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DESIGN FOR OPERABILITY: A REVIEW OF APPROACHES AND SOLUTION STRATEGIES

DISEÑO PARA OPERABILIDAD: UNA REVISION DE ENFOQUES Y ESTRATEGIAS DE SOLUCION

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Abstract

In the last decades the chemical engineering scientific research community has largely addressed the design-for-operability problem. Such an interest responds to the fact that the operability quality of a process is determined by design, becoming evident the convenience of considering operability issues in early design stages rather than later when the impact of modifications is less effective and more expensive. The necessity of integrating design and operability is dictated by the increasing complexity of the processes as result of progressively stringent economic, quality, safety and environmental constraints. Although the design-for-operability problem concerns to practically every technical discipline, it has achieved a particular identity within the chemical engineering field due to the economic magnitude of the involved processes. The work on design and analysis for operability in chemical engineering is really vast and a complete review in terms of papers is beyond the scope of this contribution. Instead, two major approaches will be addressed and those papers that in our belief had the most significance to the development of the field will be described in some detail.

Keywords: design, operability, interaction.

Resumen

En las últimas décadas, la comunidad científica de ingeniería química ha abordado intensamente el problema de diseño-para-operabilidad. Tal interés responde al hecho de que la calidad operativa de un proceso esta determinada por diseño, resultando evidente la conveniencia de considerar aspectos operativos en las etapas tempranas del diseño y no luego, cuando el impacto de las modificaciones es menos efectivo y más costoso. La necesidad de integrar diseño y operabilidad esta dictada por la creciente complejidad de los procesos como resultado de las cada vez mayores restricciones económicas, de calidad de seguridad y medioambientales. Aunque el problema de diseño para operabilidad concierne a prácticamente toda disciplina, ha adquirido una identidad particular dentro de la ingeniería química debido a la magnitud económica de los procesos involucrados. El trabajo sobre diseño y análisis para operabilidad es realmente vasto y una revisión completa en términos de artículos supera los alcances de este trabajo. En su lugar, se discutirán los dos enfoques principales y aquellos artículos que en nuestra opinión han tenido mayor impacto para el desarrollo de la disciplina serán descriptos con cierto detalle.

Palabras clave: diseño, operabilidad, interacción.

1. Introduction

In this section, the basics of *Process Design* and *Process Operability* are introduced and the importance of their interaction stressed. Current philosophies to design-for-operability are also described and future trends within the chemical engineering discipline identified. A brief outline of the vision from industry of the design-for-operability problem along the last decades is also presented in order to illustrate the practitioners point of view.

1.1 Chemical process design

Engineering has to do with the production of goods that are beneficial to mankind. In chemical engineering the goal is the manufacturing of chemical products from

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raw materials by means of chemical processes. A chemical process project roughly verifies the following stages:

1. Novel Commercially Attractive Commodity Identification
2. Abstract Description of the Process
3. Process Design
4. Plant Construction
5. Start-up and Commissioning
6. Plant Operation
7. Debottlenecking
8. Decommissioning

Process design is perhaps the most challenging stage from an intellectual point of view since design problems are usually under-defined; i.e., very little information is available from the Abstract Description stage (perhaps just chemical reaction related data) in order to precisely define the design problem. Therefore design problems become very open-ended.

Natural goals of process design are economic optimality and satisfactory operational features of the resulting design, among others. In order to meet the desired goals and to cope with the lack of information, the most intuitive way to address such a complex task is to provide the missing information on an engineering basis, and to evaluate the generated process for economic optimality and operability. If the resulting design is not satisfactory, improvements are introduced and re-evaluation performed. This iterative refining procedure, known as *sequential process design*, is carried out until a satisfactory design is achieved. Fig. 1 roughly sketches this process design procedure. Such an approach to chemical process design is justifiably considered to be a rather artistic activity. It has even been nicely compared by Douglas (1988) with the process of developing a painting by a painter.

There exists, however, a strong trend to automate the design process and to tackle it as an algorithmic activity rather than an artistic activity, relying on the availability of computational power. Since the goals of process design are economic optimality and satisfactory operability features, it seems reasonable to mathematically pose the process design problem as an optimization problem, giving rise to the so called optimization approaches to process design (Biegler *et al*., 1997).

This is an *algorithmic process design* philosophy (in opposition to the *sequential process design* approach in Fig. 1), whose mathematical formulation for continuous plants is that of problem (P1) in Section 3 of this article. The solution of problem (P1) provides the optimal process topology, the optimal process design and the optimal operating point for the expected value of the objective function, and at the same time satisfies the feasibility constraints over the whole time horizon. Problem (P1) is a multiple-objective semi-infinite-dimensional, mixed-integer, dynamic optimization problem. Such a formulation is very ambitious from both, modeling and resolution points of view and attempts to solve even simplified versions of this problem have only recently appeared.

Current practice in process design, is probably a certain degree of combination of both approaches: knowledge based "artistic" skills of the designer in order to perform an early screening of alternatives to significantly reduce the combinatorial problem (Fig.1) and algorithmic optimization techniques (simplified versions of ambitious problem (P1)) to search among a still large number of alternatives but based on more detailed mathematical models. It is our belief, however, that process design evolves to be a completely automated (algorithmic) activity, strongly dependent on problem representation, modeling, and solution strategies. There exists a necessity; a "driving force" for automation as societies become more complex.

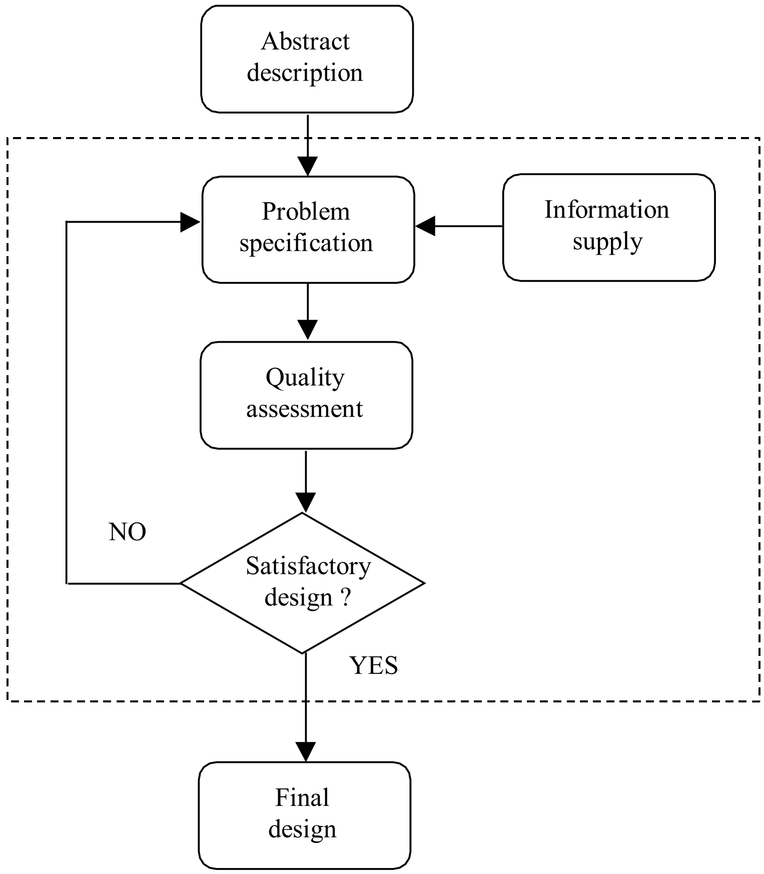

Fig.1: Sequential process design procedure.

1.2 Process operability

Besides economic optimality, the final design should verify certain desirable features. Such features include adequate dynamic behavior, safety and environmentally acceptable operation and visual amenity among others. Particular emphasis should be placed on Health and Safety Hazards, Loss Prevention, Environmental Protection, Plant Location, Plant Layout and of course Plant Operability (Peters and Timmerhaus, 1991). For example, in order to consider Health and Safety Hazards, issues as exposure, fire and explosion sources should be identified and evaluated. Loss Prevention is usually addressed by hazard and operability studies (HAZOP), fault-tree analysis (FTA), failure mode and effect analysis (FMEA), safety indexes and safety audits. Environmental Protection should consider air and water pollution abatement, solid waste disposal and thermal and noise pollution control, based on local policies and international regulations, for example those of the Environmental and Protection Agency (EPA). Plant geographical location should be chosen according to raw materials and energy availability, water and labor supply, transportation facilities, climate, taxation and legal restrictions, community factors, etc. Proper plant layout includes arrangement of processing areas, storage areas and handling areas in efficient coordination.

In particular we are interested here in "operable" designs. Operability is a wide and rather subjective concept that may be defined as "*the ability of the plant (together with the control strategy) to achieve acceptable static and dynamic operation*". This is a slightly modified version of Wolff's definition (Wolff *et al.,* 1994). In order to provide a more precise definition of operability, it is usually split into a number of properties (elements) of more intuitive meanings:

- *Stability:* Condition of the steady state operating points of the plant to be locally stable.
- *Flexibility:* The ability of the design to remain steady state feasible in the face of parametric and disturbance uncertainty.
- *Controllability:* The ability of the plant to move dynamically between operating points in a smooth and feasible fashion, as result of set-point changes (often referred as switchability) and disturbances.

