INTEGRATED DESIGN AND CONTROL OF CHEMICAL PROCESSES – PART I: REVISION AND CLASSIFICATION

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***Abstract—T*his work presents a comprehensive classification of the different methods and procedures for integrated synthesis, design and control of chemical processes, based on a wide revision of recent literature. This classification fundamentally differentiates between "projecting methods", where controllability is monitored during the process design to predict the trade-offs between design and control, and the "integrated-optimization methods" which solve the process design and the control-systems design at once within an optimization framework. The latter are revised categorizing them according to the methods to evaluate controllability and other related properties, the scope of the design problem, the treatment of uncertainties and perturbations, and finally, the type the optimization problem formulation and the methods for its resolution.**

***Keywords*—Process synthesis, process control, integrated design, controllability, process optimization.**

1. INTRODUCTION

The *Integrated Design and Control* is a comprehensive design methodology where the systematic analysis of plant dynamics is incorporated into the process design procedure in order to obtain a compromise solution between economic and control aspects.

In the process industry, the main objective is to deliver products which fulfil the specifications achieving the maximum economic benefit with the minimum cost. In a competitive market scenario, the plants must be operated as flexibly as possible in order to adapt satisfactorily to changes in product specifications, demand, different feed conditions and raw material quality variations. In such context, the application of appropriate process control strategies allows for the successful operation of the plants improving profitability by increasing product throughput and yield of higher valued products and by decreasing energy consumption and pollution (Edgar, 2004).

The traditional design procedure is sequential. Process synthesis is carried out first for determining the plant structure, the process parameters and operating conditions are calculated in a subsequent stage considering steady state and economic objectives and process constraints. Finally, the control system is designed to achieve the desired dynamic behaviour. A flow diagram representing the classical design procedure is shown in figure 1.

The integrated process design approach relies on the fact that the achievable plant dynamic performance is a property inherent to process design. In such sense, designing chemical processes based only on economic criterions and steady-state assumptions can lead to plants difficult to control and to operate exhibiting poor dynamic performance and unexpected behaviour under disturbances and uncertainties. The empirical overdesign as a solution to ensure resiliency and flexibility in the chemical plants is not attractive from the economical viewpoint and there is no guarantee of achieving efficient operation. Moreover, conservative design based on the worst operating conditions, may fail because the proper selection is far from trivial and seemingly logical choices can lead to systems with higher costs (Grossmann and Morari, 1983). Therefore, the integrated design philosophy can produce significant economic benefits as well as the improvement of the plant operation contemplating the important relationship between profitability and controllability by incorporating the assessment of plant dynamics from the initial steps of the process design procedure.

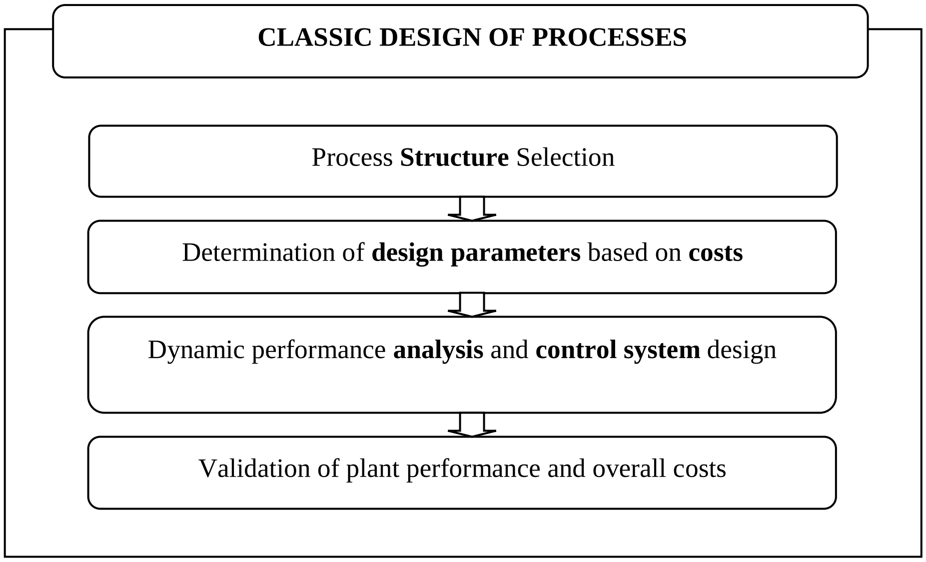

Figure 1. Classic Design of Processes

The interactions between process design and process control have been documented since 1940s (Ziegler and Nichols, 1943) motivating a number of works that have provided theoretical background about properties as controllability, flexibility, operability, switchability, stability and the selection of measurements and manipulated variables which are used to quantify the effect of process dynamics in process control design Some initial works are Stephanopoulus et al. (1979), Morari et al. (1980a,b), Morari et al. (1987) and the series "Design of Resilient Processing Plants" (Lenhoff and Morari, 1982; Marselle et al., 1982; Morari, 1983; Saboo and Morari, 1984; Holt and Morari, 1985a,b; Morari et al., 1985; Saboo et al., 1985; Skogestad and Morari, 1987). They deal mostly with controllability assessment and its incorporation into process synthesis and the selection of the control structure. Some other studied the flexibility and the operability properties (Grossmann and Morari, 1983; Perkins and Wong, 1985). Although, controllability and flexibility are strongly related concepts (Grossmann and Morari, 1983), the controllability deals with dynamic operation and it is a measure of the achievable dynamic performance, while flexibility is focused on the steady-state operation and it is the capability to handle alternate operating conditions. Moreover, the operability which is the ability of the plant to provide acceptable static and dynamic operational performance, includes controllability and flexibility analysis. All those studies motivated also the development of strategies to incorporate controllability and operability insights into the practice of process design.

In the 90's, the availability of improved computational resources allowing more powerful optimization and computing methods, together with mature controllability analysis tools and advanced control technologies, provide the necessary driving force to develop a wide variety of integrated design and control methodologies following the foundations given by those pioneering works.

Several approaches where systematic actions are taken to improve some controllability measures of plant performance and economic indicators have appeared in the literature. They screen preliminary alternatives either by constraining some controllability and flexibility indicators or by optimizing them, carrying out the process and control design concurrently. Since the stated optimization problems allow for the consideration of process and control specifications as well as constraints, this feature is used eventually for accommodating decision variables within a unique integrated-optimization framework to solve at once the process design and the control-systems design (Walsh and Perkins, 1996).

The different possibilities of the integration of design and control philosophy are evidenced in the reviews of the state of the art that have been published (Lewin, 1999; Sakizlis et al. 2004; Ricardez-Sandoval et al., 2009a; Jain and Babu, 2009; Yuan et al., 2012a, Sharifzadeh, 2013). Nowadays, the integration of design and control is a mature field of research and it is possible to distinguish the main research trends defined by the different working groups.

It is clear that an actual and extensive classification of the existing integrated design and control methodologies is necessary due to the number of works addressing the problem with different viewpoints. Some authors have manifested the necessity of a classification of the different approaches. One of the first to make a separation is Lewin (1999), who distinguish the methods that screen the controllability of the possible alternatives resulting from the preliminary design procedure from the optimization based simultaneous design and control methodologies. In Seferlis and Georgadis (2004) a compilation of the contributions of some of the most important research groups in the area is presented. It contemplates the efforts made in the integrated design and control field organized in four categories: process characterization and controllability, methods of integrated process design and control, plantwide interactions of design and control and extensions of the integrated process design and control.

The recent reviews on the state of the art and classifications concentrate on the optimization based simultaneous design and control methodologies. Sakizlis et al. (2004) distinguish two categories into the optimization problem formulation: (1) the methods that attempt to design economically optimal processes that can operate in an efficient dynamic mode within an envelope around the nominal point and (2) the methods that consider a single economics-based performance index, while representing the system operation and system specifications with dynamic rather than steady-state models. Ricardez-Sandoval et al. (2009a) adopted a classification based on the way that the dynamic behaviour and its impact on the cost are quantified in the optimization framework, as follows: (1) controllability index-based approach, (2) dynamic optimization-based approach and (3) robust model-based approach. Yuan et al., (2012a), presented a complete and recent review. They separate the controllability-indicators-based frameworks that are able of screening alternative designs from optimization-based frameworks. However, the main focuses of their work are the formulations and solving strategies of the optimization-based simultaneous design and control, which they classify in: controllability-index based optimization, mixed integer dynamic optimization, robust based approach, embedded control optimization and black-box optimization. Finally Sharifzadeh (2013) presents an extensive, thematic review, where the classification only separates classical from integrated design. Eight main types of integrated design methods are enumerated, describing the important features and the advantages and disadvantages of each method.

In this work, a classification considering the most important contributions from the wide-ranging developments related to the integration of process and control design presented in the literature is proposed. An ample variety of approaches, above and beyond the optimization-based methods are considered. The contributions are organized contemplating "projecting" and "integrated-optimization" design methods. The classification includes aspects as the scope of the problem formulation, the methods to evaluate the controllability and other related properties, the introduction of advanced control strategies, the treatment of uncertainties and perturbations, the type of optimization problem and the methods for its resolution. The all-inclusive classification presented is meant to help readers and researchers in the identification of methodologies and/or research groups that are working on the different approaches to perform the integration of design and control.

