI calculations.
5. **Assess control structures:** With all simulations performed, each control structure comprehended within each SIS will have a respective value for the OI. All SISs are then ranked in descending order and the control structure with the highest OI is selected for implementation in the actual process.

In the schematic in Fig. 4, it can be seen in this illustrative example that control structure #2 (SIS_{CS_2}) has an AOS that intersects the most with the DOS, followed by SIS_{CS_1}, then SIS_{CS_3} and lastly SIS_{CS_4}, which has no intersection with the DOS and hence, an OI of 0%. Therefore, the structures can be ranked as $OI_{CS_2} \geq OI_{CS_1} \geq OI_{CS_3} \geq OI_{CS_4}$. This analysis is general and works for any process, although a large-dimensional example may result in a combinatorial problem that still needs to be systematically addressed (by tailoring optimization-based algorithms, for example) rather than by exhaustive enumeration, which is running each case individually, as performed in this work. Lastly, if there are any multiplicities between the SIS-AOS mapping for a control structure, this is an indicator that the SIS yields multiple operable regions in terms of the overall objectives encapsulated within the AOS.

4. Case study - Depropanizer distillation column

A depropanizer distillation column is used to test the proposed framework. This process has been studied in the context of Self-Optimizing Control (SOC) (Alves et al., 2018; Lima et al., 2020; Skogestad, 2000), for which the results can be analyzed and compared against the newly introduced approach. Instead of ranking control structures based on the loss incurred by not employing real-time optimization as in SOC (Skogestad, 2000), here the control structures are to be ranked based on their operability characteristics, quantified by the OI. The process example studied is depicted in Fig. 5, in which all six degrees of freedom are highlighted in red, and the system is modeled in Aspen Plus®.

From the six available degrees of freedom, three need to be consumed to guarantee stable operation (reboiler, condenser holdups, as well as pressure inventory control Skogestad, 2000) and have no steady-state effect, and the feed is considered as given. Thus, there are two remaining degrees of freedom available to keep the process

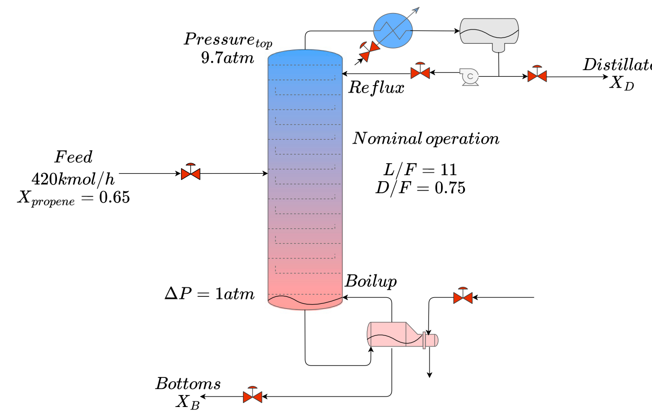

Fig. 5. Depropanizer distillation column based on Alves et al. (2018), Lima et al. (2020) and Skogestad (2000). Degrees of freedom are highlighted in red. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Candidate controlled variables (CV) for depropanizer case study that compose the SIS.

Controlled Variable (CV)	Lower bound	Upper bound
Reflux ratio (RR) [mol basis]	10	15
Distillate-to-feed ratio (D/F) [mol basis]	0.6	0.9
Sensitive tray temperature (T_{133}) [°C]	25	29
Reflux-to-feed ratio (L/F) [mol basis]	8.5	12
Boilup-to-feed ratio (V/F) [mol basis]	8.5	12

at the desired operation. Following Alves et al. (2018), the economic operation per hour is given by Eq. (12).

$$J = 20D + (10 - 20x_B)\, B - 70Q_R \text{ [\$/h]} \tag{12}$$

In which D and B are molar flow rates [kmol/h], x_B molar composition and Q_R the reboiler duty [GJ/h]. In addition, there is a purity constraint for propene, $x_D \geq 99\%$. The plant's objective function and the purity constraint will form the AOS/DOS. The next step is to select candidate controlled variables (CV) that will form each SIS. The following variables are selected and shown in Table 1 with no loss of generality, based on the literature (Alves et al., 2018; Lima et al., 2020; Skogestad, 2000).