Operability is therefore strongly related with the dynamic performance of the process.

1.3 The interaction between process design and process operability

In order to ensure satisfactory design features operability considerations, among many others as commented before, should be taken into account at the design stage. All these issues should be considered in the assessment stage of the sequential process synthesis procedure (Fig. 1), or explicitly included within the algorithmic process design formulation (P1), or somehow handled in a hybrid approach, in order to achieve a satisfactory design.

It should be emphasized the fact that process operability assessment is of outstanding importance since the sought of steady state economic optimality only (as historically done) may lead to processes that are difficult or impossible to operate. Such a situation has been reported for example in Anderson (1966). In that article, the re-design of a poorly designed heat exchanger network, impossible to operate at nominal conditions, is described.

Design for dynamic operability become particularly critical since, mainly due to economical reasons, modern chemical plants tend to be highly mass and energy integrated. This implies mass recycles from separation stages back to reaction stages in order to maximize raw material conversion throughout the whole process, and the use of hot streams to heat cold in order to optimize energy consumption ones (energy recycles). Mass and energy integration however, although desirable from an economic point of view is highly detrimental regarding operability, since the dynamics of integrated processes are far more involved than those of cascaded unit processes. Usual practice to cope with the difficult dynamics of plants with recycles is to install large buffer tanks to isolate sequences of units in order to allow the use of conventional single-unit control strategies. However, this practice is expensive in both, capital and operative costs. On the other hand, large material inventories are undesirable due to safety and environmental reasons, especially if dangerous or environmentally unfriendly chemicals are involved. It is also detrimental of the plant's capacity to rapidly change product grades. These issues gave rise to the notion of "plantwide" control, which addresses the control problem of chemical process from a global framework, visualizing the plant as a whole, rather than an interconnection of individual process units.

The above comments pretend to stress the importance of proper operability considerations at the early stages of the process design procedure in order to generate inherently operable processes.

As already discussed, the process design procedure evolves from a synthesis-artistic activity, Fig. 1, towards an algorithmic activity (problem P1).

In order to generate intrinsically operable designs from the algorithmic approach, operability elements should be explicitly included within (P1) type formulations. This may be described as the *integration of process design and process operability* in contrast with the process operability analysis of the sequential approach to process design.

The integration between process design and process controllability, a particularly important sub-field of the integration between process design and process operability, has been widely addressed in the last decades. It is known that controllability, which may be defined as the "achievable control performance", is dependent on the design itself rather than on the final control strategy. Therefore, poor control strategies are often able to perform acceptably on easily controlled processes. On the other hand, even complex control strategies may not be good enough to control poorly designed processes. Similar considerations can be argued regarding operability as an integrating concept.

As well as the design/operability problem it can be identified the design/risk problem, the design/environmental problem, the design/plant-layout problem, etc. In fact they are all sub-problems of the general design/operability-risk-environmental-plant layout-etc. problem. Just partial solutions to the particular problems have been conceived up to now. Much work still remains in each area to achieve conclusive results and far more to solve the whole process design problem.

1.4 The vision from industry

During the last decades, several critical papers to current process design and control theory from an industrial point of view appeared.

Foss (1973) identified the unique features of chemical processes in the spectrum of control problems: large dimensionality, strongly interactive nature, poorly known characteristics, high uncertainty and undetermined control system structure. The major limitations of the available theories: single input single output linear theory, non-interacting control, modal control and optimal control were also analyzed. The author also emphasized the issue of the determination of the control system structure: "An acceptable, broadly applicable solution to the control structure problem cannot be achieved by the dreaming up of a number of candidate configurations for a given process and then testing them."…"Rather, the method must have its basis in a broadly applicable representation of the process dynamics and control objectives. It must acknowledge and address quantitatively problems of sparse and poor measurements and imprecisely known process characteristics".

Later, Lee and Weekman (1976) also described the challenging features of chemical processes and the limitations of available control theories from an industry standpoint. Again research is encouraged towards integration, "… the process design and control design have to be integrated so that the dynamics and control configuration could be considered in the process design stage. New techniques must acknowledge the problems of sparse and poor measurement, imprecise process knowledge and computational difficulties in parameter estimation " … "High priority should be assigned to new techniques designed to aid modeling of chemical processes".

The necessity of integration of process and control system design was also identified and addressed by industry during the eighties as described for example by Sheffield (1992). The author comments the decision at Shell Oil Co. of physically locate the control team with the design team to allow their interaction from the early stages of the process design project.

Hernández *et al.* (1994) described the approach adopted by Shell Oil Co. for industrial control system design and posed challenges to the academic community. It is claimed in the article that up to that time, a procedure that treats plant economics and closed loop performance within the same framework was not available. Main tools for control strategy design (variable selection and variable pairing) and controller tuning were reviewed and their advantages and limitations for practical purposes identified. The development of time domain rather than frequency domain analysis tools is suggested as an area of future academic research.

J. A. Miller from DuPont (Miller, 1995) gave a vision from industry on the new plants design issue: "One major problem continues to be the lack of a completely integrated set of computer tools which will support concurrent engineering design instead of doing almost everything serially. A second problem is that chemical plants, designed on the basis of steady-state operation, rarely run at steady state in practice and sometimes end up being very hard to control. Rather than trying to use process control to correct a poor design, we need better methods to evaluate the controllability and operability of competing process alternatives as early as possible in the design process."

Some contributions from industrial practitioners made meaningful points in the control research and educational areas. Benson and Perkins (1997) commented that "The academic challenge in the future is to match the synergy in the process design with that of process control to exploit each to the mutual benefits of the customer. The evidence suggests that it is rarely done at the moment yet it also suggests that where it is done the benefits are significant".

Ramaker *et al.* (1997) from Shell Oil Co. posed an interesting (and rather shaking) thought in chemical engineering control education: "… we feel that frequency domain analysis and design should be taught at a graduate level, maintaining the undergraduate curriculum as closely tied as possible to the time domain".

In the remainder of this paper, we review the two major approaches to design-for-operability. In Section 2 most important Controllability and Resiliency (C&R) metrics based approaches are reviewed. Section 3 presents the simultaneous approach for process and control system design, based on state of the art mathematical formulations and solution strategies for the integrated problem. In Section 4 some conclusions are drawn and future trends identified.

2. C&R approaches to design-for-operability

2.1 Basics on C&R theory

In this section, linear systems theory in the Laplace and frequency domains and its implications in operability are briefly reviewed. For a comprehensive analysis on the subject see Skogestad and Poslethwaite (1996).

The dynamics of a process may be accurately described by a set of (generally non-linear) differential algebraic equations in the state space:

$$\dot{\mathbf{x}} = \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{d}_s) \tag{1}$$

$$\mathbf{y}_s = \mathbf{g}_s(\mathbf{x}, \mathbf{u}, \mathbf{d}_s) \tag{2}$$

where $\mathbf{u}$ is the vector of manipulations, $\mathbf{y}_s$, the vector of outputs, $\mathbf{x}$ is the vector of states and $\mathbf{d}_s$, the vector of disturbances (all vectors represent deviation variables from some nominal value). Performing linearization on such models:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} + \mathbf{E}\mathbf{d}_s \tag{3}$$

$$\mathbf{y}_s = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u} + \mathbf{F}\mathbf{d}_s \tag{4}$$

By applying Laplace transforms to (3) and (4) it is possible to obtain the transfer function representation of the system:

$$\mathbf{y}_s(s) = \mathbf{G}(s)\mathbf{u}(s) + \mathbf{G_d}(s)\mathbf{d}_s(s) \qquad (5)$$

where

$$\mathbf{G}(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D} \qquad (6)$$

$$\mathbf{G_d}(s) = \mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1}\mathbf{E} + \mathbf{F} \qquad (7)$$

It should be remarked that state space and transfer function models are different representations of the real system. The state space model (3), (4) has always a transfer function counterpart in (5), (6) and (7) but the opposite is not true for improper and /or time delayed systems expressed as transfer functions.

Most linear input-output controllability tools are based on appropriate scaled models of $\mathbf{G}(s)$ and $\mathbf{G}_d(s)$.

"Perfect control" (not realizable in practice) is achieved when the output, $\mathbf{y}_s$, is able to perfectly follow a certain reference, $\mathbf{r}$, this is $\mathbf{y}_s = \mathbf{r}$. Solving for $\mathbf{u}$, the corresponding perfect control input is:

$$\mathbf{u} = \mathbf{G}^{-1}\mathbf{r} - \mathbf{G}^{-1}\mathbf{G_d}\mathbf{d}_s \qquad (8)$$

The single-input single-output (SISO) case is particularly insightful, and allows the identification of those elements that impose limitations to achieve "perfect control". Let us consider the following SISO model:

$$y_s = Gu + G_d d_s \qquad (9)$$

where G and G_d have the general (pole-zero-time delay) form:

$$g_{pz\tau} = \frac{k_{pz\tau}\prod_{i=1}^{m}(s - z_i)}{\prod_{j=1}^{n}(s - p_j)} e^{\tau s}$$

where z_i are the zeros of the system, p_j are the poles of the system and τ is the time delay.

