

An Overview on Controllability Analysis of Chemical Processes

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Controllability is one of the most important aspects of chemical process operability, because it can be used to assess the attainable operation of a given process and improve its dynamic performance. The purpose of this article is to outline the main methodologies that have been developed to deal with the assessment of process controllability and the improvement of its controllability characteristics. Several existing controllability assessment methods are reviewed and discussed. For improving the controllability characteristic of a process, there are two main design methods: the optimization-based method and the controllability indices-based anticipating sequential method. Advantages and disadvantages of these techniques are discussed. It has been emphasized that bifurcation analysis, as a powerful nonlinear analysis tool, could provide important guidance for making processes more controllable by eliminating or avoiding some undesirable behaviors of processes. Further challenges and developments in the field of process controllability are identified. © 2010 American Institute of Chemical Engineers AIChE J, 57: 1185–1201, 2011

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Introduction

Chemical processes are nonlinear dynamic systems that are subject to considerable uncertainties and variations during their design and operation. They are usually designed to operate at a steady-state that has been determined to be economically optimal. However, ambient perturbations cause deviations and elicit dynamic responses from processes. Additionally, the start-up and shut-down of a process, as well as switching from one operating state to another, involves the dynamic operation of the process. Chemical engineering must confront these issues of how the process changes over time during its operation. Thus, the operability of the process, or its ability to adapt to changes, is an important quality index of the process that must be considered during the design stage.

There are many incentives for considering the operability analysis of a process during the design phase. First, increasing standards in product quality, stricter environment regulations and tighter safety requirements compel the process to maintain the specified strict operational constraints. Second, the fluctuating economy, characterized by varying customer demands, leads to changes in the process specifications. The process design must be able to adapt to these changes. Third, in efforts to improve the chemical processes' efficiency, the industrial trend has been toward more highly integrated and complex plants having processes with interacting process units, which causes more interactions between processes and complicates the design of the control system. However, the most important incentive is that when the traditional sequential design approach is used, the operability issues are usually ignored and the effects of the operability on the economics of the plant are neglected, leading to severe operating problems and significant economic penalties.^{1,2}

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The traditional chemical process design is a sequential one which evolves through a sequence of decisions and evaluations. There is a three step approach. First, the operational policy is determined, i.e., continuous, periodic or batch. The process is then designed by chemical engineers. Finally, the control system is designed by control engineers. Therefore, the control system design only begins once the main features of the process have been established. If there is no acceptable control system for the process, the process must be redesigned, leading to iterations between the process design and the control system design. Obviously, these iterations are undesirable because they cost time and money. Therefore, it is necessary to consider the controllability property, which is viewed as one of the inherent characteristics of chemical processes, at an early stage of the process design. Controllability analysis precedes the control system design during the chemical process design and it describes the best achievable control quality, independent of the controller design. It is well known that chemical process controllability depends on many different aspects, such as plant design and specific process dynamics, sensitivity to uncertainty, measurement location, actuator constraints, and disturbance characteristics. It is important to reflect how these aspects affect the process controllability. Fisher et al.³⁻⁵ described a systematic procedure for assessing process controllability at the preliminary stages of a process design. Since then, various approaches to the incorporation of controllability analysis into the stages of process design have been developed. These existing methods can be classified as: (1) methods that enable the screening of alternative designs based on controllability and (2) methods that simultaneously design the process and its control system. The latter approach to process design is now attracting increasing attention.

In this article, we focus on recent developments in controllability analysis for chemical processes, including controllability assessment and process design approaches, aiming to improve controllability characteristics. This article is structured as follows. First, concepts of operability, switchability, flexibility, and controllability in relation to similar concepts are reviewed in the section of Basic concepts. In the second section, methodologies for controllability assessments are outlined to encourage the integration of controllability analysis into chemical design at an early stage. Then the progress in design methods for improving controllability is described. Bifurcation analysis-based process design is discussed in the next section. Challenges and future research directions in the field of controllability analysis are also discussed. Finally, the main conclusion of the article is given.

Basic Concepts

Controllability is one of the most important aspects of chemical process operability. Some other aspects, such as flexibility and stability, should be considered simultaneously when assessing the controllability of a chemical process. To clarify the discussions of this article, a number of terms that appear in the next sections are defined as follows.

Operability

The ability of a process to cope with uncertainty and disturbances and also with issues of reliability and maintenance.

Operability includes flexibility, switchability, controllability, and several other issues.

Switchability

The ability of a process to move between operating points in a dynamically feasible and safe manner.

Flexibility

The ability to accommodate uncertainties over a range of uncertain parameters.

Controllability

Controllability has several different meanings, depending on the background and experiences of the user. As far back as in 1943, Zieger and Nichols⁶ devoted an entire paper to the topic of controllability and realized that the process design and the control system design should be considered simultaneously. In their paper, they defined controllability as the ability of a process to achieve and maintain a desired equilibrium value. Rosenbrock⁷ defined controllability as follows: a system is called controllable if it is possible to achieve the specified aims of control. By extension, the system is said to be more or less controllable according to the ease or difficulty of exerting control. Also, Rosenbrock⁷ introduced the term “functional controllability” as meaning that the system is functionally controllable if, given any suitable vector y of output functions defined for $t > 0$, there exists a vector u of inputs defined for $t > 0$, which generates the output vector y from the initial condition $x(0) = 0$. Later, the term “controllability” became synonymous with the rather narrow concept of state controllability and this meaning is still used by the system theory community. State controllability is the ability to bring a system from a given initial state to any final state within a finite time.⁸ A state is termed controllable if, for any initial state $x(0) = x_0$, any time t_1 and final state x_1 , there exists an input $u(t)$ such that $x(t_1) = x_1$. In control theory literature, a system is termed controllable if all states of the system are state controllable. The concept of state controllability is important for realizations and numerical calculations but it has little practical significance if all the unstable modes are both controllable and observable.⁹ To avoid confusion between practical controllability and state controllability, Morari introduced the term “dynamic resilience” as the quality of the regulatory and servo behavior, which can be obtained by feedback.¹⁰ Structural controllability is based on the concept that structural information gives insights into the pathways of disturbances in the process.¹¹ If each flow in a process is not interconnected and independent, then the disturbance in a flow does not propagate through other parts of the process, and thus, this process is well controllable. Skogestad gave a definition of input–output controllability as the ability to achieve acceptable control performance.¹² That is, to keep the outputs within specified bounds or displacements from their references, in spite of unknown but bounded variations, such as disturbances and process changes, using available inputs and available measurements. Nowadays input–output controllability is used widely in system theory. There are two other controllability definitions often invoked in the literature: the first is that

controllability can be defined as the ease with which a continuous process can be held at a specified steady state. The other states that controllability may be viewed as a property of the process, which indicates how easy it is to control the process to achieve the desired performance. Generally, the concept of controllability can be qualitatively defined as follows: controllability is an inherent property of the process that accounts for the ease with which a continuous plant can be held within a specified operating regime despite bounded external disturbances and uncertainties.