The basic categorization that emerges when considering integrated design methods separates the works where the design of the process and the controllability analysis are carried out by examining systematically the dynamic properties of alternative designs, from the works that perform design and control at once by solving an integrated-optimization problem. The basis of this classification can be found in Lewin (1999) and Meusse (2002). The former methods are named *projecting* methods in this paper, since they rely on the forecasting of the dynamics of the process of different design alternatives in order to guide the design decisions. They are the earliest methodologies proposed to solve the conflicts between process-design and control-design. Nonetheless this research area is still very active nowadays. In the latter category, denoted *integrated-optimization* methods in this work, the dynamic performance measures are introduced within the process design, originating a comprehensive, dual-objective optimization scenario which produces at the same time the best economical and controllable plant, including structure and tuning of the control systems in the general case.

Flow diagrams representing classical design and integrated design methodologies are shown in Figures 2 and 3.

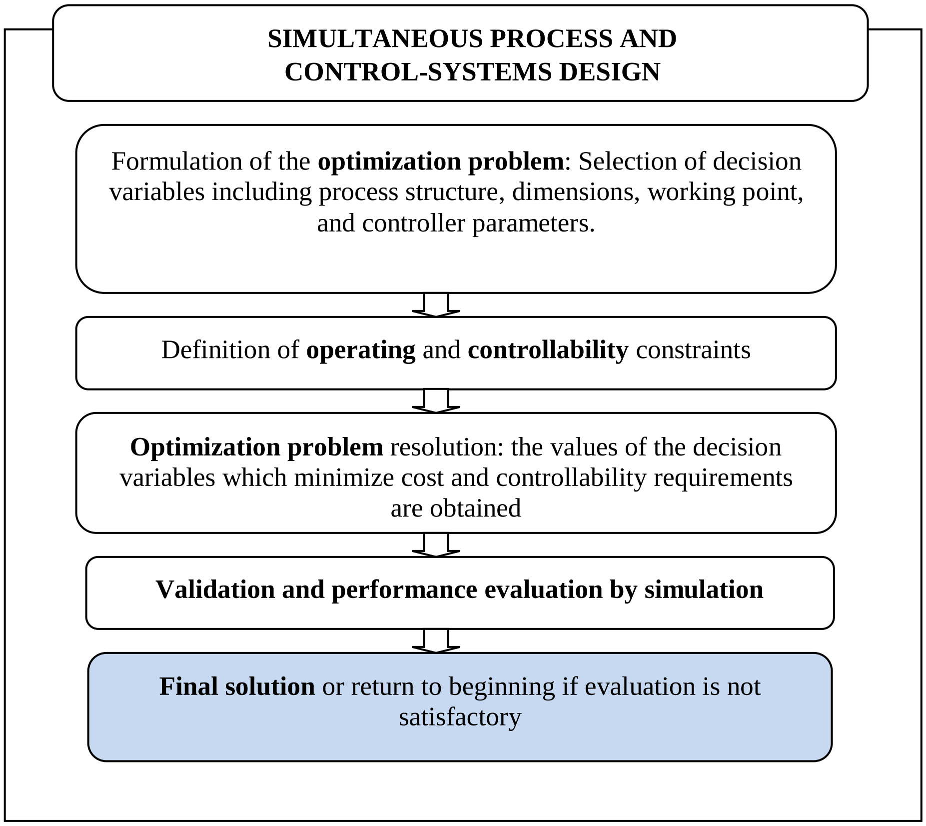

Figure 2. Simultaneous Process Design and Control

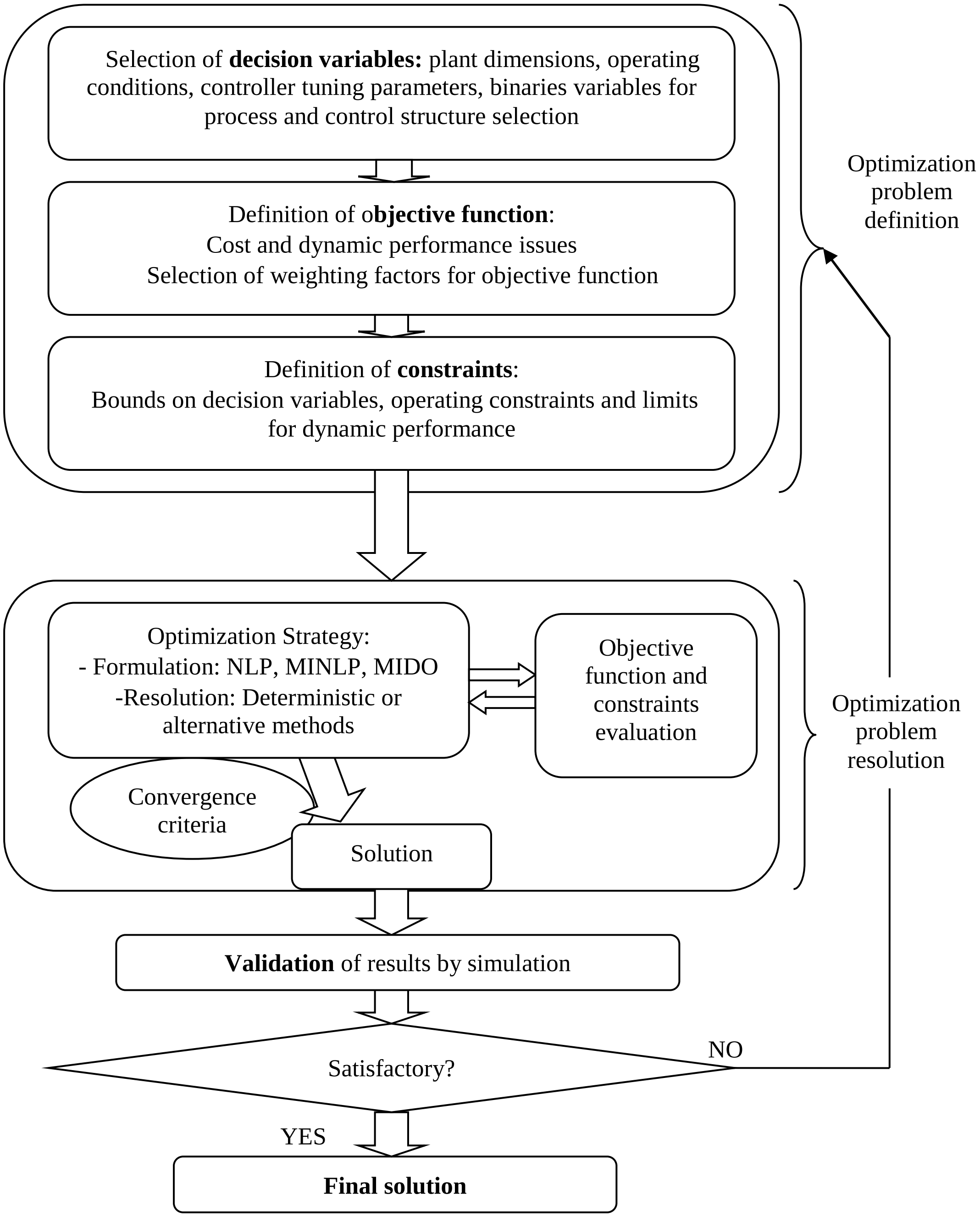

Figure 3: Integrated-Optimization Methods process design and control

The paper is organized in four sections. Section 2 is devoted to the *projecting methods* for integrating process design and control issues, presenting a complete revision from the earlier contributions to the current ones. Section 3 contains a survey of the *integrated-optimization methods* for integrated design. A wide classification is also proposed for them. Finally, conclusions of this work and different open issues are included, along with a link to a following companion paper presenting illustrative examples of integrated design applied to a waste-water treatment plant process.

2. PROJECTING METHODS

Projecting methodologies introduce the study of process dynamics, since the initial stages of process design, in order to obtain plants that are more easily controlled. They focus on the analysis of controllability and similar properties of alternative plant designs, generally obtained from a preliminary economic evaluation. The design of the process and the analysis of the process dynamics are integrated into a systematic procedure, achieving a final plant design after comparing alternatives with different control quality.

The strength of these methods is the thoughtful study of controllability issues and the theoretical background that supports them. A wide variety of studies has been developed integrating dynamical behaviour analysis within the process design and also imposing constraints or modifying operating conditions to ensure the controllability and similar properties.

The revision of the *projecting methods* is organised according to the controllability and related operability properties of the processes and generally the kind of dynamic analysis used to evaluate alternative designs, as follows:

- Methods based on input-output controllability and related properties
- Methods based on state controllability
- Process oriented methods. Systems with recycle.
- Methods based on steady-state multiplicity analysis
- Methods based on phenomenological models.

2.1 Methods based on input-output controllability and related properties

The studies included in this category address the interactions between design and control adopting the qualitative input-output controllability definition (Skogestad and Postlethwaite, 1996) that is the ability to achieve acceptable control performance. This concept is wider and more qualitative than the classical "state controllability" defined by Kalman (1960). However, attention is also paid to other concepts as functional controllability and dynamic resilience. Many types of frequency domain indexes using the process linear model have been developed for evaluating the dynamic resilience, the impact of manipulated variable constraints and the effect of process disturbances and model uncertainties (Holt and Morari, 1985a,b; Perkins and Wong, 1985; Morari et al., 1987; Skogestad and Morari, 1987; Psarris and Floudas, 1991; Skogestad, 1994a,b; Lewin,1996; Cao and Rossiter, 1998), as well as a variety of static and dynamic interaction measures, for identifying favourable pairings of manipulated inputs and controlled outputs (Bristol, 1966; Niederlinski, 1971; Manousiouthakis et al., 1986; Hovd and Skogestad, 1992; Hovd and Skogestad, 1994; Zhao and Skogestad, 1997). Some of those traditional linear indices are the maximum and minimum singular values, the process condition number, the disturbance condition number, the Relative Gain Analysis (RGA) and the Disturbance Cost (DC). Extensions of these indices to non-linear processes controllability can be found in Daoutidis and Kravaris (1991), Daoutidis and Kravaris (1992) and Manousiouthakis and Nikolau (1989).