- The poles of the system are the eigenvalues of the state space Jacobian matrix.
- The zeros of the system may be found as the non-trivial ($\mathbf{u_z} \neq \mathbf{0}$ and $\mathbf{x_z} \neq \mathbf{0}$) solutions of the following generalized eigenvalue problem:

$$(z\mathbf{I_g} - \mathbf{M})\begin{bmatrix}\mathbf{x}_z \\ \mathbf{u}_z\end{bmatrix} = 0$$

$$\text{where} \quad \mathbf{M} = \begin{bmatrix}\mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D}\end{bmatrix}; \quad \mathbf{I_g} = \begin{bmatrix}\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}\end{bmatrix}$$

- Time delays do not have a state space representation.

"Perfect control" is achieved when the output, y_s, is able to perfectly follow a certain reference, r, this is $y_s = r$. Solving for u, the corresponding perfect control input is:

$$u = G^{-1}r - G^{-1}G_d d_s \qquad (10)$$

As evident, "perfect control" requires the inverse of G, which cannot be obtained, if:

- G contains right-half-plane zeros (RHPZ) (G^{-1} unstable)
- G contains time delays (G^{-1} contains a prediction)
- G contains more poles than zeros (G^{-1} is unrealizable)
- G is uncertain (G^{-1} cannot be obtained exactly)

In order not to exceed physical constraints on the value of u, perfect control is limited by:

- $\left|G^{-1}\right|$ large
- $\left|G^{-1}G_d\right|$ large

Additional limitations to control are imposed by:

- G contains right half plane poles (RHPP) (open loop instability)
- $\left|G_d\right|$ large (outputs move too far from their desired values in controller absence)

From the analysis of the SISO case in the Laplace domain (transform function) a number of elements which are detrimental for control purposes have been identified.

- RHPPs are associated with unstable plants and feedback control is required for stabilization.
- Significant dead-times are sources of instability for closed-loop responses and advanced control systems (dead time compensation) are necessary for proper closed-loop performance.
- Inverse response behavior, associated with RHPZs, also presents challenging features from a control point of view and inverse response compensation is required for satisfactory closed-loop performance.
- The presence of uncertainty (in G and G_d) makes necessary the use of feedback control.

Although the separate effects of the aforementioned elements are well understood, they occur concurrently, making the analysis much more difficult. For example, the performance of SISO systems is poor if the plant has a RHPP located close to a RHPZ.

For the general multiple-input/multiple-output (MIMO) case, the following considerations hold:

- RHPZs, RHPPs and delays have directions associated with them introducing additional difficulties.
- Time delays pose limitations on MIMO systems. Surprisingly, however, an increased time delay may sometimes improve the achievable performance.
- As for SISO systems RHPZs impose poor control performance in the MIMO case.
- Feedback stabilization is also necessary in the presence of MIMO RHPPs.
- As in the SISO case, the performance of a MIMO plant with close RHPP and RHPZ is poor if the directions coincide.

2.1.2 Non-minimum phase elements

RHPPs, RHPZs and time delays are usually known as non-minimum phase elements. As described above, their presence impose severe control limitations and their inclusion within process design formulation have been considered in a number of ways as described later in this section.

2.1.3 Singular value techniques

Singular value techniques have been also applied to study the size or gain introduced by the linear transformation (5). The singular values of matrix **G** may be calculated as the square roots of the eigenvalues of the Hermitian matrix $\mathbf{G}(s)^*\mathbf{G}(s)$).

In particular, the minimum singular value of the steady state (zero frequency) transfer function matrix, **G**:

$$\sigma_{\min}(\mathbf{G}) = \min_{\|\mathbf{u}\|\neq 0} \frac{\|\mathbf{Gu}\|_2}{\|\mathbf{u}\|_2}$$

Indicates how close this matrix is to being singular and represents the smallest gain of the process among possible input directions. A large value of this measure implies that the process is resilient to disturbances.

The maximum singular value of **G**(s), $\sigma_{max}(\mathbf{G}(s))$, (square root of the maximum eigenvalue of the Hermitian matrix $\mathbf{G}(s)^*\mathbf{G}(s)$) indicates the largest gain of the process among possible input directions.

2.1.4 Condition number

The condition number of matrix **G**(s) characterizes model uncertainty. Perfect control cannot be realized in the presence of model uncertainty, since modeling errors in **G**(s) lead to errors in the manipulated input **u**(s) in Eq. (8). Such modeling errors are always present, and result from the linearization process, unmodelled dynamics and poorly known parameters. These errors are related by:

$$\frac{\|\delta\mathbf{u}\|}{\|\mathbf{u}\|} \leq \gamma(\mathbf{G})\frac{\|\delta\mathbf{G}\|}{\|\mathbf{G}\|}$$

Where $\gamma(\mathbf{G})$ is the condition number of matrix **G**, defined as $\sigma_{max}(\mathbf{G})/\ \sigma_{min}(\mathbf{G})$. A small condition number indicates that model uncertainty does not cause large manipulated variable errors.

2.1.5 Disturbance condition number

The disturbance condition number, $\gamma_d(\mathbf{G})$, is defined as:

$$\gamma_d(\mathbf{G}) = \frac{\|\mathbf{G}^{-1}\overline{\mathbf{d}}\|_2}{\|\overline{\mathbf{d}}\|_2}\sigma^*(\mathbf{G})$$

and quantifies the effect of rejecting disturbances. Here, $\overline{\mathbf{d}}$, corresponds to a particular disturbance $\overline{\mathbf{d}} = \mathbf{G}_{\mathbf{d}_i}\mathbf{d}_i$. A large value of $\gamma_d(\mathbf{G})$ means that the disturbance has a large directional effect and produces therefore large actions in manipulated variables.

2.1.6 Relative gain array

Finally, another valuable tool related to operability assessment is the Relative Gain Array (RGA). The RGA is a square matrix, which implies that the number of manipulations and outputs is the same, say N. It is applied to identify those control loops that verify minimal interaction among the possible pairings (N!). The relative gain between an output y_{si}, and a manipulated variable u_j is defined by:

$$\lambda_{ij} = \frac{(\Delta y_{si} / \Delta u_j)_u}{(\Delta y_{si} / \Delta u_j)_{y_s}}$$

The subscript u denotes constant values for all manipulated variables except u_j, while subscript y indicates that all outputs except y_{si} are kept constant by the control loops. It is recommended to form control loops pairing controlled outputs y_{si} with manipulated variables u_j such that the relative gains λ_{ij} are positive and as close as possible to unity.

Despite linear operability analysis techniques dominate the design-for-operability approaches, they present several limitations (Chenery, 1997). First of all, linear approximations may not be reliable enough for the usually highly non-linear process systems in the face of uncertainty. Some of the measures assume square (Laplace domain) plants (same number of controlled and manipulated variables), which may be unrealistic. These indices are defined in the frequency domain while the performance requirements are established in the time domain and the translation may no be straightforward. Finally, the application of these tools requires the use of heuristics and experience in order to overcome the subjectivity of their definition.

2.1.Design for C&R approaches

Several approaches for design-for-controllability have been presented regarding non-minimum phase elements.

Psarris and Floudas (1990) investigated the effect of MIMO systems with time delays, and proposed there a rigorous strategy to minimize the detrimental effects of time delays by performing the minimum necessary increases in the delays of the plant transfer function matrix, within the framework of mixed-integer linear programming (MILP).

Psarris and Floudas (1991) studied the dynamic operability of MIMO systems with time delays and transmission zeros. In that work, a mathematical formulation that removes the infinite RHP transmission zeros by increasing the delays of the process by the minimum amount necessary is presented.

Kokossis and Floudas (1994) proposed a systematic methodology applicable to the optimal design of stable processes. An iterative algorithmic approach was applied to solve the design optimization problem while constraining the eigenvalues of the jacobian matrix of the dynamic system (open loop poles) to lie in the left half plane of the complex domain. The methodology was applied in that article, to the synthesis of complex reactor networks.

In Blanco and Bandoni (2003a), the problem of open-loop dynamic stability has been also addressed by means of eigenvalue optimization strategies. The proposed approach makes use of the direct relation between system dynamics and eigenvalue theory, in order to ensure the open loop poles of the system to lie in the left half of the complex space. Parametric and disturbance uncertainty is considered in that contribution in the framework of a multi-period formulation.

Other C&R measures have been considered within a multiple objective design approach. Multiple objective optimization problems arise when it is necessary to deal with competing objectives, this is, when one of the objectives can be improved only at the expense of the others. This is rather common in design and it is indeed the case in design-for-controllability. The main advantage of multiple objective optimization to address the design-for-operability problem is that the objectives use to have very intuitive meanings and the tradeoff among them can be clearly traced. The set of solutions that reflect this tradeoff among the different objectives is known as the non-inferior solution set or pareto optimal solution. Common practice in multiple objective optimization is to generate somehow the non-inferior solution set, and then select among its members according to a certain decision-maker's preference.

