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Application of dynamic flexibility index for evaluation of process control system designs

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ABSTRACT

Traditionally, the process control systems have been evaluated on the basis of nominal model parameters and operating conditions. However, sole reliance on such criterion does not always guarantee operability if some uncertain parameters deviate from their assumed levels. Flexibility analysis has long been successfully adopted to quantify the ability of a given process to maintain its feasibility. This paper presents the use of the dynamic flexibility index (FI_d) for assessing the capability of PID controller of any given process system. In order to calculate FI_d efficiently, the computation strategy proposed by Ali et al. (2021) has been adopted. In particular, the dynamic flexibility index has been used as an additional criterion along with the integrated square of error, to determine suitable controller parameters. It has been shown in the case studies presented that FI_d can effectively complement the traditional tuning methods to enhance both operability and controllability in practical applications.

1. Introduction

The chemical process systems have traditionally been designed according to the nominal operating conditions and nominal parameter values, while their performances are usually evaluated with economic criteria. However, due to the complex and dynamic nature of the realistic operations in the plant, design uncertainties are inevitable. Such uncertainties are not always stochastic, as they may arise either from the unexpected exogenous disturbances (such as those in feed qualities, product demands, and environmental conditions) or from the inexplicable errors in estimation of model parameters (such as heat transfer coefficients, reaction rate constants, and other physical properties). Therefore, there is a need to account for uncertainties at the design stage. The ability of a chemical process to maintain uninterrupted operation over a definite range of uncertain conditions is usually referred to as its operational flexibility. Several computation approaches to facilitate quantitative flexibility analysis have already been proposed and were made readily available in literature (Zhou et al., 2009; Chang and Adi, 2018).

The steady-state flexibility index, usually denoted as FI_s, has been used basically as a gauge of the feasible region in the parameter space for the continuous processes (Swaney and Grossmann, 1985a, 1985b; Lima et al., 2010). This index is associated with the maximum allowable deviations of the uncertain parameters from their nominal values, throughout which a feasible operation can be ensured with proper adjustment of the manipulated variables. It was also shown by Swaney and Grossmann (1985a) that, under certain convexity assumptions, the critical points that limit a system's variability must lie on the vertices of the hypercube inscribed in the parameter space. This particular insight is the foundation of the so-called "vertex method" for computing the flexibility index. In a later study, Grossmann and Floudas (1987) tried to simplify the bi-level optimization problem in the vertex method by exploiting the fact that the active constraints represent bottleneck of a flexible design, and developed a mixed integer linear program (MILP) and a mixed integer nonlinear program (MINLP) corresponding to the linear and nonlinear system constraints respectively. This development was facilitated by formulating the Karush-Kuhn-Tucker (KKT) necessary conditions for optimization in the lower-level problem of the bi-level formulation and then by using them as constraints in the upper-level problem. The calculation procedure has been referred to as the "active set method."

Dimitriadis and Pistikopoulos (1995) later suggested characterizing flexibility of an unsteady system with the dynamic flexibility index (FI_d). This index represents the largest scaled deviation of the uncertain parameter profile that the design can tolerate while remaining feasible throughout the operation horizon. Two computation algorithms, which

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are the extended versions of the aforementioned vertex method and active set method, have been proposed by Kuo and Chang (2016) and Wu and Chang (2017), respectively. Basically, most of the recent works in this area have focused upon improving the computational efficiency of flexibility index and its application for process design. There have been attempts to improve the efficiency of operational flexibility analysis through quantifier elimination, cylindrical algebraic decomposition and derivative free optimization in the studies carried out by Zhao and Chen (2018), Zheng et al. (2020) and Zhao et al. (2021), respectively. There have also been a significant number of studies performed to integrate economic and environment assessment with flexibility analysis (Pretoro et al., 2019, 2022; Eini et al., 2020; Cortes-Pena et al., 2020). Liu et al. (2021) applied flexibility analysis to the heat exchanger network (HEN) design with the downstream path method to ensure production stability under process disturbances. Tang and Daoutidis (2019) proposed a computation method which made use of the Lyapunov function for facilitating artificial design decisions so as to improve the efficiency of dynamic flexibility quantification in non-linear process systems.

Considerable work has also been done in the area of integrated process design and control in previous decades (Mohideen et al., 1996; Bahri et al., 1997; Malcolm et al., 2007; Yuan et al., 2012). With the advancement of computation capabilities, this area has regained the attention of many PSE researchers. Specifically, Pretoro et al. (2021) proposed the evaluation of switchability index, which may be defined as the ratio of dynamic and steady-state flexibility indices of a process and can be used to quantify the ability of the process to maintain its feasibility during the transient state. In another study, Gaspar et al. (2016) performed simultaneous controllability and flexibility analysis for a carbon capture process.

Although successful applications on specific examples were reported in the literature, the aforementioned methods are still not mature enough for the dynamic flexibility analysis in practice. It is often tedious to compute FI_d with the vertex method even for moderately complex dynamic systems. This is due to an overwhelmingly large number of vertices created by the need to discretize the differential equations in implementing the extended vertex method. In particular, if n_θ is the number of uncertain parameters and M is the number of discretized intervals over the entire time horizon, then $(2^{n_\theta})^{M+1}$ should be the total number of vertices. As mentioned before, in the case of the active set method, the KKT conditions of the lower-level optimization problem of the bi-level formulation must be incorporated to formulate the mathematical model in the upper level. These auxiliary constraints, which include the lagrangian and the complementarity requirements for the stationary conditions, help in determining the set of active constraints. Since an extremely large number of binary variables are introduced in developing this formulation due to discretization over the entire time domain, convergence to the existing global optimum may take an overwhelming amount of time with the currently available well-established solvers (Sahinidis and Grossmann, 1991; Ali et al., 2021). As a result of the aforementioned computational complexities, the literature available in this area still lacks systematic and explicit applications of the dynamic flexibility analysis for process control system designs under uncertainties.

To circumvent the above-mentioned deficiency, a genetic algorithm (GA) assisted vertex enumeration technique was proposed by Ali et al. (2021) to improve the computation efficiency of the dynamic flexibility index. As FI_d can be estimated more easily with this approach, it becomes more convenient to use it as an extra performance measure for process control enhancement. Therefore, the main objective of the current study is to show that utilization of the dynamic flexibility index as an additional criterion is both effective and necessary for selecting practically suitable controller parameters.