With five measurements and two degrees of freedom, there are

$$C_2(5) = \binom{5}{2} = \frac{5!}{2!(5-2)!} = 10 \tag{13}$$

possible control structures, which are the following:

$$CS_1 = \begin{pmatrix} RR \\ D/F \end{pmatrix}, \quad CS_2 = \begin{pmatrix} L/F \\ T_{133} \end{pmatrix}$$
$$CS_3 = \begin{pmatrix} RR \\ T_{133} \end{pmatrix}, \quad CS_4 = \begin{pmatrix} V/F \\ T_{133} \end{pmatrix}$$
$$CS_5 = \begin{pmatrix} RR \\ L/F \end{pmatrix}, \quad CS_6 = \begin{pmatrix} RR \\ V/F \end{pmatrix}$$
$$CS_7 = \begin{pmatrix} D/F \\ T_{133} \end{pmatrix}, \quad CS_8 = \begin{pmatrix} D/F \\ L/F \end{pmatrix}$$
$$CS_9 = \begin{pmatrix} D/F \\ V/F \end{pmatrix}, \quad CS_{10} = \begin{pmatrix} L/F \\ V/F \end{pmatrix}$$

For the DOS, the lower bound for the economic objective function is chosen to be the optimally nominal value reported in Ref. Alves et al. (2018) of 2760 \$/h for a slighlty overpurified operation of $x_D = 99.5\%$ and an upper bound of +25% of the economic optimum under nominal disturbances is employed. The EDS is comprised of the propene

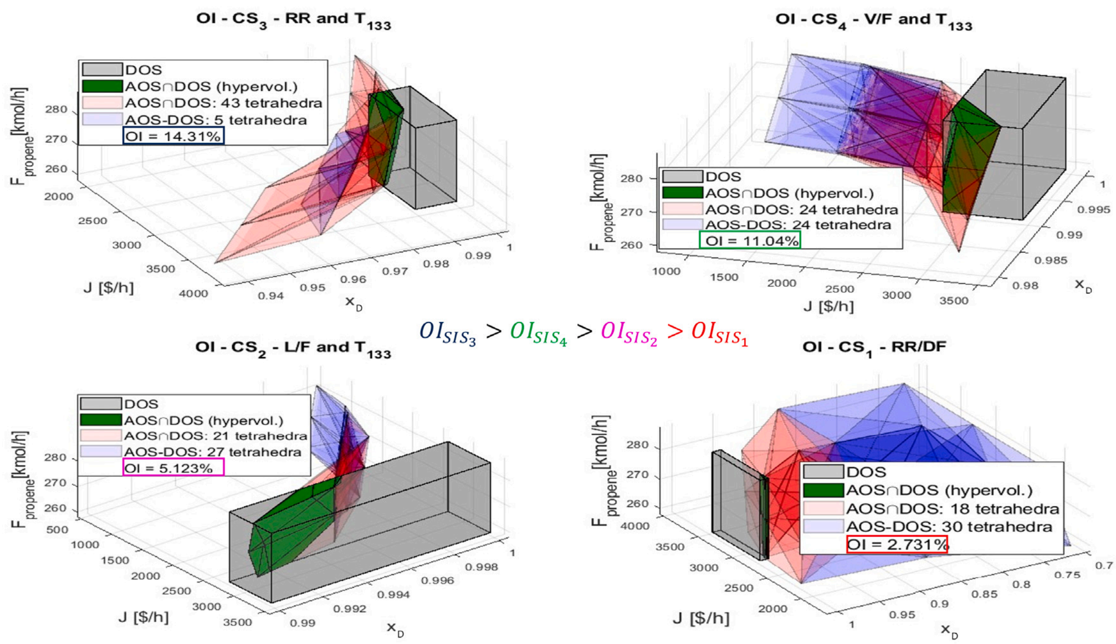

Fig. 6. Operable control structures: $OI_{SIS_3} > OI_{SIS_4} > OI_{SIS_2} > OI_{SIS_1}$.

flow rate in the feed under a ±10% variation. With the definition of all SISs representing each control structure, as well as the EDS and the plant's desired operation represented in the DOS, each scenario is run to obtain the plant's AOS for each SIS. The multimodel approach in Gazzaneo, Carrasco, and Lima (2018) and Gazzaneo and Lima (2019) is then used to evaluate the OI for each case, aided by the Process Operability App in MATLAB® (Gazzaneo et al., 2020), by establishing an ActiveX/COM connection between MATLAB® and Aspen Plus®. The results of this analysis are depicted in Figs. 6–7, which are separated between operable and non-operable control structures, respectively.