Palazoglu and Arkun (1986) is one of the first approaches that recognized the multiple objective nature of the chemical process design problem in order to consider dynamic operability characteristics besides steady-state feasibility and economics. For a given flowsheet (no structural design is performed), a multiple objective optimization problem is formulated considering an economic objective and a couple of robustness indices (singular values of the transfer function model) as dynamic operability objectives.

Luyben and Floudas (1994) proposed a multiple objective optimization framework for the interaction of design and control. In their approach steady state cost and steady state controllability measures such as minimum singular value, condition number, disturbance condition number and relative gain array, were considered as the competing objective functions. A mixed integer nonlinear design optimization model (binary distillation column) and a nonlinear design optimization model (reactor-separation-recycle system) were addressed in their contribution.

Blanco and Bandoni (2003b) implemented eigenvalue optimization techniques to cope with the controllability objective, namely the minimum singular value of the zero frequency process transfer function matrix, within a multiple objective optimization problem. In that work the possibilities of eigenvalue optimization were introduced to the chemical engineering community and its features shown through the important design-for-operability problem and illustrated by means of the reaction-separation-recycle process, of outstanding importance in chemical engineering.

3. Dynamic optimization approach to design-for-operability

3.1. Problem formulation

This approach considers process design and process operability simultaneously as one integrated optimization problem. This is an attractive approach indeed since both, flowsheet synthesis and operability analysis, are fully automated.

Process synthesis reduces to develop a superstructure of process flowsheets, which may include the possible control schemes, introducing binary decision variables within the formulation. Satisfactory process controllability is ensured since the dynamics of the (closed-loop) system is explicitly considered through the set of differential equations, giving rise to a dynamic optimization problem. Steady state and dynamic process feasibility are also ensured by taken into account disturbance and parametric uncertainty.

A closed-loop dynamic system can be described by a set of differential and algebraic equations (DAEs) in terms of continuous and discrete variables (11).

Note that for consistence the following relations must verify in (11):

$$\mathit{dim}\ \{\mathbf{x}_d\} = \mathit{dim}\ \{\mathbf{h}_d\} = \mathit{dim}\ \{\mathbf{h}_0\}$$

$$\mathit{dim}\ \{\mathbf{x}_a\} = \mathit{dim}\ \{\mathbf{h}_a\}$$

A subset of the dynamic state variables $x_d(t)$ are the controlled variables which have a desired value or set-point. Some or all u(t) are the variables manipulated by the controllers to reject disturbances and effects of uncertain parameters.

Additional sets of constraints can also exist in the design-for-operability model (12): sets h_d, h_a and h_0 represent a DAE system for the closed-loop dynamic model of the process. Equations g impose constraints on state variables. Interior- and end-point constraints (h_{dk}, h_{ak} and g_k) and static equality and inequalities constraints ($\hat{h}$ and $\hat{g}$) when present, add a further level of limitation in the process state variables. Altogether Eqs. (11) and (12) constitute a constrained DAE system, whose input/output structure is roughly sketched in Fig. 2.

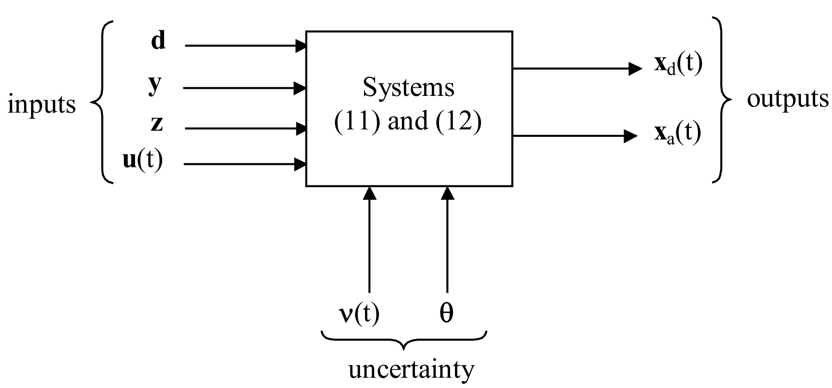

Fig. 2. Constrained DAE system.

In the design-for-operability problem it is in general desired to simultaneously optimize an amount of, usually conflicting, objective functions, $J = (J_1,\ldots,J_M)$, which involve costs, profits and product quality, leading to a multiple objective optimization problem.

The presence of uncertainties and disturbances makes the formulation semi infinite dimensional, due to the infinite values that these parameters can take. Such a situation requires the inclusion of the expectation operator, E, in the formulation.

The integrated design-for-operability problem can therefore be formulated as (P1).

Formulation (P1) is a Semi Infinite Multiple Objective Mixed-Integer Dynamic Optimization problem (SIMOMIDO) which is very difficult to solve due to the following complicating issues:

- Its multiple objective nature
- Its stochastic nature
- Its mixed integer dynamic nature

In order to cope with these issues several strategies have been proposed. In the following, we review the classical approaches devised to this end.

3.2. Multiple objective nature

Vector $\mathbf{J} = (J_1,\ldots,J_M)$ comprises M different objective functions. If there are several conflicting objectives in J, the most straightforward approach is to measure the objectives on a same basis by weighting them with appropriate factors, and set as objective function the weighted sum of the individual objectives. Alternatively, the multiple objective problem can be addressed through the ε-constrained method. This strategy provides a non-inferior set of optimal solutions known as pareto-optimal solution set. This approach is quite practical in the case of two or three conflicting objectives, because the tradeoff among them can be graphically traced.

The ε-constrained method leads to the optimization of a selected objective, J_m, while the others are included as constraints of the form $J_i \leq \varepsilon_l$ (i=1,…, M, l≠m). In order to develop the pareto-optimal solution set, several optimization runs for different values of parameter ε must be performed. Problem (P1) can therefore be reformulated as a single objective optimization problem, where J represents either a weighted sum of the objectives or one particular objective if the ε-constrained method is applied.

$$\begin{aligned}
&\mathbf{h}_d(\dot{\mathbf{x}}_d(t),\mathbf{x}_d(t),\mathbf{x}_a(t),\mathbf{u}(t),\mathbf{z},\mathbf{v}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)=\mathbf{0}\\
&\mathbf{h}_a(\mathbf{x}_d(t),\mathbf{x}_a(t),\mathbf{u}(t),\mathbf{z},\mathbf{v}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)=\mathbf{0}\\
&\mathbf{h}_0(\dot{\mathbf{x}}_d(t_0),\mathbf{x}_d(t_0),\mathbf{x}_a(t_0),\mathbf{u}(t_0),\mathbf{z},\mathbf{v}(t_0),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_0)=\mathbf{0}
\end{aligned} \tag{11}$$

$$\begin{aligned}
&\mathbf{g}(\mathbf{x}_d(t),\mathbf{x}_a(t),\mathbf{u}(t),\mathbf{z},\mathbf{v}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)\leq\mathbf{0}\\
&\mathbf{h}_{dk}(\dot{\mathbf{x}}_d(t_k),\mathbf{x}_d(t_k),\mathbf{x}_a(t_k),\mathbf{u}(t_k),\mathbf{z},\mathbf{v}(t_k),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_k)=\mathbf{0}\\
&\mathbf{h}_{ak}(\mathbf{x}_d(t_k),\mathbf{x}_a(t_k),\mathbf{u}(t_k),\mathbf{z},\mathbf{v}(t_k),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_k)=\mathbf{0}\\
&\mathbf{g}_k(\mathbf{x}_d(t_k),\mathbf{x}_a(t_k),\mathbf{u}(t_k),\mathbf{z},\mathbf{v}(t_k),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_k)\leq\mathbf{0}\\
&\hat{\mathbf{h}}(\mathbf{z},\mathbf{d},\mathbf{y})=\mathbf{0}\\
&\hat{\mathbf{g}}(\mathbf{z},\mathbf{d},\mathbf{y})\leq\mathbf{0}
\end{aligned} \tag{12}$$

$$\min_{\mathbf{d},\mathbf{y},\mathbf{z},\mathbf{u}(t)} \ \underset{\boldsymbol{\theta}}{E}\left\{\mathbf{J}(\mathbf{x_d}(t_f),\mathbf{x_a}(t_f),\mathbf{u}(t_f),\mathbf{z},\boldsymbol{\nu}(t_f),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_f)\right\}$$

s.t.