The rest of the paper is organized as follows. Firstly, in Section 2, a brief review of the genetic algorithm based FI_d evaluation strategies is outlined. A generalized procedure for flexibility analysis based controller design is presented in Section 3. Section 4 depicts the numerical results obtained by applying the proposed design strategies to two dynamic processes of different natures and complexities. Section 5 highlights the significance of dynamic flexibility analysis in feedback controller tuning, while the concluding remarks are given in the last section.

2. Review of GA-assisted vertex enumeration strategy for FI_d evaluation

To implement the genetic algorithm (Holland, 1992), every chromosome in the aforementioned vertex enumeration based evaluation procedure is encoded with the time points at which the critical corner of the feasible region of uncertain parameters shifts. Specifically, the chromosome can be constructed with a sequence of n_zN_z+1 genes, i.e., $(\widetilde{t}_1,\widetilde{t}_2,\cdots,\widetilde{t}_{n_zN_z+1})$, where $\widetilde{t}_l$ denotes the l^{th} $(l=1,2,\cdots,n_zN_z+1)$ time point at which the corner shift takes place. Note that the total number of such time points (i.e. $\widetilde{t}_1,\widetilde{t}_2,\cdots,\widetilde{t}_{n_zN_z+1}$) is bounded by the maximum number of inequality constraints that might go active (Grossmann and Floudas, 1987), i.e. n_zN_z+1, where n_z and N_z respectively denote the number of manipulated variables and the number of time intervals in each of which the corresponding manipulated variable is maintained at a constant level. This is because of the fact that an inequality constraint most likely goes active in response to drastic change(s) in one or more uncertain parameter. The GA-assisted vertex enumeration procedure was implemented via GAMS, MATLAB platforms and their interface. This two-stage procedure can be summarized as follows:

1. The individuals (chromosomes) in the first generation are created with the random number generator embedded in MATLAB. The lower-level maximization problem in Eq. (A12) in Appendix and the corresponding constraints is solved with GAMS for every individual in each generation. The upper-level minimization in Eq. (A12) for each generation is performed through genetic algorithm in MATLAB by selecting the smallest value among all δ_k. The smallest δ_k value amongst all generations is chosen as the dynamic flexibility index FI_d corresponding to the given N_z.
2. The above evaluation steps of FI_d are performed repeatedly by gradually increasing the number of manipulated-variable pieces, N_z. The computation is terminated when the FI_d value converges. The resulting FI_d is considered to be the dynamic flexibility index for the given system.

To better understand the advantages of incorporating GA to the vertex based strategy for the FI_d evaluation, let's consider the scenario of a simple dynamic system with a single uncertain parameter (θ) and 800 discretized intrevals (M) over the entire time horizon. In such case, if the exhaustive vertex enumeration tecnique, i.e., Eqs. (A10) and (A11) in the Appendix, is followed, $2^{801}(=1.33\times10^{241})$ ietrations are needed before reaching the final solution. On the other hand, if the GA-assited vertex enumeration technique is utilized in a 100-generation run with 20 individulas in each generation, then only 2000 iterations are required. Also, in a previous study performed by Ali et al. (2021), it was found that the GA-assited vertex enumration technquie can speed up FI_d quantification by almost 20 times, while it still maintains the solution accuracy at a very high level.

3. Flexibility analysis for process control system design

After obtaining the dynamic flexibility index of a given process with the aforementioned computational strategy, this FI_d value may then be utilized for checking the feasibility of the corresponding control system. Specifically, $FI_d<1$ implies that the process system is operable only up to a fraction of the expected ranges of uncertain parameters. On the other hand, for the process system to be feasible over the entire range of each expected uncertain deviations, the FI_d value should be greater than or equal to one. Moreover, notice that the integrated squared error (*ISE*), defined by Eq. (1) below, has been extensively used as a parameter for characterizing the controller performance (Luyben and Luyben, 1997; Seborg et al., 2004; LebLanc and Coughanowr, 2009; Romgnoli and Palazoglu, 2012).

$$ISE = \int_0^\infty e(t)^2 dt \tag{1}$$

Therefore, through simultaneous evaluation of these two aforementioned measures (FI_d, ISE), a quantitative approach can be developed to ensure that the given control system is operable throughout the time horizon and also that satisfactory controller performance can still be achieved during operation. Specifically, the PID controller is first tuned with the standard prevalent methods such as, Ziegler Nichols (ZN) (Ziegler and Nichols, 1942), Tyreus Luyben (TL) (Tyreus and Luyben, 1992), Direct Synthesis (DS) (Chen and Seborg, 2002) and Internal Model control (IMC) (Rivera et al., 1986), etc., and then the dynamic flexibility indices of the controlled process are evaluated, respectively. The corresponding *ISE* values are also determined accordingly. The resulting design procedure can be summarized as follows:

1 Evaluate FI_d and *ISE* values of the controlled systems constructed with the same uncontrolled process and different PID controllers (which are tuned with various standard tuning methods).
2 Select the control systems for which $FI_d \geq 1$ and, also, *ISE* is the smallest among all candidates.

The resulting process control system design should be feasible throughout the entire operation horizon and also superior to the other alternatives in terms of control performance. Additionally, if none of the tuning methods under consideration allow for $FI_d \geq 1$, it can therefore be inferred that all given controller designs cannot guarantee the system to remain feasible throughout the operation horizon and other more qualified candidates should be sought after. Therefore, the proposed controller design procedure is not only able to guide the designers toward the best plausible controller (through *ISE*), but also warn them against the probable operation infeasibilities (through FI_d). The above design procedure is also summarized in the flowchart shown in Fig. 1.

4. Numerical examples

The control system design procedure described in the previous section has been applied to two dynamic processes for illustration purpose. The first example is a mixing tank process, while the second is a semi-batch reaction process.