Within this classification are also included works on *process synthesis*, this is, the analysis of how the process structure affects controllability and even the effects of the control systems structure on the dynamic behaviour of the designs obtained. In fact, the problems more frequently considered in the early literature on integrated design are those related to the synthesis of the process and the control structure.

Among the opening contributors, Morari and Stephanoupoulus (1980) discuss the structural design of alternative regulatory control schemes to satisfy a posed objective. They use structural models to describe the interactions among the units of a plant and the physicochemical phenomena occurring in the various units. They discuss the relevance of controllability and observability in the synthesis of control structures, and use modified versions to develop all the alternative feasible regulatory structures in an algorithmic fashion. Various examples are presented to illustrate the developed concepts and strategies, including the application of the overall synthesis method to an integrated chemical plant.

Marselle et al. (1982) present a heat exchanger network synthesis technique that takes into account aspects of flexibility and resiliency, leading to networks flexible to changes in the plant operating conditions. The method involves the structural and parametric design of the network and the synthesis of the regulatory control structure. The objective is to find the structure able to operate feasibly in a specific range of uncertain parameters while achieving the maximum energy recovery. Saboo and Morari (1984) develop a rigorous synthesis technique based on the fundamental properties for maximum energy recovery in heat exchanger systems which leads to networks that can handle specific inlet temperature variations and also guarantee maximum energy recovery. In Morari et al. (1985) these techniques are extended to the synthesis of the heat exchanger network and the control structure for a sequence of two exothermic open-loop unstable continuous stirred tank reactors.

On a more extensive vision, the subject of the process synthesis as such is usually tackled with systematic methods as the *hierarchical decomposition* and the *superstructures optimisation*. The *hierarchical* method, more frequently used in plant-wide design, allows the decomposition of the design problem in a sequence of sub-problems ordered by level of detail. In general five levels are considered, namely, the type of operation (batch or continuous), the input-output structure of the process, the recycles needed, the design of the separation-processes and finally, the design of the heat exchanger systems (Douglas, 1988). One of the leading works that proposes a systematic procedure for a controllability analysis in the hierarchical synthesis of chemical processes is Fisher et al. (1988). They introduce control objectives in the procedure of *hierarchical synthesis,* evaluating the impact of typical perturbations on the operation costs and constraints. Thus in each possible design and in every level of the process synthesis, the degrees of freedom between the control and manipulated variables and the impact of perturbations are examined, in order to decide on design modifications aimed at improving controllability.

In Barton et al. (1992), the controllability of plant designs previously obtained by economic optimization of stationary models is evaluated, the steady-state Relative Gain Array (RGA) is used to determine the best input-output pairings, and the limitations to the functional controllability are analysed. Then, the designs are modified in order to improve their deficiencies. Narraway et al. (1991) present a method to evaluate the impact of disturbances on plant economic performance in alternative process structures or alternative control schemes for a given process. The best operating point in the absence of disturbances is obtained by non-linear steady-state optimization, and frequency response analysis of a linearized plant dynamic model is used to estimate the effects of disturbances on this ideal performance under a variety of control strategies. A modification of this method is presented in Narraway and Perkins (1993). In this work, they provide a measure of the best achievable economic performance as the amount that the operating point must be backed off from constraints active at the optimal operating point to accommodate the effects of disturbances. The back-off idea is also used to measure the effect of dynamical performance on economics because the required back off represent the necessary extra cost to ensure that none of the operating constraints which affects controllability is violated. Perfect control is assumed and integer programming techniques are used for screening the potential control structures which are then all subjected to controllability analyses or are used as control structures for nonlinear dynamic economic analysis.

The work of Luyben (1993d) dealing with the design of a continuous-stirred-tank reactor (CSTR) clearly illustrates how the different structural alternatives of a process can produce opposite effects on investment costs and control performance. In a CSTR system, the most economical structure, with the smaller total reaction volume and heat transfer area, exhibits the worst closed loop dynamical performance and the poorer heat exchange capacity. It is shown that other structures with larger heat transfer areas result in better trade-off solutions between investment cost and dynamical performance.

Also Wolff et al. (1992), Wolff et al. (1994) and Wolff (1994) propose interesting procedures using analysis tools to evaluate the inherent control properties of chemical plants. Wolff et al. (1992) present a method to assess linear controllability, combining different controllability measures that complement each other for enhanced understanding of the process behaviour. In Wolff et al. (1994) a systematic study of the operability and decentralized control system design of the total plant is presented. It involves the selection of manipulated and controlled variables, and flexibility and controllability analysis using linear indices.

Focusing on the synthesis of a control system structure, Lin et al. (1991) establish the concept of Output Structural Controllability (OSC) and derive a condition to ensure Output Structural Controllability of a process explaining how to use it for the selection of the control schemes in chemical plants. Later, Hopkins et al. (1998) make use of this index (OSC) for integrating process design and control in the process and control structure synthesis. Also, Lee at al. (2001) study the structural controllability concept in relation to the propagation paths of the perturbations. They use only the structural digraph of the plant and their relative order matrices, without knowledge of other process details, to select the best flowsheets and discard non-controllable alternatives.

Vinson and Georgakis (2000; 2002) define the Output Controllability Index (OCI) or Operability Index (OI) which is a steady state and non-linear measure of the ability of a design to reach all points of the desired output space and to reject the expected disturbances using input actions not exceeding the available input space. It has been proven to be effective for both linear and nonlinear processes. Its extension to dynamic analysis called Dynamic Operability Index (DOI) is presented in Uzturk and Georgakis (2002). These operability analysis tools are exploited in Subramanian et al. (2001) for examining the inherent steady state operability of continuous processes, using as example a CSTR system. They propose an approach that further extends the original OI formulation to include nonsquare systems, distinguishing different categories for process outputs: (1) set-point controlled, with outputs to be controlled at a desired value, and (2) set-interval controlled, with outputs to be controlled within a desired range. In Georgakis et al. (2003) a similar methodology is presented. An extension of the operability analysis for plantwide systems is applied to the Tenesse Eastman process in Subramanian and Georgakis (2005).

A steady state resiliency analysis of chemical processes is presented in Solovyev and Lewin (2000) for linear systems. Later, in Solovyev and Lewin (2003a, 2003b) the analysis is extended to the non-linear case and an extension of the Disturbance Cost (DC) (Lewin, 1996; Weitz and Lewin, 1996) to non-linear systems is suggested. Those resiliency concepts are used by the authors for screening alternative process flowsheets (Soloyev and Lewin, 2004), showing that larger manipulated variable range requirements are associated with more expensive process designs.

2.2 Methods based on state controllability

Some recent works are found in the literature where the methodology to integrate design and control focuses in analyzing the state-space controllability of non-linear systems. Some particular concepts on controllability and observability for non-linear systems in state-space are developed in Hermann and Krener (1977).

The works by Ochoa (2005) and Ochoa and Alvarez (2005), are interesting contributions where the integrated design is carried out to ensure the local controllability of input affine, non-linear systems, by means of some metrics for *practical controllability* based on state-space theory. They concern different aspects of the process, such as the available degrees of freedom for control, the rank of the *local controllability* matrix, the system inversibility, the range of available control actions and the existence of a linear reachability trajectory. These indices are examined to address problems such as misleading interactions between inputs and states, wrong selection of manipulated variables or final control elements and physical restrictions of the states, which preclude the assurance of practical controllability. The procedure uses the phenomenological model of the process and selects the manipulated variables and the best structure (pairing) for control. It also includes the determination of the *available operation range* for the input variables and the selection of perturbations tolerances under different scenarios. The method addresses the plant optimization as a function of the investment and operation costs, while including the evaluation of the controllability metrics and considering the restrictions imposed by them. At last, the control system is designed to suit the optimal plant, knowing that its controllability is assured at the desired operating point. They present an ammonium-water separation process with a reactor-flash-exchanger plant, as a design example.

An extension of this work to undertake the integrated design of coupled systems is found in Muñoz et al. (2008), where a methodology is proposed to verify the controllability of coupled systems based on the computation of the accessibility distribution and the controllable/non-controllable states decomposition. In Alvarez (2008) the Hankel Matrix is proposed as controllability measure. In Lamanna et al. (2009) the state-space practical controllability analysis is used as a pre-factibility step to impose certain restrictions in the integrated design of a sulfitation tower by integrated-optimization methods. Calderón et al. (2012a) propose the redesign for a wastewater treatment plant based on the results of the non-linear state controllability analysis of the system. The set theory is used to check the controllability limits of the system including disturbances limits and constraints on control inputs. In Calderón et al. (2012b) a comparison between differential geometric and set theoretical (randomized algorithms) methods to consider the nonlinear state controllability is presented. Finally, a detailed description of the methodology to assess non-linear state controllability in the integrated design framework, named by the author: *Simultaneous Process and Control Design (SPCD),* can be found in Alvarez (2012).