$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{h_d}(\dot{\mathbf{x}}_\mathbf{d}(t),\mathbf{x_d}(t),\mathbf{x_a}(t),\mathbf{u}(t),\mathbf{z},\boldsymbol{\nu}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)\right\}=\mathbf{0}$$
$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{h}_a(\mathbf{x_d}(t),\mathbf{x_a}(t),\mathbf{u}(t),\mathbf{z},\boldsymbol{\nu}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)\right\}=\mathbf{0}$$
$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{h}_0(\dot{\mathbf{x}}_d(t_0),\mathbf{x_d}(t_0),\mathbf{x_a}(t_0),\mathbf{u}(t_0),\mathbf{z},\boldsymbol{\nu}(t_0),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_0)\right\}=\mathbf{0}$$
$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{g}(\mathbf{x_d}(t),\mathbf{x_a}(t),\mathbf{u}(t),\mathbf{z},\boldsymbol{\nu}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)\right\}\le\mathbf{0}$$
$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{h}_{dk}(\dot{\mathbf{x}}_d(t_k),\mathbf{x_d}(t_k),\mathbf{x_a}(t_k),\mathbf{u}(t_k),\mathbf{z},\boldsymbol{\nu}(t_k),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_k)\right\}=\mathbf{0}$$
$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{h}_{ak}(\mathbf{x}_d(t_k),\mathbf{x}_a(t_k),\mathbf{u}(t_k),\mathbf{z},\boldsymbol{\nu}(t_k),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_k)\right\}=\mathbf{0}$$
$$\underset{\boldsymbol{\theta}}{E}\left\{\mathbf{g}_k(\mathbf{x_d}(t_k),\mathbf{x_a}(t_k),\mathbf{u}(t_k),\mathbf{z},\boldsymbol{\nu}(t_k),\boldsymbol{\theta},\mathbf{d},\mathbf{y},t_k)\right\}\le\mathbf{0}$$
$$\hat{\mathbf{h}}(\mathbf{z},\mathbf{d},\mathbf{y})=\mathbf{0}$$
$$\hat{\mathbf{g}}(\mathbf{z},\mathbf{d},\mathbf{y})\le\mathbf{0}$$
$$\mathbf{d}\in D=\{\mathbf{d}:\mathbf{d}^L\le\mathbf{d}\le\mathbf{d}^U\}$$
$$\mathbf{z}\in Z=\{\mathbf{z}^L\le\mathbf{z}\le\mathbf{z}^U\}$$
$$\mathbf{u}(t)\in U=\{\mathbf{u}^L\le\mathbf{u}(t)\le\mathbf{u}^U\}$$
$$\boldsymbol{\theta}\in\Gamma$$
$$\boldsymbol{\nu}(t)\in V$$
$$t\in[t_0,t_f] \qquad \text{(P1)}$$
$$t_k\in[t_0,t_f]$$
$$\mathbf{y}\in\{0,1\}$$

3.3. Stochastic nature

It is difficult to find examples of problems in chemical engineering that do not include some level of uncertainty on the values to assign to some or all of the parameters of the model. There are cases where the uncertain parameters play a central role in the decision making process, thus it is not possible to ignore their character without taking the risk of invalidating the conclusions that may be drawn from the analysis. In particular, the design-for-operability problem becomes a stochastic programming problem, whose most general formulation is that of (P1).

The classic approach to address the solution of problem (P1) regarding uncertainty is to remove the expectation operator from the objective function and model equations, as described below. It is assumed that the dynamic functional form of the disturbances, ν(t), are fully known and that can be generally expressed as $\boldsymbol{\nu}(\boldsymbol{\theta},\mathbf{z},\mathbf{d},t)=\mathbf{0}$ becoming a subset of $\mathbf{h}_a$. They are therefore removed from subsequent formulations.

3.3.1 Objective function

Let's consider the definition of the expectation operator:

$$\underset{\boldsymbol{\theta}\in\Gamma}{E}\left\{J(\mathbf{v},\boldsymbol{\theta})\right\}=\iint_{\boldsymbol{\theta}\in\Gamma} J(\mathbf{v},\boldsymbol{\theta})\cdot P(\boldsymbol{\theta})\cdot d\boldsymbol{\theta}$$

Where $\mathbf{v}=\{\mathbf{x}_d(t_f),\mathbf{x}_a(t_f),\mathbf{u}(t_f),\mathbf{z},\mathbf{d},\mathbf{y},t_f\}$ and P(.) is a probability density function. Despite the characterization of uncertainty can be addressed in different ways (Nemhauser *et al.,* 1989), one of the most general approaches is to assign a probability distribution function to the uncertain parameters. Even with a non rigorous statistical base for the choice of a particular distribution, a "probability space" may be established as consisting of a number of scenarios, and the probability measure could only be a subjective measure of the reliability to attach to these scenarios. Therefore the stochastic optimization problem under uncertainty can be visualized as extensions of the deterministic optimization model.

The direct resolution of the integral is not practical in process systems engineering, either because a closed (or explicit) definition of the function P(.) is not available, or there are not enough historical records of the process uncertainties as to develop probability density functions for each single parameter. Consequently, the discrete approximation through a weighted sum for each uncertain parameter is a more useful, simple and practical methodology for many applications:

$$\underset{\boldsymbol{\theta}\in\Gamma}{E}\left\{ J(\mathbf{v},\boldsymbol{\theta}) \right\} \cong \sum_{i=1}^{Q} w^i \cdot J(\mathbf{v},\boldsymbol{\theta}^i)$$

Where w^i is a weight factor for each realization i of the uncertain parameter, and Q is the number of considered scenarios.

Under no further available information, a common assumption in chemical engineering is to consider that they follow a constant density function equal to one, where each single realization or scenario is equally probable, i.e. every weight factor is equal to the unity.

The discretization approach outlined above is the most popular to address uncertainty in engineering. It is mostly concerned with problems that require a "here-and-now" decision without making further observations of the quantities modeled as random variables. This approach is supported in the fact that there is a rather important number of applications in engineering where can be assumed, without loosing too much precision in the results that the uncertain quantities are known, either because the level of uncertainty is low, or because it is good enough to assign only some discrete values for these quantities. In mathematical statistics, on the other hand, it is mostly the "wait-and-see" analysis that is of interest.

A more elaborated approximation, assuming that independent continuos probability density functions are known for each parameter, can be determined using an integration scheme as proposed by Pistikopoulos (1988), based on a Gaussian quadrature formula (Carnahan *et al.,* 1969). Here, the multiple integral of the expected value operator is approximated by a series of one dimensional integrals in terms of each single parameter at each node of the quadrature formula. The advantages are that sometimes it is possible to make the analytical integration for each parameter (if the required information is available) and it also provides a systematic way to choose the discretization points. Its major limitation is that the number of quadrature points grows very rapidly with the number of uncertain parameters.

3.1.2 Model constraints

A max-min-max operator is usually included within the constraints (feasibility condition), in order to remove the expectation operator from the model equations in (P1), thus leading to problem (P2). The max-min-max operator accounts for feasible operation and it should be interpreted as follows: for a fix process design and structure (**d** and **y**), algebraic and dynamic operating variables ($\mathbf{z}$ and $\mathbf{u}(t)$) can be selected in order to minimize the objective function J (when embedded in an optimization problem) and satisfy every inequality constraint over the whole time horizon in the face of uncertainties $\boldsymbol{\theta}$.

Problem (P2) is a Semi Infinite Mixed-Integer Dynamic Optimization problem (SIMIDO) whose resolution is still quite complicate. A classic approach to address problem (P2) involve the following steps, also illustrated in Fig. 3.

$$
\begin{aligned}
&\min_{\mathbf{d},\mathbf{y},\mathbf{z},\mathbf{u}(t)} \sum_{i=1}^{Q} w^i J(\mathbf{x_d}(t_f), \mathbf{x_a}(t_f), \mathbf{u}(t_f), \mathbf{z}, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t_f) \\
&\text{s.t.} \\
&\quad \chi(\mathbf{d},\mathbf{y}) = \max_{\boldsymbol{\theta}} \min_{\mathbf{z},\mathbf{u}(t)} \max_{j} g_j(\mathbf{x_d}(t), \mathbf{x_a}(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) \le 0 \\
&\quad \mathbf{h_d}(\dot{\mathbf{x}}_\mathbf{d}(t), \mathbf{x_d}(t), \mathbf{x_a}(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) = \mathbf{0} \\
&\quad \mathbf{h}_a(\mathbf{x_d}(t), \mathbf{x_a}(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) = \mathbf{0} \\
&\quad \mathbf{h}_0(\dot{\mathbf{x}}_d(t_0), \mathbf{x_d}(t_0), \mathbf{x_a}(t_0), \mathbf{u}(t_0), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_0) = \mathbf{0} \\
&\quad \mathbf{h}_{dk}(\dot{\mathbf{x}}_d(t_k), \mathbf{x_d}(t_k), \mathbf{x_a}(t_k), \mathbf{u}(t_k), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0} \\
&\quad \mathbf{h}_{ak}(\mathbf{x_d}(t_k), \mathbf{x_a}(t_k), \mathbf{u}(t_k), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0} \\
&\quad \mathbf{h}(\mathbf{z}, \mathbf{d}, \mathbf{y}) = \mathbf{0} \\
&\quad \mathbf{d} \in D = \{\mathbf{d} : \mathbf{d}^L \le \mathbf{d} \le \mathbf{d}^U\} \\
&\quad \mathbf{z} \in Z = \{\mathbf{z}^L \le \mathbf{z} \le \mathbf{z}^U\} \\
&\quad \mathbf{u}(t) \in U = \{\mathbf{u}^L \le \mathbf{u}(t) \le \mathbf{u}^U\} \\
&\quad \boldsymbol{\theta} \in \Gamma = \{\boldsymbol{\theta}^L \le \boldsymbol{\theta} \le \boldsymbol{\theta}^U\} \\
&\quad t \in [t_0, t_f] \\
&\quad t_k \in [t_0, t_f] \\
&\quad \mathbf{y} \in \{0,1\} \\
&\quad j \in [1, \ldots, \dim\{\mathbf{g}\} + \dim\{\mathbf{g}_k\} + \dim\{\hat{\mathbf{g}}\}]
\end{aligned}
\qquad \text{(P2)}
$$

