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Flexibility analysis of a distillation column: Indexes comparison and economic assessment

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The worldwide shared definition of “optimal design” refers to the cheapest and simplest design able to perform the required job; most of the time this definition is strictly related to given operating conditions, i.e. the input variables are seldom subjected to considerable variations. However, in process engineering, plenty of cases don't fit this definition due to the uncertain nature of the feedstock needed to be processed. Therefore, if a system is likely to undergo several and substantial perturbations, an a priori flexibility assessment can be crucial for the good performance of the operation. In chemical engineering the leading separation process is distillation. Hence the first purpose of this paper is to define a procedure and compare the different flexibility indexes found in literature in order to perform a simple distillation column flexibility assessment. The second goal of this paper is to couple the flexibility and economic aspects related to the distillation column investment costs and again to compare the different indexes economic behaviours.

1. Introduction: A measure of flexibility

Flexibility analysis is a step of process design procedure that is often skipped. Sometimes a sensitivity analysis is performed with features similar to the flexibility one but in general they don't overlap.

The standard procedure for chemical plants design consists of the assessment of the optimal design according to the economic and operational aspects. Nevertheless this optimal design is strictly related to the operating conditions, i.e. perturbations, when present, can seriously turn the tables. In these cases an a priori flexibility analysis could be of critical importance to assess in which range of operating conditions a system design is effectively better performant than another one.

The word flexibility commonly refers to the ability to change in order to cope with variable circumstances both in a passive and an active sense; to be more detailed, in process engineering, flexibility can be defined as the ability of a process to accommodate a set of uncertain parameters (Hoch and Eliceche, 1996). This concept looks easily understandable but actually the definition standalone says nothing about how we can deal with it. Thus we need an opera-

tional definition and to know what flexibility means through the way it could be measured.

The very first publication about the definition of a flexibility index is provided by Swaney and Grossmann (1985a) and soon after Saboo et al. (1985) proposed another possible index to quantify the flexibility of a process design (called in this case “resiliency”). Moreover there exists an additional paper by both Grossmann and Morari (1983) where the flexibility related problems and solution are thoroughly analyzed with a pioneering methodology.

The Swaney and Grossmann flexibility index (F_{SG}) mathematically states as follow:

Given that:

- θ^N : nominal values of uncertain parameters (base point);
- $\Delta\theta^+$, $\Delta\theta^-$: expected deviations for each parameter;
- d : design variables associated to the equipment capacities;
- z : control variables.

The flexibility index, for a given design d , is the solution of the problem:

$$F_{SG} = \max \delta \quad (1.1)$$

$$s.t. \max_{\theta \in T(\delta)} \min_z \max_{j \in J} f_j(d, z, \theta) \leq 0 \quad (1.2)$$

If $F=1$, the deviations $\Delta\theta^+$ and $\Delta\theta^-$ can be accommodated. In order to have a clearer idea of what these statement means we can help ourselves with the plot in Fig. 1.

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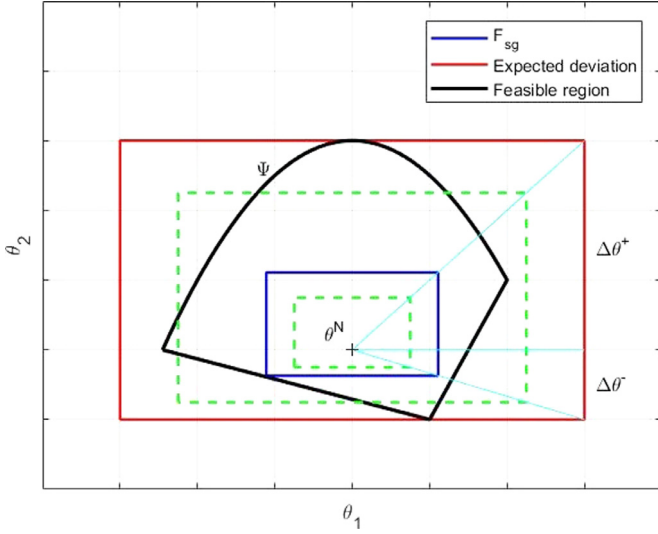


Fig. 1. Feasibility domain - F_{SG} (Swaney and Grossmann, 1985a).

The curve $\Psi(d, \theta)$ is the so called feasibility domain defined by the constraints. Constraints can be physical, legal, operational, economic etc. and in general a deeper study about the way this region is outlined and the conditions to be satisfied, as well as the degrees of freedom analysis, is needed. This step precedes the flexibility analysis since the domain shape is strictly related to the nature of the case study.

As shown by the optimization problem, the flexibility index defined as above (1.1, 1.2), is the maximum fraction of the expected deviation δ that can be accommodated by the system; it graphically represents the minimum among the maximum fractions of the hyperrectangle sides' lengths that is bounded by the feasible zone.

Moreover, for constraints jointly quasi convex in z and 1D quasi convex in θ the problem can be decomposed into two level optimization problem:

$$F_{SG} = \min_k \delta^k \quad (1.3)$$

$$\delta^k = \max_z \delta \quad (1.4)$$

$$f_j(d, z, \theta^k) \leq 0 \quad j \in J \quad (1.5)$$

$$\theta^k = \theta^N + \delta \cdot \Delta\theta^k \quad (1.6)$$

and the solution lies at a vertex of the hyperrectangle allowing us to solve the optimization problem by evaluating the feasibility of the design at each vertex. In this way, it can be noted that the explicit solution of the min-max problem can be circumvented; on the other hand certain types of non-convex domains may lead to nonvertex solutions (Grossmann and Floudas, 1987).

Before the introduction of the flexibility study, to move from feasibility study towards the design phase, we just need to know whether the project is feasible under the nominal operating conditions or not, but once we deal with flexibility the qualitative answer yes/no is not sufficient anymore. We need to quantify "how much" the project is feasible and the independent variables ranges enclosing the possible operating conditions.

As anticipated at the beginning, the same year Morari et al. proposed a "resiliency index" defined as the capability to easily recover or adjust to misfortune or change, that is more or less the passive alter ego of the capability to adapt to new, different or changing requirements, i.e. flexibility.

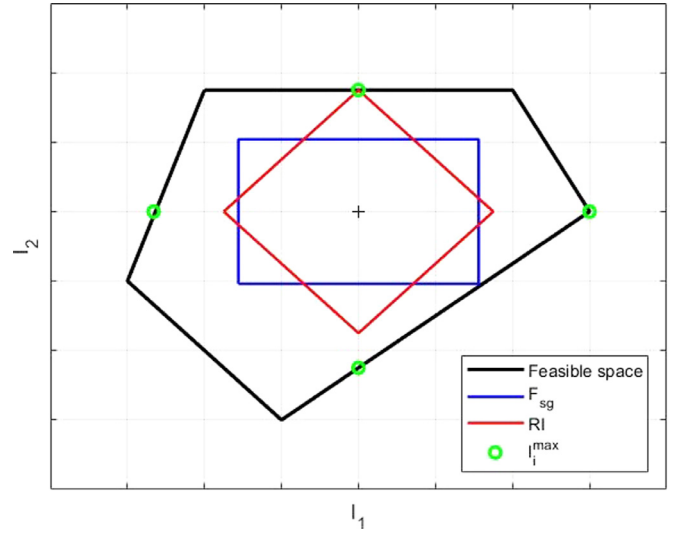


Fig. 2. Feasibility domain - F_{SG} vs RI (Saboo et al., 1985).

This index is based on the same premises of the F_{SG} , i.e. even in this case the very first step to perform is the definition of the feasibility domain. Then the resiliency index RI is defined as the largest total disturbance load, independent of the direction of the disturbance, a system is able to withstand without becoming infeasible.

It mathematically stands as:

$$RI = \min_i \{|l_i^{max}|\} \quad (1.7)$$

$$s.t. \{ \max_j f_j(\theta) \leq 0, \forall l : \sum_i |l_i| \leq RI \} \quad (1.8)$$

this corresponds to inscribing the largest possible polytope inside the feasible region defined by the inequalities here above. The RI is then equal to the distance between a vertex V of the polytope and the nominal operating point 0 as shown in Fig. 2.

The main advantage of the RI compared to the F_{SG} is that it requires a lower computational effort; this can be easily figured out in the case of an n -dimensional problem where a vertex analysis has to be performed: in the hyperrectangle case we have 2^n vertices to calculate while in the polytope case we have just $2n$ of them.

Moreover, the disturbance region measured in the first case might be practically more interesting because it expresses directly the disturbance load allowed in the direction of each parameter independently on the others.

For the same reason, since the hyperrectangles sides have to be parallel to the axes even if this configuration doesn't allow the biggest possible rectangle, the F_{SG} index results to be very conservative and significantly underestimate the actual flexibility of the system.

This representation of the feasible and expected possible zones does not reflect thoroughly the real world since not all the possible operating conditions are equally probable; hence this kind of analysis results in rather conservative estimates. In many real world applications, however, data are usually available that allow a better definition of uncertainty in a statistical sense.

For this reason a novel flexibility analysis approach for processes with stochastic parameters was then proposed in 1990 by Pistikopoulos and Mazzuchi (1990). It's shown that the flexibility index can correspond to a multivariate cumulative distribution function transforming the original constraint space to the space of stochastically dependent flexibility function by mean of the analytical properties of the flexibility problem.

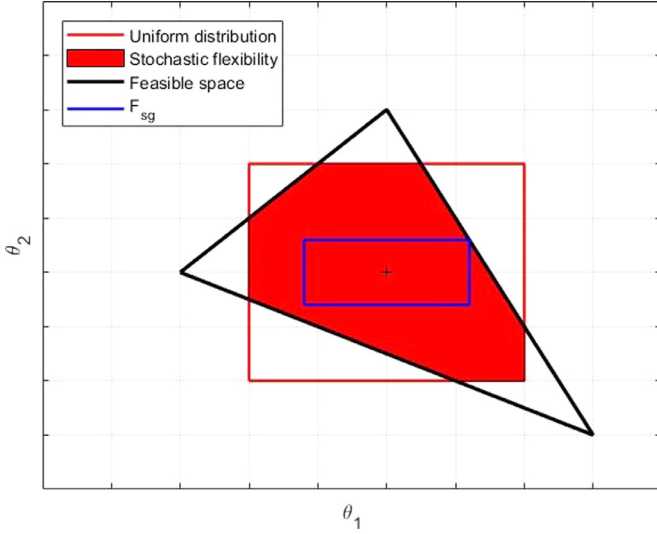


Fig. 3. Feasibility domain - F_{SG} vs SF (Pistikopoulos and Mazzuchi, 1990).

Given the feasibility region constraints inequalities as:

$$\Psi(d, \theta) \leq 0 \quad (1.9)$$

the equality defines the boundary of the feasible zone.

The stochastic flexibility index SF can be defined as:

$$SF = Pr\{\Psi(d, \theta) \leq 0\} = \int_{\{\theta: \Psi(d, \theta) \leq 0\}} \dots \int P_D(\theta) d\theta \quad (1.10)$$

where P_D is the joint distribution function of the uncertain parameters θ .

The comparison between the stochastic flexibility index SF and the Swaney and Grossmann is better shown in Fig. 3.

With this methodology we can calculate a weighted estimation of flexibility. Thus, if something is unlikely to happen and our system cannot withstand this operating conditions, it only slightly affects the final value of the flexibility index providing a measurement less conservative and more adherent to reality.

Obviously, the other side of the coin is the strict dependency of this index on the availability of probability distribution data, that is if no data are available this methodology is clearly unusable.