2.3 Process-oriented methods. Systems with recycles

Modern chemical plants are highly integrated and interconnected which invariably introduce a dynamic coupling between the process units. Material and energy recycle affects process performance leading to complex dynamic behavior, such as inverse response, open loop instability and chaotic behavior. Several authors propose different strategies to quantify these effects (Denn and Lavie, 1982; Morud and Skogestad, 1994; MacAvoy and Miller, 1999, Jacobsen, 1997; Dimian et al., 1997; Semino and Giuliani, 1997; Bildea and Dimian, 2003; Lakshminarayanan et al, 2004; Bildea et al., 2004).

Luyben and coworkers present a series of papers devoted to the study of dynamics and control of recycle systems in chemical processes (Luyben, 1993a; Luyben, 1993c; Tyreus and Luyben,1993; Luyben, 1994; Luyben,1999). The special dynamic behaviour of recycle systems, identified in the works just mentioned, are important in the development of process design methodologies, in the subsequent works of the authors. Particularly, Elliot and Luyben (1995) present a capacity-based economic approach which allows comparing and screening quantitatively conceptual plant designs assessing both, steady state economics and dynamic controllability of the process. The alternative plant designs are evaluated considering their ability to maximize annual profit in the presence of their associated peak disturbances. The method deals explicitly with the impact of product quality variability on plant profits, considering the losses generated in the fraction of time that the product is outside the limits of desired specifications. A reactor/ stripper recycle system is considered as case study. The methodology is applied in the design of a complex recycle system consisting of one reactor and two distillation columns in Elliot and Luyben (1996). In this case study the approach is used to design parameter alternatives, conceptual design flowsheet alternatives, and control structure alternatives for the system.

Luyben and Luyben (1996) deal with the plantwide design and control of a complex process containing two reaction steps, three distillation columns, two recycle flows, and six chemical components. A heuristic design procedure and a nonlinear optimization are used to determine an approximate economically optimal steady-state design; the sensitivity to design parameters and specifications is evaluated and control strategies are developed using guidelines from previous plantwide control studies. In Luyben (2000), the trade-off between the reactor size, recycle flowrate and reactor inlet temperature of a gas-phase reactor /recycle plant in the steady state design is studied, as well as the economic impact of inert components in the feed stream. In a second step, alternative control structures are evaluated and basic control strategies are applied in the presence of large disturbances. Reyes and Luyben (2000a) present a similar study for an irreversible reaction system with a reactor feed preheating system (feed effluent heat exchanger and furnace) where the steady-state economics and the dynamic controllability of this dual-recycle system are compared with those of single-recycle processes. Reyes and Luyben (2000b) and Reyes and Luyben (2001) focused on processes with more realistic separation systems (a distillation column) for gas-phase tubular reactors with liquid recycle and with a dual recycle system.

Zheng and Mahajanam (1999) have pointed out that there are very few indices available which establish a direct relation between cost and controllability. They propose an index to quantify the cost associated with dynamic controllability of a process with a given control structure, focusing on the additional surge volume (or overdesign) required to achieve the control objectives. Such cost/controllability index is used to quantify the cost associated with dynamic controllability. Zheng et al. (1999) propose a hierarchical procedure where alternative plantwide control systems are synthesized and compared in terms of economics. They describe the design procedure for an existing plant (a simple reactor-separator-recycle system) and also show how the most interesting problem of determining the optimum surge capacities of a process can be addresses with a simple modification.

Other contributions are found in the works of Cheng and Yu (2003) and Kiss et al. (2005). The former explores the dynamics of simple recycle plants under different process designs using different control structures. The recycle dynamics is evaluated using transfer-function-based linear analysis and also validated using rigorous nonlinear simulation; finally, implications to control structure design are specified for different levels of reactor conversions. Kiss et al. (2005) address the design of recycle systems involving multiple reactions. They use the mass-balance model of the plant to capture the interaction between units and to predict the main pattern of behaviour. After choosing the method of controlling the plantwide material balance, nonlinear analysis reveals regions of unfeasibility, high-sensitivity, state multiplicity, and instability.

2.4 Methods based on steady-state multiplicity analysis

Some interesting works are focused on integrating operability criterions into chemical reactors design based on the steady state multiplicity analysis. Several preliminary results by Russo and Bequette (1995;1996; 1997; 1998) use the bifurcation based approach to study the behaviour of CSTRs showing that the infeasible operation regions that affect open loop and closed loop performance can be avoided with some parameter modifications in the design stage. More recently, Altimari and Bildea (2009) tackle the integrated design and control of plantwide systems. Their methodology evaluates the steady state multiplicity and allows selecting possible flowsheets and admissible control structures in terms of feasibility.

The influence of input/output multiplicity on stability and non-minimum phase behaviour of chemical reaction systems is studied in Yuan et al. (2009), Yuan et al. (2011), Wang et al. (2011) and Wang et al. (2013). Focusing on inherently safer designs, their study reveals how the essential properties of a process change with variations in its operating conditions. A systematic framework that includes multiplicity and phase behaviour together with open loop stability analysis over the entire feasible operation region of plantwide processes is presented in Yuan et al. (2012b).

Yuan et al. (2009), address a strategy for classifying the process operating region into distinct zones at the early stage of process design, based on stability/instability and minimum/non-minimum phase behaviour analysis. Wang et al. (2011) conclude that stability and phase behaviour should be analysed considering the overall system rather than individual units because those properties may differ from the global system. Yuan et al. (2011) present a methodology that explores the open and closed-loop controllability of the liquid-phase catalytic oxidation of toluene. They evaluate set-point tracking and disturbances rejection in various sub-regions with different controllability characteristics.

2.5 Methods based on phenomenological models

Grouped in this paragraph are procedures where the phenomenological knowledge of the process is used to distinguish the designs with best dynamic performance, using sensibility analysis of the thermodynamic properties of the chemical process or specifically passivity theory.

In Gani et al. (1997), different process flowsheets and equipment design parameters are generated through simulations using simple or rigorous models of the process, analyzing at every step different process features, and including environmental aspects and controllability. In Rusell et al. (2002), more emphasis is given to the analysis of the process model as a preliminary solution step for integration of design and control problems. In Li et al. (2003), a systematic sensitivity analysis of the process model is developed to select the best control structure. In Ramírez and Gani (2007a,b), a model based analysis methodology for the integrated-design and control is presented, using first-principles phenomenological models of different complexities to identify the interactions between process and design variables. Parametric sensitivity analysis is performed in order to determine the control structure.

In Hamid et. al. (2010) the simultaneous process and control system design of a process is addressed by the reverse design algorithm approach. The formulation of the integrated-optimization process design and process control problem is decomposed in four sub-problems easier to solve. The search space is reduced by considering thermodynamic and feasibility aspects, the concepts of attainable region (AR) and driving force (DF) are used to locate the optimal process-controller design in terms of optimal condition of operation from design and control viewpoints. The AR concept is used to find the optimal (design target) values of the process variables for any reaction system. The DF concept is used in this methodology to find the optimal (design target) values of the process variables for separation systems. The final selection and verification is performed according to the value of the objective function. Alvarado-Morales et al. (2010) extend this methodology, proposing a framework that combines the simultaneous process design and controller design methodology and the process-group contribution (PGC) methodology. A process flowsheet can be described by means of a set of process-groups bonded together to represent the structure. The PGC methodology has been used to generate and test feasible design candidates based on the principles of the group-contribution approach used in chemical property estimation. It is applied to the bio-ethanol production process, however, this is a general framework that can be applied to different processes.

The possibilities to include the controllability analysis within the process synthesis, in terms of sensibility to perturbations, particularly using thermodynamic-models and passivity theory, have been studied by Meeuse et al. (2000, 2001), Meusse (2002) and Meeuse and Grievink (2002). The passivity systems are a class of processes that dissipate certain types of physical or virtual energy, defined by Lyapunov-like functions. The authors use the passivity framework, linked to process thermodynamics, in process input-output controllability analysis. This approach allows for studying the stability of distributed systems and the selection of the manipulated and measured variables pairing alternatives that ensure stability and efficient plant operation by relating the entropy production sensibility of the plant with its sensibility to perturbations. Specifically, in Meusse (2002) and Meeuse and Grievink (2004) controllability conditions are incorporated in the process synthesis by considering thermodynamic aspects of the process, in order to derive some design guidelines.

In conclusion, the literature about projecting methodologies in integrated design introduces the controllability analysis in the early stages of the process design to guarantee a good dynamic behaviour of the system. The analysis, when based on input-output models, is accomplished evaluating different alternatives of the plant obtained by economic optimization of the steady-state process, using open-loop controllability indexes. The controllability criterions employed in the works previously described, are focused mainly on the effects of perturbations on the operation constraints and their propagation through the process, concerning the analysis of the information contained in different indexes based on the linear model. When the state-space models are used, the controllability analysis focuses on measures that assure a controllable closed loop structure and operating conditions, with methods that allow fixing a priori the controllability conditions in non-linear systems. Finally works can be found in the literature that take advantage of the phenomenological information in the process mathematical models or the thermodynamical properties of the process to improve the synthesis and process design integrating sensitivity to perturbations and other control aspects. Additionally, a special mention deserve the works to include controllability analysis in the process synthesis, exploring different operability and sensitivity qualities of a process flowsheet to determine the structure of the process even at plantwide level, and including also the control schemes structure.

3. INTEGRATED-OPTIMIZATION METHODS

In the integrated-optimization of process and control design, the dynamic performance measures are introduced within the process design, originating a single optimization scenario containing additionally the tuning of the controllers and even the selection of the control structure. The formulation of the optimization problem contains decision variables, objective functions and constraints related to economics as well as operating and control performance aspects. Thus, this approach provides the possibility of carry out at once the process and the control system design by solving the optimization problem, providing the plant design that best satisfies the compromise between economic and control aspects and all the criterion considered in the problem formulation.