Zero dynamics

Zero dynamics^{13,14} is analogous to the right half plane (RHP) zeros of a linear system and can be characterized as the remaining dynamics of a nonlinear system in the case where the output remains at zero (constant) for all times.

Methodologies for Controllability Analysis

To prevent a process from failing to meet the required performance specifications, it is important to analyze the controllability at a design stage when modifications of the process are still possible. Controllability analysis includes the assessment of the attainability of a given process and the improvement of the dynamic performance of the process. In this section, an overview will be given on existing methods for controllability assessment. Particularly, the switch from one operating point to another is analyzed. The major work on controllability analysis and recent advances are summarized in Table 1.

In general, these measures can be classified into two main sets: linear model-based approaches and nonlinear model-based approaches. It can be seen from the above table that most tools relied on the use of steady states or linear dynamic models before 2000. In recent years, more and more tools based on nonlinear dynamic models have appeared. Next, a brief overview based on the sets of linear model-based approaches and nonlinear model-based approaches for controllability assessment is given and the limitations of these methods are also pointed out.

Controllability analysis for linear processes

A great amount of effort has been placed on the assessment of controllability based on linear dynamic models. Most controllability assessment studies based on linear models have been concerned with the attainability of perfect plant control, limited by factors that prevent physically realizable inversions of the plant transfer function, such as time delays, RHP zeros, model uncertainties, and manipulated variable constraints.⁵⁵ Two main approaches along these lines are the dynamic resilience method, as proposed by Grossmann and Morari⁵⁶ and the functional controllability method. These approaches for analyzing and measuring controllability are summarized in the next two subsections.

Dynamic Resilience. The IMC controller structure presented by Garcia and Morari⁵⁷ is a powerful tool for measuring controllability. Its assumption that the ideal controller is the inverse of the chemical process transfer function gives an upper bound on controllability. Dynamic resilience uses

Table 1. Summary of the Controllability Analysis Measures in the Literature

Authors	Merits	Model
Morari ¹⁰	RHP zeros, time delay, IMC	LD
Holt and Morari ^{15,16}	RHP zeros, dead-time	LD
Wong and Perkins ¹⁷	RHP zeros, time delay, CN	LD
Palazoglu and Manousiouthakis ¹⁸	CN	LD
Morari et al. ¹⁹	RHP Zeros	LD
Russell and Perkins ²⁰	Time delay	NLD
Skogestad and Morari ^{21,22}	CN	LD
Bogle and Rashid ²³	CN	LD
Psarris and Floudas ^{24,25}	Time delay	LD
Naraway and Perkins ²⁶	Economic back-off	LD
Skogestad and Hovd ²⁷	RGA, CLDG	LD
Weitz and Lewin ²⁸	Disturbance cost	LD
Soroush ²⁹	Time delay	LD
Zafriou E, Chiou ³⁰	Process zeros	LD
Cao and Perkins ³¹	Output deviation	NLD
Lewin and Bogle ³²	RGA	LD
Young and Swart ³³	Economic back-off	LD
Ross and Swartz ³⁴	Closed-loop performance	LD
Havre and Skogestad ³⁵	NMP performance	NLD
Gal and Varga ³⁶	Structural controllability	LD
Chenery and Walsh ³⁷	Output deviation	LD
Zheng and Mahajanam ³⁸	Dynamic controllability	LD
Kim and Yoon ³⁹	Structural controllability	NLD
Byungwoo et al. ⁴⁰	Structural controllability	NLD
Kuhlman and Bogle ⁴¹	NMP performance	NLD
Karafyllis and Kokossis ⁴²	Disturbance resiliency	NLD
Meeuse and Tousain ⁴³	Closed-loop performance	LD
Maya-Yescas and Aguilar ⁴⁴	RGA	NLD
Kuhlman and Bogle ⁴⁵	NMP performance	NLD
Cao and Yang ⁴⁶	Singular value, zeros	LD
Engell et al. ⁴⁷	RPN	LD
Meel and Seider ⁴⁸	NMP performance	NLD
Santoso et al. ⁴⁹	Passivity	NLD
Srinivasan and Bonvin ⁵⁰	Output controllability	NLD
Kaymak and Luyben ⁵¹	Dynamic controllability	NLD
Santoso et al. ⁵²	Passivity	LD
Papadopoulos and Seferlis ⁵³	Sensitivity analysis	NLD
Kaistha et al. ⁵⁴	Closed-loop performance	NLD

the IMC structure to represent the best possible controller that is achievable. Holt used the IMC concept as a framework to measure controllability, and also found the effects of nonminimum phase elements, input saturation, and model plant mismatch on controllability.^{15,16} Skogestad and Morari used the RGA as a framework to measure the effect of uncertainty for linear systems.²² For a perfectly controlled process, the controller must be the inverse of the process transfer function. However, the physical realizability of such a controller is limited and dynamic resilience may be used to generate an index that measures the attainability of perfect control or the limits on the physical realization of the perfect controller.

The effect of RHP zeros on the controllability of chemical processes has been studied by Holt, based on the IMC framework.¹⁶ RHP zeros become unstable poles in the inverse of the process transfer function, and therefore, render the ideal controller unstable. Also, RHP zeros exhibit inverse response behavior. Even if they do not exhibit an inverse response, they provide a challenge for control engineers. The effect of the location of RHP zeros on the controllability of chemical processes is similar for SISO and MIMO linear systems. The severity of control deterioration increases with

increasing proximity of the zeros to the imaginary axis. Studies⁵⁸ have shown that RHP zeroes cannot be shifted to different locations by output feedback. In other words, no controller can vary their location. Similar to time delays, one can only modify them by redesigning the chemical processes.

Morari proposed the corresponding minimum singular values σ_{\min} and input magnitudes to judge the attainable process performance. A small singular value implies the requirement of large input magnitude.¹⁰ Plants with higher minimum singular values should be favored because they can handle larger disturbances.¹⁰ As σ_{\min} is applicable only to unstructured uncertainty assumption, a structured singular value which was defined as the smallest perturbation that made the process singular at each frequency was also proposed.²² The magnitudes of the disturbances that can be rejected are limited by the actual constraints on the manipulated variables which have a negative effect on the controllability of the process.

Functional Controllability. Functional controllability is defined by considering a linear state space system. A linear system is functional controllability if, given the smooth and causal output functions and zero initial conditions of the state variables, there exists a smooth manipulation profile that generates the output functions.⁷ It has some advantages over state controllability for the evaluation of controllability of chemical processes.²⁰ State controllability does not guarantee that it is possible to independently specify arbitrary trajectories of the selected set of output variables, whereas functional controllability does. This is important because the main goal of regulatory control is usually to maintain the process at a given steady state. Functional controllability offers an attractive tool to evaluate controllability; whatever inhibits process inversion limits the controllability. The basic limitations to process inversion are RHP zeros, time delays, manipulated variable constraints, and model uncertainty. Wong and Perkins characterized the effect of time delays with the parameter Δ_{\min} , which is the minimum time before a trajectory for any output can be specified.¹⁷ Δ_{\min} is calculated based on the magnitudes and locations of delays in the process transfer function. Also the singular value decomposition (SVD) analysis of the transfer function G can be used to characterize the effects of manipulated variable constraints and model uncertainty.

