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State-of-the-Art and Progress in the Optimization-based Simultaneous Design and Control for Chemical Processes

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Significant progress in the area of simultaneous design and control for chemical processes has been achieved and various methodologies have been put forward to address this issue over the last several decades. These methods can be classified in two categories (1) controllability indicator-based frameworks that are capable of screening alternative designs, and (2) optimization-based frameworks that integrate the process design and control system design. The major objective is to give an up-to-date review of the state-of-the-art and progress in the challenging area of optimization-based simultaneous design and control. First, motivations and significances of simultaneous design and control are illustrated. Second, a general classification of existing methodologies of optimization-based simultaneous design and control is outlined. Subsequently, the mathematical formulations and relevant theoretical solution algorithms, their merits, strengths and shortcomings are highlighted. Last, based on the recent advances in this field, challenges and future research directions are discussed briefly. An attempt is made with the help of this review article to stimulate further research and disseminate the simultaneous design methods to challenging problem areas. In particular, the application of optimization-based simultaneous design and control methods to large-scale systems with highly inherent nonlinear dynamics often the case in industrial chemical processes remains a challenging task and yet to be solved. © 2012 American Institute of Chemical Engineers *AIChE J,* 58: 1640–1659, 2012
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Introduction

In an economic context characterized by fierce competition and concerns about future energy supply, modern chemical processes are becoming more and more highly integrated and have more interactions among various process units to improve the efficiency of energy/mass transfer and to reduce capital and operating cost. These integrated processes have two characteristics, the first feature is that they are complex networks of substantial number of interconnected process units with material and energy recycle streams; and the second one is that the individual units are generally nonlinear, as the feedback interactions among these units included by recycle, typically give rise to more complex overall network dynamics,[1–3] so in the integrated plants, economic gains come at the cost of an increased dynamic complexity and control challenges.

Traditionally, chemical processes are designed by a sequential approach involving a sequence of decisions and evaluations,[4] and the steps for sequential design and control of chemical process is shown schematically in Figure 1. As can be seen, the process is initially designed by chemical engineer based on steady-state economic calculations followed by the synthesis of a control structure that is generally based on heuristic controllability measures. Hence, the control system design only begins once the main features of the process have been established. This approach sometimes may lead to iterations between the process design and the control system design, and may also lead to poor dynamic operability in face of disturbances and uncertainties. Conflicts between the process design and inherent characteristics and for dynamic performance are illustrated in the next section. Although a closed-loop control system can be used to tackle the undesirable factors, including external disturbances and parameter/model uncertainties that affect the chemical process, studies in literatures[5,6] have shown that process design decisions may have a large impact on the process dynamics and the capability of the control systems. Improving the dynamic performance and functionalities of control systems is a key element in this case. Therefore, it is valuable and important to investigate the interactions between the process design and process control design and process

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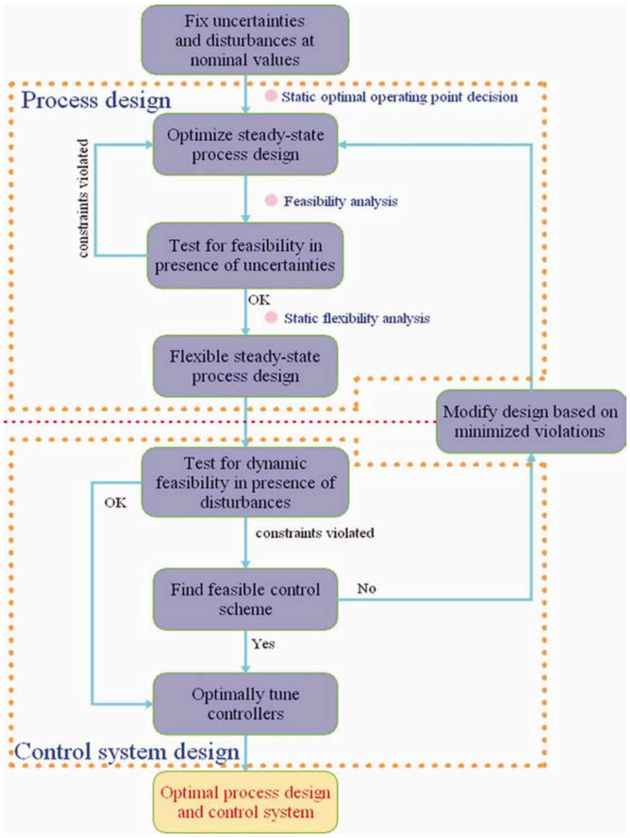

Figure 1. Framework for sequential design and control of chemical process.