4.1. Mixing tank system

Let's consider the mixing tank system (Mohideen et al., 1996) shown in Fig. 2. The corresponding dynamic model can be written as:

$$\frac{dV}{dt} = F_h + F_c - F(V) \tag{2}$$

$$F(V) = z\left(V^{1/2}\right) \tag{3}$$

$$V\frac{dT}{dt} = F_h(T_h - T) + F_c(T_c - T) \tag{4}$$

where, F_h is the flowrate of hot process stream and it is considered to be uncertain due to upstream variations. Also, T_h denotes the temperature of the hot stream and it is subject to random disturbances (noise). Two corresponding manipulated variables include: (1) the valve coefficient, z, which is assumed to be piecewise constant and can be determined arbitrarily, and (2) the flowrate of cold process stream, F_c, to which the controller is deployed. There are two state variables, i.e., the volume and

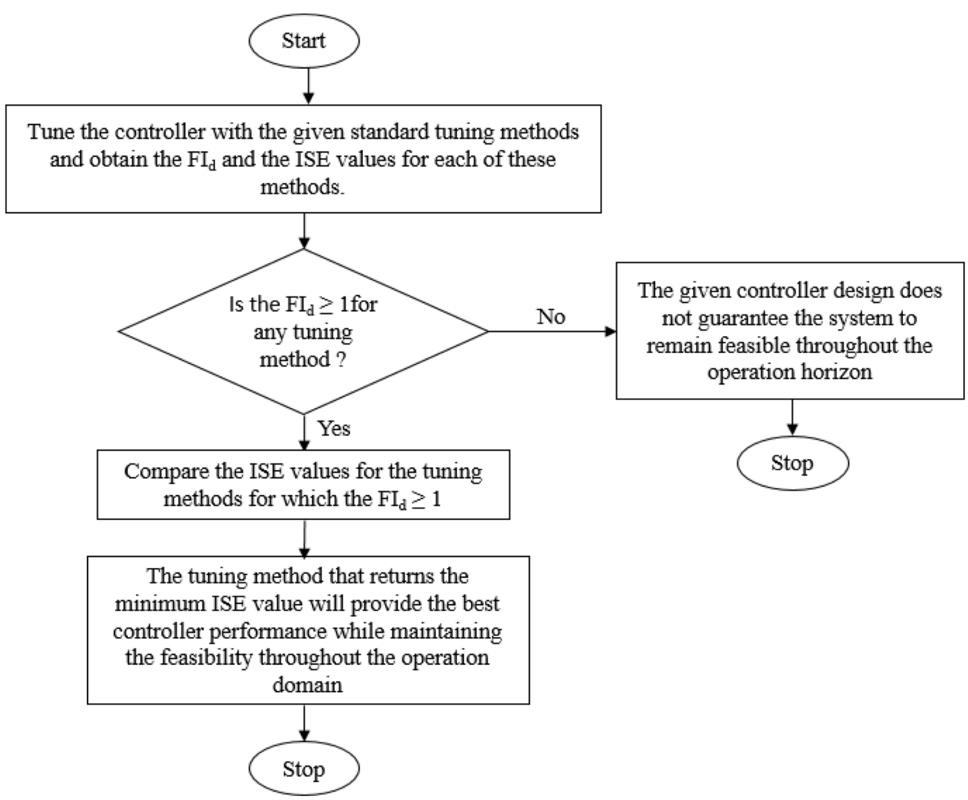

Fig. 1. Flexibility analysis based controller tuning procedure.

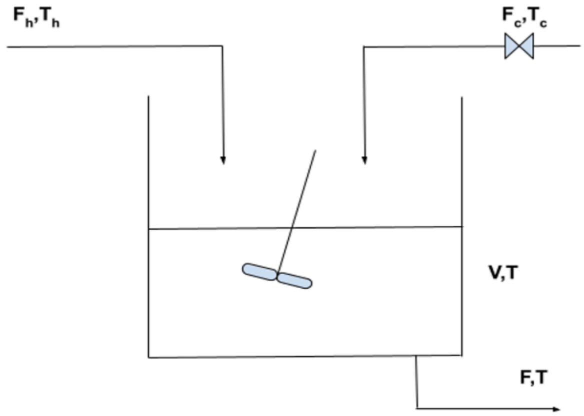

Fig. 2. A mixing tank system.

temperature of liquid in tank (denoted as *V* and *T* respectively). Finally, *F* denotes the flowrate at tank outlet. The process parameters are adopted from Mohideen et al. (1996). The initial values and allowed ranges of the system variables are summarized in Table 1.

A PI controller (Luyben and Luyben, 1997; Seborg et al., 2004; LebLanc and Coughanowr, 2009; Romgnoli and Palazoglu, 2012) is applied to manipulate the flowrate of the cold stream, F_c with a bias of 0.02 (m^3/h). The liquid load in tank (*V*) is chosen to be the corresponding controlled variable with a set point of 1.2 m^3. To facilitate the FI_d and *ISE* quantification, let us assume that the time horizon covers a span of 48 hours, i.e., $0 \leq t \leq 48$. Note that, the number of generations adopted in GA was taken to be 50, whereas the probabilities for cross-over and mutation were chosen to be 0.7 and 0.5, respectively.

A summary of the computation results obtained in the present example can be found in Table 2. In this table, the tuning method, the corresponding controller parameters, the dynamic flexibility index and the integrated squared error are listed in column 1–column 4, respectively. It can be observed that out of the two tuning methods with which the dynamic flexibility indices are greater one, the IMC tuning method returns the smallest integrated squared error. Specifically, with this tuning method, the FI_d and *ISE* values obtained are 1.05 and 0.43, respectively. Clearly, in this example, the IMC tuning method produces the best control performance while still maintains operability throughout the time horizon.

For better visualization of the system dynamics with the IMC-tuned controller, the time profiles of the worst-case uncertain parameter variation, the random disturbance, the two manipulated variables and the controlled variable are shown in Fig. 3(a)–(e), respectively. Notice that the dashed line in Fig. 3(e) denotes the set point adopted in the present case study. It can be observed that the manipulated variables behave well within their respective bounds (see Fig. 3(c)(d) and Table 1) to counter the extreme variations in uncertain parameter (see Fig. 3(a)) and random system disturbances (see Fig. 3(b)). Also, it can be observed from Fig. 3(e) that the controller performs effectively to drive the controlled variable toward the set point. From the aforementioned results, it is clearly seen that, amongst the tested tuning methods, the IMC-based approach provides the best controller performance under the condition that the system's operability can be ensured throughout the time horizon.

Table 1
System variables for example 4.1.

Variables		*Initial Value*	*Range (l.b., u.b.)*	*Units*
State Variables:	V	1	(0.9, 1.5)	m^3
	T	360	(350, 370)	K
Disturbance:	T_h	N.A.	(350, 390)	K
Uncertainty:	F_h	N.A.	(0.05, 0.15)	m^3/h
Manipulated Variables:	z	N.A.	(0, 0.3)	$m^{4.5}$/h
	F_c	0.02	(0.015, 0.05)	m^3/h

Table 2
Controller performance for example 4.1.