As discussed above, the concept of functional controllability is closely related to dynamic resilience, there are differences between them,⁵⁹ functional controllability only provides a “yes or no” type answer; also, there is no indication of how far it is from the achievable performance when the process is not functionally controllable. Dynamic resilience includes a quality measure of the achievable performance.

Applications. Palazoglu and Arkun proposed a multiobjective function-based methodology that applies the SVD technique to measure the process closed-loop dynamic performance.⁶⁰ However, the SVD-based robust controllability indices are only considered as inequality constraints within the formulation and do not appear in the economic cost function to be optimized. Skogestad and Wolff presented the evaluation of process sensitivity to sinusoidal disturbances for open-loop, decentralized control, partial control and regulatory control.⁶¹ Wolff et al. demonstrated the controllability

assessments for a fluid catalytic cracking reactor and a hydrodealkylation of toluene (HDA) process.^{62,63} Weitz and Lewin introduced the disturbance cost (DC) for dynamic controllability, which was similar in principle to the disturbance condition number.²⁸ Trierweiler and Engell⁶⁴ introduced the robust performance number (RPN) and the robust performance number of a plant set (RPPN), which allowed a systematic analysis of the controllability of the system including many different aspects that must be considered in control structure design. Zhao and Skogestad applied the partial disturbance gain (PDG) to assess the controllability of continuous bioreactors for the control configuration selection.⁶⁵ Hernandez and Jimenez analyzed the controllability properties of thermally coupled distillation sequences.⁶⁶ Vaca compared two different steady-state designs for a direct thermally coupled distillation sequence for ternary separations, using controllability indices, which were provided by condition number (CN) and SVD.⁶⁷ All of these indices rely on a linear model describing the effect of control variable on the process outputs. Therefore, they are readily integrated with existing design procedures.

Remarks. Linear analysis is normally performed around a nominal operating condition that is normally the most common operating regime in the process but can also be calculated from a prior static optimization of the process.^{68–70} There are several limitations of these techniques. First, both functional controllability and dynamic resilience may be used to rank different processes with similar economics but it may be impossible to compare processes with quite different economics and robustness indices. This is because chemical process typically exhibit more than one inherent property that presents limitations on the performance of the control system, in which case comparisons based on single controllability indicator become ambiguous. To address this drawback, Swartz and coworkers proposed a methodology where they attempted to pose controllability assessment within an optimization framework.^{71–73} Second, the relationship between the indices and the closed-loop performance is often unclear. Although the use of these indices may be adequate in some cases, it is quite unpredictable whether the conclusions drawn are correct or not. Third, these indices are based on input–output linear static systems. In particular, when nonlinear characteristics are important, closed-loop dynamic simulations are usually required. Finally, most of the indices are based on the frequency domain specification. Recently, Gabor and Mizsey presented a methodology for the simple determination of controllability indices in the frequency domain,⁷⁴ with this methodology, the process of making open loop simulations to approximate transfer function matrices can be avoided. However, most of existing methods to calculate these indices are complex. In practice, time domain performances are more favorable. It is worth highlighting here that limited work has resolved the relationship between measures and scaling satisfactorily. Therefore, controllability analysis that is directly applicable to the nonlinear model of the chemical process would be more useful.

Controllability analysis for nonlinear processes

Most of the above methods are based on frequency domain analysis. They are not applicable to nonlinear methods.

However, it appears that controllability evaluation based on a linearized model gives correct information even for strongly nonlinear systems.⁷⁵ This is true for regulatory performance around a specified steady state but is not satisfactory for problems with a high degree of nonlinearity, ranged throughout wide operating regions, such as start-up, shut-down, and batch or semi-batch-processes, which are not easily correctable with simple nonlinear transformations. Thus, methods for the evaluation of controllability may be somewhat different.

If complex nonlinear behaviors of a process are understood and effects of parameters and operation conditions are analyzed at the design stage, several undesirable characteristics, such as limit cycles can be avoided. The potential control problems associated with these characteristics could be eliminated or avoided by modifying the process design itself.⁷⁵ Although many complex nonlinear behaviors can be efficiently dealt with using modern control algorithms like the nonlinear model predictive control (NMPC) algorithm,^{76,77} it is important for analyzing the controllability of a system to fully identify all potential problems associated with the complex behavior and to assess how easy the design is to control when the alternatives are considered during the design stage.⁷⁸

The existing nonlinear controllability analysis methods can be divided into those which are analytical and those which are optimization based. Some insights into analytical nonlinear controllability analysis are given below, followed by a review of the optimization methods. Passivity/dissipativity-based controllability analysis is an emerging research area. This methodology is also discussed in this section.

Analytical Method. A selection of nonlinear controllability analysis techniques are based on the concept of functional controllability. In nonlinear dynamics, a nonlinear inverse may be evaluated. Because there are no direct methods for quantifying the effect of inverse dynamics, the nonlinear inverse must be analyzed instead. A fundamental limitation on perfect control for linear systems is the presence of RHP transmission zeros, which give rise to an unstable inverse. However, for nonlinear systems there are no zeros or poles. The analogous problem for a nonlinear system is unstable zero dynamics. The zero dynamics of a nonlinear system is given by the dynamics of its reduced inverse, which is a minimal-order realization of the systems inverse.⁷⁹ Therefore, an investigation of the zero dynamics of a nonlinear system will reveal whether or not a nonlinear system has a stable inverse. Trickett provided an approach that concerned the evaluation of controllability of nonlinear nonminimum phase systems.⁸⁰ In this approach, the main goal was to rule out the possibility of unstable zero dynamics inside the entire operating region. Although they have assessed qualitatively that a system has an unstable inverse, they still cannot quantitatively determine the actual best achievable performance for this nonlinear system. The relative order of a system has been introduced as an analysis tool for the structural evaluation of alternative control configurations.^{81,82} The technique was subsequently extended to nonlinear discrete systems.⁸³ This method allowed the coupling and interaction for specific control structures to be assessed but it did not indicate whether or not specific performance requirements might be achievable.

Similarly to the use of RGA for linear systems to assess the interaction of input/output pairings, the static RGA could also be calculated for general nonlinear process.⁸³ It was shown that the formulae used for computing the nonlinear RGA were of the same form as those used for the linear case. The block relative gain (BRG) was extended to nonlinear systems by Nikolau,⁸⁴ giving the steady state nonlinear block relative gain (NBRG) and dynamic nonlinear block relative gain (DNBRG), which provided a measure of the interaction between decentralized feedback loops for dynamic nonlinear systems. The steady state NBRG was shown to be a lower bound for the CN of a nonlinear system. Recently, Moaveni and Khaki-Sedigh gave a detailed introduction and discussion about applying these controllability indices to control configuration assessment.⁸⁵

However, it is not clear how these measures relate to the achievable control performance and whether or not it can satisfy certain performance specifications. None of these analytical techniques addresses more than one of fundamental characteristics on controllability and they only incorporate one at a time.