An additional problem to be solved was pointed out in 1995 by Dimitriadis and Pistikopoulos (1995) and it consists in the evaluation of flexibility taking into account the dynamics of the studied system. This topic was already pointed out by Grossmann and Morari (1983) few years before but Pistikopoulos is the very first one to define a specific index namely Dynamic Flexibility (DF) that takes into account the evolution of the system. Actually the definition itself of DF is not so different since it is a modification of the previous index F_{SG} . However, its introduction allows the study of a system taking into account its control loops and their tuning, therefore from an operational point of view its introduction is of critical importance.

The Dynamic Flexibility problem is introduced here below for literature coverage reasons. Nevertheless this index will not be taken into account in the flexibility analysis proposed in the next section both because no other dynamic flexibility indexes to compare it with have been found in literature and because the analysis refers to steady state conditions.

The definition of the Dynamic Flexibility follows the path of the F_{SG} considering the uncertain and control parameters namely θ and z as a function of time, therefore the dynamic flexibility index evaluation problem becomes:

$$DF(d) = \max \delta \quad (1.11)$$

$$s.t. \chi(d) = \max_{\theta(t) \in T(\delta, t)} \min_{z(t) \in Z(t)} \max_{j \in J, t \in [0, H]} f_j(d, x(t), z(t), \theta(t), t) \leq 0 \quad (1.12)$$

$$s.t. h(d, x(t), z(t), \theta(t), t) = 0 \quad (1.13)$$

$$x(0) = x^0 \quad (1.14)$$

$$\delta \geq 0 \quad (1.15)$$

$$T(\delta, t) = \{\theta(t) | \theta^N(t) - \delta \cdot \Delta\theta^-(t) \leq \theta(t) \leq \theta^N(t) + \delta \cdot \Delta\theta^+(t)\} \quad (1.16)$$

$$Z(t) = \{z(t) | z^L(t) \leq z(t) \leq z^U(t)\} \quad (1.17)$$

Qualitatively, the dynamic flexibility index, DF, represents the largest scaled deviation of the uncertain parameter profile that the design can tolerate while remaining feasible within the horizon considered.

The dynamic flexibility index problem is a two-stage, semi-infinite, dynamic optimization problem with an infinite number of decision variables. Therefore, in order to solve it, an ad hoc methodology to reduce the dimension of the problem has to be implemented.

Finally, the most recent flexibility index found in literature is provided by Lai and Hui (2007, 2008). It has the aim to overcome the problems related to previous indexes, i.e. the requirement of nominal point and the consideration of the critical uncertainty only (causing an underestimation) for F_{SG} and RI, as well as the availability of the probability distribution of all uncertain parameters at the design stage for the SF. This new flexibility metric is much easier to use and does not need a lot of computational effort or available data and it is defined as follow.

Let V_0 be the volume defined by the uncertain parameters:

$$V_0 = \prod_{i=1}^N (\theta_{iU} - \theta_{iL}) \quad (1.18)$$

and V_f the feasible volume defined as the intersection of the constrained volume and V_0 .

Then the flexibility index F_V is defined as the ratio between the feasible space and the uncertain space:

$$F_V = \frac{V_f}{V_0} \quad (1.19)$$

However, S_f is usually irregular in shape and its volume (V_f) determination is not straightforward. To estimate V_f , a constructed space (S_e , the region outlined by the thick solid line), whose volume determination is less difficult, can be inscribed inside S_f . With a careful selection of the shape of S_e , its volume (V_e) can be used as a close estimate of V_f .

As illustrated in Fig. 4, S_e can be constructed by first picking a reference point (P_R), which is not necessarily the nominal point, within S_f . Auxiliary vectors v_j with selected directions can be radiated from P_R . The interception points (P_j) of v_j and the feasible space boundary are obtained. The S_e can then be constructed by joining these P_j points according to their positions in space. Since different S_e can be generated by different auxiliary vector direction selection schemes, estimation accuracy of V_f and F_V will depend on the selection scheme employed. The general formulation for the auxiliary vectors' positions in a 3D space is as follows:

$$\max_{x_j, y_j, z_j} V_e(x_j, y_j, z_j) \quad (1.20)$$

$$f_k(\theta_{ij}) \leq 0 \text{ and } 0 \leq x_j, y_j, z_j \leq 1 \quad (1.21)$$

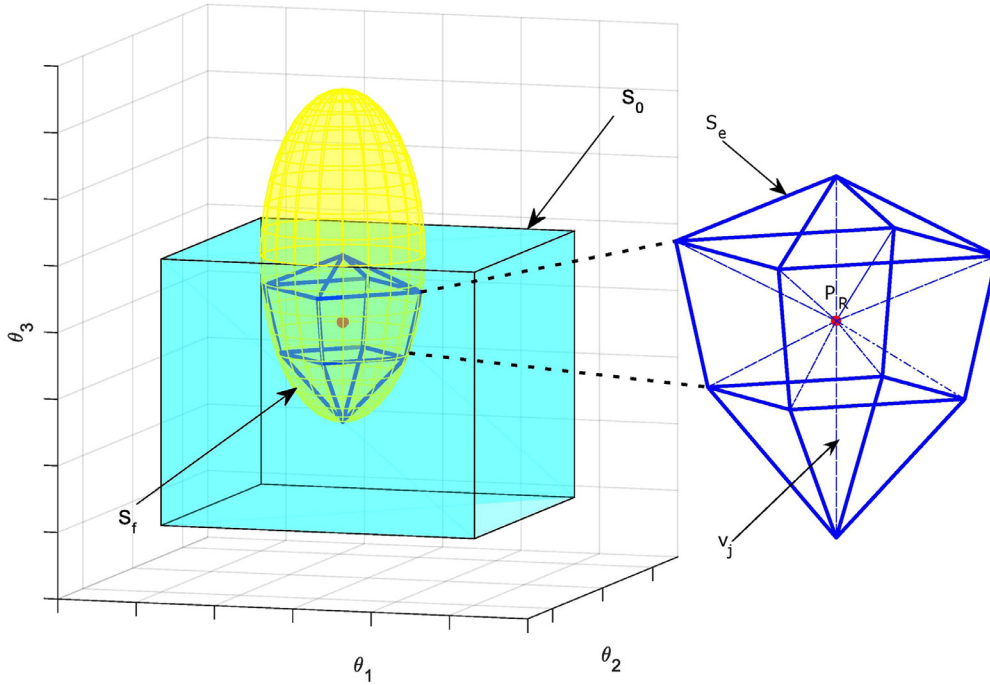


Fig. 4. Feasibility domain - F_v (Lai and Hui, 2008).

$$s.t. \theta_{i,j} = v_{ij} i_j \Delta_{ij} + \theta_i^R, \Delta_{ij} = \begin{cases} \Delta^+ \cdot \theta_i & (v_{ij} \geq 0) \\ |\Delta^- \cdot \theta_i| & (v_{ij} < 0) \end{cases} \quad i = x, y, z \quad (1.22)$$

However, whether the feasibility domain is well defined and the constraints equations are known, there's no need to approximate anymore since we can get the exact value of the S_f volume through a multiple integral at the cost of a higher computational effort.

An additional remark is worth to be done: the volumetric flexibility index takes into account no perturbation outside the uncertain space and treat every point as equally possible. Therefore, given its definition, we can write it as:

$$F_v = \frac{V_f}{V_0} = \frac{1}{V_0} \int_{V_f} d\theta = \int_{V_f} \frac{1}{V_0} d\theta \quad (1.23)$$

that is the same definition as the stochastic flexibility index for a probability step function. A practical application of this analogy between SF and F_v will be shown in the following chapters.

Finally, on one hand we can say that several flexibility indexes have been found in literature but, on the other hand, except the steady state debutanizer case study proposed by Hoch et al. (1995) (F_{SG}), no case studies about distillation have been provided (cf. Table 1). Most of the systems found in literature subjected to flexibility analysis have linear constraints or at least a quasi convex feasibility domain; whether a higher complexity can be detected, the flexibility analysis has been conducted with the simple F_{SG} that, due to its straightforward application, results to be the index used in the vast majority cases. However, the behaviour of less used and more complex indexes is worth to be studied in deeper and for a wider range of systems as well; therefore, a complete flexibility analysis of a distillation column, inspired by the aforementioned debutanizer example (Hoch et al., 1995), is proposed here below with all the four steady state indexes. An accurate results comparison and economic assessment will follow.

2. The debutanizer case study

In order to better understand the distillation related application of these indexes, the simple debutanizer case study proposed by Hoch et al. (1995), with few modifications, has been analyzed in detail.

In short, the system is made up of a standard distillation column, i.e. total condenser, no intermediate feeds/withdrawals and partial reboiler (Fig. 5).

The feed stream is defined by the composition and conditions shown in Table 2 while the given design parameters are listed in Table 3.

Finally the uncertain parameters are reported in Table 4, their expected variation ranges $\Delta\theta^{k\pm}$ are the same in either positive or negative direction and equal to 10% of their nominal value as suggested in the paper. The feed variations are related to the nature of the upstream process, the performances of the heat exchangers to the tubes fouling, the water temperature to the seasonality and finally the flooding and weeping velocity are function of the trays technology and status.

The specifications are given by the paper as three inequality constraints, namely:

- Maximum molar fraction of butane in the bottom product = 0.01786;
- Maximum molar fraction of pentane in the distillate = 0.025;
- Minimum pentane recovery in the bottom = 0.97.

In this paper the two most restrictive equality relationships have been selected to fulfill the two remaining degrees of freedom:

- Molar fraction of butane in the bottom product = 0.01786;
- Pentane recovery in the bottom = 0.97.

The controlled variables are respectively the reflux and distillate flowrates.

3. Flexibility analysis

Flexibility analysis can be performed either during the design phase or for an already existing equipment (or plant). In the next

Table 1
Flexibility studies in literature.

Case study	Authors	Index
Pump and pipe	Grossmann and Morari (1983)	F_{SG}
	Swaney and Grossmann (1985a)	F_{SG}
	Floudas et al. (2001)	F_{SG}
	Lai and Hui (2008)	F_V
	Swaney and Grossmann (1985b)	F_{SG}
Refrigeration cycle	Swaney and Grossmann (1985b)	F_{SG}
Reactor-recycle	Swaney and Grossmann (1985b)	F_{SG}
Heat exchanger network	Grossmann and Morari (1983)	F_{SG}
	Swaney and Grossmann (1985b)	F_{SG}
	Saboo et al. (1985)	RI
	Pistikopoulos and Mazzuchi (1990)	SF
	Dimitriadis and Pistikopoulos (1995)	DF
	Floudas et al. (2001)	F_{SG}
	Lai and Hui (2008)	F_V
	Dimitriadis and Pistikopoulos (1995)	DF
	Wu and Chang (2017)	DF
	Debutanizer	Hoch et al. (1995)
Reactor + cooler	Hoch and Eliceche (1996)	F_{SG}
	Floudas et al. (2001)	F_{SG}
Chemical process with recycle	Floudas et al. (2001)	F_{SG}
Solar-driven membrane distillation desalination (SMDD) process	Wu and Chang (2017)	DF
Benzene chlorination reaction system	Huang (2017)	DF
Batch reactor system	Huang (2017)	DF

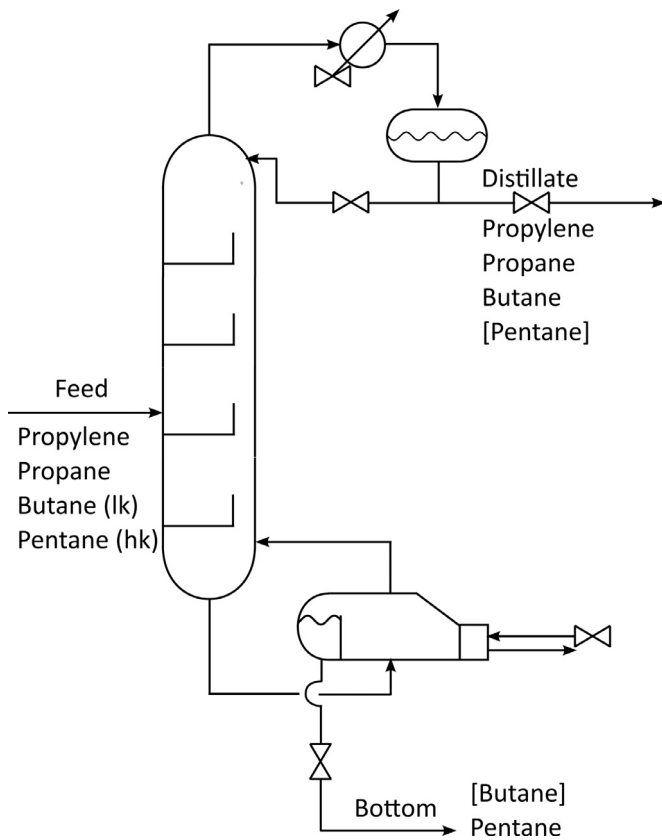


Fig. 5. Debutanizer column layout.