Tuning Method	*Controller Parameters*	*Dynamic Flexibility Index(FI_d)*	*Integrated Square of Error(ISE)*
ZN	K_c=0.045; τ_i=17.500	0.747	0.403
TL	K_c=0.031; τ_i=46.200	0.921	0.339
DS	K_c=0.015; τ_i=8.000	1.112	0.448
IMC	K_c=0.016; τ_i=8.000	1.050	0.430

4.2. Semi-batch reactor system

The second case study is concerned with a semi-batch reactor as shown in Fig. 4, which has been adopted from Ingham et al. (1994). An exothermic reaction between reactant 'A' and 'B' takes place in this reactor to produce product 'C.' The reactor is run in semi-batch mode, i.e., the entire amount of the former reactant is placed in the vessel initially while the latter is then fed continuously over a period of time. The mathematical model of the uncontrolled system can be described as follows

$$\frac{d(VC_A)}{dt} = -kC_AC_BV \tag{5}$$

$$\frac{d(VC_B)}{dt} = F_BC_{Bf} - kC_AC_BV \tag{6}$$

$$\frac{d(VC_C)}{dt} = kC_AC_BV \tag{7}$$

$$\frac{dV}{dt} = F_B \tag{8}$$

$$k = k_o e^{-E/RT} \tag{9}$$

$$\frac{dT_R}{dt} = F/V(T_f - T_R) - UA/V\rho C_{Pr}(T_f - T_R) + \Delta H/\rho C_{Pr}(kC_AC_B) \tag{10}$$

$$\frac{dT_C}{dt} = F_C/V_C(T_{Cin} - T_C) + UA/V_C\rho C_{Pc}(T_R - T_C) \tag{11}$$

where, C_A, C_B and C_C denote the concentrations of A, B and C in the reactor respectively; *V* is the volume of liquid in the reactor; *A* is the heat transfer area. All of them are treated as the state variables in the given dynamic system. Due to upstream variations, the inlet composition of the feed B, i.e. C_{Bf}, is uncertain and, thus, considered as the uncertain parameter in the present example. On the other hand, the temperature of the feed stream (T_f) fluctuates due to random noise. The corresponding manipulated variables in this example include: (1) the cooling water flowrate ($F_{C,}$), which is approximated with a piecewise-constant time profile to reduce the computation load and the constant values in this profile can be adjusted arbitrarily and (2) the inlet feed flowrate F_B, which is used as the manipulated variable of a controller. The parameter values of the aforementioned mathematical model are adopted from Ingham et al. (1994). The initial values and allowed ranges of the system variables are shown in Table 3.

A PI controller is used to manipulate the inlet feed flowrate (F_B) with a bias value of 1 (m^3/h). The temperature of the reactor load (T_R) is the corresponding controlled variable with a set point of 25 °C. Also, the GA parameters were kept the same as those adopted in the previous example.

The results obtained for this case study are summarized in Table 4. It

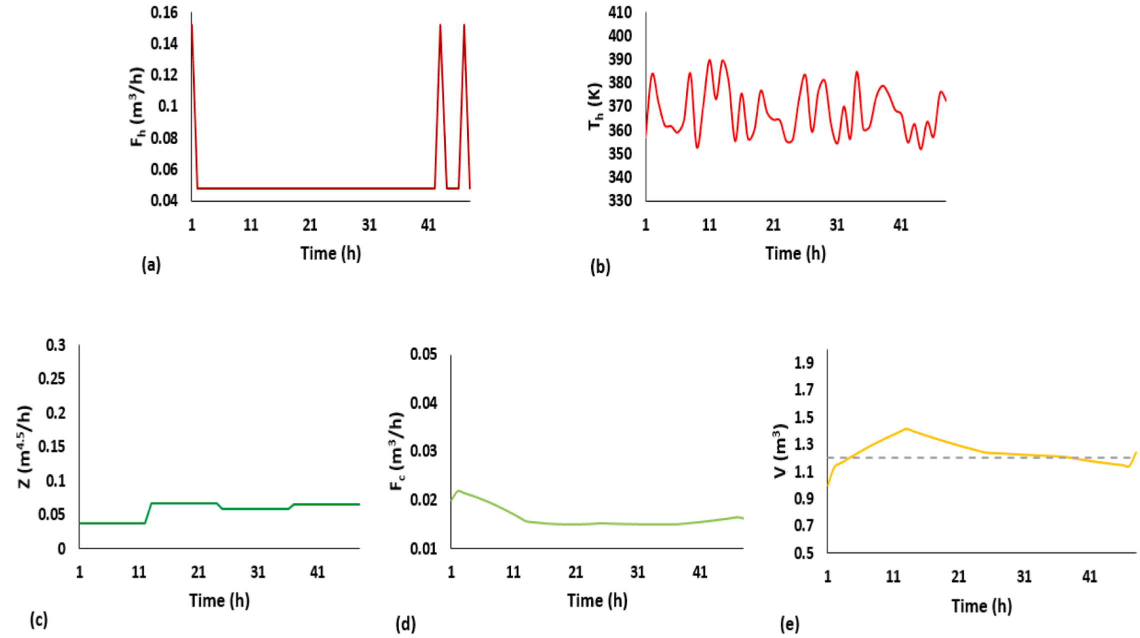

Fig. 3. Variable time profiles with IMC tuning for example 4.1. (a) Uncertainty, F_h.

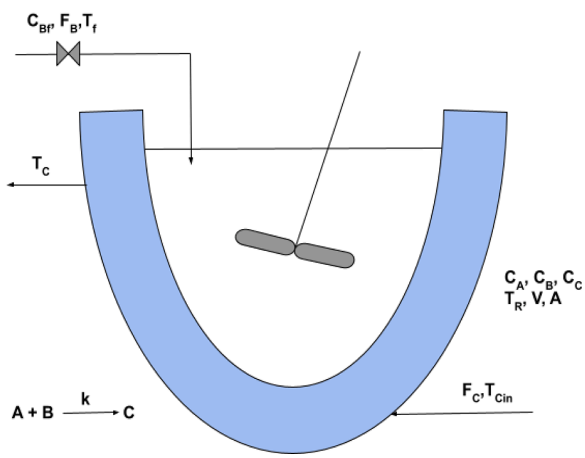

Fig. 4. A semi-batch reactor system.

Table 3
System variables for example 4.2.