Optimization Method. The optimization methods may be the most successful ones for integrating process design and controllability analysis. The important factor is their ability to consider multiple specifications. This capability enables the method to quantify process controllability or to integrate one or more controllability indices into process control synthesis. Reviews of these methods have been published.^{86,87} Approaches for optimization problems are discussed in many papers.^{88–90} In this section, brief introductions are given. In optimization-based frameworks the problem is formulated as a mathematical superstructure capable of attaining a given steady state economic objective as respecting at the same time dynamic operability, model uncertainty and the synthesis of optimal controllers. Because controllability analyses are performed in the time domain, the performance specifications and the limitations on the control performance, such as the constraints on state, manipulated and output variables, are easily incorporated into the formulation. Naturally, the solution of superstructures is difficult and time consuming, most of the time requiring a simplified process model to avoid numerical intractability. Linear controllability measures⁹¹ also can be integrated into superstructures as part of their formulations. Therefore, this feature can be employed further to produce a controllability assessment that is applicable for a given set of alternative processes and control structures. For example, Nongluk presented a preliminary case study on the SISO nonlinear system of the depropanizer column where IMC is used as the controller and the variability cost was calculated and added into the cost function.⁹² The optimization of a single objective function is performed subject to the robust stability and manipulated variable constraints, so it can improve the controllability characteristics of the process. Many researchers have pointed out the fundamental idea concerning the interaction between design and control and have suggested incorporating controllability measures into the early stages of the process design, allowing design alternatives to be compared on a common basis. Several methodologies for process design to improve controllability characteristics have been presented, which will be reviewed in detail in the section of process design methods for improving controllability.

Passivity/Dissipativity-Based Method. Passivity/dissipativity-based methodology is a new development for plant-wide operability analysis. Bao and coworkers^{93–100} have done a great deal of research in the field of controllability analysis based on passivity.¹⁰¹ In 2007, they gave a detailed introduction to this approach.¹⁰² Recently, based on dissipativity or passivity of each process unit and the topology of the process network, Bao and coworkers analyzed the dynamic controllability characteristic for plant-wide processes from a network perspective.^{103–106} According to the concept of dissipative systems,^{107–109} the approach described could deal with nonlinear processes directly and could quantify how the disturbance to one unit propagates throughout the entire network, influencing other variables of interest. This approach showed links between process dissipativity and operability and provided new insights into how the structure of the process units affects plant-wide operability. As dissipativity or passivity of chemical processes can be linked to their thermodynamic properties,^{110–116} it is possible to determine process controllability from the irreversible thermodynamics of process systems. This may lead to heuristic design rules for better process controllability for chemical engineers. However, there are two limitations to this approach: first, an effective controllability analysis approach for nonlinear unstable processes is still required. Second, at present, this approach is applied to controllability analysis of relatively simple processes. Although it has been successfully applied to the glass manufacture process,¹¹⁷ when faced with other more complex chemical flowsheets, the question of how to establish passivity requires further study.

Switchability Analysis. To minimize power consumption and loss of product or to follow load variations, as required by the demands of a downstream customer, certain chemical processes must move between different operating points. This leads to the switchability problem, which is an important aspect of controllability. Because these moves occur frequently, it is essential that the optimal and safe movement between multiple operating points with varying throughput or product grades be met by the process design.

Several researchers^{118–120} proposed a switchability analysis based on an operability analysis that results in economically desirable steady state conditions at the beginning and the end of the transition. To ensure safe and feasible moves, the switchability problem is formulated as a dynamic optimization problem where the trajectories of the manipulated variables and the state variables for the switching between two stationary points are found by minimizing the integrated squared deviation of the variables from their desired final steady state values, subject to the model equations and path constraints. The problem can generally be posed in the following generic manner

$$\begin{aligned} \min_{x(t), u(t), t_f, \theta} \quad & J(x(t), y(t), u(t), t_f, d) \\ \text{s.t.} \quad & f(x'(t), x(t), y(t), u(t), t, d) = 0 \\ & \eta_1(x(t), y(t), u(t), t, d) = 0 \\ & \eta_2(x(t), y(t), u(t), t, d) \leq 0 \end{aligned} \quad (\text{P1})$$

In these equations, x is the differential variables and y is the algebraic variables, respectively; f refers to the set of dif-

ferential and algebraic equations that describe the process being studied. The quantities η_1 and η_2 are equality and inequality constraints. The design parameters d are also incorporated into the formulation to allow for design modifications to improve switchability. The formulation simply determines the optimal move between operating points.

The difficulty of switchability analysis is, in general, not the formulation of the optimization problem but rather the reliable computation of the problem solution in reasonable computing times. The dynamic optimization problems are often converted to nonlinear algebraic optimization problems and solved by existing NLP methods. Methods that apply NLP solvers can be separated into two groups: sequential^{121–125} and simultaneous strategies.^{126,127} In the sequential method, also known as control vector parameterization, only the control variables are discretized. Despite the success of sequential methods for dynamic optimization problems, repeated numerical integration of the DAE model is required at each iteration, which may become time consuming for large scale problems. Moreover, it is well known that sequential approaches cannot handle open loop instability. To avoid the requirement for solving differential equations at each iteration, the method of simultaneous optimization is introduced, which fully discretizes the state and control variables, leading to large-scale NLP problems that usually require special optimization strategies.^{128–131} The DAE system is solved only once at the optimal point. Also, simultaneous approaches have advantages for problems with unstable modes but the NLP grows with size of the DAE system, and solution of such a large NLP problem requires careful initialization of the optimization variables.^{132,133} The simultaneous optimization approach provides a promising research area for the future. However, to date, not many applications have been found in solving switching problems.

Few applications of switchability analysis are reported. Vu et al. solved an optimal control problem for determining the optimal switch for a system of two CSTRs, including back-off from constraints to allow for controllability issues.¹¹⁸ White and Perkins examined the effect of plant characteristics on switchability by determining the optimal switching trajectory for the plant through setting up and solving an optimal control problem.¹¹⁹ The feature of this optimization formulation is the ability to include parameters characterizing the design of the plant as decision variables. When the plant is designed by the optimal switching algorithm, flexibility of the design is ensured because the solution will be feasible at the operating points. Also, the feasibility of the plant in the duration of the switch will be guaranteed.¹³⁴ Kuhlman and Bogle presented a design strategy for optimally switchable nonminimum phase (NMP) processes based on a method for the evaluation of switchability for nonlinear NMP processes and demonstrated the method with a reactor-separator case study.¹³⁵ The problem was formulated as a dynamic optimization problem, with special emphasis placed on the possible presence of input multiplicities. According to this study, small parameter changes may change the character of a process entirely, including switchability characteristics. Recently, Hartwich and Marquardt discussed the load change problem of a real large-scale industrial chemical process, which was closely related to switchability analysis of technical systems.¹³⁶ However, this work did not approach

the fastest possible load change, but the most economical one.