For the first group (operable control structures) shown in Fig. 6, it can be seen that some of the control structures using the sensitive tray temperature have the highest operability index values, namely

$$\begin{aligned} SIS_3 &= \begin{pmatrix} RR \\ T_{133} \end{pmatrix} > SIS_4 &= \begin{pmatrix} V/F \\ T_{133} \end{pmatrix} > \\ SIS_2 &= \begin{pmatrix} L/F \\ T_{133} \end{pmatrix} > SIS_1 &= \begin{pmatrix} RR \\ D/F \end{pmatrix} \end{aligned} \tag{14}$$

This is an important result that validates the proposed approach against the result in the literature (Alves et al., 2018) since it is known that for distillation processes, the use of sensitive tray temperatures, as well as feedforward strategies should enable improved control performance. The remaining control structures are not operable ($OI = 0\%$) considering the EDS bounds and their operability analyses as shown in Fig. 7.

To directly compare the proposed approach against the well-established work in Self-Optimizing Control (SOC), a study was performed by generating the control structures from the SOC perspective. Results for a similar study from the SOC standpoint have been generated in literature (Alves et al., 2018) for a similar distillation column problem (Skogestad, 2000). For a fair comparison, the same study conducted here from an operability perspective is reassessed from a SOC perspective to compare the control structures obtained. The expectation is that the most promising control structures from an operability standpoint (e.g., the ones with the highest OI) will incur in the lowest loss from a SOC perspective.

In order to accurately compare both operability-based and SOC-based control structure selections, the metacontrol software (Lima et al., 2020) is employed as it allows the connection with the process simulator and generation of the best SOC-based control structures after creating a surrogate model based on a computational experiment. The SOC-based analysis employed uses the exact local method with analytical solution from the literature (Alstad, Skogestad, & Hori, 2009) coupled with a bidirectional branch-and-bound algorithm tailored for SOC (Cao & Kariwala, 2008; Kariwala & Cao, 2009, 2010) that automatically pre-screens the most promising CV candidates for control structures, including linear combinations of measurements as CVs. For the sake of simplicity, only single measurements were taken into consideration here. However, this is not a constraint to the proposed approach, as linear and even nonlinear expressions can be constructed as CV candidates and incorporated into the SIS, as long as the constituents of these expressions can be evaluated from the process model (M).

Table 2 shows the most promising control structures in descending order of the OI, which were (as expected) the same order for the top structures in terms of economic loss from a SOC standpoint.

In addition, these results show that even though some of the control structures from a SOC standpoint are theoretically possible (e.g., CS_6 and CS_5), as they might be controllable around the nominal setpoint assuming the active constraints do not change (a premise of the exact local method Alstad et al., 2009), they are not operable from an operability standpoint as it can be evidenced by Fig. 7, for the selected DOS. As the OI corresponds to a metric that encapsulates the achievability of a (possibly) multidimensional region, its use as a metric is more comprehensive to quantify how promising a control structure will be when disturbances and setpoint changes happen as opposed to the SOC-loss evaluation which compares exclusively optimal operation (RTO) against a constant setpoint policy. In addition, it is worth mentioning that the SOC approach employed is based on local linearization of the nominal economic optimal point, and the farthest from that point, the worst the prediction of the loss. On the other hand, the operability approach uses the full nonlinear model to generate polytopic regions in which the computational geometry operations are employed, which might yield a more accurate depiction of the control structures feasible region.

These results show that process operability metrics can be used to systematically assess promising control structures early in the design phase of a chemical process. The proposed approach offers a significant benefit as it allows for safely discarding control structures that do not