Variables		*Initial Value*	*Range(l.b., u.b.)*	*Units*
State Variables:	C_A	10	(0, 10)	kmol /m^3
	C_B	0	(0, 10)	kmol /m^3
	C_C	0	(0, 10)	kmol /m^3
	T_R	20	(18, 35)	°C
	T_C	15	(15, 30)	°C
	V	6	(1, 15)	m^3
	A	3	(3, 15)	m^2
Uncertainty:	C_{Bf}	N.A.	(2, 18)	kmol /m^3
Disturbance:	T_f	N.A.	(17, 19)	°C
Manipulated Variables:	F_B	1	(0.01, 2)	m^3/h
	F_C	N.A.	(9, 11)	m^3/h

can be observed that these results are similar to those in the previous example. Specifically, the DS and IMC tuning methods yield better system flexibility indices than those produced with the ZN and TL tuning approaches. This observation can be attributed to the fact that the former two methods are model based and therefore can lead to relatively better controller parameters (Seborg et al., 2004). On the other hand,

Table 4
Controller performance for example 4.2.

Tuning Method	*Controller Parameters*	*Dynamic Flexibility Index(FI_d)*	*Integrated Square of Error(ISE)*
ZN	K_c=0.037; τ_i=1.670	0.988	65.610
TL	K_c=0.025; τ_i=4.400	0.965	73.336
DS	K_c=0.095; τ_i=3.200	1.019	25.110
IMC	K_c=0.100; τ_i=3.200	1.023	27.323

notice that in this example, the DS method outperforms the IMC method due to a lower *ISE* value while the FI_d values are greater than 1 in both cases. Again, to be able to visualize the system dynamics resulting from adopting the PI controller tuned with the DS approach, the time profiles of the worst-case uncertain parameter variation, the random disturbance, the two manipulated variables and the controlled variable are shown in Fig. 5(a)–5(e), respectively. Notice also that the dashed line in Fig. 5(e) represents the set point of the controlled variable. It can be observed that the manipulated variable F_C stays at the upper bound throughout the entire time horizon (see Fig. 5(c) and Table 3), and the other manipulated variable (F_B) stays within the designated bounds (see Fig. 5(d) and Table 3). Also, it can be seen from Fig. 5(e) that the controller performs effectively to keep the reactor temperature close to the set point of 25 °C. This is achieved even when the uncertain feed composition dips past the expected lower bound (see Fig. 5(a) and Table 3). From these results, it can be inferred that amongst the tuning methods studied in this example, the DS tuning method can produce the best plausible controller, while still maintaining the system's operability throughout the time horizon.

5. Significance of flexibility analysis in controller tuning

As stated before in Section 3, it is imperative to evaluate the dynamic flexibility index while tuning the system controllers. This practice is adopted to check whether the given dynamic system is able to withstand the maximum degree of uncertainty without becoming inoperable. To delineate the advantages of flexibility-based controller design, a

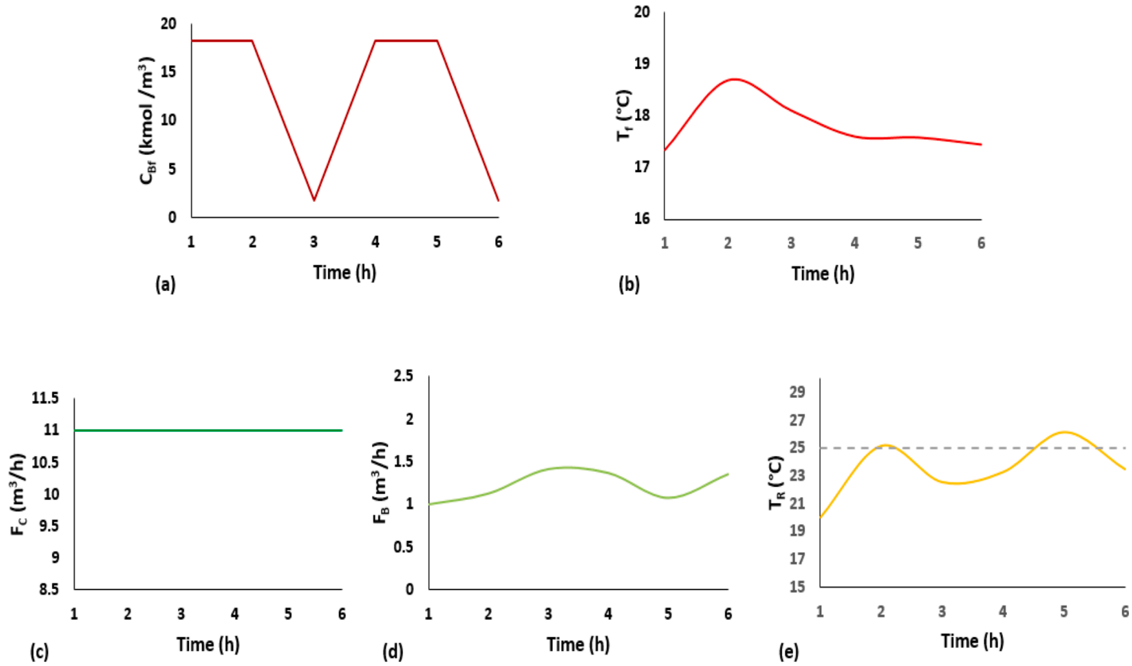

Fig. 5. Variable time profiles with DS tuning for example 4.2. (a) Uncertainty, C_{Bf}. (b) Disturbance, T_f. (c) Manipulated variable, F_C. (d) Manipulated variable, F_B. (e) Controlled variable, T_R.

comparison between the performances of two standard tuning methods corresponding to $FI_d < 1$ (TL) and $FI_d > 1$ (IMC) is presented here on the basis of results obtained in Example 4.1. Firstly, notice that the uncertain parameter and disturbance profiles used for this comparison are taken from Fig. 3(a) and 3(b), respectively, which are the time profiles generated by a PI controller tuned with the IMC based method. Secondly, notice that the time profiles of the state, manipulated and controlled variables for the two tuning methods, which are obtained under the influence of the same uncertain parameter and disturbance profiles, i.e., Fig. 3(a) and (b), can be found in Fig. 6. Note that the dashed line in Fig. 6(a) represents the lower bound of the corresponding state variable, while that in Fig. 6(b) represents the set point for the controlled variable. It can be observed that if the tuning method is chosen solely on the basis of *ISE* (see Table 2) and if the system is under