Table 2
Feed conditions and composition.

Partial molar flowrates	Value	Unit
Propylene	0.055	mol/s
Propane	0.053	mol/s
Butane (lk)	6.863	mol/s
Pentane (hk)	2.743	mol/s
Temperature	Bubble	K
Pressure	$15 \cdot 10^5$	Pa

Table 3
Design parameters.

Desing variables	Symbol	Value	Unit
Rectification stages	N_r	9	1
Stripping stages	N_s	10	1
Column diameter	D_{col}	0.634	m
Condenser area	A_{cond}	40.00	m^2
Reboiler area	A_{reb}	26.83	m^2
Top pressure	P_{top}	$4 \cdot 10^5$	Pa

chapters flexibility will be both assessed for the debutanizer column as shown in the previous paragraph and for a distillation column to be designed; the results will be then compared.

Moreover, the analysis will be conducted separately for the deterministic and stochastic indexes in order to highlight analogies and differences.

3.1. Deterministic indexes: Swaney Grossmann F_{SG} and resilience index RI

First of all, in order to evaluate the Swaney and Grossmann flexibility index F_{SG} , we need to estimate the variation ranges of

Table 4
Uncertain parameters θ^k .

Parameter θ	Symbol	Value θ^N	Expected deviation $\Delta\theta^{k\pm}$	Unit
Butane flowrate	F_4	6.863	$\pm 10\% \pm 0.686$	mol/s
Pentane flowrate	F_5	2.743	$\pm 10\% \pm 0.274$	mol/s
Condenser heat transfer coefficient	U_{cond}	473.77	$\pm 10\% \pm 47.377$	$W/m^2/K$
Inlet cooling water temperature	T_w	20	$\pm 10\% \pm 2$	$^\circ C$
Reboiler heat transfer coefficient	U_{reb}	552.90	$\pm 10\% \pm 55.29$	$W/m^2/K$
Max vapor velocity	G_f	0.38	$\pm 10\% \pm 0.038$	m/s
Min vapor velocity	G_w	0.13	$\pm 10\% \pm 0.013$	m/s

Table 5
Flexibility analysis results: F_{SG} .

Deviation [%]	Condenser area [m ²]	Reboiler area [m ²]	Minimum diameter max [m]	Maximum diameter min [m]
0.00	32.91	22.26	0.603	0.782
5.00	38.08	24.59	<u>0.634</u>	0.744
6.66	<u>40.00</u>	25.43	0.644	0.732
9.35	43.35	<u>26.83</u>	0.662	0.712
15.00	51.53	30.09	0.701	0.673
21.00	62.30	34.05	0.746	<u>0.632</u>

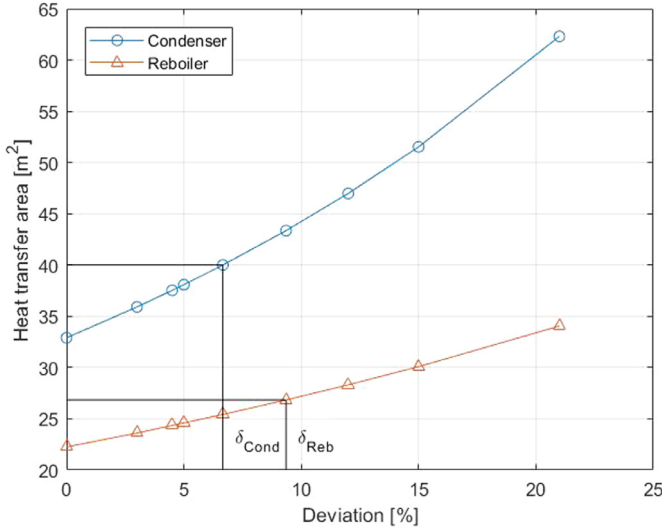


Fig. 6. Heat transfer areas (F_{SG}).

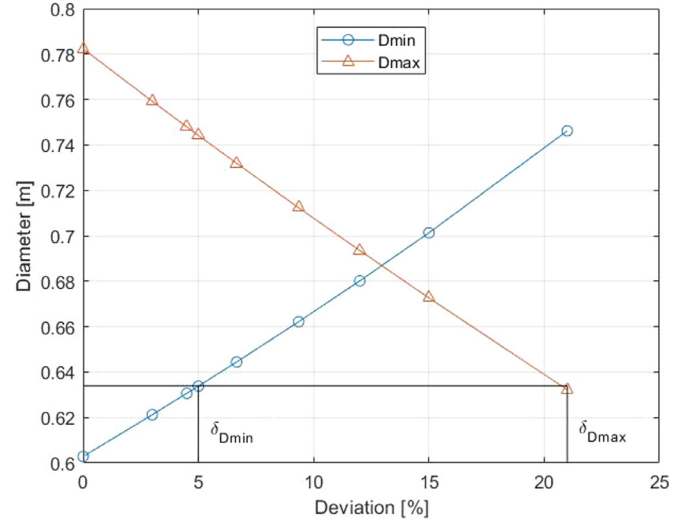


Fig. 7. Column max & min diameters (F_{SG}).

the uncertain variables as shown in Table 4, called from here on out “expected deviations”.

Since the system is rather simple (i.e. convex feasibility domain), for the moment there’s no need of outlining the whole feasible space as discussed in the first section; the vertex analysis, by increasing the parameters variation percentages until the expected values and keeping constant the ratios between them, can be then easily and effectively performed. Since there are 7 changing parameters, the hyperrectangle has 7 dimensions that means $2^7 = 128$ vertices should be theoretically calculated for each simulation but, thanks to the possibility to decouple some independent parameters, the computational effort can be substantially reduced.

The complete flexibility analysis results and the corresponding plots are shown respectively in Table 5 and Figs. 6 and 7, the debutanizer related values are indicated.

The resulting Swaney and Grossmann flexibility index for this case study is then given by:

$$F_{SG} = \frac{\text{allowed deviation}}{\text{expected deviation}} = \frac{5\%}{10\%} = 0.5 \quad (3.1)$$

The bottleneck of flexibility is given by the column minimum diameter equal to 0.634 m, i.e. by the flooding conditions. However, the analysis has been carried out for all the other design parameters standalone as well. The condenser results to be the second most constraining variable, while the reboiler the third one; for a value between 12 and 15% of the allowed deviation we can notice that the maximum diameter becomes lower than the minimum one causing the column design to be impossible with a single diameter column. This last phenomenon occurs because flexibility indexes refer both to positive and negative perturbations causing the range of diameter values able to ensure operable conditions to become smaller for higher flexibility requirements.

The conditions that cause the hyperrectangle to exceed the feasibility domain boundaries, i.e. which vertex is tangent one, for each design variable are reported in Table 6; “+” and “-” indicate respectively a positive or negative deviation of the uncertain parameter while “/” indicates that the parameter does not affect the constraining design variable.

For the “Condenser area”, “Reboiler area” and “Minimum column diameter” critical conditions are achieved because of overfed column and underperforming equipment while for the maximum diameter, i.e. weeping conditions, criticalities are present in case of underfeeding as expected according to the physics of the problem.

Beside the design and sizing, an economic assessment has been performed as well. The purpose is to couple flexibility and investment costs in order to make the best decision during the design phase and avoid the plant underperform; operational costs have not been taken into account since they’re univoquely determined due to the fact that we’re not changing the number of trays. For more detail about equipment costs correlations cf. Appendix B

The capital costs trends (normalized to the lowest value) as function of F_{SG} flexibility are plotted for each equipment in Figure 8. All of them increase as flexibility increases (according with their size). The most expensive equipment is the Kettle reboiler that has a much more accurate technology than the other heat exchangers and that works under pressure, while the column is relatively cheap because of its small diameter.

In Fig. 9 three series of percentage data as function of flexibility have been plotted; they refer namely to:

- $\frac{dC}{C_0}$: the additional investment referred to a column designed in nominal operating conditions, i.e. 0% flexibility (Blue trend);
- $\frac{dC}{C_{eff}}$: the cost differences with respect to the case study column design (Red trend);

Table 6
Critical vertices.

Parameter vs design	Condenser area	Reboiler area	Minimum diameter	Maximum diameter
Butane flowrate	+	+	+	-
Pentane flowrate	+	+	+	-
U_{cond}	-	/	/	/
T_w	+	/	/	/
U_{reb}	/	-	/	/
G_f	/	/	-	/
G_w	/	/	/	+

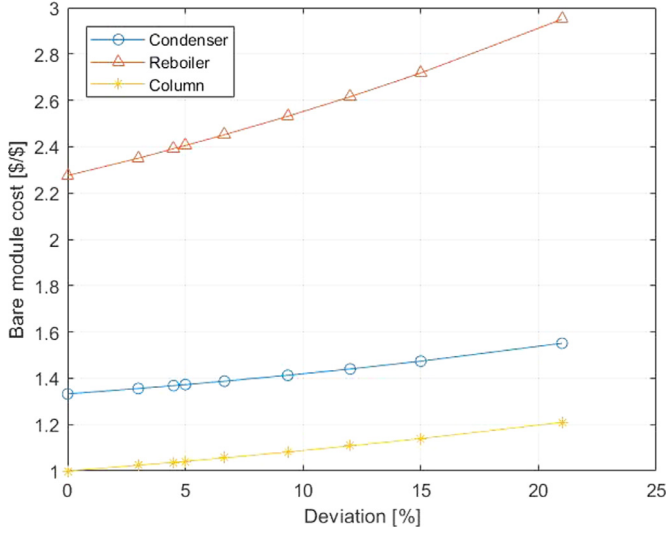


Fig. 8. Equipments bare module cost (F_{SG}).

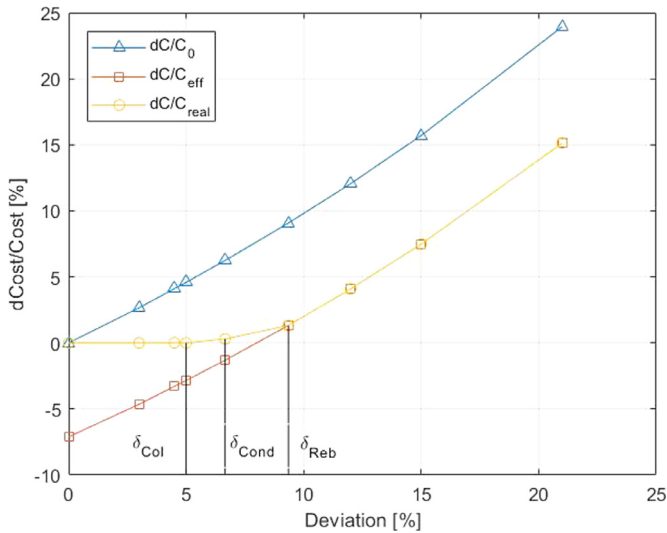


Fig. 9. Capital costs comparison (F_{SG}).