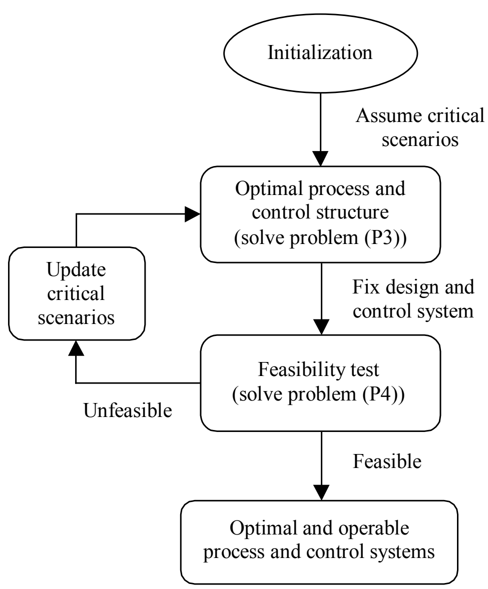

Fig. 3. MIDO solution strategy.

Step 1: Choose an initial set of scenarios for the uncertain parameters, θ^i. A critical issue is how to appropriately select a finite number of realizations for the uncertain parameters, to ensure an optimal and feasible operation. Some approaches have been proposed (Halemane and Grossmann, 1983; Floudas and Grossmann, 1987).

Step 2: Solve multiperiod problem (P3). This formulation is a Mixed-Integer Dynamic Optimization (MIDO) problem. Details about its solution are provided in Section 3.3.

Step 3: Perform the feasibility test (P4) for the optimal solution found in Step 2.

Details about the solution of the flexibility test are provided later in this paper (Section 3.4).

Step 4: If $\chi(\mathbf{d},\mathbf{y}) \leq 0$ then the system is feasible and the procedure terminates; otherwise the solution of (P4), determines a critical uncertain parameter realization that should be added to the set of current scenarios and the control returns to Step 2. This scheme proceeds until the feasibility condition verifies.

3.4. Mixed integer dynamic nature

As already discussed, a further complication in the solution of problem (P1) is how to address its mixed integer dynamic nature. This issue has to do with the resolution of the MIDO problem (P3) in Step 2.

There are two major "complications" in a MIDO problem: the presence of binary variables and the presence of differential variables. Therefore the different solution strategies that have been proposed for MIDO problems can be classified according to the way they deal with these "complicating variables", as it is shown in Fig. 4. According to the chosen procedure, the solution of MIDO problems reduce to the solution of Dynamic Optimization (DO) problems, Mixed Integer Linear Programming (MILP) problems or Mixed Integer Non linear Programming (MINLP) problems (Floudas, 1995). Furthermore, available algorithms for MIDO problems in each route of Fig. 4 also differ regarding on the algorithm applied in the solution of the DO and MI problems. Major approaches are briefly discussed below:

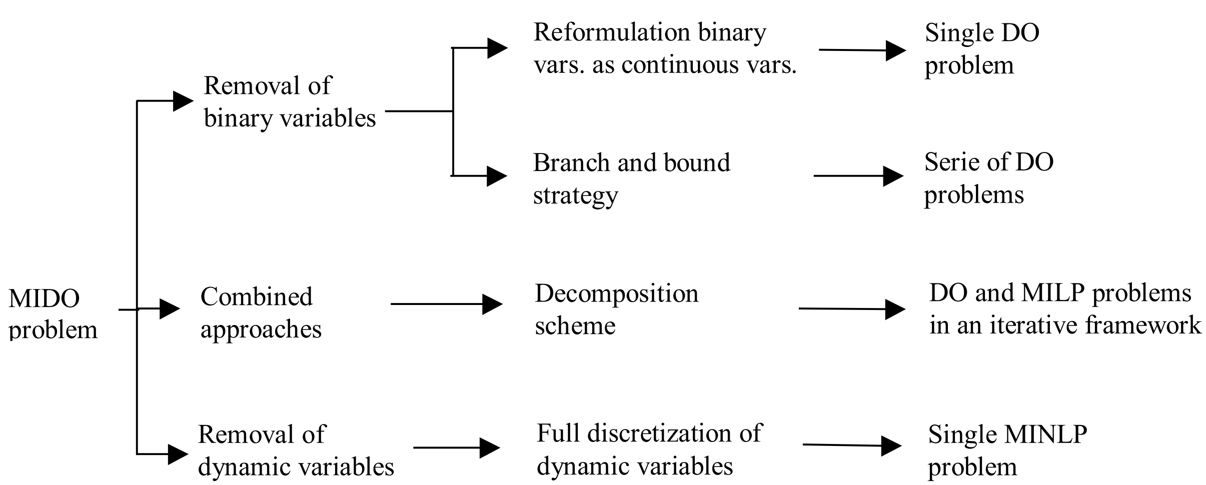

Fig. 4. Classification of MIDO problems according to the different solution strategies.

$$\min_{\mathbf{d},\mathbf{y},\mathbf{z},\mathbf{u}(t)} \sum_{i=1}^{Q} w^i J(\mathbf{x_d}(t_f), \mathbf{x_a}(t_f), \mathbf{u}(t_f), \mathbf{z}, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t_f)$$

s.t.

$$\begin{aligned}
&\chi(\mathbf{d},\mathbf{y}) = \max_{\boldsymbol{\theta}} \ \min_{\mathbf{z},\mathbf{u}(t)} \ \max_{j} \ g_j(\mathbf{x_d}(t), \mathbf{x_a}(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) \le 0\\
&\mathbf{h_d}(\dot{\mathbf{x}}_\mathbf{d}(t), \mathbf{x_d}(t), \mathbf{x_a}(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) = \mathbf{0}\\
&\mathbf{h}_a(\mathbf{x_d}(t), \mathbf{x_a}(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) = \mathbf{0}\\
&\mathbf{h}_0(\dot{\mathbf{x}}_d(t_0), \mathbf{x_d}(t_0), \mathbf{x_a}(t_0), \mathbf{u}(t_0), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_0) = \mathbf{0}\\
&\mathbf{h}_{dk}(\dot{\mathbf{x}}_d(t_k), \mathbf{x_d}(t_k), \mathbf{x_a}(t_k), \mathbf{u}(t_k), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0}\\
&\mathbf{h}_{ak}(\mathbf{x_d}(t_k), \mathbf{x_a}(t_k), \mathbf{u}(t_k), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0}\\
&\mathbf{h}(\mathbf{z}, \mathbf{d}, \mathbf{y}) = \mathbf{0}\\
&\mathbf{d} \in D = \{\mathbf{d} : \mathbf{d}^L \le \mathbf{d} \le \mathbf{d}^U\}\\
&\mathbf{z} \in Z = \{\mathbf{z}^L \le \mathbf{z} \le \mathbf{z}^U\}\\
&\mathbf{u}(t) \in U = \{\mathbf{u}^L \le \mathbf{u}(t) \le \mathbf{u}^U\}\\
&\boldsymbol{\theta} \in \Gamma = \{\boldsymbol{\theta}^L \le \boldsymbol{\theta} \le \boldsymbol{\theta}^U\}\\
&t \in [t_0, t_f]\\
&t_k \in [t_0, t_f]\\
&\mathbf{y} \in \{0,1\}\\
&j \in [1,..., \dim\{\mathbf{g}\} + \dim\{\mathbf{g}_k\} + \dim\{\hat{\mathbf{g}}\}]
\end{aligned} \tag{P2}$$

$$\min_{\mathbf{d},\mathbf{y},\mathbf{z},\mathbf{u}(t)} \sum_{i=1}^{Q} w^i J(\mathbf{x_d}(t_f), \mathbf{x_a}(t_f), \mathbf{u}(t_f), \mathbf{z}, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t_f)$$

s.t.