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operability to improve the dynamic performance of chemical processes at the early design stage.

The need to simultaneously design, evaluate and control chemical process systems has been widely recognized by the abundant literature published on this subject. These methods can be classified as follows[7] (1) methods that enable the screening of alternative designs based on controllability indicators, and (2) methods for integrating the design of the process and the control system based on optimization. The first class of methods focus on controllability analysis for chemical processes based on open and closed-loop controllability indicators. Two approaches are identified: linear model-based approaches and nonlinear model-based approaches.[8] In the first approach, a large effort is dedicated to the integration of design and control.[9–24] They have the advantage that the controllability indicators are often easy to compute based on linear or linearized nominal models. However, they suffer from a number of deficiencies, for example, while most of the linear model based controllability indicators may give correct information (even for strongly nonlinear systems) around a specified steady state,[25] they fail for problems with a high degree of nonlinearity, such as in startup, shutdown and batch or semi-batch-processes that are not easily correctable with simple nonlinear transformations. Although controllability indicators generally provide useful insights into the limiting effects on achievable performance, they fail to establish a systematic connection to rigorous performance specifications such as effects to plant design and economics. Thus, extensive closed-loop dynamic simulations are again required to verify the validity of the controllability issues. Also, controllability indicators only give an approximate ranking of design alternatives. Recently, a detailed overview on controllability analysis for chemical processes, which outlines the main methodologies that have been developed to deal with the process controllability evaluation and the improvement of its controllability properties, has been published.[8] In order to overcome the weaknesses of methods that enable the screening of alternative designs, optimization-based simultaneous design and control for chemical processes has attracted an increased attention over the last decade.

The principal purpose of this presented article is to provide an up-to-date review of the state-of-the-art and progress in optimization based simultaneous design and control of chemical processes. Different formulations as well as their relevant applications, advantages and disadvantages are discussed. Challenges and further developments in this field are also identified. This article is structured as follows. Following the Introduction, motivations and significances for addressing simultaneous design and control for chemical processes are presented. In the next section, developed methodologies for optimization-based simultaneous process design and control design are discussed together with their merits/blemishes. Challenges and future research directions are then discussed briefly followed by the conclusion.

Motivations and Significance for the Simultaneous Design and Control

When referring to simultaneous design and control for chemical process, the word "design" means process decisions regarding flow sheet topology structure, process design/operating parameters and nominal operating conditions based on the steady-state mathematical model. The word "control" on the other hand, refers to the design of control system resulting in optimal closed-loop dynamic performance. There is no guarantee that the conceptually designed optimal operating conditions and steady-state based economic objectives of a process flow sheet will still be optimal and/or has good plant-wide dynamic performance when met with external disturbances and parametric/model uncertainties. In this section, two simple examples are considered to demonstrate the conflict between design and inherent characteristics and between steady state economics and dynamic controllability, respectively.

Conflict between design parameters and inherent characteristics

When the process topology structure, the feed and process specifications are fixed, under certain design/operating parameters, the chemical process may exhibit highly inherent nonlinear behavior, including input/output multiplicities, limit cycles, sustained oscillations, hysteresis and chaos.[26,27] All of these have been identified as the main cause for destabilization of the control system. In other words, process design decisions define the inherent process and the control performance of the chemical process.