- $\frac{dC}{C_{real}}$: the effective cost differences if the case study column is already available (Yellow trend).

We can notice first that the trends are more or less linear; moreover, we can also point out that part of the investment (about 3%) could have been saved if the reboiler was properly designed, from a flexibility point of view, since its oversizing is practically useless considering the bottleneck of 5.00% given by the column diameter.

Differently from the F_{SG} index, the resilience index defines the largest total disturbance load a system is able to withstand independently of the direction of the disturbance.

It was originally defined for heat exchangers networks, therefore some modifications are needed in order to adapt it to every type of system. First of all the Resilience Index has a dimension that usually is an “heat” related value (kW, K etc.); in this case, in order to make the comparison with the other indexes possible and because of the several perturbations we have to cope with, each one with its different dimension, the percentage deviation value will be used. Then, since we’re dealing with a simple system (i.e. quasi-convex domain), we’re sure we’re going to solve a so called “Class 1 problem”, i.e. the standard vertex analysis procedure can be performed successfully.

The complete Resilience analysis results are shown in [Tables 7 and 8](#) and [Figs. 10 and 11](#).

The resulting Resilience Index (RI) for this case study is then given by:

$$RI = \min_i \{ |l_i^{max}| \} = 9.64 \quad (3.2)$$

First of all we can notice that there are no problems even if the intervals are only half-bounded because we’re looking for the minimum of the maximum withstood perturbations. The ∞ values don’t mean that we really calculated results for infinite percentage values of parameter deviation, but it means that the withstood percentage perturbation is large enough not to affect the flexibility analysis or enough to fulfill all the physically possible (not only expected) deviation range in that direction.

Then we can focus our attention on the limiting design factor that is, as for F_{SG} index, the column diameter whose corresponding parameter is the flooding velocity. The Resilience Index calculated this way has an higher value than the F_{SG} since we perturbate only one parameter at time leaving unchanged the others. Vice versa, in order to attain a given flexibility value, a smaller oversizing than F_{SG} case is needed.

Even the crossover of the minimum and maximum diameter values, i.e. the completely infeasible conditions with a single diameter column, was more conservative in the F_{SG} analysis where it was about 13% (cf. [Fig. 7](#)), while in the RI this condition is attained for a 24% (cf. [Fig. 11](#)) flexibility more or less.

Moreover, it is worth noticing that, beside the column diameter, the second most constraining variable is the reboiler while for the F_{SG} analysis was the condenser. This is the most representative difference between the two indexes because the variables acting on the condenser are U_{cond} and T_w in both cases but, while in the RI analysis they are perturbed one at a time, in Swaney and Grossmann analysis they change all at once causing the equipment affected by an higher number of uncertain parameters (in this case the condenser) to be more critical.

As well as the Swaney and Grossmann index costs analysis, the capital costs trends (normalized to the lowest value) as function of RI flexibility are plotted for each equipment in [Fig. 12](#). All of them increase as flexibility increases (according with their size). The most expensive equipment is the Kettle reboiler that has

Table 7
Allowed disturbances loads.

Parameter	Maximum deviation [%] I_i^{max+}	Minimum deviation [%] I_i^{max-}	Limiting constraint
Butane flowrate	11.80	∞	D_{min}
Pentane flowrate	81.00	∞	D_{min}
Inlet cooling water temperature	18.28	∞	A_{cond}
Condenser heat transfer coefficient	∞	17.74	A_{cond}
Reboiler heat transfer coefficient	∞	17.02	A_{reb}
Max vapor velocity	∞	9.64	D_{min}
Min vapor velocity	52.18	∞	D_{max}

Table 8
Flexibility analysis results: RI .

Deviation [%]	Condenser area [m^2]	Reboiler area [m^2]	Minimum diameter max [m]	Maximum diameter min [m]
0.00	32.91	22.26	0.603	0.782
9.64	36.42	24.64	0.634	0.745
17.02	39.65	26.82	0.662	0.715
17.74	40.00	27.06	0.665	0.712
24.00	43.30	29.29	0.691	0.686

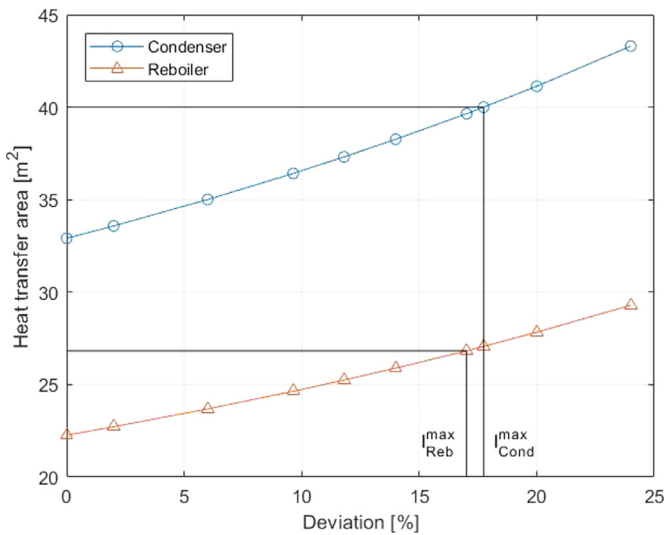


Fig. 10. Heat transfer areas (RI).

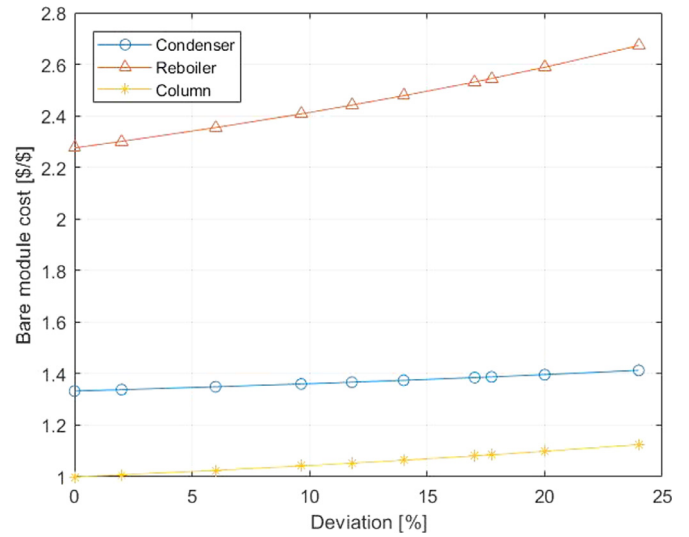


Fig. 12. Equipments bare module cost (RI).

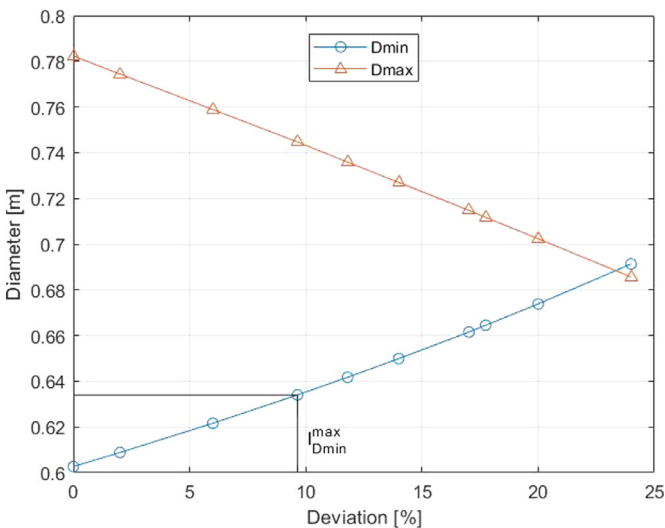


Fig. 11. Column max & min diameters (RI).

a much more accurate technology than the other heat exchangers and that works under pressure, while the column is relatively cheap because of its small diameter.

In Fig. 13 the three series of percentage data as function of Resilience Index analogous to those in Fig. 9 are reported.

Even in this case the trends are more linear, the differences between F_{SC} and RI indexes economical analysis reflects the differences highlighted in the equipment design analysis as well as the analogies, i.e. for a given flexibility value the capital cost is lower if we consider the Resilience Index flexibility. Obviously it doesn't mean that we can save money just by changing the index we use, it only means that by selecting a different index we are measuring different performances; so for each process the more suitable the index is the more accurate the economical analysis will be, where with the word "suitable" refers to the performances demanded to cope with the possible disturbances.

The Swaney and Grossmann flexibility measures the ability of the system to withstand an overall parameters deviation of $F_{SC} \cdot \Delta\theta^{k\pm\%}$, the Resilience Index measures the case of a single variable, it doesn't mind which one, deviation of $RI\%$, therefore, in order to find the most suitable index, we need to evaluate which of the two kinds of deviation our system is more likely to undergo to. This idea of "disturbance likelihood" leads

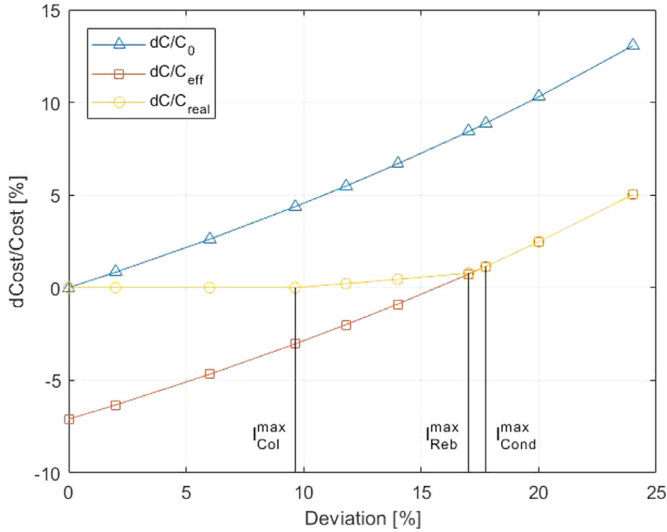


Fig. 13. Capital costs comparison (RI).

us then to the stochastic characterization of the flexibility indexes discussed in the following section for the same debutanizer case study.

3.2. Stochastic indexes: Pistikopoulos and Mazzuchi SF and Lai and Hui F_V

When we move from a deterministic point of view to a stochastic one we have to transform the idea of perturbation expected or not, defined by a well bounded deviation range, into a continuous function describing how much expected the deviation is. To do this we need to use a probability distribution function relating a probability value to each condition “x”, i.e. the independent variable(s) (cf. Appendix C for more details).

The probability density function are usually parametric functions, the probability of the independent variable falling within a particular range of values is given by the integral of this variable’s PDF over that range. The probability density function is nonnegative everywhere and its integral over the entire space is equal to one.

Before going any further with the application of these principles to our debutanizer case study, a few observations about the chosen PDF and its properties will be remarked here below.

First of all, in order to univocally define the PDFs we need to set the parameters; the selected values are:

- μ = operating conditions for each variable;
- σ or b = 20% of μ for each variable.

For this case study a 20% variance has been selected since it is about the maximum allowed individual deviation for the variables taken into account in the stochastic flexibility analysis. This choice makes the analysis sensible enough to appreciate the features of the coupling of flexibility and economics, that is the main goal of the paper. A very small σ value would result in a useless flexibility analysis since almost all possible perturbations would be withstood; on the other hand a higher σ value has poor reliability since variables uncertainty range would be too wide and a significant stochastic flexibility value would be never attained. Therefore 20% results a good compromise allowing an analysis more sensible and unbiased by excessive optimism, keeping us as conservative as needed.

We have then to choose which type of PDFs would better describe the system under analysis. Probability reflects the state of the information therefore, since we actually have no data about the

probability functions of our parameters deviations, the most general PDF possible should be used in order to have the more unbiased possible results. The condition of “general validity” is satisfied by the Gaussian or normal probability distribution. It is symmetrical with respect to its mean and the 99.73% of cumulative probability falls in the range $[-3\sigma, +3\sigma]$.