$$\begin{aligned}
&\mathbf{h}_d^i(\dot{\mathbf{x}}_d^i(t), \mathbf{x}_d^i(t), \mathbf{x}_a^i(t), \mathbf{u}^i(t), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t) = \mathbf{0}\\
&\mathbf{h}_a^i(\mathbf{x}_d^i(t), \mathbf{x}_a^i(t), \mathbf{u}^i(t), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t) = \mathbf{0}\\
&\mathbf{g}^i(\mathbf{x}_d^i(t), \mathbf{x}_a^i(t), \mathbf{u}^i(t), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t) \le \mathbf{0}\\
&\mathbf{h}_0^i(\mathbf{x}_d^i(t_0), \mathbf{x}_a^i(t_0), \mathbf{u}^i(t_0), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t_0) = \mathbf{0}\\
&\mathbf{h}_{dk}^i(\dot{\mathbf{x}}_d^i(t_k), \mathbf{x}_d^i(t_k), \mathbf{x}_a^i(t_k), \mathbf{u}^i(t_k), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, V) = \mathbf{0}\\
&\mathbf{h}_{ak}^i(\mathbf{x}_d^i(t_k), \mathbf{x}_a^i(t_k), \mathbf{u}^i(t_k), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0}\\
&\mathbf{g}_k^i(\mathbf{x}_d^i(t_k), \mathbf{x}_a^i(t_k), \mathbf{u}^i(t_k), \mathbf{z}^i, \boldsymbol{\theta}^i, \mathbf{d}, \mathbf{y}, t_k) \le \mathbf{0}\\
&\hat{\mathbf{h}}^i(\mathbf{z}^i, \mathbf{d}, \mathbf{y}) = \mathbf{0}\\
&\hat{\mathbf{g}}^i(\mathbf{z}^i, \mathbf{d}, \mathbf{y}) \le \mathbf{0}\\
&\mathbf{d} \in D = \{\mathbf{d} : \mathbf{d}^L \le \mathbf{d} \le \mathbf{d}^U\}\\
&\mathbf{z}^i \in Z = \{\mathbf{z}^L \le \mathbf{z}^i \le \mathbf{z}^U\}\\
&\mathbf{u}^i(t) \in U = \{\mathbf{u}^L \le \mathbf{u}^i(t) \le \mathbf{u}^U\}\\
&\boldsymbol{\theta}^i \in \Gamma = \{\boldsymbol{\theta}^L \le \boldsymbol{\theta}^i \le \boldsymbol{\theta}^U\}\\
&t \in [t_0, t_f]\\
&t_k \in [t_0, t_f]\\
&\mathbf{y} \in \{0,1\}\\
&j \in [1,..., \dim\{\mathbf{g}\} + \dim\{\mathbf{g_k}\} + \dim\{\hat{\mathbf{g}}\}]\\
&i \in [1,..., Q^i]
\end{aligned} \tag{P3}$$

$$\chi(\mathbf{d},\mathbf{y}) = \max_{\boldsymbol{\theta}} \min_{\mathbf{z},\mathbf{u}(t)} \max_{j} \; g_j(\mathbf{x}_d(t), \mathbf{x}_a(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t)$$

s.t.

$$\left.\begin{aligned}
&\mathbf{h}_d(\dot{\mathbf{x}}_d(t), \mathbf{x}_d(t), \mathbf{x}_a(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) = \mathbf{0}\\
&\mathbf{h}_a(\mathbf{x}_d(t), \mathbf{x}_a(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t) = \mathbf{0}\\
&\mathbf{h}_0(\dot{\mathbf{x}}_d(t_0), \mathbf{x}_d(t), \mathbf{x}_a(t), \mathbf{u}(t), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_0) = \mathbf{0}\\
&\mathbf{h}_{dk}(\dot{\mathbf{x}}_d(t_k), \mathbf{x}_d(t_k), \mathbf{x}_a(t_k), \mathbf{u}(t_k), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0}\\
&\mathbf{h}_{ak}(\mathbf{x}_d(t_k), \mathbf{x}_a(t_k), \mathbf{u}(t_k), \mathbf{z}, \boldsymbol{\theta}, \mathbf{d}, \mathbf{y}, t_k) = \mathbf{0}\\
&\hat{\mathbf{h}}(\mathbf{z}, \mathbf{d}, \mathbf{y}) = \mathbf{0}\\
&\mathbf{z} \in Z = \{\mathbf{z}^L \le \mathbf{z} \le \mathbf{z}^U\}\\
&\mathbf{u}(t) \in U = \{\mathbf{u}^L \le \mathbf{u}(t) \le \mathbf{u}^U\}\\
&\boldsymbol{\theta} \in \Gamma = \{\boldsymbol{\theta}^L \le \boldsymbol{\theta} \le \boldsymbol{\theta}^U\}\\
&t \in [t_0, t_f]\\
&t_k \in [t_0, t_f]\\
&j \in [1, \ldots, \dim\{\mathbf{g}\} + \dim\{\mathbf{g}_k\} + \dim\{\hat{\mathbf{g}}\}]
\end{aligned}\right\} \quad (13) \qquad \text{(P4)}$$

3.4.1 Removal of binary variables

1. *Binary variables reformulation*. The approach includes the reformulation of the binary variables using some smoothing function such those proposed by Samsatli *et al*. (1998). Each single binary variable is approximated with some kind of continuous function, using an adjusting parameter to regulate the approximation. A limitation in this approach is that it is not always possible to obtain a full integral-value 0-1 for the binary variables, rendering to engineering problems in some applications.

2. *Branch and Bound (B&B) strategy*. This approach involves the direct use of a B&B strategy as proposed by Androulakis (2000). A DO optimization problem has to be solved at each node of the B&B tree, where the binary variables are treated as continuous ones, using their relaxed (between 0 and 1) and fixed (in 0 or 1) values as constraints. The inconvenient with this scheme is that it is not adequate for large scale engineering problems, because of the large time requirements of the B&B strategy.

3.4.2 Removal of differential variables

1. *Full discretization of the differential variables*. This approach converts a MIDO problem, into a large scale MINLP problem by complete discretization of the dynamic variables using orthogonal collocation on finite elements. The continuous variables are the dynamic variables of the original MIDO formulation plus the set of parameters introduced by the discretization procedure. The advantage of this approach is that since it is based on a fully equation oriented framework, it is more natural to handle general inequality constraints. The major limitation is that even for small MIDO problems, the resulting MINLP are quite large regarding continuous variables as results of the discretization process.

3.4.3 Combined approach

1. The combined approach takes the advantages of both previous strategies. The MIDO problem is decomposed into a *Primal* DO problem for fix values of the binary variables, which are updated in a *Master* MILP problem. Both problems must be solved in an iterative scheme as shown in Fig. 5. The main difference among the different implementations of this strategy relies on the way the DO problem is solved and the Master problem formulated.

In relation to the solution of MINLP problems, there exist two major approaches:

- The Outer Approximation / Equality Relaxation / Penalty Function (OA/ER/PF) algorithm of Viswanathan and Grossmann (1990) (implemented as solver DICOPT++, available under the commercial modeling package GAMS (Brooke *et al*., 1992).
- Generalized Benders Decomposition (GBD) (Geoffrion, 1972) which can be programmed in modeling languages like GAMS.

Regarding strategies for DO problems there exist:

- Complete discretization approach of the dynamic variables (decision and state variables) in order to convert the DO problem into a large scale Non Linear Programming (NLP) problem, which can be solved with any standard large scale NLP algorithm (like MINOS and CONOPT also available under GAMS).
- Partial discretization approach. Here only the dynamic decision variables **u**(t) are parameterized, in terms of time-invariant parameters ("reduced space discretization" or "control vector parameterization"). For a parameterized **u**(t) and values for the other decision variables (**z** and **d**), the resulting DAE system is integrated to evaluate the profiles of the dynamic variables using standard integration routines. Additionally, gradient information of the objective function and constraints with respect to decision variables is obtained, either by finite difference perturbations (brute force strategy), or through integration of sensitivity equations (Vassiliadis et al., 1994 a,b), or via the solution of the adjoint equations (Sullivan and Sargent, 1979; Pytlak, 1998; Bloss *et al*., 1999). A NLP solver uses this information to adjust the values of the decision variables, and the iteration continues. Fig. 6 shows schematically how this strategy works.

An available commercial package to solve this problem is gPROMS/gOPT (Process Systems Enterprice Ltd., 2000).

3.5.Solution of the feasibility condition

A further important issue in the solution of problem (P2) is how to address the solution of the flexibility condition of problem (P4). Several strategies have been proposed.

Mohideen *et al*. (1996) proposes a methodology based on the active set strategy of Grossmann and Floudas (1987) for solving problem (P4), which results in a MIDO problem. Its solution provides the optimal control action **u**(t) and the optimal operators' manipulated variables, **z**. This optimal operating point however, might not be practically achieved for some operating conditions since, although proper control action, **u**(t), is always possible for any uncertainty realization, such is not the case for operators' manipulated variables, **z,** who do not know in advance the incoming uncertain parameters realization.

Some authors overcome this problem by searching a single operating decision for any realization of the uncertain parameters, defining a scenario that does not depend on previous knowledge of the uncertainty realization. This is equivalent to say that there are no operating decision variables or that they are treated as design variables.