Remarks. As stated above, chemical processes are always subjected to disturbances and uncertainties during operation. Determining the inherent-process characteristics that enable the process to operate with acceptable performance is the ultimate objective of any controllability analysis. Controllability assessment precedes the control system design during the process design procedure. Thus, the controllability assessment deals with whether the plant is controllable and, ideally, also with what is the achievable controlled performance of the process. How the process actually is controlled is subsequently dealt with during control structuring and controller design. Accordingly, this analysis is independent of the control system imposed on the chemical process.

Process Design Methods for Improving Controllability

Controllability analysis can be broken into three separate stages: assessment, diagnosis, and design. The controllability assessment is used to rank alternatives and highlight shortcomings. Diagnosis is used to explain any of the shortcomings in the analysis phase, whereas design is used to modify the process to improve the figure of merit and/or remove shortcomings. The last stage describes the relationship between controllability and process design. Consideration of the controllability of a process at an early phase of the process design is now being widely accepted in both academia and industry. Many methodologies and tools have been reported for considering the interactions between process design and process control.

Optimization-based approaches

Several approaches that include the question of controllability into the design problem formulation are the optimization-based methods for synthesis and design.

Optimization-Based Flexibility Analysis. The optimization-based steady-state flexibility approach was presented and extended by Grossmann and Haleman and Swaney and Grossmann.^{137,138} They first checked the feasible operation for a range of operating conditions, including uncertainties, and determined the design variables accordingly. A formulation was used that included operating variables that are allowed to be varied to compensate for the effect caused by the uncertainties at steady state. They then extended the above work to measure the flexibility of a process by maximizing a scalar value called the flexibility index, which evaluated the flexibility of a process at steady state. Steady flexibility typically considers the feasibility issue and an index for flexibility but does not consider feedback control built into virtually every chemical process operation. Over the last decade, the focus has been on the dynamic flexibility analysis for chemical processes. Chacon-Mondragon and Himmelblau discussed the integration of process flexibility with control in process design.¹³⁹ Dimitriadis and Pistikopoulos¹⁴⁰ extended the steady state flexibility analysis and flexibility index to dynamic processes. The dynamic flexibility problem of the process is as follows

$$\begin{aligned}\chi(z, y) &= \max_{\theta \in \Theta} \psi(z, y, x, x', u, w, \theta(t), t) \\ s.t. \psi(z, y, x, x', u, w, \theta(t), t) &= \min_{z \in Z} v \\ s.t. h_i(z, y, x, x', u, w, \theta(t), t) &= 0 \\ g_i(z, y, x, x', u, w, \theta(t), t) &\leq v \\ \Theta(t) &= \{\theta(t) | \theta^L(t) \leq \theta(t) \leq \theta^U(t)\} \\ i &\in E \\ j &\in I\end{aligned}\quad (P2)$$

In problem (P2), the process dynamics are represented by a set of DAEs, subject to a single time-varying uncertainty, where x and x' are the vectors of state variables and their derivatives, u is the vector of manipulated variables and $\theta(t)$ is the uncertainty profile. If $\chi \leq 0$, the design is dynamically feasible in $\Theta(t)$. Otherwise, the process is not feasible. Mohideen et al. further extended this work by using an economic objective.^{141,142} The objective of this approach is to select design variables and a control scheme to optimize the cost, whereas remaining feasible over the finite time horizon under both parametric uncertainty and disturbances. Because the class of controllers is restricted, in this approach PID controllers are included in the formulation, such that the result is actually a pessimistic bound on the solution. Further work following this measure has been presented by Bansal et al.^{143,144} Linninger and coworkers used dynamic flexibility analysis as a tool for integrating systems design and control.^{145,146} The methodology presented in their article allows designers to arrive at key structural decisions for process flowsheet and control layout and to optimize them simultaneously for high performance under realistic, uncertain operating conditions. Zhou et al. formulated problems of dynamic flexibility problems as dynamic optimization problems to analyze the effect of the initial operation condition on the dynamic flexibility of batch processes.¹⁴⁷ Although the dynamic flexibility function guarantees flexibility and controllability, it does not quantify them. It should be used along with the complementary dynamic flexibility index, which identifies the critical disturbance combination. With the calculation of a corresponding penalty, such as an economic penalty, the index is calculated relative to the optimum steady-state objective and associated with the maximum magnitude of the critical dynamic profile. Over the time horizon, this indicates that the dynamic is bounded.

Back-Off Optimization Method. Chemical plants are faced with uncertain conditions and disturbances during its operation. The operating point needs have the flexibility to achieve feasible operation over a range of uncertain conditions to efficiently handle these uncertainties, one way to accomplish this, is by moving the nominal optimum to some permanently feasible operating point inside the feasible region (back-off point). Narraway and Perkins utilized the back-off from the steady-state economic optimum to assess alternative plant designs and control structures based on economic.¹⁴⁸ To assess the potential economic benefits of any given control structure, Narraway and Perkins¹⁴⁹ proposed a modification approach, which consists of identifying the optimum steady-state operating point and estimating the back-off required from constraints active at this optimum to accommodate the effects of disturbances, applying these

back offs gives a modified operating point whose economics may be computed. Bahri et al. developed a dynamic operability framework for operability assessment and process synthesis based on the back-off optimization formulation for both linear and nonlinear of steady-state and open-loop dynamic processes.^{150–152} Both uncertainties and disturbances are considered in this method. The objective is to maximize the process economy, subject to the feasible regulatory dynamics. Therefore, an economic penalty is determined by the distance between the steady-state optimum and the dynamic operating point, which are calculated based on nonlinear steady-state and nonlinear dynamics models, respectively. The ideals were further developed by Figueroa et al.¹⁵³ where a recovery factor was defined as the ratio of the amount of penalty recovered with control to the penalty with no control. The back-off approach was then applied to a variable structure control case.¹⁵⁴ One feature of the back-off approaches is that they determine the cost increase associated with moving to the back-off position due to uncertainties and disturbance. The limitation of this approach is that it leads to conservative design, because the framework considers the worst-case uncertainty scenario, even though the probability of the worst-case uncertainty may not be high. Ekawati and Bahri¹⁵⁵ presented the integration of the output controllability index¹⁵⁶ within the dynamic operability framework to facilitate controllability and economic assessment of process system design for regulatory cases. This framework utilizes a geometric representation of the feasible operating region. The approach is made simpler by replacing multiple maximization problems in the inner level and the inequalities in the outer-level with a single geometric operation and equality constraint, respectively.