For the sake of completeness, in order to prove that the results of the stochastic flexibility analysis are not qualitatively PDF dependent, it will be conducted with a different probability distribution function as well, i.e. the Laplace one. This distribution satisfies, in a sense, the same requirements needed by the system description, that is:

- The maximum probability is attained at the operating conditions;
- the probability value is not dependent on the deviation direction.

For further details about Normal and Laplace probability distribution functions cf. Appendix C.

In order to have a visual approach with the stochastic flexibility index meaning, a 2D analysis for the condenser perturbation has been performed first (Figs. 14 and 15). Then, once dealt with it, the analysis is shifted to higher dimensions; it is nonetheless worth remarking that the analysis methodology is independent on the dimension of the problem. As we can notice, the two selected parameters, i.e. heat transfer coefficient and cooling water temperature, act on the same design variable, i.e. heat exchanger transfer area. Therefore a single constraint representing the heat balance is present.

However, since we don’t want to perform the flexibility analysis of a heat exchanger, on one hand we need to increase the dimension of our problem on the other hand we don’t want the computational effort to be too high. To match these two purposes we could, for instance, add the most constraining parameter (according to the previous flexibility analysis), i.e. the flooding velocity. This way we have a 3D domain with a variable (G_f) related to the column design (D_{min}) and the other two (T_w and U_{cond}) acting on the same design variable (A_{cond}) (Fig. 16); the independence of the third parameter on the other two can be immediately noticed since the yellow plane, i.e. flooding constraint, is parallel to the $T_w \times U_{cond}$ plane.

An additional difference between this index and the previous ones we’ve got to deal with is that, even if a given design defines univocally a stochastic flexibility value, a given stochastic flexibility value does not define univocally a system design. The two constraints can be shifted in several configuration keeping constant the value of the integral function indeed. Therefore we’ll refer as the “x” stochastic flexibility value design to the optimal configuration that attains that value, where optimal simply means cheaper. This need of economical optimization directly links flexibility with design and economic aspects whose trends will be anticipated with respect to the sizing ones.

The results of the stochastic flexibility analysis for each 1% cost increase are reported in Figs. 17 and 18, the optimal design variables in Figs. 19 and 20.

First of all it’s worth highlighting that, differently from previous flexibility indexes, the stochastic one has a non-zero value at operating conditions design.

Moreover the optimal design according to flexibility could be different from the operating conditions design or the economical optimal design.

An additional difference between SF and F_{SC} or RI is that its trend is highly non-linear if expressed as function of the equipments’ size, that means that for big oversized equipment the flexibility increase due to a further oversizing is only slightly appreciable. The relative optimal oversizing trend between the condenser

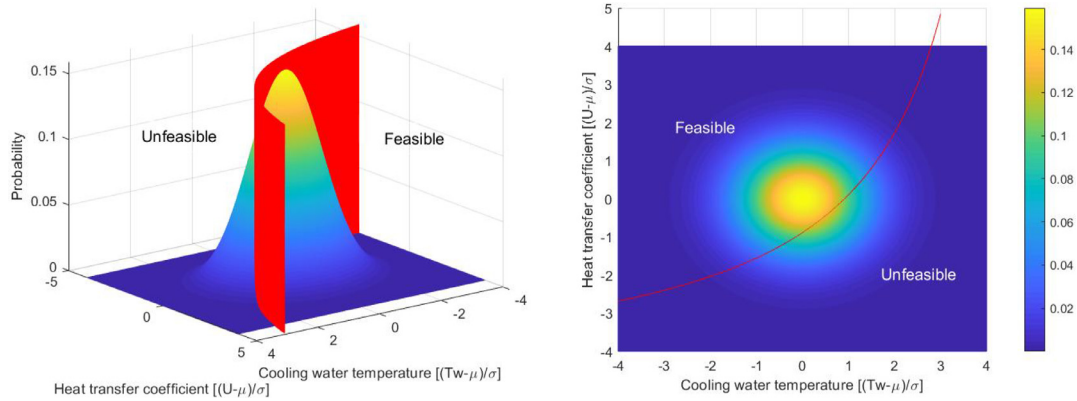


Fig. 14. Condenser SF: Normal PDF.

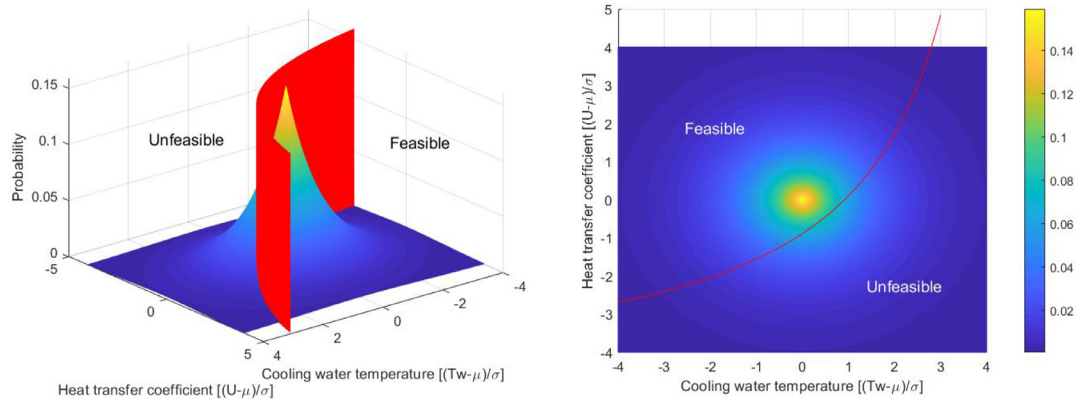


Fig. 15. Condenser SF: Laplace PDF.

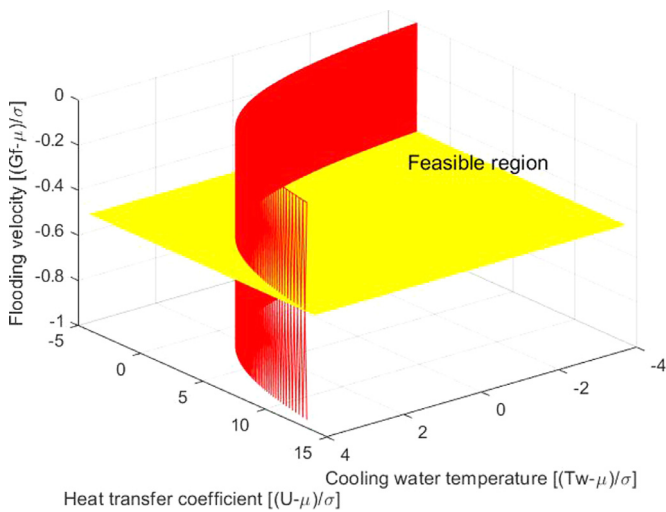


Fig. 16. 3D SF analysis domain.

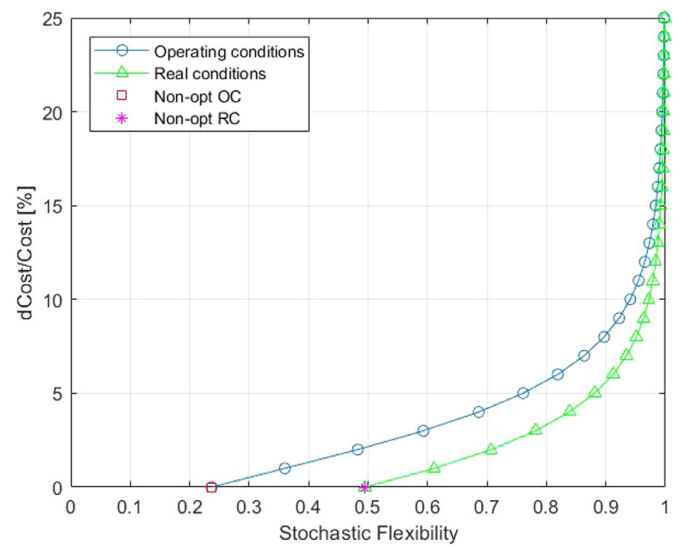


Fig. 17. SF results normal PDF.

and the column keeps being nonetheless almost linear and furthermore it follows the same line independently on the starting design condition as expected.

Finally if we compare the two different distributions results we can immediately notice that they reflect the nature of the distributions themselves. Laplace distribution converges more slowly than the Normal one, therefore the related SF approaches the value 1 only for a bigger oversizing. Nonetheless their trends are qualitatively as similar as the PDF are.

The same sizing related remarks are valid if we talk about costs since they're directly related.

For two different equipment design the starting points of the $\frac{dC}{C}$ vs. SF lines are different but, after a while, the ending branches of the two curves overlap each other approaching the asymptote.

Additional costs are higher for the Laplace distribution case than Normal distribution, as expected, because the deviation likelihood is slightly higher even far from the operating conditions.

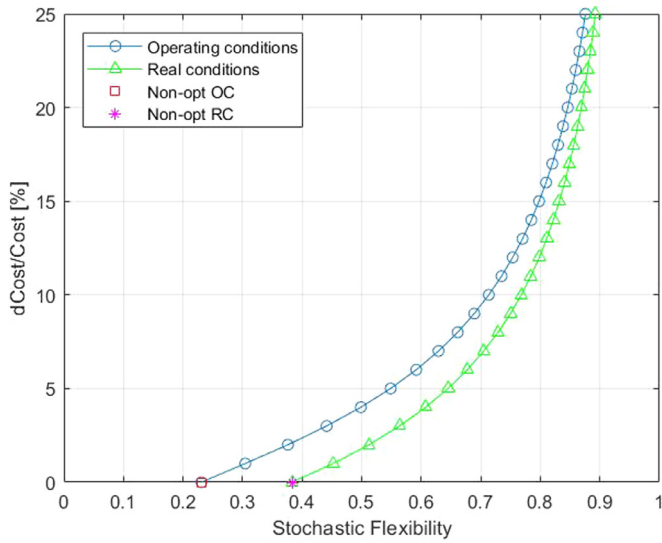


Fig. 18. SF results Laplace PDF.

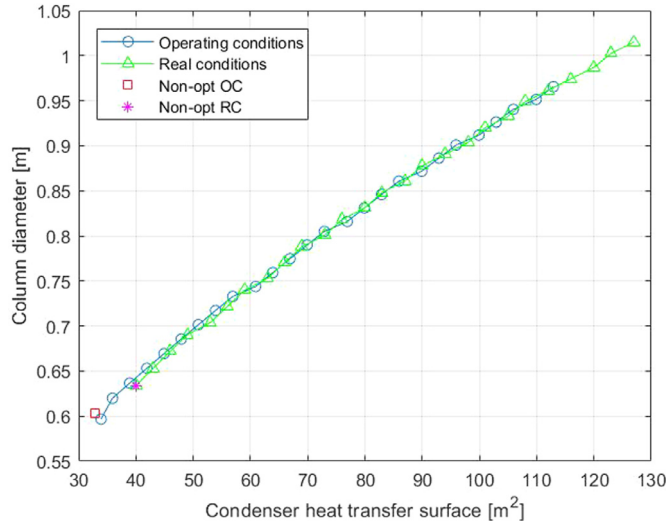


Fig. 19. SF optimal sizing NDF.