Pioneer works that introduced the idea of integrating the process design and the controllability issues in a comprehensive optimization problem were those by Lenhoff and Morari (1982), Palazoglu and Arkun (1986) and Georgiou and Floudas (1989), among others. In Lenhoff and Morari (1982) an optimization based design approach considering economic and dynamic aspects simultaneously is proposed, taking into account process structural decisions, parametric changes and the control structure selection which leads to a multiobjective optimization problem. Palazoglu and Arkun (1986) formulate a multiobjective optimization using robustness indices as constraints to quantify the dynamic operability which is illustrated by solving design and operability problems of a CSTRs system. Georgiou and Floudas (1989) developed a systematic framework for control system synthesis. They used the generic rank of a process structural matrix as an index of structural controllability to select the best process configuration, computed by solving an integer-linear optimization problem.

Perkins and Walsh (1996) pointed out the notable trend towards the use of optimization as a tool for the integration of process design and process control, which was enabled by advances in computational hardware and optimization methods and driven by the need to place control design decisions on the same basis as process design decisions.

The most relevant contributions using methods based on an integrated optimization problem are classified first in terms of the methods to evaluate controllability or other properties related to process dynamic performance. Due to the number of works dealing with the simultaneous process design and process control procedure within an optimization framework, other criterion can be considered to classify the works, namely the scope of the design problem, the control strategies, the treatment of perturbations and uncertainties, and the formulation of the optimization problem.

The most relevant contributions using methods based on an *integrated-optimization* problem are classified in terms of all the different edges of the problem, namely:

- The scope of the design problem
    - Synthesis and design
    - Process design only
- The methods to evaluate controllability or other properties related to process dynamic performance
    - Methods based on controllability indices
    - Methods based on numerical indices and the dynamic non-linear model.
    - Robust methods
    - Probabilistic based methods
- The control strategies
    - Classical feedback PID type
    - Model Predictive Control
    - Others
- The treatment of uncertainties and perturbations
    - No treatment
    - Worst-case scenarios
    - Robust-approach based methods
- The formulation of the optimization problem
    - Multiobjective optimization
    - Formulations with an economic objective function and controllability constraints.
- The methods of resolution of the optimization
    - Classical
    - Stochastic or alternative optimization methods

3.1 The scope of the design problem

The most complete formulation of the integrated design of a process includes in addition to the determination of the plant dimensions and operating conditions, the selection of the plant topology (process synthesis) and the selection of the control structure (input-output pairing and control scheme). When the synthesis is considered, the optimization problem is posed based on a superstructure containing all the possible alternatives of the process (algorithmic synthesis or automatic synthesis), aimed to find the optimal flowsheet in the economic and controllable sense. The selection of the control system configuration can also be embedded in a superstructure. This formulation involves continuous variables, representing the dimensions and operating conditions, and discrete variables, related to the process/controller structure.

Different formulations of the integrated design including the process synthesis and the selection of the control structure are found in the literature. Luyben and Floudas (1994a) present a general formulation of the problem considering a superstructure for the process synthesis that include all possible design alternatives of interest and open-loop steady-state controllability measures. Mohideen et al. (1996a) propose a unified process synthesis optimization framework for obtaining process designs together with the control structure and controller design. The objective is to design the process and the required control scheme at minimum total annualized cost which comprises investment and operating costs including controller costs. It results in an optimum set of design variables, the best selection/pairing of controlled-manipulated variables and the optimal values of the controller parameters. Some other works addressing the complete integrated design problem involving close loop behaviour analysis into the optimization are Mohideen et al. (1996b), Bahri et al. (1996a), Bansal et al. (2000b), Kookos and Perkins (2001), Ekawati (2003) and Flores-Tlacuahuac and Biegler (2007), Revollar et al., (2012). The most recent papers dealing with the full integrated design formulation are Sanchez-Sanchez and Ricardez-Sandoval (2013a), Trainor et al. (2013) and Sharifzadeh and Thornhill (2013).

A number of works carry out the integrated design considering only the process synthesis and the determination of the optimal plant dimensions, operating conditions and even the controller parameters: Schweiger and Floudas (1997), Bahri et al. (1997), Gutierrez (2000), Sakizlis et al. (2003), Sakizlis et al. (2004), Malcom et al., (2007), Revollar et al. (2008b) and the recent contributions of Revollar et al. (2010a), Revollar (2011) and Sanchez-Sanchez and Ricardez-Sandoval (2013b). Some other works focuses on process dimensioning and determination of optimal operating conditions including the selection of the control structure and controller tuning: Narraway and Perkins (1994), Asteasuain et al. (2005), Asteasuain et al. (2006), Asteasuain et al. (2007), Patel et al. (2007), Flores-Tlacuahuac and Biegler (2008).

In the literature are found very interesting papers where the integrated design methodology is limited to the determination of the optimal design for a given process structure and an specific control structure. Most of them undertake challenging issues in the integrated design framework such as alternative procedures to evaluate controllability, uncertainties handling techniques, the inclusion of advance control strategies or address a complex application. For instance, Brengel and Seider (1992) performing the integrated design of a fermentation process with a strong non-linearity and an instability trend with model predictive control (MPC), Ricardez-Sandoval et al. (2008, 2009b) introducing robust modelling approach in the design of a mixing process with great parametric uncertainties, Bahakim and Ricardez-Sandoval (2014) who tackle the integrated design of a wastewater treatment plant in the presence of stochastic disturbances using advanced model-based control schemes. Other works considering fixed structures are Lenhoff and Morari (1982), Palazoglu and Arkun (1986), Luyben and Floudas (1994b), Gutiérrez and Vega (2000), Blanco and Bandoni (2003), Chawankul et al. (2007), Miranda et al. (2008), Grosh et al. (2008), Kim and Linninger (2010), Francisco et al. (2011) and Ricardez-Sandoval (2013). Large scale systems are addressed in recent works as Exler et al. (2008), Moon et al. (2011), Ricardez-Sandoval et al. (2009c, 2010, 2011) and Muñoz et al. (2012).

3.2 The methods to evaluate controllability or other properties related to process dynamic performance.

An important classification of the integrated-optimization methods arises separating them in four groups according to the techniques used within the optimization framework to quantify controllability or more generally the dynamic performance of the process. This classification is adopted from Ricardez-Sandoval et al. (2009).

a. <u>Methods based on controllability indices</u>

The classical input-output controllability indices can be easily included as objectives or constrains within the optimization formulation. Most of the indices are based on steady state models or linear models, which allows the evaluation of process dynamic performance with a minimun computing effort, however, it limits the applicability and accuracy of the indices to an enveloped around the nominal operating point. Additionally, most of those the linear input output controllability indices do not provide a clear relation to process economics.

In the work of Luyben and Floudas (1994a), controllability indexes based on stationary linear models which are described as functions of the process parameters are applied. Some examples of these indexes are the Relative Gain Matrix (RGA), the minimum singular value and the condition number. Previous to them, Palazoglu and Arkun (1986), apply the singular values analysis. Blanco and Bandoni (2003) also consider the minimum singular value of the stationary transfer matrix as a measure of controllability.

Some authors have introduced procedures that include practical controllability analysis based on state controllability indices in the Integrated Design framework (Lamanna et al., 2009; Revollar et al., 2010b).

b. *Methods based on numerical indices and the dynamic non-linear model*

Some techniques based on the simulation of the full nonlinear dynamic model of the process have been proposed to introduce the dynamic performance evaluation within the integrate optimization methods for the simultaneous design and control. These approaches allow an appropriated representation of process nonlinearities and make possible to carry out the direct evaluation of performance requirements in terms of plant and controller parameters. Moreover, the dynamic effect of external time-dependent perturbations can be rigorously taken into account within the problem formulation and some methods considers the critical profile in the disturbance that produces the largest (worst-case) variability in a process variable due to critical realizations in the disturbance and uncertainty in the system's parameters. (Ricardez-Sandoval et al., 2009a).

The controllability analysis based on the dynamic model is carried out by computing some indicator of the evolution of the model output(s) throughout a predefined time horizon. A typical technique is to obtain the integral of the square control error (ISE) using the dynamic non-linear model. Some examples of the use of this index can be found in Schweiger and Floudas (1997), Bansal et al. (1998), Asteasuain et al. (2006), Asteasuain et al. (2007), Revollar et al. (2010a). Also in Flores-Tlacuahuac and Biegler (2007), where aside from the ISE, they use additionally the time to steady state. In Exler et al. (2008) a set of performance indexes is evaluated, including the ISE and other open loop measures related to the activated sludge process considered, as the pumping energy and the aeration energy in the system.

Some of these approaches consider the flexibility or even the operability analysis in the process performance evaluation. The flexibility analysis involves two important problems: the feasibility test and the quantification of the inherent flexibility of a process (Grossmann and Morari, 1983). The feasibility test problem determines the existence of at least one set of manipulated variables that can be selected during plant operation, such that, for every possible realization of the uncertain parameters all the process constraints are satisfied (Halemane and Grossmann, 1983). Bansal et al. (2000a) propose an approach for the flexibility analysis and design of linear systems, based on parametric programming which provides explicit information about the dependence of the system flexibility on the values of the design variables. Bansal et al. (2002a) generalize and unify this approach for the flexibility analysis and design of nonlinear systems. Recent works dealing with flexibility evaluation are Lima et al. (2010a,b), Chang et al. (2009) and Adi and Chang (2011).