This conflict between design parameter decisions and inherent process properties is highlighted below through a methyl methacrylate polymerization reactor.[28] Our previous work has investigated the influence of design parameters on the inherent process properties including open-loop stability properties and (non) minimum phase behavior.[29] As shown in Figure 2, when the reactor volume $V = 0.1$, the process

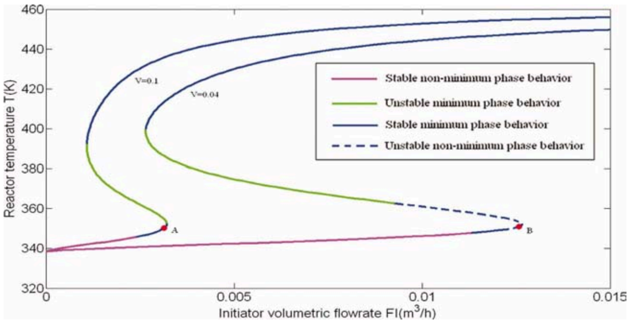

Figure 2. Extended bifurcation diagrams for the polymerization reactor.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

exhibits open-loop stable and minimum phase behavior at the operating point (Point A), whereas when the reactor volume $V = 0.04$, the process shows open-loop unstable and nonminimum phase behavior that would adversely affect the process dynamic performance at the operating point (Point B), proving the need for managing the complexity in control system design.[30] Also, it is well-known that increasing the reactor volume will improve the investment costs.

The aforementioned results obviously indicate that the design parameters that lead to the most economical from a steady-state point of view are not necessarily the best from a nonlinear analysis and control system design point of view. Therefore, this simple example illustrates the need and importance of addressing the problem of process design and operability analysis simultaneously to avoid undesirable inherent process characteristics for achieving good dynamic performance.

Conflicts between process flow sheet topology structure and steady-state economics and dynamic controllability

Inherent conflicts between steady-state economics and control objectives have been recognized. Here, a simple example adapted from Luyben is given to illustrate this issue.[31] Luyben compared the steady state economic design and the dynamic closed-loop performance of two alternatives designs: Case I is a single large reactor; Case II are two smaller reactors operating in series, in both cases, an irreversible liquid-phase exothermic reaction A→B occurs.

According to the steady state economics indicator,[4] Case II is the better process since it has a lower capital cost. However, based on the same control structures for both cases, dynamic simulations are carried out to compare load rejections. Oscillation amplitude in Case II during the initial transient period is much larger than in Case I when restraining the disturbance of 50% increase in the heat of reaction.[31] This result implies that the process that is the most economical from a steady-state point of view is not necessarily the best from a dynamic performance point of view.

The aforementioned two simple examples provide convincing arguments for employing simultaneous design, control and operability analysis for chemical process with the aim to identify design decisions that would potentially generate and/or inherit unacceptable dynamic performance of the control system. Also, the aim is to exploit the synergistic powers of a simultaneous approach to ensure the economic profit at steady state and smooth operation of the plant in a desirable manner even under the influence of disturbances and the existence of uncertainties. Rijnsdorp proposed the concept for an ideal integrated process and control system design, where they suggested that process designers and control engineers should work together to determine the final optimal process design.[32]

Following the aforementioned discussion, it can be concluded that the interaction between design specifications and process inherent characteristics have a profound effect on the optimal process dynamic performance. Great systematic efforts in the context of interactions of design and control toward better economic and operability benefits have been made. These are discussed in the next sections.

State-of-the-Art of the Optimization-based Simultaneous Design and Control

To remain competitive, low-cost integrated plants with stringent safety requirements and stricter environmental regulations need to be designed to maintain the specified strict operational constraints. To guarantee that the plant meets a desirable dynamic performance criterion, controllability analysis considering the selection of a suitable control structure, as well as the specification of the tuning parameters for the selected control algorithm is needed. Due to the complexity associated with this problem, there are not general approaches in the literature that address the simultaneous design and control, instead, several methodologies have been proposed to solve partial aspects of this problem. Seferlis and Georgiadis provided a detailed review on the recent contributions and new techniques that have emerged in the integration of design and control field.[33] Current approaches to simultaneous chemical process design and control can be loosely categorized as optimization-based approaches, heuristic-based approaches, evolutionary based approaches and a combination of the above approaches.[31,34] In general, most of the methodologies focus on some aspects of the problem such as process flexibility, stability and controllability while ignoring others. The remainder of this section is dedicated to provide an up-to-date review on the optimization-based simultaneous design and control for chemical processes.