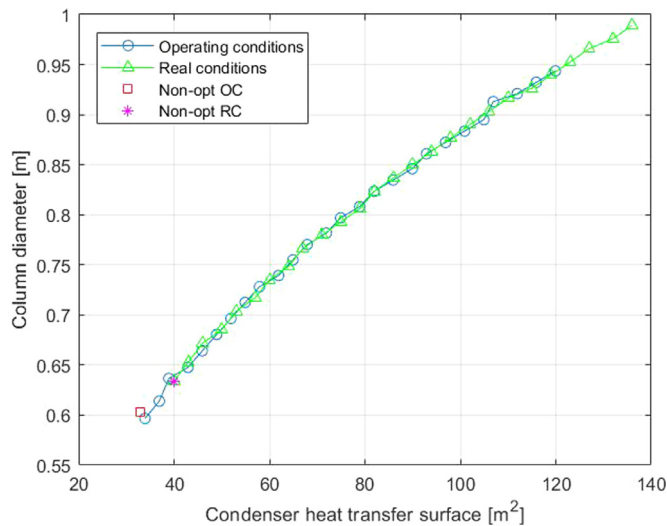


Fig. 20. SF optimal sizing LDF.

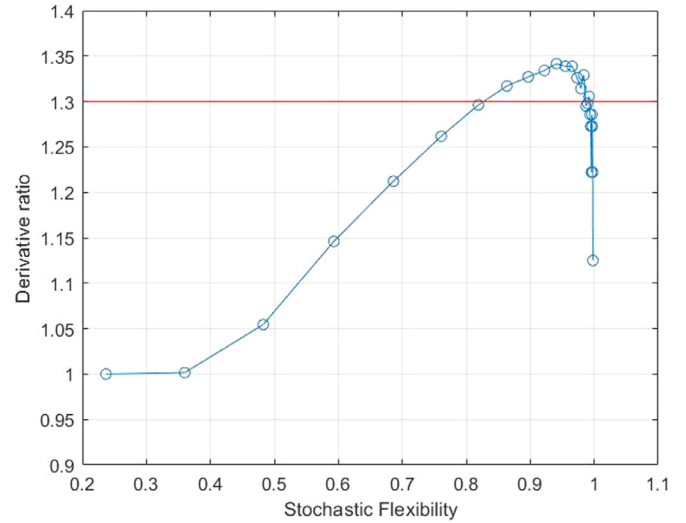


Fig. 21. $\frac{dC}{C}$ vs. SF derivatives ratio.

Differently from F_{SG} and RI , costs increase as function of stochastic flexibility index shows a non-linear trend, this means that once a certain point of the curve has been passed the ratio between the increase in flexibility and costs starts declining fast.

The main purpose of Process System Engineering is to enhance the decision making capability of the chemical engineer, therefore we'd like to identify the "certain point" after whom it's not worth keeping spending money in overdesign. The range of convenient oversizing is visible to the unaided eye: the first part of the curve gives a high flexibility increase with a small additional costs but the unwitstood deviation probability is still relevant; on the other hand the last part, even withstanding almost the whole possible deviations, needs a consistent oversizing (i.e. additional costs) to be achieved. Finally we can then conclude that the middle range of the curve is a good compromise between high flexibility and affordable additional cost.

The thorough procedure we propose to assess the optimal range is based on the curve properties: tangent lines have almost the same slope (i.e. derivative) at the beginning and at the end of the curve while it considerably changes within the interval we're interested in.

The procedure then consists in plotting the ratio between the derivative calculated at each point and the derivative calculated at the previous one as illustrated in Fig. 21 for the case of NDF and operating conditions.

This way, given the $\frac{dC}{C}$ vs. SF plot only, we can obtain a new plot whose trend shows a maximum corresponding to the value $SF = 0.9409$, i.e. 10% of additional cost.

However even the other values near there can be considered good conditions for a flexibility based design, more important than the optimal value itself is to avoid the conditions corresponding to very first and very last part of the plot. The chronologically last flexibility index proposed in scientific literature is the volumetric flexibility index F_V . It is defined as the feasible fraction of the uncertain space, that is a line for 1D case, a surface for 2D case, a volume for 3D case and a hypervolume for higher dimensions.

The reason why the volumetric flexibility index is included among the stochastic indexes is that it can be also thought as a SF index particular case whose deviation probability function is described by a step function (Fig. 22) defined as:

$$\begin{cases} 1 & \text{if } |x_i| < \Delta\theta_i^\pm \\ \frac{1}{\prod_{l=1}^N (\theta_{lU} - \theta_{lL})} & \text{if } |x_i| > \Delta\theta_i^\pm \\ 0 & \end{cases} \quad (3.3)$$

therefore the same SF analysis rules and remarks can be applied.

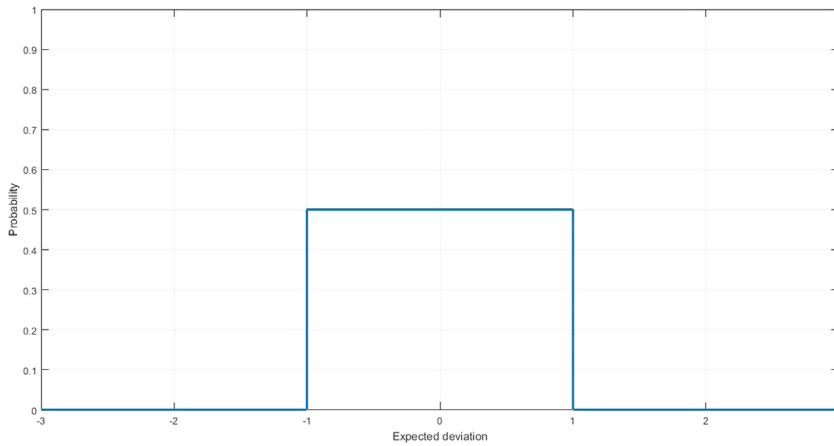


Fig. 22. F_V probability distribution function.

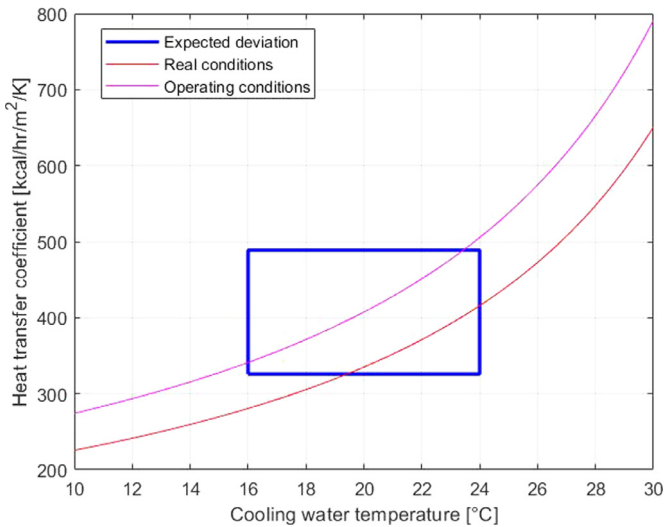


Fig. 23. 2D F_V analysis.

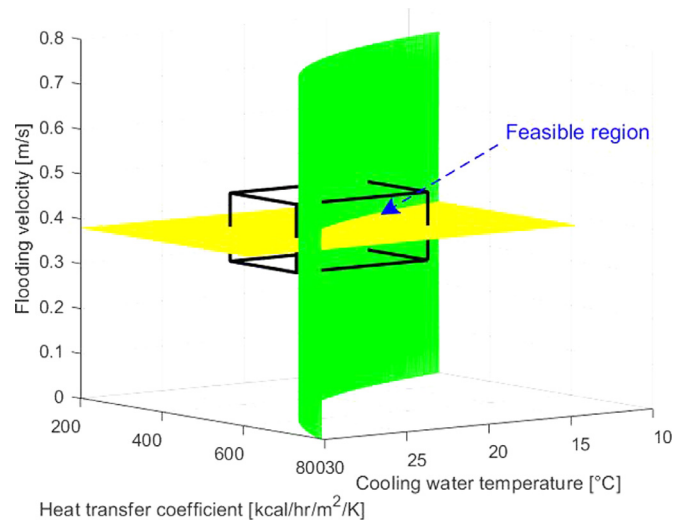


Fig. 24. 3D F_V analysis domain - operating conditions.

Thus, in order to perform this kind of analysis, two parameters have to be set: the nominal point to the operating conditions and the expected deviation value to 20%.

For this index as well a 2D analysis for the condenser perturbation has been performed first (Fig. 23) and then, once dealt with it, the analysis is shifted to higher dimensions. The same SF analysis remarks apply, i.e. the analysis methodology is independent on the dimension of the problem, the two selected parameters act on the same design variable, i.e. heat exchanger transfer area, therefore a single constraint representing the heat balance is present.

The results of this 2D case study are $F_V = 0.4714$ for operating conditions and $F_V = 0.8584$ for real conditions.

For the F_V index the analysis has been shifted in the same SF 3D domain (Fig. 24). The flooding velocity has then been included in the analysis; since it is the most constraining parameter, it reduces significantly the feasibility of the system. The triple integral required by the SF index actually becomes a volume integral since the probability distribution is constant on each interval where it is defined; due to the complexity of PDF to be integrated in stochastic flexibility analysis, the computational effort for the F_V analysis prove much lower (seconds vs. minutes).

Even in this case a given volumetric flexibility value does not define univocally a system design, therefore the “x” volumetric flexibility value design refers to the optimal, i.e. cheapest, configuration that attains that value.

The results of the volumetric flexibility analysis for each 0.5% cost increase are shown in Figs. 25 and 26.

On one hand we have the analogies with the SF that are non-zero values at operating conditions, optimal sizing independent on the starting conditions and asymptotes at $F_V = 1$. On the other hand we've got to notice that the trends of the F_V analysis results are rather peculiar and very distinctive of this kind of index. In Fig. 26 we can mainly distinguish three zones:

1. Linear trend: In the very first overdesign part both the column diameter and condenser area affect the flexibility of the system, therefore the optimal design strategy is to split the investment according to the proportion expressed by the slope of the line.
2. Horizontal (or vertical) trend: After a while the flooding constraint is almost outside the uncertain parallelepiped. The only thing to do is then to shift the condenser constraint until it exits the parallelepiped as well. In the end a little adjustment of both the design variables is observed and the value $F_V = 1$ is finally attained.
3. Overpayment zone: After the $F_V = 1$ value has been achieved the whole uncertain domain is contained within the feasible boundaries therefore any additional oversizing is, considering flexibility, practically useless. The $A_{cond} = 50.90 \text{ m}^2$ and $D_{col} = 0.686 \text{ m}$ condition corresponds definitely the maximum achievable flexibility.

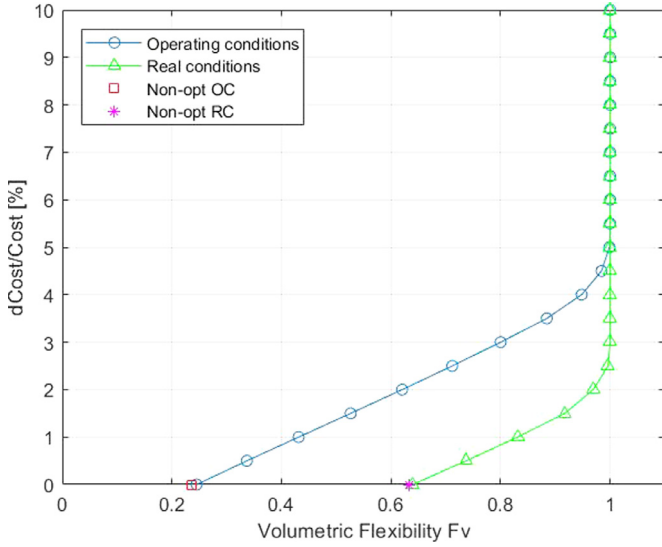


Fig. 25. F_V analysis economic results.