In Mohideen et al. (1996a) the dynamic feasibility analysis is included in the integrated design problem, verifying the operation and control constraints all over the uncertainty range of the parameters in the established time horizon. Bahri et al. (1996a) and Bahri et al. (1997) propose the dynamic operability analysis within the process synthesis and control structure selection problem. This analysis includes aspects as stability, controllability and flexibility, its objective is to optimize the process economy subject to feasible regulatory dynamics. Stands out the use of the backward margin based on the dynamic non-linear model. It relates the economic aspects with the operability, by fixing the distance between the optimal steady-state operating point and the dynamic operating point of the plant. They also consider the dynamic feasibility and indexes as the ISE and the steady-state time. In Ekawati and Bahri (2003) this analysis is completed by introducing the output controllability index, OCI (Vinson and Georgakis, 2000).

In Novak and Kravanja (2004) the flexibility and static operability analysis is introduced in the problem formulation by determining in a first stage, the optimal flexible structure and optimal oversizing of the process units that guarantee feasibility of design for a fixed degree of flexibility. In a second stage, the structural alternatives and additional manipulative variables are included in the mathematical model in order to introduce additional degrees of freedom for efficient control. Malcom et al. (2007) and Moon et al. (2011)

test the process and control design over the set of uncertain parameters by solving the dynamic feasibility test problem.

A particular work, where the study of process behaviour is performed considering the process model to evaluate thermodynamic insights is Hostrup et al. (2001). In this work a methodology is proposed that combines flowsheet generation based on thermodynamic insight and structural optimization.

c. *Robust methods.*

In the recent years robust approaches have been introduced in the integrated optimization formulations. They take into account the uncertainties existing in real processes in order to provide robustness properties to the obtained plants and the worst case variability. The robust approach-based methodologies have been emerged as an alternative to alleviate the computational demands associated with the dynamic optimization-based methodologies. In this approaches, the process non-linear dynamic model is represented as uncertain models that can be used to calculate bounds on the variables that are involved in the objective function and the constraints of the problem under consideration (Ricardez-Sandoval et al., 2010).

In Monnigmann and Marquardt (2005) is proposed a method that establishes robust measures based on a minimal distance between the uncertain parameter space region and the critical boundaries. Later, in Grosch et al. (2008), constraints are imposed simultaneously on time-domain performance indicators and on the asymptotic dynamic process behavior while optimizing the steady state profit of the plant, accounting for the effect of uncertainty in both, design and model parameters. This approach is difficult to apply in the presence of more than one disturbance, then, in order to overcome its disadvantages, Muñoz et al. (2012) uses an extension of the normal vector approach proposed in Monnigmann and Marquardt (2002) to consider simultaneously robust asymptotic stability of steady states despite parametric uncertainty and robust feasibility of the transient behaviour despite disturbances.

In particular, several articles by Ricardez-Sandoval and coworkers present a robust-approach based methodology that performs the simultaneous design and control under disturbances and process model parameters uncertainties. In Chawankul et al. (2007) a measure of the closed loop output performance is introduced based on the output widest variability caused by model uncertainties and constraints related to the robust stability of the plant are imposed. Furthermore, this performance indice is added to the objective function as a cost associated to the variability. In Ricardez-Sandoval et al. (2008, 2009a, 2009b) a new technique is presented to assess the flexibility, stability and controllability of a process. In this method, the infinite time horizon bounds are estimated for the worst case scenarios, enforcing process feasibility constraints by using the Structured Singular Value analysis (SVA), avoiding expensive dynamic optimizations. This methodology is improved in Ricardez-Sandoval et al. (2009c) to reduce the computational requirements of the method toward its application to large-scale processes; the methodology is referred as the Analytical Bounds Worst-case Approach (BWA). However, a disadvantage of this approach is the conservatism resulting from the use of analytical bounds. In Ricardez-Sandoval et al. (2010) a method named hybrid worst-case approach (HWA) is proposed. It combines the analytical calculation of the worst-case disturbance and dynamic simulations using the mechanistic closed-loop process model to calculate variability. It is expected to reduce the conservatism in the final design at the expense of additional computational time in the calculations. Ricardez-Sandoval, et al. (2011) have expanded hybrid worst-case approach considering time-varying disturbances and parametric model uncertainties, making it suitable for application to large-scale systems.

In Sanchez-Sanchez and Ricardez-Sandoval (2013a) is presented a method for optimal process synthesis and control structure selection that simultaneously evaluates dynamic flexibility and dynamic feasibility in the presence of the worst-case (critical) time-trajectories in the disturbances. Furthermore, a robust stability test based on Quadratic Lyapunov theory is included in this methodology to ensure that the optimal design is asymptotically stable for any of the magnitude-bounded perturbations considered in the analysis. The disturbances are treated as stochastic time-discrete unmeasured inputs. The work of Trainor et al. (2013) adopt this methodology for the design of a ternary distillation system treating disturbances as random time-dependent bounded perturbations. In Sanchez-Sanchez and Ricardez-Sandoval (2013b) an approach for the integration of process flowsheet and control design methodology incorporating a multivariable model predictive control (MPC) strategy in the analysis is proposed. It contemplates an iterative decomposition strategy comprising of a dynamic flexibility analysis, a robust dynamic feasibility analysis, a nominal stability analysis, and a robust asymptotic stability analysis.

In Gutierrez et al., (2013) an integrated design methodology focused on the selection of an optimal control structure is addressed by adding a communication cost function within the overall cost function. Different control structures composed of centralized and fully decentralized predictive controllers are considered in the analysis. A cost function related to the worst-case closed-loop variability is calculated using analytical bounds derived from tests used for robust control design.

In Matallana et al. (2011) a design methodology based on the optimization of the domain of attraction is proposed. The idea is to simultaneously ensure asymptotic stability and an optimum domain of attraction of the resulting operating point in a certain sense. The approach consists in maximizing the radius of a ball in the states space within which negative definiteness of the time derivative of a quadratic type Lyapunov function can be ensured.

In Francisco et al. (2011) and Francisco (2011) norm based indexes for controllability are considered. They allow for including robust performance conditions within the integrated design procedure by using a polyhedral uncertainty region, limited by multiple linearized models. The multi-objective problem is stated include investment, operating costs, and dynamical indexes based on the weighted sum of some norms of different closed loop transfer functions of the system.

d. Probabilistic based methods

Some of the recent works presented in literature for optimal design considers a stochastic or probabilistic based approach. Most of design procedures ensures the appropriated process performance in the presence of uncertainties and disturbances focusing on the worst case scenario given by the critical realizations in the disturbances and the uncertain system's parameters that produce the largest deviations in the controlled variables, demanding major control efforts to maintain the desired operating conditions. This is called the worst-case process variability (Bahakim and Ricardez-Sandoval, 2014). The overestimation of the uncertainties, typical in process design methodologies, leads to conservative design decisions resulting in an unnecessary deterioration of the objective function, In such sense, probabilistic programming is a promising solution for solving optimization problems under uncertainty in the process industry (Li et al, 2008) allowing to take into account the probability of occurrence of the worst-case variability in the process variables.

Few works have introduced such considerations in the integrated design formulation. Ricardez-Sandoval (2013) introduce a distribution analysis on the worst-case variability in the integrated design framework. The work case variability is approximated by normal distribution functions in order to estimate the largest variability expected for the process variables at a user-defined probability limit. Thus, the user is able to rank the goals of design according to its particular criterion. The worst-case variability estimates are used to evaluate the process constraints, the system's dynamic performance and the system's cost function enabling the assessment of the optimal process design by assigning different probability levels to the process variables used to evaluate the process constraints and the process economics. In Bahakim and Ricardez-Sandoval (2014) an optimization framework for achieving a feasible and stable optimal process design in the presence of stochastic disturbances while using advanced model-based control scheme is proposed.

3.3 The control strategies

The optimization based integrated design of process and control system usually introduces the tuning of the controllers and the evaluation of their performance within the optimization framework. In most works classical feedback control systems are used; even so, some applications with advanced control techniques, particularly predictive control (MPC), have been proposed (Brengel and Seider, 1992; Loeblein and Perkins, 1999; Sakizlis et al. 2003; Sakizlis et al. 2004; Chawankul et al., 2007; Francisco et al., 2011).

In several formulations of the integrated optimization of process design and control the controller parameters are introduced as decision variables in the optimization, while in others they are tuned empirically. Some formulations focuses in the analysis of the open loop system in order to obtain an optimal and controllable design for any possible controller, as in Luyben and Floudas (1994a), Grosh et al. (2008), Matallana et al. (2011), Guerra et al. (2012). In some works, the notion of perfect control is assumed in the optimization formulation avoiding the complexity associated to the controllers evaluation. Sharifzadeh and Thornhill (2012) propose a simplified optimization framework with a multiobjective function taking advantage of the perfect control concept, which is the best performance that a given control structure can achieve. Later this approach is introduced in the integrated design formulation in Sharifzadeh and Thornhill (2013). Perfect control is supposed also in Narraway and Perkins (1993, 1994) and Blanco and Bandoni (2003).