General formulation for optimization-based simultaneous design and control

Extensive research in this field has resulted in impressive advances and significant new technologies.[35,36] All of the proposed methodologies address issues such as follows[35] (1) robust design under external disturbances and parametric uncertainties, (2) selection of the suitable control structure and the control tuning parameter for multivariable processes that will be optimized in terms of both control and design objectives, and (3) formulation of an appropriate optimization framework and selection of an efficient optimization solution algorithm. The strategies reported in the literature vary in their level of complexity and in the assumptions/simplification made to solve the resulting optimization problem. The general formulation of the problems can be written as

$$\min_{x,y,u} \quad F(\dot{x}, x, y, u) = \begin{bmatrix} F_1(x, y, u) \\ F_2(x, y, u) \end{bmatrix} \tag{1}$$

Subject to

$$f(x, y, u, t) = 0 \tag{2}$$

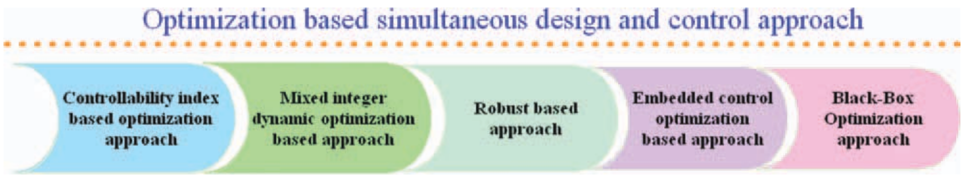

Figure 3. Classifications of existing techniques addressing the optimization-based simultaneous design and control.

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$$h(x, y, u) = 0 \tag{3}$$

$$g(x, y, u) \geq 0 \tag{4}$$

$$x^L \leq x \leq x^U \tag{5}$$

$$x(t_0) = x_0 \tag{6}$$

$$u(t_0) = u_0 \tag{7}$$

where x is the vector of state variables, y is the vector of process variables, and u is the vector of design variables. x_0 is the vector of initial conditions of the state variables, and u_0 is the vector of initial conditions of the design variables, the objective function (Eq. 1) to be minimized includes (the combination of capital and operating costs), and F_2 (the controllability measure, i.e., controllability index, integral square error), f means the set of differential and algebraic equality constraints. Equations 3–5 are possible equality and inequality path and/or point constraints, which express additional requirements for the process performance.

From this general formulation of the optimization-based simultaneous design and control problem, the remaining algorithms are derived or formulated as particular cases. Current frameworks for treating the solution of the optimization-based simultaneous design and control that has been published can be classified as shown in Figure 3.

Controllability index-based optimization approach

This approach takes advantages of the controllability indicators such as relative gain array, condition number and disturbance condition number to quantify the process closed-loop dynamic performance. In order to design economically optimal chemical processes that can run in an efficient dynamic mode within an operating window around a nominal operating point, an economic cost function is defined as the combination of the process steady-state economics and an economic cost correlated with a controllability indicator. Consequently, controllability index-based optimization methodologies offer tradeoffs between economic benefits and operability items of the process. A summary of works that have been carried out in this area is given in Table.1, organized in terms of controllability index, objective function, and the type of model for optimization.

Different optimization frameworks have been proposed for the controllability index-based optimization approach. For instance, through taking into dynamic control performance in the form of matrix norms or dynamically calculated controller error, Floudas and coworkers presented a methodology for analyzing the interaction of design and control.[42,58] A design framework was proposed as a multiobjective mixed-integer optimal control problem. Hence, decisions of the process design, control structures and PI control-tuning parameters could be made simultaneously. Seferlis and Grievink developed an optimization framework for assessing alternative process flow sheet configurations and control structures based on economic potential and static controllability characteristics,[52] the economic optimization was defined as a function of design variables, model parameters and external specified disturbances to minimize the process cost.