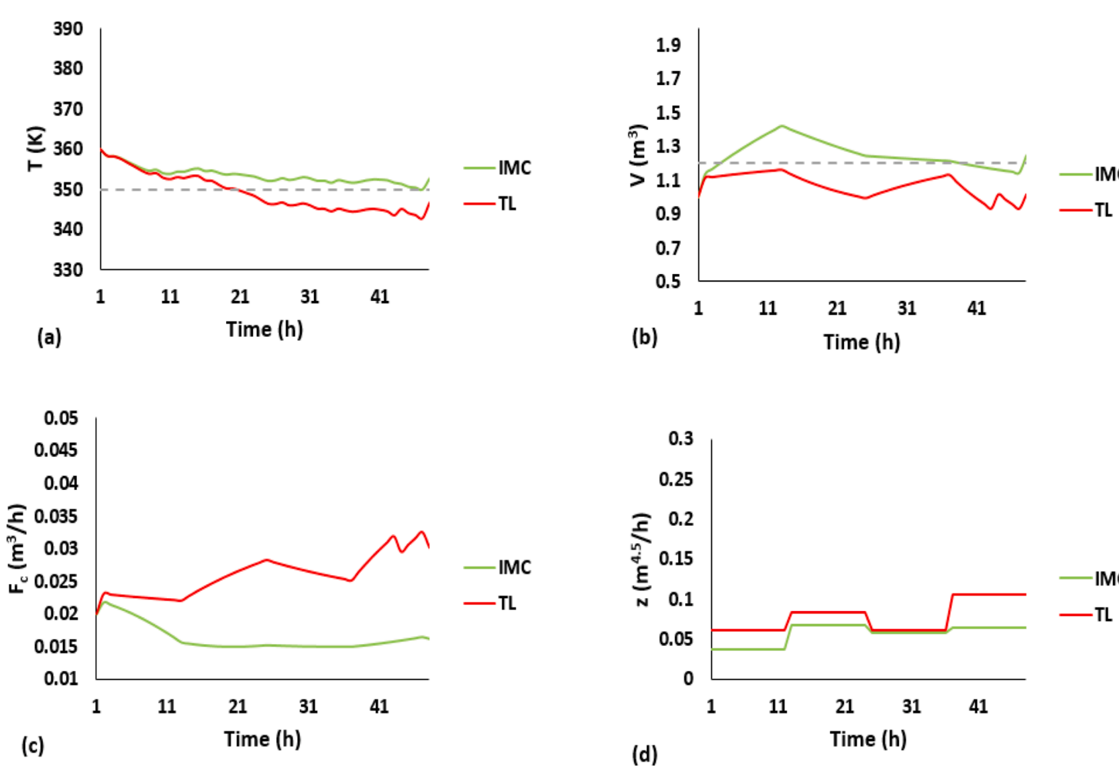

Fig. 6. Variable time profiles with IMC and TL tuning for example 4.1. state variable, T. (b) Controlled variable, V. (c) Manipulated variable, F_c. (d) Manipulated variable, z.

the influences of the worst-case uncertain condition in Fig. 3(a) along with the random disturbance in Fig. 3(b), the control system may fail to comply with the temperature constraint. Specifically, Fig. 6(a) shows that the temperature in the tank drops well below the designated lower bound, i.e., 350 °C, for a considerable duration of time. Moreover, in such case, the controller struggles to maintain the controlled variable, i.e. liquid load, close to its set point of 1.2 m^3 (Fig. 6(b)). Therefore, it is evident that the flexibility analysis should be adopted to rule out unsuitable controller parameters corresponding to $FI_d < 1$, and it is possible to ensure that, with the final controller design obtained, the system is able to withstand the uncertain variations without breaking down during the entire time horizon.

6. Conclusion

In this study, an efficient computation strategy, namely the GA-assisted vertex enumeration method (Ali et al., 2021), was applied to two dynamic systems to demonstrate the advantages of using flexibility analysis for process control system design with the aim to ensure operability throughout the time horizon. A generalized procedure was developed to select the appropriate controller parameters with the standard tuning methods, namely, ZN, TL, DS and IMC. This was done by using the dynamic flexibility index (FI_d) as an additional criterion along with the integrated squared error (*ISE*), to obtain the best plausible controller. The numerical results from the two case studies show that a robust controller design could be systematically achieved with the proposed procedure.

CRediT authorship contribution statement

Shoeb Moon Ali: Conceptualization, Methodology, Visualization, Software, Writing – original draft. **Chuei-Tin Chang:** Supervision, Conceptualization, Visualization, Writing – review & editing. **Jo-Shu Chang:** Supervision, Writing – review & editing.

Declaration of Competing Interest

The authors declare no competing interests.

Appendix: Vertex enumeration based computational strategies for FI_d evaluation

Two index sets, $\mathbb{I}$ and $\mathbb{J}$, are introduced to enumerate and classify all constraints in the given model:

$$\mathbb{I} = \{i \mid i \text{ is the index of an equality constraint in the design model}\} \tag{A1}$$

$$\mathbb{J} = \{j \mid j \text{ is the index of an inequality constraint in the design model}\} \tag{A2}$$

The i^{th} equality constraint in the model can be expressed in general as

$$h_i(\mathbf{d}, z(\mathrm{t}), \boldsymbol{x}(\mathrm{t}), \dot{\mathbf{x}}(\mathrm{t}), \boldsymbol{\theta}(\mathrm{t})) = \dot{x}_i(\mathrm{t}) - \varphi_i(\mathbf{d}, z(\mathrm{t}), \boldsymbol{x}(\mathrm{t}), \boldsymbol{\theta}(\mathrm{t})) = 0 \tag{A3}$$

where, $x_i(0) = x_i^0$; $i \in \mathbb{I}$; $t \in [0, H]$ and H is the length of time horizon; d represents a constant vector with all the design specifications; $z(\mathrm{t}) \in R^{n_z}$ denotes the manipulated variables at time t, $x(\mathrm{t}) \in R^{n_x}$ denotes the state variables at time t and $\theta(\mathrm{t}) \in R^{n_\theta}$ denotes the uncertain parameters at time t. Also, φ_i is a given function of three types of functions of time, i.e., $z(\mathrm{t})$, $x(\mathrm{t})$, $\theta(\mathrm{t})$, and it is established to model the dynamic behaviour of an unsteady process over the given time horizon. Let the total number of equality constraints be denoted by n_e.

Similarly, the j^{th} inequality constraint in this model can be written as

$$g_j(\mathbf{d}, z(\mathrm{t}), \boldsymbol{x}(\mathrm{t}), \boldsymbol{\theta}(\mathrm{t})) \le 0 \tag{A4}$$

where, $j \in \mathbb{J}$ and g_j is also a given function. The Eq. (A4) is usually adopted to reflect the physical and/or chemical boundaries in a given process (e.g. the product quality). Let the total number of inequality constraints be denoted by n_i.