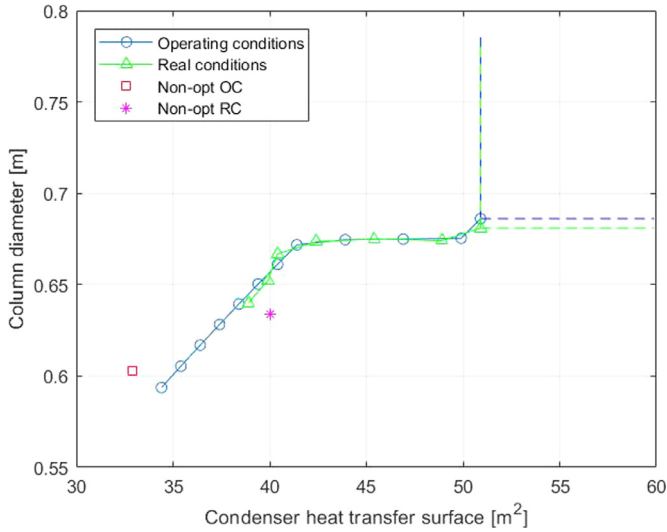


Fig. 26. F_V analysis optimal sizing.

In the end it is worth remarking that the shape of the oversizing curve is strictly related to the system features and to the expected deviations, the flexibility analysis procedure has nonetheless general validity.

The cost related remarks are the direct consequence of the combination of sizes related ones. The increase in investment costs as function of volumetric flexibility shows an almost linear trend. Since the equivalent probability distribution has a constant value, the F_V index tendency results more similar to the F_{SG} and RI indexes one, even if the domain considerations, the way we compute its value and the properties of the oversizing curves practically make it analogous to the SF index.

In the end we can conclude that a 5.5% additional cost (w.r.t. operating conditions) is definitely the maximum investment worth to be done according to a flexibility improvement purpose.

4. Conclusion

After these four flexibility analysis an indexes comparison is necessary to summarize and comment the relationships between all the results.

First of all we can mainly distinguish two typologies of indexes according to their approach towards the feasible domain: the indexes assessing the minimum of the maximum performance and the ones giving a global assessment within the uncertain or feasible domain.

The F_{SG} and RI indexes are generally more conservative, they're based on n-D hyperpolygons that can be inscribed within the feasible domain, where n is the dimension of the uncertain zone (i.e. the number of possibly perturbed parameters). The first one is more suitable if the expected perturbation involves several variables at the same time, the second one for bigger variations referred to single variables. However, they're both very conservative (specially F_{SG}) since the described geometrical objects can only scale up or down but their structure is not flexible at all, it doesn't coast the domain, it just stops whether one point is tangent. This way two completely different systems could have the same flexibility index value just because they allow the same perturbation intensity for the most constraining parameter only; on the other hand given a certain starting design, a flexibility index defines univocally the system configuration.

On the other hand we have more optimistic indexes with non-null value at operating conditions that require integration to be calculated: SF and F_V . Even in this case one of them refers to an expected deviation while the other one needs an a priori knowledge or estimation of perturbation likelihood. F_V results are similar to the linear ones until the index achieves its maximum value of 1 after whom every kind of oversizing is useless; on the other hand the SF index is very sensitive and smart, it takes into account all the possible deviations proportionally to their likelihood, showing an hyperbolic trend in oversizing/cost vs. flexibility plots that reflects well the real capability of the system to better withstand small and likely deviations than big and unlikely ones. Several configurations may have the same SF or F_V index value since they assess a global system property, not the most constraining one; therefore during the flexibility assessment we could need to solve an optimization problem according to the analysis purpose.

In the end it's worth remarking that the value of F_{SG} and F_V strictly depends on the expected deviations, nevertheless F_{SG} can be generalized and compared to the whole feasible domain as shown while F_V cannot.

Then, from a design point of view we can definitely conclude that the most suitable flexibility index for the particular analyzed system is a function of the expected deviation nature.

An advice of general validity is to perform the flexibility analysis using more than one index, combining this way their advantages; for instance the first two indexes are quite easy to compute while the ones requiring an integral calculation have a higher computational effort demand. Thus we can perform the flexibility analysis with F_{SG} or RI first in order to identify the most constraining variables in order to be able to reduce the dimension of the problem and perform the SF or F_V analysis on a smaller domain. Obviously this is a good procedure if some parameters perturbations affect variables whose constraints are very loose; if the order of magnitude of all the F_{SGi} or RI_i is almost the same, this preliminary analysis is of little help since we cannot be sure that the most constraining variable for one index will be the most constraining for the other indexes as well unless much less relevant deviations are allowed with respect to the others.

In order to compare the four indexes more immediately, the Table 9 resuming all their main features has been outlined.

On the other hand, from an economic perspective, the introduction of the Capital costs vs. Flexibility relationship and its relative plots let the decision maker, i.e. the engineering, take a more informed decision whatever the adopted flexibility index. Moreover, it clearly shows how an a priori flexibility analysis during the

Table 9
Steady state flexibility indexes comparison.

	Pros/Cons	F_{SG}	RI	SF	F_V
Need for data	Expected deviation	-	+	+	-
	Feasibility region outline	-/+	-/+	-	-
	Probability distribution			-	
Computational effort	Bounded domain	-/+	-/+	+	+
	Vertex analysis	+	+	-	-
	Computational effort	++	+	4+	++
Results accuracy	Conservative	-	-/+	+	+
	Accuracy	-	-/+	+	-/+

design phase could have allowed to save part of the investment keeping unchanged the flexibility performance of the system.

Appendix A. List of acronyms and symbols

Symbol	Definition	Unit
A	Characteristic dimension	m^p
A_{cond}	Condenser heat transfer area	m^2
C_{BM}	Equipment bare module cost	\$
C_p^0	Purchase equipment cost in base conditions	\$
CDF	Cumulative distribution function	Function
d	Design variables	/
D_{col}	Column diameter	m
D_{min}	Minimum column diameter	m
DF	Dynamic flexibility index	1
f_j	Inequality constraint	Function
F_4	Butane partial flowrate	mol/s
F_5	Pentane partial flowrate	mol/s
F_{BM}	Bare module factor	1
F_M	Material factor	1
F_P	Pressure factor	1
F_q	Column trays factor	1
F_{SG}	Swaney and Grossmann flexibility index	1
F_V	Lai & Hui flexibility index	1
G_f	Flooding velocity	m/s
G_w	Weeping velocity	m/s
h	Equality constraint	Function
$i_i^{max\pm}, i_i^{\pm}$	(Maximum) i-th direction disturbance load	1
LDF	Laplace distribution function	Function
$M\&S$	Marshall & Swift cost index	1
N, N_r, N_s	Overall, rectifying and stripping stages	1
NDF	Normal distribution function	Function
P	Pressure	Pa
Pr	Probability	1
PDF	Probability distribution function	Function
RI	Resilience index	1
S_e	Polygonal feasible space approximation	/
S_f	Feasible space	/
SF	Stochastic flexibility index	1
T	F_{SG} n-D hyperrectangle	/
T_w	Inlet cooling water temperature	$^{\circ}C$
U_{cond}	Condenser heat transfer coefficient	$W/m^2/K$
U_{reb}	Reboiler heat transfer coefficient	$W/m^2/K$
V_0	F_V uncertain volume	/
V_e	Polygonal feasible volume approximation	/
V_f	Feasible volume	/
z	Control variables	/
Z	Control variables space	/
z^U, z^L	Control variables upper and lower limits	/

Greek letters	Definition	Unit
δ	hyperrectangle vs. expected deviation ratio	1
δ^k	k-th rectangle ratio	1
θ^k	Uncertain parameters values	/
θ^N	Nominal conditions	/
$\Delta\theta^{k\pm}$	Expected deviation	1
θ_{U}, θ_{L}	F_V upper and lower expected deviation	1
μ	PDF mean value	1
σ	PDF variance	1
χ	Most restrictive dynamic constraint	Function
Ψ	Feasible space	/

Appendix B. Capital costs estimations

In order to evaluate the investment cost required for the whole system or make any kind of economic consideration and comparison, we need to estimate the costs of every single equipment.

For this purpose the Guthrie-Ulrich-Navarrete correlations described in the next paragraphs will be used (Guthrie, 1969; 1974; Navarrete and Cole, 2001; Ulrich, 1984).

B.1. Purchase equipment cost in base conditions

The purchase equipment cost in base conditions is obtained by mean of the following equation:

$$\log_{10}(C_p^0[\$]) = K_1 + K_2 \cdot \log_{10}(A) + K_3 \cdot [\log_{10}(A)]^2 \quad (B.1)$$

where A is the characteristic dimension ad the K_i coefficients are relative to the equipment typology (cf. Table 10).

The provided coefficients refers to the year 2001 and to a M&S index equal to 1110. In order to update the costs value to the year 2016 we'll refer to a M&S index equal to 1245.2 by mean of the correlation:

$$C_{P,2}^0 = \frac{M\&S_2}{M\&S_1} \cdot C_{P,1}^0 \quad (B.2)$$

B.2. Bare module cost

The equipment bare module cost can be calculated according to the following correlation:

$$C_{BM} = C_p^0 \cdot F_{BM} \quad (B.3)$$

where the bare module factor is given by:

$$F_{BM} = B_1 + B_2 \cdot F_M \cdot F_P \quad (B.4)$$

The F_M and F_P factors refers to the actual constructions materials and operating pressure while the B_i coefficients refers to the equipment typology (cf. Table 11).

The $F_{P,Kettle}$ value is given by:

$$\log_{10}(F_P) = 0.03881 - 0.11272 \cdot \log_{10}(P) + 0.08183 \cdot [\log_{10}(P)]^2 \quad (B.5)$$

where P is the relative pressure in 10^5 Pascal.

For column trays bare module cost a slightly different correlation should be used:

$$C_{BM} = N \cdot C_p^0 \cdot F'_{BM} \cdot F_q \quad (B.6)$$

where N is the real trays number, $F_{BM} = 1$ e F_q is given by the correlation:

$$\log_{10}(F_q) = 0.4771 + 0.08561 \cdot \log_{10}(N) - 0.3473 \cdot [\log_{10}(N)]^2 \quad (B.7)$$

if $N < 20$

$$F_q = 1 \quad \text{if } N \geq 20 \quad (B.8)$$

Appendix C. Probability distributions

C.1. Normal probability distribution function

As already mentioned, the condition of "general validity" is represented by the gaussian or normal probability distribution. It is symmetrical with respect to its mean and the 99.73% of cumulative probability falls in the range $[-3\sigma, +3\sigma]$.

The single variable Normal PDF (Fig. 27) states as:

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (C.1)$$

where μ is the mean and σ is the variance.

Table 10
Equipment cost in base conditions parameters.

Equipment	Typology	K_1	K_2	K_3	A
Heat exchanger	Fixed tubes	4.3247	-0.3030	0.1634	Heat transfer area [m ²]
	Kettle	4.4646	-0.5277	0.3955	Heat transfer area [m ²]
Columns (vessel)	Packed/tray	3.4974	0.4485	0.1074	Volume [m ³]
	Trays	Sieved	2.9949	0.4465	0.3961

Table 11
Bare module parameters.

Equipment	Typology	B_1	B_2	F_M	F_P
Heat exchanger	Fixed tubes	1.63	1.66	1	1
	Kettle	1.63	1.66	1	$F_{P,Kettle}$
Columns/vessel	/	2.25	1.82	1	1
Pumps	Centrifugal	1.89	1.35	1.5	1

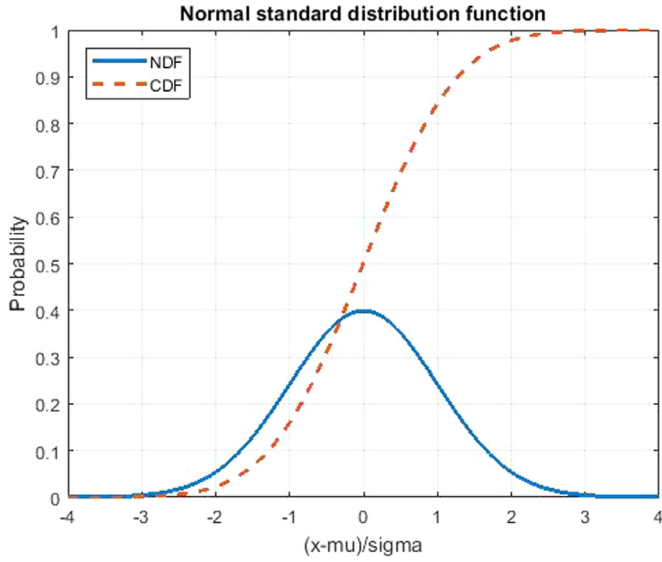


Fig. 27. 1D NDF and its CDF.