In the aforementioned methods, controllability indicators are usually treated as constraints of the mathematical optimization problem or considered in the cost function through using the weighted functions. Although these methodologies can integrate process design and control aspects, it should be pointed out that they fail to determine precisely the importance of the two competing objectives and fail to treat the dynamic behavior of the plant systematically as the selection of weighting factors multiplying each objective has been generally performed arbitrarily. Besides, these methods investigate the closed-loop controllability properties by using quantities which are calculated based on steady-state models or linear nominal dynamic models. This defect, thus, limits their further applicability to those systems that exhibit highly nonlinear dynamic behavior. Furthermore, in the aforementioned framework, due to the use of multiobjective cost function, and to the linearity assumptions, the application of the multiobjective optimization-based simultaneous design and control to chemical processes may result in a suboptimal design.

Another work, although belonging to the classification of controllability index-based optimization approach, deserves some attention as it is different from the other methods that listed in Table.1. Focusing on integrating a model predictive control with a process design scheme, a coordinate strategy was developed by Brengel and Seider.[59] The presented framework not only evaluated the economic objective, but also assessed alternative designs for their controllability properties based on the integral of the squared error of the closed-loop response to different kinds of disturbances. Moreover, the aforementioned conclusions were simulated with model predictive control algorithms. Obviously, this methodology shows two advantages compared with those listed in Table.1. First, the complete process dynamic mathematical model is utilized; and second, advanced model-based controller is adapted to control the process. However, this approach cannot derive explicitly the associated control law, so it is forced to make certain simplifications in the optimal control problem that remove some of the advantageous features of the model predictive control algorithm.[35]

Mixed integer dynamic optimization-based approach

As discussed earlier, the need for considering process operability issues at an early phase of process design is now becoming widely accepted in both academia and industry. A number of dynamic optimization-based methodologies have been proposed. Here, the simultaneous design and control problem is cast as a mixed-integer dynamic optimization (MIDO) problem where discrete (flow sheet topology structures, number of control loops, and continuous variables

Table 1. Summary of Controllability Index Approach in the Literature

Authors	Controllability index	Type of model for optimization	Optimization	Objective function
Morari[37]	Integral of the squared error	Linear model	Multi-objective optimization	Minimize an economic cost + control cost
Palazoglu[38]	Singular Value Decomposition	Nominal linear model	Multi-objective optimization	Minimize an economic cost + control cost
Palazoglu[39]	Singular Value Decomposition	Nominal linear model	Two-stage steady state optimization	Minimize an economic cost + control cost
Figueroa[40]	Structure singular value	Nominal linear model	Multi-objective optimization	Maximize an economic objective
Perkins[41]	Worst case disturbance	Nonlinear model	Steady-state optimization	Minimize design cost
Floudas[42,43]	Relative Gain Array	MINLP models	Multi-objective optimization and MINLP	Minimize capital cost +operating cost + control cost
Pistikopoulos[44,45]	Structural Controllability	MINLP models	Multi-objective optimization and MINLP	Minimize total annualized cost+ operating cost
Perkins[46]	Worst-case disturbance	Linear model	MILP	Minimize operating cost + cost of control instrument
McAvoy[47]	Relative Gain Array	Nominal linear model	MILP	Minimize the valve movement to compensate
Zheng[48]	Controllability Index *v*	Nominal linear model	Steady state optimization	Minimize the annualized cost
Lee[49]	Gap metric	Nominal linear model	Gap metric minimize	Minimize gap metric
Jorgensen[50]	Relative Gain Array	Nominal linear model	Steady state optimization	Minimize the close loop error
Seferlis[51,52]	Controllability performance index	Nonlinear model	Steady state optimization	Minimize the annualized cost
Meeuse[53]	Closed loop controllability	Linear model	Multi-objective optimization	Minimize the economic cost+operating cost
Ekawati[54]	Output controllability index	Nonlinear model	Iterative dynamic optimization	Maximum profits
Blanco[55,56]	Eigenvalue of *Jacobian* matrix	Nonlinear model	Steady state optimization	Minimize the capital+operating cost
Alhammadi[57]	Relative Gain Array	Nonlinear model	Multi-objective optimization and MINLP	Minimize an economic cost + control cost
Douglas[58]	Structured singular value	Nonlinear model	Steady state optimization	Minimize the economic cost

(design/operating parameters, controller tuning parameters, etc.) are incorporated into a single optimization framework.