The expected upper and lower bounds on the uncorrelated uncertain parameters can be included in the present model as follows.

$$\boldsymbol{\theta}^N(\mathrm{t}) - \Delta\boldsymbol{\theta}^-(\mathrm{t}) \le \boldsymbol{\theta}(\mathrm{t}) \le \boldsymbol{\theta}^N(\mathrm{t}) + \Delta\boldsymbol{\theta}^+(\mathrm{t}) \tag{A5}$$

These bounds are approximated from historical records for specific applications.

Let us next introduce a feasibility functional Ψ, whose *scalar* value is dependent upon the given design specifications in d and also the chosen feasible time profiles of parameters in $\theta(t)$. Specifically, this functional must be determined by solving a two-level optimization problem described below:

$$\Psi\big(\mathbf{d}, \boldsymbol{\theta}(\mathrm{t})\big) = \min_{\boldsymbol{x}(\mathrm{t}), \boldsymbol{z}(\mathrm{t})} \max_{j,t} g_j\big(\mathbf{d}, \boldsymbol{z}(\mathrm{t}), \boldsymbol{x}(\mathrm{t}), \boldsymbol{\theta}(\mathrm{t})\big) \tag{A6}$$

subject to the constraints in Eqs. (A3) and (A4) for both the lower and upper-level optimization problems. Note that the given system can be guaranteed to be always operable only if the feasibility functional value is non-positive, i.e., $\Psi \le 0$.

To facilitate the evaluation of dynamic flexibility index, FI_d, a scalar variable δ is introduced to adjust the ranges mentioned in Eq. (A5), I.E.

$$\boldsymbol{\theta}^{\mathrm{N}}(\mathrm{t}) - \delta\Delta\boldsymbol{\theta}^-(\mathrm{t}) \le \boldsymbol{\theta}(\mathrm{t}) \le \boldsymbol{\theta}^{\mathrm{N}}(\mathrm{t}) + \delta\Delta\boldsymbol{\theta}^+(\mathrm{t}) \tag{A7}$$

The corresponding dynamic flexibility index FI_d can be computed by solving another multi-level optimization problem (Dimitriadis and Pistikopoulos, 1995) i.e.

$$FI_d = \max \delta \tag{A8}$$

subject to Eq. (A7) and the inequality constraint presented below

$$\max_{\boldsymbol{\theta}(t)} \Psi(\mathbf{d}, \boldsymbol{\theta}(t)) \leq 0 \tag{A9}$$

Under the assumption that the manipulated variables can be adjusted arbitrarily, an extended version of the traditional vertex method was developed by Kuo and Chang (2016) for computing FI_d. It was assumed that the critical points must be located at the vertices in a functional space formed by $\boldsymbol{\theta}(t)$. Based on this assumption, a two-level optimization problem was developed for computing the dynamic flexibility index, i.e.

$$FI_d = \min_{k} \max_{\delta, \mathbf{z}(t), \mathbf{x}(t)} \delta \tag{A10}$$

subject to Eqs. (A3) and (A4) for the lower-level optimization problem and also the following constraints in a function space formed by all possible time profiles of $\boldsymbol{\theta}(t)$:

$$\boldsymbol{\theta}(t) = \boldsymbol{\theta}^k(t) = \boldsymbol{\theta}^N(t) + \delta \Delta \boldsymbol{\theta}^k(t) \tag{A11}$$

where, $\Delta\boldsymbol{\theta}^k(t)$ denotes a vector pointing from the nominal point $\boldsymbol{\theta}^N(t)$ towards the k^{th} vertex ($k = 1, 2, \cdots, 2^{n_\theta}$) at time t. Note that each element in $\Delta\boldsymbol{\theta}^k(t)$ should be obtained from the corresponding entry in either $-\Delta\boldsymbol{\theta}^-(t)$ or $\Delta\boldsymbol{\theta}^+(t)$.

After discretization, (A3), (A4), (A10) and (A11) can be replaced with the following formulation:

$$FI_d = \min_{k} \max_{\delta_k, \mathbf{Z}, \mathbf{X}} \delta_k \tag{A12}$$

subject to the discretized equalities and inequalities in (A3) and (A4) along with the following

$$\boldsymbol{\theta}(t_p) = \boldsymbol{\theta}^N(t_p) + \delta_k \Delta \boldsymbol{\theta}^k(t_p) \tag{A13}$$

where, $p = 0, 1, 2, \cdots, M$; $\mathrm{k} = 1, 2, \cdots, (2^{n_\theta})^{M+1}$; $\mathbf{X} = [\, \mathbf{x}(t_1),\ \mathbf{x}(t_2),\ \ldots.. \ \mathbf{x}(t_M) \,]$; $\mathbf{Z} = [\, z(\widehat{t}_1),\ z(\widehat{t}_2),\ \ldots..\ z(\widehat{t}_{N_z}) \,]$.

Notice that, although $z(\mathrm{t}) \in R^{n_z}$ are considered to be unspecified arbitrary functions of time over $[0, H]$ in (A3) and (A4), it is computationally more convenient and practically more feasible to view them as piecewise-constant profiles. Consequently, the dimension of space formed by the manipulated variables can be transformed from infinite to finite at $n_z N_z + 1$ (where N_z is the number of horizontal line segments in the time profiles of manipulated variables) and, furthermore, the upper limit of the number of aforementioned *active* constraints in an optimum solution may be set to be this particular finite value. Finally, notice that $z(\mathrm{t})$ should reduce to the original arbitrary functions of time in (A3) and (A4) if N_z approaches infinity. As a result, the flexibility index value should increase as the number of manipulated-variable pieces, i.e., N_z, increases. Furthermore, in most cases, this number does not have to be raised to a very high level for the corresponding FI_d to saturate and such a stabilized value should be taken as the actual dynamic flexibility index of the given system

References

Ali, S.M., Hwang, S.W., Chang, C.T., Chang, J.S., 2021. An effective numerical procedure for evaluating flexibility indices of dynamic systems with piecewise constant manipulated variables. Comput. Chem. Eng. 154, 107464.

Bahri, P.A., Bandoni, J.A., Ramagnoli, J.A., 1997. Integrated flexibility and controllability analysis in design of chemical processes. AIChE J. 43 (4), 997–1015.