The usual type of controller included in most of the integrated optimization based formulations independently of the scope of the problem is the feedback decentralized PI or PID (Narraway et al., 1991; Walsh and Perkins, 1994; Bahri, 1996; Schweiger and Floudas, 1997; Bansal et al., 2002b; Exler et al., 2008; Grosch et al., 2008; Ricardez-Sandoval et al., 2011; Sanchez-Sanchez and Ricardez-Sandoval, 2013; Gutierrez et al., 2013; Trainor et al., 2013; Ricardez-Sandoval, 2013). An early step toward the application of advanced control schemes is observed in Kookos and Perkins (2001) where a multivariable PI is implemented. Asteasuain et al. (2006) combine a scheme of feedback PI and feedforward multivariable control, while Asteasuain et al. (2007) uses a PI multivariable controller and a relation control scheme is used. Generally, the parameters of the PI controller are considered decision variables in the optimization problem. Nevertheless, in Bahri (1996) and Bahri et al. (1997) pre-designed PI controllers that are more fined tuneg after the procedure, in Dominguez et al. (2009) the PID IMC tuning method (Skogestad, 2003) is used to include the controller design within the integrated design framework.

Brengel and Seider (1992) are the first to propose advanced strategies, introducing a non-linear predictive controller in the *integrated design* problem. In Loeblein and Perkins (1999) a non-constrained MPC is used, then Sakizlis et al. **(**2003) and Sakizlis et al. (2004) implement a parametric predictive controller (MPC) that directly computes the control actions avoiding the on-line optimization of the controller. A constrained linear MPC is considered in Baker and Swartz (2006). Francisco and Vega (2006), Francisco et al. (2011), Gutierrez et al., (2013) and Bahakim and Ricardez-Sandoval (2014) include advanced control strategies based on MPC in for the integrated design of wastewater treatment processes considering a fixed process and control structure. A non linear MPC based on a non-linear model Revollar et al. (2010b) introduced

Most of the MPC-based approaches reported in the literature are limited to a fixed process and control structure. However, some works addressing the complex integrated design problem with MPC including the selection of the process structure and the controller tuning (determination of the weights of the controller cost function) are Revollar et al. (2008b), Francisco et al. (2009) and Sanchez-Sanchez and Ricardez-Sandoval (2013b).

Some works include other advanced control strategies, different from MPC, in the optimization based *integrated design* of processes*:* Chawankul et al. (2005) uses an internal model controller (IMC) and (Swartz, 2004) considers Q-parameterized controllers.

Terrazas-Moreno et al. (2008), Patel et al. (2007), Miranda et al. (2008) apply optimal control schemes. Malcolm et al. (2007) and Moon et al. (2011) use Linear Quadratic Regulators (LQR). Finally, Lu et al. (2010) considers a fuzzy-model-based controller which estimate the process behaviour and derive fuzzy rules to guarantee stability, robustness and feasibility.

3.4 The treatment of uncertainties and perturbations

In many works the effects of uncertainties and perturbations are ignored or else very simple perturbations profiles are considered (Narraway and Perkins, 1994; Schweiger and Floudas, 1997; Bahri, 1996; Kookos and Perkins, 2001). Nevertheless, in Bandoni et al. (1994) an algorithm of the worst case is presented, in order to compute the maximum variation of the uncertain parameters that can take place without impairing the feasibility of the process. Another group of publications can be found, focused on studying the effects of different settings of perturbations and parameter uncertainties on the process economics and dynamic performance (Mohideen et al., 1996a; Mohideen et al., 1996b; Bahri et al., 1996b; Bahri et al., 1997; Bansal et al., 2000b; Asteasuain et al., 2007).

In Chawankul et al. (2007) robust integrated design has been developed; particularly quantifying the uncertainties as a family of linear models around the nominal model. These uncertain models have been typically used in robust control, and they have also been used for integrated design in Francisco et al. (2011). However, most of the robust integrated design methods consider parametric uncertainty. In Moon et al. (2011) some uncertain scenarios are considered varying process parameters. In Muñoz et al. (2012), an extension of the normal vector method is developed to consider simultaneously disturbances and uncertain model and process parameters. Ricardez-Sandoval et al. (2008, 2009a), consider model parametric uncertainty, that is translated to an uncertain state space model, and later to a robust Finite Impulse Response model with uncertain parameters Ricardez-Sandoval et al. (2009b, 2009c, 2010). In Ricardez-Sandoval et al. (2011), the uncertainty has been extended to process physical parameters uncertainty. Sanchez-Sánchez et al. (2013a, 2013b) includes process synthesis and control structure decisions, but using again the uncertain Finite Impulse Response model.

As for the treatment of disturbances, Chawankul et al., (2007) only considers sinusoidal time-varying disturbances, and Gerhard et al. (2005) and Monnigmann and Marquardt (2005) are also limited to particular disturbances. Other works consider a general form of the disturbances, by means of their maximal magnitude. Particularly, Ricardez Sandoval et al. (2008, 2009a, 2009b, 2009c, 2010, 2011) assumes general disturbances of bounded magnitude, calculating carefully the worst case disturbance. Francisco et al. (2011) also considers the maximal magnitude of the disturbances based on the actual weather profiles.

3.5 The formulation of the optimization problem and the methods of resolution

The mathematical formulation of the optimization depends on the scope of the problem, the techniques used for introducing the quantification of controllability and other related properties related to dynamic performance, the control scheme and the treatment of disturbances and uncertainties.

The multi-objective nature of the integrated process and control design can be addressed by means of an optimization problem with different cost functions, or problems with just one objective function based on economic aspects and constraints related to dynamic performance indices. Representative works of the different formulation are classified here.

a) *Multi-objective formulations*

In Luyben and Floudas (1994a) a mixed-integer non-linear (MINLP), multi-objective programming problem is posed, where economic objectives and some linear controllability indexes are optimized. Blanco and Bandoni (2003) introduce controllability measures in this type of formulation using the eigenvalues optimization theory. Matallana et al. (2011) maximizes the region of asymptotic stability of the equilibrium point, which results in a bi-level optimization problem with non differentiable inner sub-problems, which is solved using a stochastic (derivative free) algorithm in the outer level. Sharifzadeh and Thornhill (2012) propose a simplified optimization framework with a multiobjective function taking advantage of the perfect control concept which is extended in Sharifzadeh and Thornhill (2013) introducing the inversely controlled process model which results in a dynamic optimization formulation that is solved by sequential integration and by full discretization.

In Schweiger and Floudas (1997) the mixed-integer optimal control problem (*MIOCP*) is simplified into a mixed integer non linear problem with differential equations (*MINLP/DAE).* Imposing different limits to the constraints, Pareto curves can be developed to reveal compromise solutions.

In Asteasuain et al. (2006), the optimization based simultaneous design and control of a polimerization reactor translates into a multi-objective, mixed-integer, dynamic optimization problem (MIDO). The two objectives are an economic function with the investment and operation costs, and a dynamic index similar to the ISE related to the product quality. The problem is solved by the application of a decomposition algorithm where there is a master mixed-integer, non-linear problem (MINLP) and an associated dynamic optimization problem.

Miranda et al. (2008) formulate the problem focusing in the application of optimal control theory, relying on Pontryagin's minimum principle. The Euler-Lagrange equations are derived from the underlying optimization problem which are then solved by using a discretization technique.

Malcom et al. (2007) and Moon et al. (2011) propose a new mathematical methodology to reduce the combinatorial complexity of multi-objective integrated design and control by embedding control for specific process designs. The optimal design problem is solved using the Nelder-Mead simplex method. Other alternative optimization formulations and methods have been applied successfully to solve the complex integrated design problem, for instance multi-objective formulations are successfully solved with stochastic optimization methods based in genetic algorithms in Revollar et al. (2010b, 2010c).

In Brengel and Seider (1992) a coordinated optimization strategy to solve the simultaneous design and control with a MPC is proposed. The economic objective function is penalized by deficient controllability. This translates into a *bilevel programming problem* (BPP) which is later on simplified to obtain a solution. A similar procedure, also using an MPC, is applied in Baker and Swartz (2006). They introduce the quadratic problem (QP) of the controller in the integrated design formulation, by replacing it with constraints associated to the Karush-Kurn-Tucker optimality conditions. Francisco et al. (2011) presents a multiobjetive formulation of the integrated design and control with an MPC considering economic and robust controllability objectives.
In the problem of integrated design including the process and control structure synthesis using MPC formulated in Sánchez-Sánchez and Ricardez-Sandoval (2013a) an iterative decomposition strategy is used. The analysis is formulated as convex problems, instead of mixed-integer nonlinear problems (MINLP), which is more convenient and efficient in these case studies.

b) Formulations with an economic objective function and controllability constraints

In these works a different formulations of the optimization problem is considered, introducing the controllability issues or dynamic performance indices as constraints. Although it is not equivalent to multi-objective formulations, it may simplify the optimization problems, once the particular bounds have been carefully selected.

In Bahri (1996) the economy of the process is optimized and feasible regulatory dynamics is ensured by means of constraints on the dynamic operability conditions. The problem is solved with the application of a two level iterative algorithm. On the first level the structure, dimensions and operating conditions are obtained through a MINLP. On the second level the feasibility of the solution is examined by means of the resolution of the associated NLP problems. This methodology is also applied in Bahri et al. (1996a) and Bahri et al. (1997), while in Ekawati and Bahri (2003) it is enlarged by adding a new controllability index to perform the dynamic operability analysis.