Areas of application of MIDO frameworks are as follows: batch process synthesis and development,[60–62] reduction of kinetic mechanisms,[63,64] solvent design in batch processes,[65] optimization of hybrid discrete/continuous systems,[66,67] biochemical process such as optimal chemotherapy.[68,69] In short, recent consistent improvement in synthesis, design, operation and control for chemical and biochemical processes have created a steadily increasing need for efficient numerical algorithms for optimizing a dynamic system coupled with discrete (binary or integer) decisions.[70–72] These advances give an excellent start-point and an incentive to the application of MIDO for simultaneous design and control framework. The next two subsections will mainly discuss the framework for MIDO problems and MIDO based simultaneous design and control.

Mixed-Integer Dynamic Optimization. MIDO problems are encountered when binary decision variables enter a dynamic optimization problem. From an optimization point of view, the algorithms for solution of dynamic optimization problems without associated binary variables can be segregated into several types as: simultaneous approaches (orthogonal collocation on finite elements,[73] multiple shooting[74]); sequential approaches (single shooting also named as control vector parameterization,[75] adaptive control vector parameterization[76]). Within the simultaneous approach, both states and controls are discretized, whereas within the sequential approach only the control variables are discretized, a more detailed review of these methods is found elsewhere.[77,78] Based on the aforementioned methods, one can convert the DAE optimization problem into a NLP problem. Through either of the two discretization methods, a MIDO problem is converted into a mixed-integer nonlinear programming (MINLP), which can be solved by branch and bound algorithm (BB),[79] generalized benders decomposition (GBD),[80] and outer approximation (OA).[81] A substantial algorithm in the open literature for dealing with MIDO problems are described in Table 2.

It is the presence of binary variables that increase the complexity of the solution procedure for a MIDO problem compared to a continuous dynamic optimization problem. In recent years, the popularity of MIDO has increased due to advances in dynamic optimization algorithms and the increasing computing power available to researchers in this area.[33]

From Table 2, we can find that a common approach to solving MIDO problems is through orthogonal collocation on finite elements discretization approach, where both state and control variables are discretized, and the overall problem is transformed into a large-scale MINLP problem and then solved by any appropriate numerical solver. Since for problems with many differential-algebraic equations, the orthogonal collocation on finite elements discretization approach typically generates a very large number of variables and equations, they result in large NLP's that may be difficult to solve reliably. On the other hand, the number of parameters to be optimized grows rapidly when encountering larger-scale process. Therefore, the efficient use of this approach is limited to relatively small-scale problems. Avraam et al.[68,82] and Mohideen[85,86] applied the orthogonal collocation on finite elements discretization approach for MIDO problems, and solved the resulting MINLP based on outer approximation and

Table 2. Summary of Methodologies for Addressing Mixed-Integer Dynamic Optimization Problems