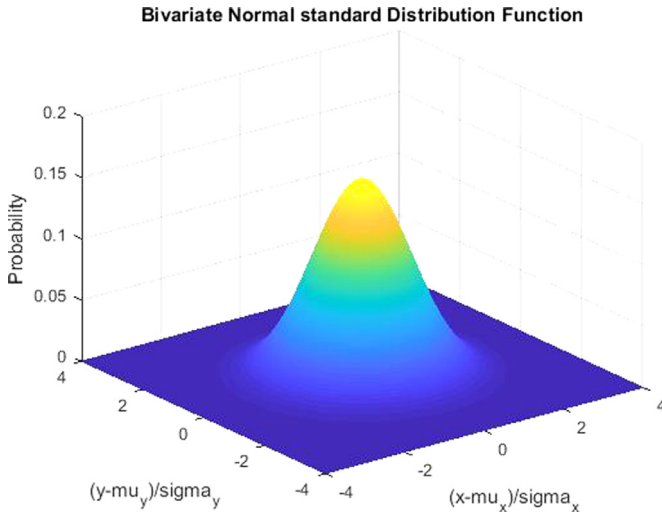


Fig. 28. 2D NDF.

The bivariate Normal PDF (Fig. 28), for a correlation between the variables $\rho = 0$, states as:

$$P(x) = \frac{1}{2\pi\sigma_1\sigma_2} e^{-\frac{y^2}{2\sigma_2^2}} \quad (C.2)$$

where y is given by:

$$y = \frac{(x_1 - \mu_1)^2}{\sigma_1^2} + \frac{(x_2 - \mu_2)^2}{\sigma_2^2} \quad (C.3)$$

Finally the most general n-variables normal PDF with can be defined as:

$$P(x) = \left(\frac{1}{2\pi}\right)^{n/2} \cdot \left|\Sigma\right|^{-\frac{1}{2}} \cdot e^{-\frac{1}{2}(x-\mu)'\Sigma^{-1}(x-\mu)} \quad (C.4)$$

where Σ is the variance-covariance matrix, Σ^{-1} its inverse and $|\Sigma|$ its determinant.

Moreover we can standardize, i.e. reconduct to a 0 mean value and variance equal to 1 (variance-covariance matrix equal to the identity matrix), the normal distribution by mean of the independent variable substitution:

$$z = \frac{x - \mu}{\sigma} \quad (C.5)$$

obtaining:

$$P(z) = \left(\frac{1}{2\pi}\right)^{n/2} \cdot \left|\Sigma\right|^{-\frac{1}{2}} \cdot e^{-\frac{1}{2}z'z} \quad (C.6)$$

for a general n variables standard normal probability distribution (Severini, 2011).

This transformation besides making the calculations easier allows to compare variables with different dimensions, e.g. temperature vs. flowrate vs. velocity etc.

The boundaries of the feasibility domain, if analytically available, have then to be rewritten as functions of the new variable z by inverting the Eq. (C.5).

C.2. Laplace distribution function

The second distribution function used for the stochastic flexibility analysis is the so called Laplace PDF.

This distribution satisfies, in a sense, the same requirements needed by the system description, that is:

- The maximum probability is attained at the operating conditions;
- the probability value is not dependent on the deviation direction.

The analytical expression of the single variable Laplace PDF (Figure 29) states as:

$$P(x) = \frac{1}{2 \cdot b} e^{-\frac{|x-\mu|}{b}} \quad (C.7)$$

where μ is the mean and b is the diversity local parameter.

Even in this case we can standardize the distribution, i.e. reconduct to a 0 mean value and diversity parameter equal to 1 by mean of the independent variable substitution:

$$z = \frac{x - \mu}{\sigma} \quad (C.8)$$

obtaining:

$$P(z) = \frac{1}{2} e^{-|z|} \quad (C.9)$$

Moreover, keeping in mind that:

$$|a| = \sqrt{a^2} \quad (C.10)$$

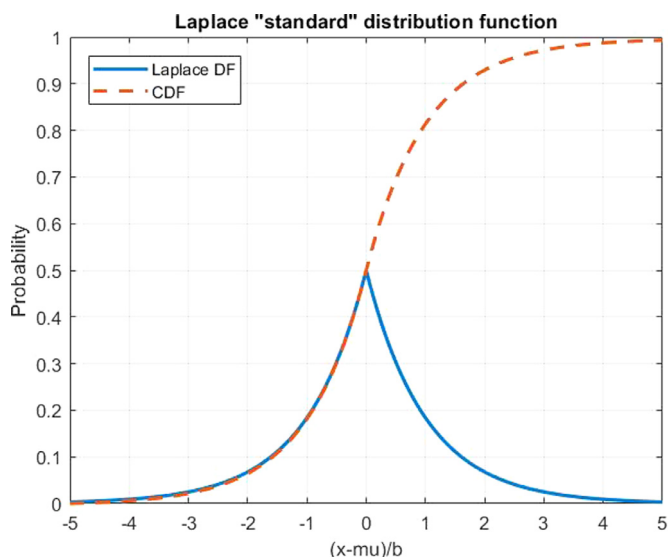


Fig. 29. 1D Laplace DF and its CDF.

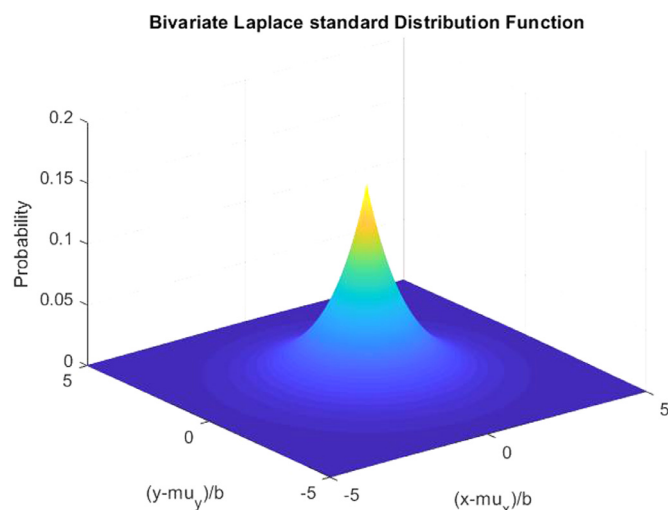


Fig. 30. 2D Laplace DF.

the trivariate Laplace PDF (for the bivariate cf. Fig. 30), for a correlation between the variables $\rho = 0$, states as:

$$P(x) = \frac{1}{8\pi} e^{-\sqrt{x_1^2 + x_2^2 + x_3^2}} \quad (\text{C.11})$$

The Laplace distribution function converges more slowly than the normal distribution, therefore we expect a lower flexibility increase by increasing the sizing, i.e. the costs.

Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:[10.1016/j.compchemeng.2019.02.004](https://doi.org/10.1016/j.compchemeng.2019.02.004).

References

- Dimitriadis, V.D., Pistikopoulos, E.N., 1995. Flexibility analysis of dynamic systems. *Ind. Eng. Chem. Res.* 34 (12), 4451–4462. doi:[10.1021/ie00039a036](https://doi.org/10.1021/ie00039a036).
- Floudas, C.A., Gümüş, Z.H., Ierapetritou, M.G., 2001. Global optimization in design under uncertainty: feasibility test and flexibility index problems. *Ind. Eng. Chem. Res.* 40 (20), 4267–4282. doi:[10.1021/ie001014g](https://doi.org/10.1021/ie001014g).
- Grossmann, I., Morari, M., 1983. Operability, Resiliency, and Flexibility: Process Design Objectives for a Changing World. Department of Chemical Engineering. <http://repository.cmu.edu/cheme/65>
- Grossmann, I.E., Floudas, C.A., 1987. Active constraint strategy for flexibility analysis in chemical processes. *Comput. Chem. Eng.* 11 (6), 675–693. doi:[10.1016/0098-1354\(87\)87011-4](https://doi.org/10.1016/0098-1354(87)87011-4).
- Guthrie, K.M., 1969. Capital cost estimating. *Chem. Eng.* 76 (3), 114–142.
- Guthrie, K.M., 1974. *Process Plant Estimating, Evaluation, and Control*. Craftsman Book Company of America.
- Hoch, P.M., Eliceche, A.M., 1996. Flexibility analysis leads to a sizing strategy in distillation columns. *Comput. Chem. Eng.* 20, S139–S144. doi:[10.1016/0098-1354\(96\)00034-8](https://doi.org/10.1016/0098-1354(96)00034-8).
- Hoch, P.M., Eliceche, A.M., Grossmann, I.E., 1995. Evaluation of design flexibility in distillation-columns using rigorous models. *Comput. Chem. Eng.* 19, S669–S674. doi:[10.1016/0098-1354\(95\)00137-Q](https://doi.org/10.1016/0098-1354(95)00137-Q).
- Huang, W., 2017. Operation feasibility analysis of chemical batch reaction systems with production quality consideration under uncertainty. *J. Chem. Eng. Jpn.* 50 (1), 45–52. doi:[10.1252/jcej.16we119](https://doi.org/10.1252/jcej.16we119).
- Lai, S.M., Hui, C.W., 2007. *Measurement of Plant Flexibility*.
- Lai, S.M., Hui, C.-W., 2008. Process flexibility for multivariable systems. *Ind. Eng. Chem. Res.* 47 (12), 4170–4183. doi:[10.1021/ie070183z](https://doi.org/10.1021/ie070183z).
- Navarrete, P.F., Cole, W.C., 2001. *Planning, Estimating, and Control of Chemical Construction Projects, Second Edition*. CRC Press.
- Pistikopoulos, E.N., Mazzuchi, T.A., 1990. A novel flexibility analysis approach for processes with stochastic parameters. *Comput. Chem. Eng.* 14 (9), 991–1000. doi:[10.1016/0098-1354\(90\)87055-T](https://doi.org/10.1016/0098-1354(90)87055-T).
- Saboo, A., Morari, M., Woodcock, D., 1985. Design of resilient processing plants 0.8. a resilience index for heat-exchanger networks. *Chem. Eng. Sci.* 40 (8), 1553–1565. doi:[10.1016/0009-2509\(85\)80097-X](https://doi.org/10.1016/0009-2509(85)80097-X).
- Severini, T.A., 2011. *Elements of Distribution Theory (1 edition)*. Cambridge University Press, Cambridge.
- Swaney, R.E., Grossmann, I.E., 1985a. An index for operational flexibility in chemical process design. part i: formulation and theory. *AIChE J.* 31, 621–630. doi:[10.1002/aic.690310412](https://doi.org/10.1002/aic.690310412).
- Swaney, R.E., Grossmann, I.E., 1985b. An index for operational flexibility in chemical process design. part II: computational algorithms. *AIChE J.* 31 (4), 631–641. doi:[10.1002/aic.690310413](https://doi.org/10.1002/aic.690310413).
- Ulrich, G.D., 1984. *A Guide to Chemical Engineering Process Design and Economics*. Wiley.
- 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. doi:[10.1016/j.jtice.2016.09.009](https://doi.org/10.1016/j.jtice.2016.09.009).