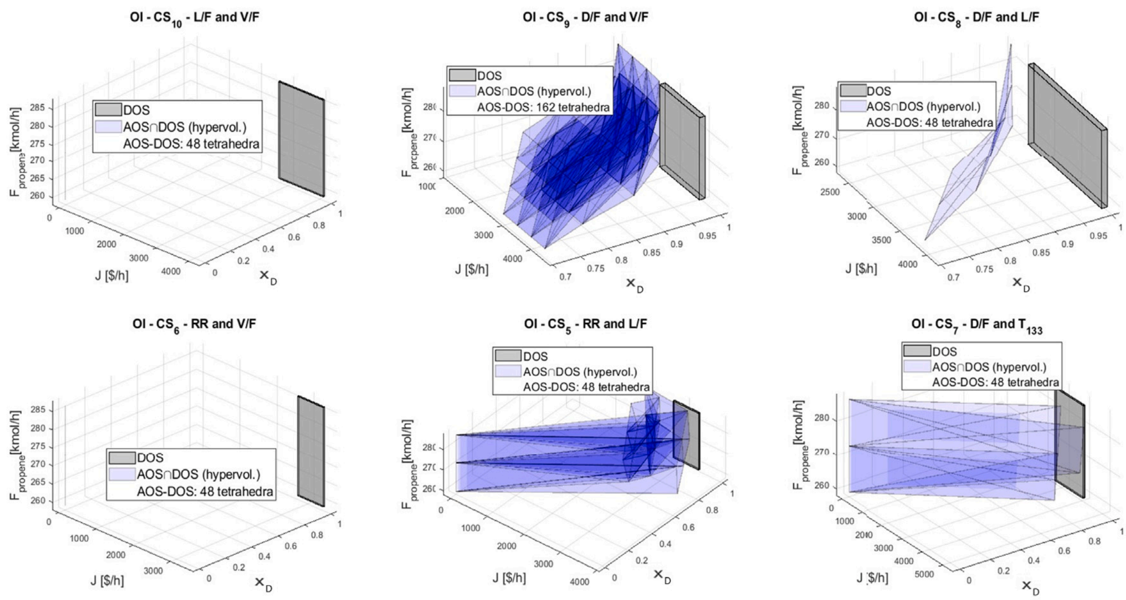

Fig. 7. Non-operable control structures: SIS_{10}, SIS_9, SIS_8, SIS_6, SIS_5, SIS_7.

Table 2
SOC-based *vs.* OI-based results for different control structures for depropanizer case study.

Control structure	Operability Index (OI) [%]	SOC average-case loss [$/h]	SOC worst-case loss [$/h]
$CS_3 - RR\,|\,T_{133}$	14.310	1.011	7.706
$CS_4 - V/F\,|\,T_{133}$	11.040	1.171	7.796
$CS_2 - L/F\,|\,T_{133}$	5.123	1.174	7.862
$CS_6 - RR\,|\,V/F$	Not operable	14.020	125.202
$CS_5 - RR\,|\,L/F$	Not operable	15.381	137.417
$CS_1 - RR\,|\,D/F$	2.731	1111.728	10 003.559
$CS_8 - D/F\,|\,L/F$	Not operable	1187.642	10 685.826
$CS_9 - D/F\,|\,V/F$	Not operable	1196.062	10 761.601
$CS_{10} - L/F\,|\,V/F$	Not operable	3633.690	32 701.619
$CS_7 - T_{133}\,|\,D/F$	Not operable	15 163.794	136 468.733

meet the plant's objectives based on the operability characteristics. This can assist both researchers and practitioners in concentrating on promising control structures for further analysis and subsequent controller design.

5. Conclusions

In this work, an approach for generating control structures based on process operability analysis was formalized and proposed for the first time. A new operability set, namely the Setpoint Interval Set (SIS) was defined in order to encapsulate the different control structures that define the possible CV candidates. The AOS and the DOS were adapted for employing the overall objectives of the industrial process studied, including economics and process constraints as needed. The application to the case study which served as a benchmark showed that the same promising control structures were found from an operability perspective, when compared against the SOC-based strategy that is well-known in the literature, thus validating the findings in this work. The proposed framework is capable of providing advances by producing systematic solutions for existing and emerging systems in which ad-hoc strategies should be avoided for the control structure selection problem. This yields a more comprehensive method for selection of control structures when compared to ad-hoc and existing strategies. Although this work contributes to formalizing the control structure selection problem from an operability point-of-view, work needs to be done to automate the pre-screening of this combinatorial problem as a future direction, following for example similar formulations (Kariwala & Cao, 2009; Kariwala et al., 2008) performed in the context of Self-Optimizing Control. Lastly, formulations of the proposed approach for dynamic systems could employ dynamic operability concepts (Dinh & Lima, 2023; Uztürk & Georgakis, 2002). Hence this work can be expanded using dynamic operability concepts to further advance the ideas here proposed.

CRediT authorship contribution statement

Victor Alves: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Fernando V. Lima:** Writing – review & editing, Writing – original draft, Supervision, Resources, Project administration, Funding acquisition, Conceptualization.

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.

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