Chang, C.T., Adi, V.S.K., 2018. Deterministic Flexibility Analysis; Theory, Design and Applications. CRC Press, Taylor & Francis Group, Boca Raton, FL, USA. ISBN: 978-1-4987-4816-2.

Chen, D., Seborg, D.E., 2002. PI/PID controller design based on direct synthesis and disturbance rejection. Ind. Eng. Chem. Res. 41, 4807.

Cortes-Pena, Y., Kumar, D., Singh, V., Guest, J.S., 2020. BioSTEAM: a fast and flexible platform for the design, simulation, and techno-economic analysis of biorefineries under uncertainty. ACS Sustain. Chem. Eng. 8 (8), 3302–3310.

Dimitriadis, V.D., Pistikopoulos, E.N., 1995. Flexibility analysis of dynamic systems. Ind. Eng. Chem. Res. 34, 4451–4462.

Eini, S., Kontogeorgis, G.M., Rashtchian, D., 2020. Cost optimization and flexibility analysis for the liquefaction of an associated natural gas stream. J. Energy Resour. Technol. 142 (6), 062801.

Gaspar, J., Sandoval, L.R., Jorgensen, J.B., Fosbol, P.L., 2016. Controllability and flexibility analysis of CO_2 post-combustion capture using piperazine and MEA. Inter. J. Greenh. Gas Control 51, 276–289.

Grossmann, I.E., Floudas, C.A., 1987. Active constraint strategy for flexibility analysis in chemical process. Comput. Chem. Eng. 11, 675–693.

Holland, J.H., 1992. Genetic algorithms. Sci. Am. 267, 66–73.

Ingham, J., Dunn, I.J., Heinzle, E., Prenosil, J.E., 1994. Chemical Engineering Dynamics. VCH, Weinheim. ISBN 3-527-28577-6.

Kuo, Y.C., Chang, C.T., 2016. On heuristic computation and application of flexibility indices for unsteady process design. Ind. Eng. Chem. Res. 55 (3), 670–682.

LeBlanc, S.E., Coughanowr, D.R., 2009. Process Systems Analysis and Control. McGraw-Hill, 3eISBN 978-0-07-339789-4.

Lima, F.V., Jia, Z., Ierapetritou, M., Georgakis, C., 2010. Similarities and differences between the concepts of operability and flexibility: the steady-state case. AIChE J. 56, 702–716.

Liu, J., Zhnag, P., Xie, Q., Liang, D., Bai, L., 2021. Flexibility analysis and design of heat exchanger network for syngas-to-methanol process. Int. J. Coal Sci. Technol. 8, 1468–1478.

Luyben, M.L., Luyben, W.L., 1997. Essentials of Process Control. McGraw-Hill. ISBN 0-07-114193-6.

Malcolm, A., Polan, J., Zhnag, L., Ogunnaike, B.A., Linninger, A.A., 2007. Integrating systems design and control using dynamic flexibility analysis. AIChE J. 53 (8), 2048–2061.

Mohideen, M.J., Perkins, J.D., Pistikopoulos, E.N., 1996. Optimal design of dynamic systems under uncertainty. AIChE J. 42 (8), 2251–2272.

Pretoro, A.D., Montastruc, L., Maneti, F., Joulia, X., 2019. Flexibility analysis of a distillation column: indexes comparison and economic assessment. Comput. Chem. Eng. 124, 93–108.

Pretoro, A.D., Montastruc, L., Joulia, X., Maneti, F., 2021. Accounting for dynamics in flexible process design: a switchability index. Comput. Chem. Eng. 145, 107149.

Pretoro, A.D., Fedeli, M., Flavia, C., Joulia, X., Motastruc, L., Maneti, F., 2022. Flexibility and environmental assessment of process-intensified design solutions: a DWC case study. Comput. Chem. Eng. 159, 107663.

Rivera, D.E., Morari, M., Skogestad, S., 1986. Internal model control for PID controller tuning. Ind. Eng. Process Design Dev. 25, 252.

Romgnoli, J.A., Palazoglu, A., 2012. Introduction to Process Control. CRC Press. ISBN 978-1-4398-5486-0.

Sahinidis, N.V., Grossmann, I.E., 1991. Convergence properties of generalized benders decomposition. Comput. Chem. Eng. 15 (7), 481–491.

Seborg, D.E., Edgar, T.F., Mellichamp, D.A., 2004. Process Dynamic and Control. John Wiley & Sons Inc, 2eISBN 0-471-45246-7.

Swaney, R.E., Grossmann, I.E., 1985a. An index for operational flexibility in chemical process design part A. AIChE J. 31, 621–630.

Swaney, R.E., Grossmann, I.E., 1985b. An index for operational flexibility in chemical process design part B. AIChE J. 31, 631–641.

Tang, W., Daoutidis, P., 2019. Lyapunov dynamic flexibility of nonlinear processes. Comput. Chem. Eng. 47, 35–40.

Tyreus, B.D., Luyben, W.L., 1992. Tuning PI controllers for integrator/deadtime processes. Ind. Eng. Chem. Res. 31, 2625.

Wu, R.S., Chang, C.T., 2017. Development of mathematical programs for evaluating dynamic and temporal flexibility indices based on KKT conditions. J. Taiwan Inst. Chem. Eng. 73, 86–92.

Yuan, Z., Chen, B., Sin, G., Gani, R., 2012. State-of-the art and progress in the optimization-based simultaneous design and control for chemical processes. AIChE J. 58 (6), 1640–1659.

Ziegler, J.G., Nichols, N.B., 1942. Optimum settings for automatic controllers. Trans. ASME 64, 759.

Zhao, F., Chen, X., 2018. Analytical and triangular solutions to operational flexibility analysis using quantifier elimination. AIChE J. 64 (11), 3894–3911.

Zhao, F., Grossmann, I.E., Garcia-Munoz, S., Stamatis, S.D., 2021. Flexibility Index of black-box models with parameter uncertainty through derivative-free optimization. AIChE J. 67 (5), e17189.

Zheng, C., Zhao, F., Zhu, L., Chen, X., 2020. Operational flexibility analysis of high-dimensional systems via cylindrical algebraic decomposition. Ind. Eng. Chem. Res. 59 (10), 467046–467087.

Zhou, H., Li, X.X., Qian, Y., Chen, Y., Kraslawski, A., 2009. Optimizing the initial conditions to improve the dynamic flexibility of batch processes. Ind. Eng. Chem. Res. 48, 6321–6326.