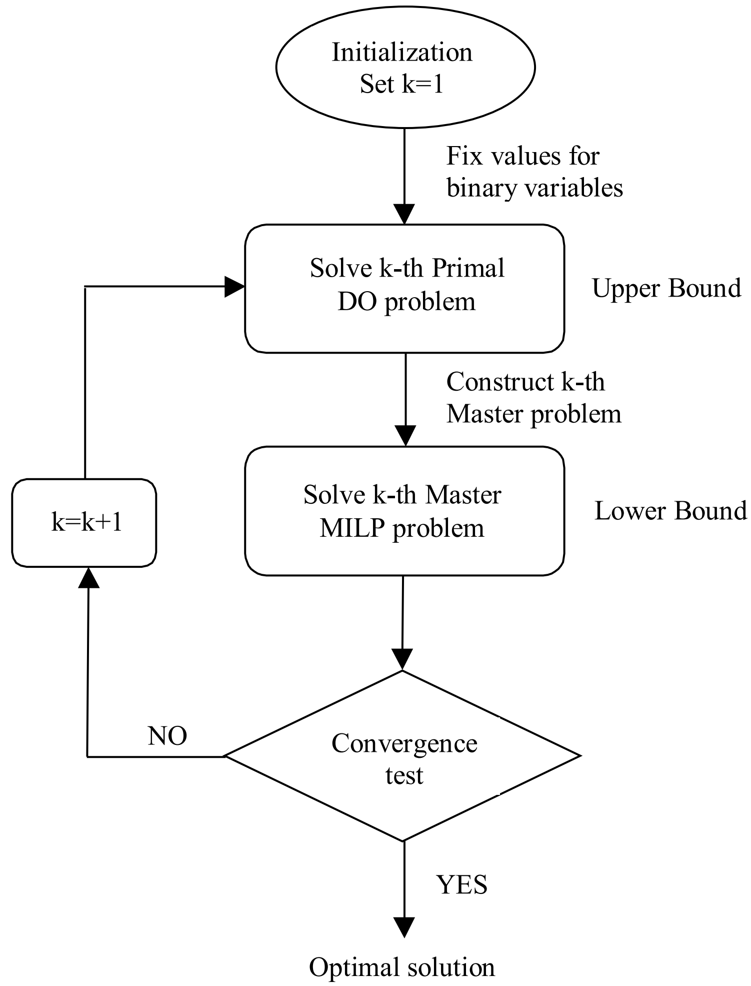

Fig. 5. Combined approach to manage the uncertainties.

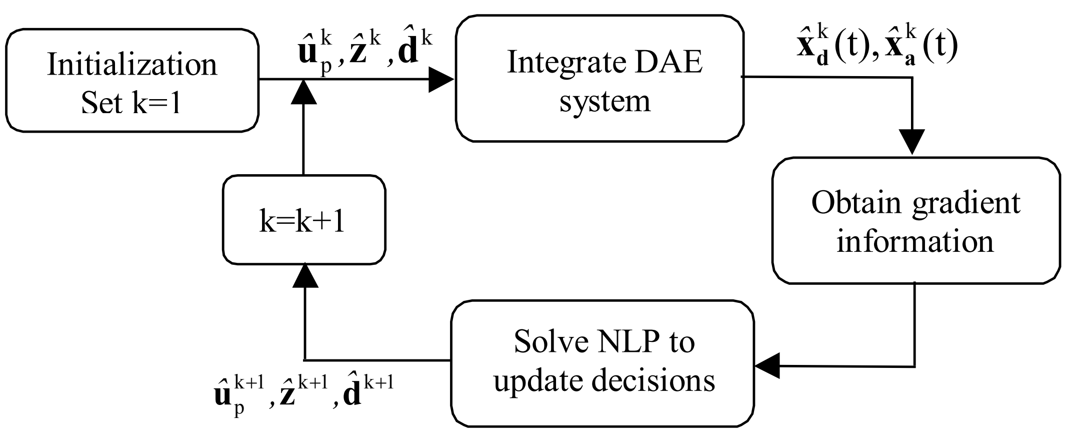

Fig. 6. DO algorithm with partial discretization (control vector parameterization).

Therefore the max-min-max operator reduces to a single maximization operator as in (P4'), which constitutes the so-called "worst-case" approach (Walsh and Perkins, 1996; Bahri *et al.*, 1997):

In general, the "worst-case" strategy presents a further simplification in the objective function: only a nominal (average or best known) point for the uncertain parameters is considered. This corresponds to the scenario where feasible operation despite the value of $\theta \in \Gamma$ is obtained, while the objective function is only evaluated relative to its nominal value. See Bandoni *et al*. (1994) for further details on the "worst-case" or "back-off" algorithm.

The "worst-case" strategy is simple and practical in many applications, but it could lead to very conservative solutions. Another drawback is that an optimization problem must be solved for each inequality constraint, which can be time consuming for large models. This issue has been addressed by Raspanti et al. (2000), where an aggregation function (the KS function) that overestimates each single constraint is used to handle the whole set of inequality constraints, and therefore only a single optimization problem must be solved in Step 3 (P4'').

In (P4''), ρ is an adjusting parameter. For larger ρ's a tighter overestimation of the constraints by the KS function is achieved. The WC strategy in problems (P4') and (P4'') have been successfully applied to asses the "worst case" steady-state operation under uncertainty of entire chemical plants (Diaz *et al.*, 2002).

Up to date, problem (P2) with its different solution strategies has been applied to several important chemical engineering design-for-operability problems. For example, Mohideen *et al.* (1997) solved a single and a double-effect heat-integrated distillation column with a simple control system. Using fixed discrete decisions and simplifications in the treatment of the uncertainties, Bansal *et al*. (2000) solved a rigorous double effect system, while Ross *et al*. (2000) addressed an industrial distillation column.

$$\begin{aligned} &\chi(\mathbf{d},\mathbf{y},\mathbf{z},\mathbf{u}(t)) = \max_{\theta}\ \max_{j}\ g_j(\mathbf{x_d}(t),\mathbf{x_a}(t),\mathbf{u}(t),\mathbf{z},\boldsymbol{\theta},\mathbf{d},\mathbf{y},t) \\ &\text{s.t.} \\ &\{\text{Eq. (13)}\} \end{aligned} \tag{P4'}$$

$$\begin{aligned} &\chi(\mathbf{d},\mathbf{y},\mathbf{z},\mathbf{u}(t)) = \max_{\theta}\ KS(g_j(\mathbf{x_d}(t),\mathbf{x_a}(t),\mathbf{u}(t),\mathbf{z},\boldsymbol{\theta},\mathbf{d},\mathbf{y},t)) \\ &\text{s.t.} \\ &KS(g_j(.)) = \frac{1}{\rho}\sum_{j=1}^{Q}\exp\left[\ln(\rho \cdot g_j(.))\right] \\ &\{\text{Eq. (13)}\} \end{aligned} \tag{P4''}$$

Conclusions

In this paper the two major successful strategies to deal with the design for operability problem have been discussed. C&R dominates the picture of operability assessment, making wide use of linear, Laplace and frequency domains indices. Several contributions incorporated those linear operability tools within the synthesis problem, for example as a multi objective optimization, which is the most intuitive step towards the integrative approach.

On the other hand, the dynamic optimization approach to design-for-operability leading to a SIMOMIDO problem, presents very attractive features since it allows the explicit consideration of most required design issues within a very elegant formulation. The major drawback of such an approach is the inherent difficulty in modeling and solving the resulting complex programming problem. However, there exist strategies and commercial solvers that allow to address the problem, and several important applications have been reported in the literature. Future research on the field includes the consideration of more advanced control strategies like Model Predictive Control, within the integrated framework.

Nomenclatura

$\mathbf{h}_d$, $\mathbf{h}_a$: Sets of differential and algebraic equations respectively, for the process and control system (material and energy balances, definitions of actuating signals, etc.).

$\mathbf{h}_0$: Equations that define the set of initial conditions at t_0 for the differential states.

$\mathbf{z}$: Static operating degrees of freedom which can only verify step-like time profile (variables manipulated by plant operators, e.g. fixed flow-rates).

$\mathbf{d}$: Static process design degrees of freedom (equipment dimensions, controller tuning parameters, etc.).

$\mathbf{u}(t)$: Dynamic control degrees of freedom manipulated variables (mainly flow-rates).

$\mathbf{x}_d(t)$: Dynamic state variables.

$\mathbf{x}_a(t)$: Algebraic state variables.

$\nu(t)$: Disturbances.

θ: Uncertain parameters (heat transfer coefficients, fouling factors, kinetic constants, etc.).

$\mathbf{y}$: Integer variables (normally 0-1 binary variables), corresponding to discrete process and control decisions (the existence or not of a process unit or control loop).

t: Independent time variable, $t \in [t_0, t_f]$.

t_0, t_f: Initial and final time of the time horizon.

$\mathbf{g}$: Inequalities that determine the constraints that the system must satisfy in order to achieve feasible operation in the face of disturbances $\nu(t)$ and uncertainties θ. They are normally called "path constraints" because they are to be verified throughout the whole time horizon of operation (design specifications, physical operating limits, etc.)

$\mathbf{h}_{dk}$, $\mathbf{h}_{ak}$, $\mathbf{g}_k$: Equalities and inequalities that define "interior- and end-point constraints" at some specific time instance t_k ($t_k \in [t_0, t_f]$).

$\hat{\mathbf{h}}$, $\hat{\mathbf{g}}$: Sets of static equality and inequality constraints.

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