Optimization-Based Control Structure for Improving Controllability. Perkins was the first to directly evaluate the effect of process dynamics on process economic performances within an optimization framework.¹⁵⁷ An optimistic bound on the disturbance rejection performance was provided by the approach of Walsh and Perkins,¹⁵⁸ who replaced operating variables with an idealized controller to assess the effect of time delays and bounded parametric uncertainty on disturbance rejection capabilities when employing optimal control. To deal with the controllability issues on an economic level, Narraway and Perkins presented a method for selecting the optimal control structure of a process without designing the process controller after determining the optimal steady-state.^{148,149} Perfect disturbances are rejected by the control system and a linear dynamic model of the process to formulate a mixed-integer linear programming technique, where the integer variables indicate the pairings between the manipulated and controlled variables. This approach was subsequently modified by Kookos and Perkins,¹⁵⁹ whereby the control objectives were posed in terms of economic penalties associated with the effect of disturbances on key process variables, aiming to identify optimal control structure selection for static output feedback controllers. Seferlis and Grievink developed a method for assessing alternative process designs and control structures based on the economic potential and static controllability characteristics and depicted the advantages of this method by multiple reactive and separation steps with recycle.¹⁶⁰ To stabilize the open loop unstable process with the minimum

control effect, a new method for control structure screening based on improving branch and bound optimization was presented by Cao and Saha,¹⁶¹ using the controllability index (Hankel singular value, HSV). According to these methods, the variations of each variable were used to estimate the required back off for ensuring the feasibility, as well as to estimate the change in process economics. The economic analysis was carried out at the expected disturbance frequencies and amplitudes, although stochastic disturbances were not involved.

It is clear that sufficient attention has been given to the complete and combined approaches of rigorous and systematic screening of alternative process design with embedded control structure characteristics based on control and economic performance. The full count of all possible combinations between potential manipulated and controlled variables may become large, especially for plant-wide control system design. Thus, the complete enumeration of all possible sets of control structures for a number of disturbances incorporating the dynamic behavior of the system within an optimization framework would require great computational effort.

Optimization-Based Design and Control Simultaneously. Modern chemical processes operate in a dynamic environment, and are expected to handle variations in ambient conditions and managers' imposed demand on production. The conventional design of first obtaining a plant configuration and initial design based on steady-state economic calculations and then using over-design factors to account for variability based on controllability measures may prove to be inadequate in today's process design activities. So simultaneously optimizing the process design and process control strategy is a very active research area in the academic world. Over the last decades, important efforts have been aimed at providing methodologies for tackling process design and control in an integrated framework, the control configuration and controller parameters are optimized together with the plant design parameters to determine the optimal design and operating conditions of a process in this integrated framework. A number of methodologies have been proposed for solving integrated process design and controller design (IPDC) problems.^{162,163} In these methodologies, a mixed-integer nonlinear optimization problem (MINLP) is formulated and solved with standard MINLP solvers. When solving this optimization problem, the reconciling conflicting design and control objectives will be required. When a MINLP problem represents an IPDC, the process model considers only steady state conditions. Although a mixed-integer dynamic optimization (MIDO) problem represents an IPDC where steady state as well as dynamic behavior are considered. A substantial algorithm have been developed to solve the *MIDO* problem,^{164–174} from an optimization point of view, these approaches can be divided into simultaneous and sequential methods. Due to the computational complexity associated with the resulting nonlinear dynamic optimization problems, applying these methodologies to large processes is restricted. In order to alleviate some of the intensive computational burden associated with dynamic optimization, in recent years, several novel approaches have been proposed. A novel decomposition method to solve the *IPDC* formulated as a mathematical programming problem is presented, and the optimization

problem is decomposed into four subproblems which are relatively easier to solve.¹⁷⁵ Douglas and coworkers^{176–179} present a robust model-based approach that is based on the calculation of estimated bounds on process variables that determine the process flexibility, stability and controllability of the system, in these approaches, although the computationally demanding task of solving a dynamic optimization problem is reduced by formulating the problem as a nonlinear optimization problem, the use of estimated bounds on variables that determine the flexibility and controllability may result in potentially conservative and suboptimal designs. Only the recent advances are discussed as above. A more comprehensive review of the exist methodologies that address the integration of process design and control problem can be found elsewhere.^{180,181}

Multiobjective Optimization Method. Brengel and Seider presented an approach for determining process designs which are both steady-state and operationally optimal.¹⁸² The controllability of potential designs is evaluated along with their economic performance by incorporating a model predictive control algorithm into the process design optimization algorithm. This coordinated approach uses an objective function that is a weighted sum of economics and controllability measures. Luyben and Floudas used a multiobjective optimization framework to simultaneously consider both open-loop controllability and economic aspects of the design.^{183,184} Schweiger and Floudas then generated a set of trade-off solutions between economy and controllability (in terms of ISE) during process synthesis.^{185,186} They considered the vector of objective functions $J = (J_1, J_2)$, where J_1 represents a design objective and J_2 a controllability objective. The problems can be formulated as

$$\begin{aligned} \min & J_1(z'_1(t_i), z_1(t_i), z_2(t_i), u(t_i), x, y) \\ \text{s.t.} & J_2(z'_1(t_i), z_1(t_i), z_2(t_i), u(t_i), x, y) \leq \varepsilon \\ & f_1(z'_1(t_i), z_1(t_i), z_2(t_i), u(t_i), x, y, t) = 0 \\ & f_2(z_1(t_i), z_2(t_i), u(t_i), x, y, t) = 0 \\ & c(z'_1(t_i), z_1(t_0), z_2(t_0), x) = 0 \\ & h'(z'_1(t_i), z_1(t_i), z_2(t_i), u(t_i), x, y) = 0 \\ & g'(z'_1(t_i), z_1(t_i), z_2(t_i), u(t_i), x, y) \leq 0 \\ & h''(x, y) = 0 \\ & g''(x, y) = 0 \\ & x \in \chi \subseteq \mathbb{R}^p \\ & y \in \{0, 1\}^q \\ & t_i \in [t_0, t_N] \\ & i = 0 \dots N \end{aligned} \quad (\text{P3})$$

where x is the vector of p time invariant continuous variables and y is the vector of q binary variables. f_1 represents the n differential equations, f_2 represents the m dynamic algebraic equations, $z_1(t)$ is a vector of n dynamic variables whose time derivatives, $z'_1(t)$ appear explicitly, and $z_2(t)$ is a vector of m dynamic variables whose time derivatives do not appear explicitly. h' is the equality point constraints, g' is the point inequality constraints, and c is the initial condition equations. This multiobjective problem is solved by assigning the ISE as a weighted point constraint to the optimization problem.

Stochastic disturbances are often not considered when use ISE, Meeuse and Tousain⁴³ proposed a new method which compares alternative designs based on the optimal closed-loop performance, taking into account stochastic disturbances and measurement noise. However, there are several drawbacks in using ISE.^{59,150} First, ISE only represents one profile at a time, for a multivariable process that has several measured and constrained output variables, it is not yet clear which variables should be assessed with ISE, due to the fact that different process structures may activate different dynamic profiles and activate different constraints. Second, ISE only reflects the dynamics of the measured variables and neglects the dynamics of the unmeasured state variables. Third, ISE only quantifies the dynamic profile against a point reference and does not, by itself, guarantees process feasibility or controllability. Finally, ISE does not directly address the question of what are the design implications of an important in the value of a particular controllability index.