Mohideen et al. (1996a) propose a general formulation containing the *Total annual cost* as the minimizing function, subject to the constraints associated with: a) the differential and algebraic equations of the process model, b) the feasibility of the operation, c) the trajectory and d) the variability of the process due to perturbations and uncertainties. This formulation results into a mixed-integer dynamic optimization (*MIDO*). The proposed algorithm for its resolution requires the decomposition in two sub-problems and the application of an iterative procedure, starting with the determination of the optimal process design and control structure to end with the evaluation of the feasibility of the process operation throughout the possible range of perturbations and uncertainties. This framework is also adopted in the works of Bansal et al. (2002b), Sakizlis et al. (2003) and Sakizlis et al. (2004). Kookos and Perkins (2001) propose another decomposition algorithm, based on upper and lower limits to the economic performance of the plant. Firstly, the optimization of the plant layout and the control structure is performed, secondly the computation of the continuous and invariant parameters with dynamic optimization. In Flores-Tlacuahuac and Biegler (2007) an algorithm based on the transformation of a MIDO problem into a mixed-integer nonlinear programming (MINLP) program is proposed. Three MINLP formulations are developed and evaluated: a nonconvex formulation, the conventional Big-M formulation and generalized disjunctive programming (GDP).

In Chawankul et al. (2007) the variability of the controlled output is included in the objective function, imposing constraints on the manipulated variables to improve disturbance rejection and to ensure robust stability. In this work the non linear plant is represented by a family of linear models.

In Asteasuain et al. (2007) is an extension of Asteasuain et al. (2006) adding uncertainties and perturbations, while using only one objective function related to the product quality. A two-level optimization algorithm is applied to solve the problem. An initial set of uncertain parameters is considered and then extended up to the complete dominion of uncertainty to find the maximum violation of the operation constraints.

It is important to note that, it is quite difficult to disconnect the formulation of the integrated optimization problems from the solution approaches. Note that some common approaches result in non linear optimization problems (NLP), mixed-integer non linear problems (MINLP) and dynamical optimization (MIDO). Nevertheless, a number of algorithms have been developed to solve the MIDO problem and can be classified depending on the reformulation of the original MIDO problem into a MINLP problem or into a bi-level optimization problem (Sakizlis et al., 2004, Hamid, 2011).

Moreover, taking into account the optimisation methods applied for the resolution of the integrated design problem a further classification can be made. Thus, the optimization strategies basically can be deterministic methods or alternative methods such as stochastic and hybrid algorithms (Egea et al., 2007). For instance, in Exler et al. (2008), Lamanna et al. (2009), Francisco et al. (2009), Revollar et al. (2010a) and Revollar et al. (2012), stochastic methods as tabu search, simulated annealing and genetic algorithms are applied for solving different problems.

4. CONCLUSIONS

Scores of advances in different aspects within the general area of *integrated design* have been reported in the recent literature. Depending on how several issues are addressed, very different procedures of integrated design can be found. A general classification is presented in this paper, which distinguishes between *projecting* methods, where controllability indices are computed during the design to predict and compare alternative expected dynamic performances, and methods where process design and control is carried out through the resolution of a joint or *integrated-optimization* problem. The latter may address additionally the optimization of the controller structure and tuning.

However, numerous aspects of the integrated design problem remain still open to research. Regarding the scope of the design problem, some successful global applications can be found, which include discrete decisions on the plant structure and closed loop dynamics evaluations. Even thought, most cases of integrated design dealt with one equipment or process units, some recent works are focused on the integrated design process and control a large-scale chemical process (e.g.Tennessee Eastman process) (Ricardez-Sandoval et al., 2009c). Nevertheless, the development of efficient methodologies that account for structural changes in the process flowsheet and the control structure is still an open field of research.

On the subject of controllability evaluation techniques, the lack of conciliation between the state-variable and the input-output approaches is notorious, as is the small number of applications based on state controllability. Some recent works by Lamanna et al. (2009) and Revollar et al. (2010b) combine the state-space analysis with the simultaneous design and control of a sulfitation tower, showing the interesting potential of the state-space methods.

When the controllability evaluation is based on the behaviour of the dynamic non-linear model under perturbations, *mixed-integer dynamic* optimization problems (MIDO) arise, and therefore the computational effort required in integrated design increases considerably. On the other hand, this type of analysis offers several advantages, because it allows to easily understand the controllability results, to directly relate the economic indexes with the dynamic performance, and to study the flexibility of the process when submitted to perturbations. It becomes evident the need of a two-fold investigation: more powerful and efficient optimization algorithms, and alternate methods to evaluate the controllability in order to lighten the computational burden imposed by the on-line resolution of the dynamic model. Also more use of process model insights and practical rules in the problem formulation.

The methods that perform integration of design and control using stochastic-based formulations are recent developments offering the flexibility to assign probabilities to the worst-case variability expected in the system (Ricardez-Sandoval, 2012; Bahakim and Ricardez-Sandoval, 2014). This methodology avoids the conservative and expensive designs obtained from classical methodologies based on the computation for the worst-case scenario. Nevertheless, this methodology is extremely demanding in terms of computational load. Future work in this field should be focused on the development of complementary strategies for the reduction of the number of the random disturbance samples that are needed in the analysis allowing for its application to large scale processes.

The other important aspect in integrated design is the type of controllers and control strategies considered. Applications of advanced control techniques introduce significant improvements in the process dynamic performance, particularly in the multivariable cases, yet they appear seldom in the literature. Only recently, several results of the use of MPC in projects of integrated design have been published.

The new techniques for analysis of the dynamic performance as well as the application of advanced control strategies in the integrated design framework are limited by the complexity of the resulting optimization problems, which of course deserve special consideration, and escape the objectives of this work. However, let us address publications of integrated design applications dedicated in particular to the study of special methods of optimization, as those on genetic algorithms by Revollar et al., 2008b and Revollar et al. (2010b). Also worth mentioning are the comparisons between classical and stochastic methods of numerical optimization, in Francisco et al. (2005) and Revollar et al. (2010a) and comparison between global optimization methods (Egea et al., 2007).

Some examples of the Integrated Design philosophy concerning the simultaneous synthesis, design and control of the activated-sludge process in a wastewater treatment plant, will be presented in a following companion paper. Model Predictive Controllers are used for the plant automation, and robust methods are included for the monitoring of the controllability properties in the problem formulation of the integrated design. Classical and stochastic techniques based on genetic algorithms are also tested for the solution of the optimization problems.

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A linear system is considered functional controllable if, given smooth and causal output functions and zero initial states, there exists an input trajectory that generates exactly the desired outputs. This concept associates the restrictions in the plant model inversion to process controllability (Rosenbrock, 1970). The Dynamic Resiliency term is proposed in Morari (1983) to describe the ability of the plant to tolerate and to recover from undesirable changes and upsets. In the same work, the idea of perfect control, related to process model invertibility, is measured by some characteristics that determine the process dynamic resilience regardless of the controller used, namely the non-minimum phase elements (RHP-zeros and delays), the constraints in the control actions and the sensitivity/robustness. A similar analysis in terms of Functional Controllability is performed in Perkins and Wong (1985).

Chemical processes are strongly nonlinear exhibiting multiple steady state solutions which differ in terms of stability and dynamical behaviour. In order to evaluate the non-linear processes controllability in a more realistic and effective way, several analysis techniques are proposed.

Hernjak and Doyle (2003) study the correlations between control-relevant nonlinearity and the achievable performance of a variety of control structures. The degree of open-loop nonlinearity of the processes is assessed using a numerical nonlinearity measure and then compared to the performance results for a set of controllers of varying complexity in disturbance rejection. Westphalen et al. (2003) propose a heat exchanger network controllability index which is a function of the network topology. The index provides information about possible controllability improvements and clearly identifies the tradeoffs between control performance and energy savings. Cao and Yang (2004) suggest a multiobjective optimization technique for controllability analysis in control structure selection. The set of performance specifications, such as minimum control error and input effort with closed loop pole placement are represented as a Linear Matrix Inequality (LMI) system. If the solution of the problem is feasible it produces at least one controller that satisfies the desired closed loop performance.

Other works dealing with the effect of multiplicities and instabilities in chemical reactors and its dynamic behaviour are Razon and Schmitz (1987), Seider et al. (1990), Razon (2006) and Kumar and Kaistha (2009).

Process design is usually approached by considering the steady-state performance of the process based on an economic objective. Only after the process design is determined are the operability aspects of the process considered. This sequential treatment of the process design problem neglects the fact that the dynamic controllability of the process is an inherent property of its design. This work considers a systematic approach where the interaction between the steady-state design and the dynamic controllability is analyzed by simultaneously considering both economic and controllability criteria. This method follows a process synthesis approach where a process superstructure is used to represent the set of structural alternatives. This superstructure is modeled mathematically by a set of differential and algebraic equations which contains both continuous and integer variables. Two objectives representing the steady-state design and dynamic controllability of the process are considered. The problem formulation thus is a multiobjective Mixed Integer Optimal Control Problem (MIOCP). The multiobjective problem is solved using an ∈-constraint method to determine the noninferior solution set which indicates the trade-offs between the design and controllability of the process. The (MIOCP) is transformed to a Mixed Integer Nonlinear Program with Differential and Algebraic Constraints (MINLP/DAE) by applying a control parameterization technique. An algorithm which extends the concepts of MINLP algorithms to handle dynamic systems is presented for the solution of the MINLP/DAE problem. The MINLP/DAE solution algorithm decomposes the problem into a NLP/DAE primal and MILP master problems which provide upper and lower bounds on the solution of the problem. The MINLP/DAE algorithm is implemented in the framework MINOPT which is used as the computational tool for the analysis of the interaction of design and control. The solution of the MINLP/DAE problems is repeated with varying values of ∈ to generated the noninferior solution set. The proposed approach is applied to three design/control examples: a reactor network involving two CSTRs, an ideal binary distillation column, and a reactor/separator/recycle system. The results of these design examples quantitatively illustrate the trade-offs between the steady-state economic and dynamic controllability objectives.