Sequential design method for improving the plant-wide controllability

The basic idea of this approach is that controllability analysis has been integrated into the process design and the control system design is conducted only after the process design. Many researchers have adopted this approach for improving the controllability characteristics of plant-wide processes.

Most modern chemical plants are complex networks of multiple interconnected, nonlinear process units, often with multiple recycle and by-pass streams and energy integration. Interactions between process units often lead to plant-wide controllability problems. Plant-wide controllability can be defined as: A process is steady-state, plant-wide controllable if and only if there exists a plant-wide control system to maintain a process at desired steady states in the presence of uncertainty and disturbances.¹⁸⁷ Because of the complexity and nonlinearity of processes, plant-wide controllability analysis is often difficult. Also it is difficult to implement the optimization approach in plant-wide process controllability analyses.

The resiliency and operability, as well as the interaction among control loops and determination of variable pairing (selection of controlled and manipulated variables), are important issues for the controllability of a plant-wide process. A large number of contributions on plant-wide controllability analysis have been published, focusing on these problems.^{188–200} Skogestad gave an excellent review and discussion of the design of a plant-wide control system and the concept of self-optimizing control.^{201–205} Therefore, in this section, a brief discussion and an outline of recent progress will be given as follows.

Many of the major issues involved in the plant-wide control problem, such as the effects of recycles and energy integration have been discussed. In many existing reports, several alternative processes and process control structures are obtained, based on economic objectives, respectively. Subsequently, the respective dynamic performances were assessed and ranked based on the ISE and the frequency domain specifications such as bandwidth, magnitude ratio, phase angle, and peak log modulus. Because of the large number of variables and a combinatorial growth in the total number

of possible control structures with respect to the number of variables, a complete dynamic evaluation of all alternative control structures is impractical for any realistic process. To deal with this disadvantage, several researchers decomposed the problem into a hierarchy of decisions,^{206–209} motivated by Douglas's hierarchical procedure for conceptual process design.²¹⁰ In this approach, some alternatives are eliminated according to economic, environmental, or controllability considerations at each level of hierarchy. Simulation-based frameworks as listed above make use of exhaustive closed-loop dynamic simulations for controllability tests that allows for realistic ranking of alternative designs. This type of framework requires extended time for performing several runs. Although a dynamic simulation is used, initially some important and complex dynamic behavior may not be observed for the specified conditions due to the limited number of simulation tests that can be performed. When the process comprises fast and slow modes, this approach is inefficient and potentially not inclusive.

Recently, Molina et al. presented a new systematic methodology for synthesizing a plant-wide control structure based on retaining the most useful ideas provided by process-based experience, engineering judgment and a rigorous mathematical framework, applied to a simple flowsheet.²¹¹ The results shown that this approach is helpful in deciding whether the equipment sizing is suitable for guaranteeing plant-wide controllability. This approach also gave useful guidelines for analysis of the effects of process structures and control structures on the operability or controllability of plant-wide processes and the improvement that controllability characteristics may reach. In the meantime, further study is required before applying it to complex flowsheets.

Remarks

Generally, the integrated design methods can be classified into two sets. The first set of approaches uses methods that enable the screening of alternative designs for controllability. The first step in these methods is the consideration of the steady-state operation that will be most desirable. They then seek to develop steady-state designs that are economically optimal but are also dynamically operable in a region around the specified steady-states. The final decision will be determined by a trade-off between an economic performance measure and controllability indices, as listed in Table 1. The main disadvantage is that the results are only reliable around the specific steady state and it is usually not clear how controllability indices are related to the real performance requirements. The second set of approaches are dynamic approaches^{212–214} that take the view that all processes are inherently dynamic and that dynamic operation is inevitable or in some cases preferable to steady-state operation. Therefore, they explicitly consider the dynamic performance using dynamic models at the design stage. These methods are not restricted to a small operating region around steady-states, thus the final decision drawn are reliable over a large region of operation in the face of disturbances. Although uncertainty or disturbances seem to be solved in the design stages, uncertainty in the models will arise in practice. Moreover, as the cost of obtaining a “detailed” dynamic model is expensive and the computational effort required is significant, their

applications are currently restricted to small scale problems.¹⁸¹

Therefore, it is desirable that a method should be one that only uses open-loop steady-state data as considering dynamic characteristics of a process design. The bifurcation analysis-based methods discussed in the next section, which use only the open-loop steady-state data, can predict some dynamic characteristics of a process design, so can also provide important guidance for making processes more controllable by eliminating or avoiding some undesirable behaviors.

Bifurcation Analysis-Based Method for Process Design

Bifurcation analysis, a method for studying how qualitative behavior of a nonlinear system changes as the parameters vary, is a powerful nonlinear analysis tool that characterizes complex nonlinearities and examines the causes of steady-state multiplicity and periodic operations by using only steady-state data and applying this to process design.

The applications of bifurcation analysis as a powerful nonlinear system analysis tool for chemical processes have been widely reported.^{215–225} Morari suggested that bifurcation analysis should be used in controllability analysis for nonlinear systems.²²⁶ Input/output multiplicity is a complex phenomenon that can be encountered in chemical processes and will adversely affect the performance of the closed-loop system, subject to the changing operating conditions. Russo and Bequette studied the effect of design parameters on the multiplicity behavior of jacketed exothermic CSTRs.²¹⁷ Gudekar and Riggs performed open-loop and closed-loop nonlinear stability analyses of an industrial ethylene oxide reactor using bifurcation analysis.²²⁷ The nonlinear stability analysis indicated that an ethylene oxide process with a detuned temperature controller is most prone to reactor runaway. Much research has shown that nonlinear dynamic phenomena due to input multiplicity can compromise the robustness of a control system. Kuhlman and Bogle addressed the question of the relationship between input multiplicity and nonminimum phase behavior and between controllability and optimal operation for nonlinear SISO systems.²²⁸ Bifurcation analysis could be sufficient to obtain a qualitative picture of the solution space for a nonlinear process as a parameter of the process variables at the design stage. This can be used to identify the potential control difficulties determined by the process design and to investigate the influences of the design and operating parameters and disturbances on control, hence providing guidance to eliminate control difficulties by modifying the process design at the design stage. Bifurcation analysis gives a guideline for modifying a process to avoid undesirable behavior.

Ma and Bogle presented an approach for modifying a process design to improve its controllability based on bifurcation analysis and optimization.^{229–231} In their work, based on bifurcation analysis, they first developed a methodology for determining potential control problems associated with the inherent characteristics of a nonlinear process over the entire operating region of interest and analyzing the parameter effects on these problems. They then presented a method for modifying an existing process design to improve controllability, as keeping modifications as minor as possible.

Recently, many papers have shown that performing detailed bifurcation and stability analysis may be very helpful for the development and implementation of nonlinear models and model-based controllers.^{232–236} Hence, bifurcation analysis provides a guide for process modifications to make processes more controllable by eliminating or avoiding undesirable behaviors.

Challenges and Future Developments

Significant progress has been made in the field of controllability analysis for chemical processes over the last several decades. Various design methodologies have been presented to improve controllability characteristics. At the same time, a critical assessment for academia and industry is what has been achieved vs. what we will do next. Some of these challenges and future developments are discussed below.

Multiobjective optimization-based analysis for chemical process design

The traditional chemical engineering design problem is no longer a single economic objective problem. In recent years, as discussed above, many papers^{237,238} have been published on process design combining control and economic considerations. Although profitability remains the key objective for shareholders and management in selecting optimal designs, other objectives such as controllability and flexibility have been gaining importance, due to tight restrictions on product quality and strict environmental regulations. These objectives are important aspects in the design of chemical processes.²³⁹ Trade-offs between these objectives has been the focus of designs that account for controllability and designs in the face of uncertainty. Alhammadi and Romagnoli discussed the problem of process design and operation incorporating environmental, profitability, heat integration, and controllability considerations.²⁴⁰ Recently, as a series of serious accidents has occurred, researchers and engineers^{241,242} have placed efforts on improving the safety of chemical processes. Meel and Seider presented a game theory-based multiobjective optimization method for designing processes, focusing on inherent safety.⁴⁸ This multiobjective optimization of design considering controllability, flexibility, and stability simultaneously would be a very interesting future development.

Recently, Yuan et al. presented an approach to segregate the operation zone of a chemical reactor into different sub-zones based on stability and nonminimum phase analysis, focusing on inherent safety.²⁴³ In many cases, operation is more profitable at an unstable steady state or involving nonminimum phase behavior. Certain operation spaces have minimum phases but instability, as seen in Figure 1, which describes the concentration of reactant x_2 varied with feed q and coolant flow rate q_c of an exothermic CSTR.²⁴³

On the basis of a series of nonlinear analyses for chemical processes,^{244–247} we will next analyze controllability involving stability, profitability, and flexibility based on the multiobjective optimization method presented by our group.²⁴⁸ Furthermore, the presented method will be extended to the design of more complex industrial processes, such as industrial polymerization reactors.²⁴⁹

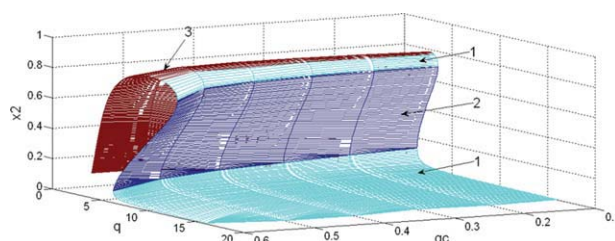


Figure 1. Zone classification for the space surface of $x_2 - q - q_c$.

1, stable minimum phase subspace; 2, unstable minimum phase subspace; and 3, stable nonminimum phase subspace. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

New methods for solving optimization problems

One of the main challenges in the successful application of optimization-based process design for improving controllability characteristics is the rigorous and efficient solution of underlying large-scale mixed integer dynamic optimization problems such as (P2) and (P3). The need for new global mixed integer dynamic optimization algorithms becomes extremely important in preventing the generation of economically or controllability unfavorable designs and fortifying the theoretical foundations of the techniques.

Switchability analysis is an important aspect of controllability analysis. To meet the demands of downstream customers, certain chemical process must move between steady state operating points in nonminimum phase zones or in unstable zones due to the high profitability/product quality in these zones. As is well known, the difficulty of switchability analysis is not the formulation of the dynamic optimization problem but the reliable computation of the problem. Sequential approaches and simultaneous approaches have their advantages and disadvantages, respectively. Therefore, methods for solving dynamic optimization problems such as (P1) efficiently, involving path constraints and unstable processes, is very helpful in switchability analysis. This is a challenging problem, especially when the operating point moves between unstable processes.

In the future, the contributions of other objectives such as energy efficiency and sustainability are expected to weigh more heavily when seeking optimal designs. Clearly, these issues will complicate the multiobjective design optimization. The main challenge is achieving high-efficiency algorithms for solving multiobjective optimization. Recent theoretical and computational advances in multiobjective optimization provide an excellent starting point for future developments.

Application to novel and realistic process

To further bridge the gap between academia and industry, substantial expansion of the boundary of application for process controllability analysis is required. Meeuse applied controllability analysis tools to the design of a monolithic reactor for Fischer Tropsch synthesis.²⁵⁰ Based on anticipating sequential design with screening of alternatives using dynamic controllability indices, Kaymak and Luyben quantitatively compared two different process flowsheets for a hypothetical reactive distillation,¹⁹⁴ not directly aimed at representing any real industrial reactive distillation system. Ydstie and

coworkers designed the control systems for improving the controllability of glass manufacture process based on passivity.¹¹⁶ Garcia et al. presented a controllability analysis of a low-temperature ethanol reformer based on a cobalt catalyst for fuel cell application.²⁵¹ Ramachandran analyzed the controllability of continuous granulation plants.²⁵² Kalbasenka analyzed the industrial batch crystallizers,²⁵³ a controllability analysis was performed to find suitable process actuators and to assess their influence on the decisive process parameters (the process yield and the product properties such as crystal size distribution and the crystal size distribution width). Perhaps such studies can provide a basis for applying controllability analysis to more novel processes. To apply controllability analysis to realistic processes, especially plant-wide processes with a high degree of nonlinearity, novel controllability analysis methods and tools should be developed.

Conclusions

This article presented an overview of controllability analysis for chemical processes. A detailed description of controllability assessments and process design methods for improving controllability characteristics were given. Switchability analysis is an important aspect of controllability analysis and was also discussed. Because incorporation of controllability measures into the early stages of a process design could make designed processes inherently safer, this has received increasing attention. The detailed classification of existing process design methods for improving controllability, including optimization-based design and controllability indices-based anticipating sequential design, were illustrated and discussed. The advantages and disadvantages of these methods were described. Because of various constraints and the development of novel and complex processes, controllability analysis should be considered together with other aspects. Future developments in the field of multiobjective optimization-based analysis for chemical process design requires further work in the development of more effective optimization algorithms and new analysis tools.

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Notation

BRG = block relative gain
 CN = condition number
 CSTR = continuous stirred-tank reactor
 DAE = differential algebraic equations
 DC = disturbance cost
 DNBRG = dynamic nonlinear block relative gain
 HDA = hydrodealkylation
 IMC = internal model control
 IPDC = integrated process design and controller design
 LD = linear dynamics
 MIDO = mixed-integer dynamic optimization
 MIMO = multi-input multi-output
 MINLP = mixed-integer nonlinear programming
 NBRG = nonlinear block relative gain
 NLD = nonlinear dynamics
 NLP = nonlinear programming
 NMP = nonminimum phase
 NMPC = nonlinear model predictive control

PDG = partial disturbance gain
 RGA = relative gain array
 RHP = right-half plane
 RPN = robust performance number
 RPPN = robust performance number of a plant set
 SISO = single input single output
 SVD = singular value decomposition

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