Discretization methods	Authors	Methods for solving MINLP
Orthogonal collocation on finite elements	Avraam[69,83]	Outer Approximation.
	Biegler[84]	
	Bahri[85]	
	Mohideen[86,87] Dimitriadis[88]	Generalized Benders Decomposition.
	Androulakis[66]	Branch and Bound.
	Flores-Tlacuahuac[89]	
	Giovanoglou[68]	Variant-2-GBD.
	Flores-Tlacuahuac[90,91]	Branch and bound algorithm combined with NLP solvers incorporated within GAMS.
	Terrazas-Moreno[92]	Solving two state stochastic programming using DICOPT based on outer approximation.
	Terrazas-Moreno[93]	Lagrangean decomposition method.
	Lopz-Negrete[94]	Solved relaxed versions of the optimization problem; using results to initialize complex problem versions.
	Terrazas-Moreno[95]	SBB solver in GAMS
	Flores-Tlacuahuac[96–99]	
	Fengqi You[100]	Using CPLEX to solve the MILP for initialization; Solving NLP sub-problems by KNITRO solver.
	Chaowei Liu[101]	Using CPLEX and CONOPT to solve the MILP master problem and the NLP sub problem.
Direct multiple shooting	Sager[102,103]	Outer convexification; Relaxation.
	Sager[104]	Combination Integral Approximation and branch and bound; MS MINTOC algorithm[105].
	Kirches[106]	Convex reformulation, Relaxation
Hybrid discretization method based on single and multiple shooting	Prata[107]	Outer approximation with extensions to account for nonconvexity.
Adaptive control vector parameterization	Oldenburg[108]	Outer approximation, CPLEX for solving MILP.
	Bush[109]	Outer approximation with Augmented Penalty extension.
Control vector parameterization	Sharif[110]	Outer approximation.
	Schweiger[59]	Generalized Benders Decomposition.
	Mohideen[111]	Integration gradient evaluation based master sub-problem formulation; Generalized Benders Decomposition.
	Allgor[73]	New integer set obtained via screening model technique.
	Bansal[112,113]	Variant-2-GBD.
	Bansal[114]	Generalized Benders Decomposition with simplified master problem and no restriction to any integration.
	Chatzidoukas[115,116]	Generalized Benders Decomposition GAMS with CPLEX MILP.
	Hirmajer[117,118]	MISQP.

generalized benders decomposition algorithms, respectively. However, the linearization of nonconvexities at infeasible points in the full discretization method can reduce the algorithm to an *ad hoc* improvement strategy when used in conjunction with a convex MINLP solver.[61]

Another approach[58,72,111] for solving MIDO problems is to use control vector parameterization and sensitivity-based arguments for solving the primal problem where the binary variables are fixed. Thereafter, an intermediate adjoint problem is solved to provide the dual information needed to formulate the relaxed master problem which determines a new configuration for the next primal problem. In the formulation, the primal problem corresponding to a dynamic optimization is solved by a reduced space approach, and the results give an upper bound on the final solution. The benefit of this approach is that the primal problem is solved in the reduced-space. However, the intermediate adjoint problem may often be expensive. To overcome this pullback, based on control vector parameterization for the control variables discretization for nonlinear dynamic system and generalized benders decomposition for solving the MINLP problem, Bansal proposed a new method for treating the integers with a simplified master problem,[113] where numerical difficulties associated with reformulating the primal problem is also circumvented with the presented algorithm. In short, based on the aforementioned control vector parameterization approach, the MIDO is decomposed into a sequence of primal problems and relaxed master problems. Due to nonconvexity of the constraints in dynamic optimization problems, the aforementioned approaches may be excluding large portions of the feasible region, and within the feasible region an optimal solution may occur, which will lead to suboptimal solutions.[71]

In summary, solving MIDO problems includes two steps: converting MIDO problems into MINLP problems and handling MINLPs through different algorithms.[125] Chachuat gave a review and description of the detailed steps of algorithms for MIDO problems.[71,120]

To reduce the incidence of convergence to the suboptimal solution in MIDO problems, stochastic and deterministic global optimization methods for MINLPs have begun to emerge. Regarding deterministic global optimization methods for MINLPs where the participating functions are nonconvex, these methods rely either on a branch and bound procedure or on a decomposition strategy.[118–120] For example, Lee and Barton proposed a procedure for solving MIDO problems with embedded linear time-varying (LTV) dynamic systems to seek the global optimal solution.[67] Unfortunately, applications of this framework were only given for linear hybrid discrete/continuous systems where the sequence of modes is optimized. A novel decomposition approach for a quite general class of MIDO problems was developed by

Chachuat[71] through this approach. The global solution of MIDO problems could be found, besides, total enumeration of the discrete alternatives could be potentially avoided even under the nonconvexities inherent in the dynamic optimization subproblem. Regarding stochastic global optimization methods such as genetic algorithm for MINLPs, sufficient works have demonstrated that the region of global solutions can be located with relative efficiency.[121–124] However, these methods meet difficulties when faced with highly constrained problems, in other words, global optimality can not be guaranteed.

Mixed-Integer Dynamic Optimization-based Simultaneous Design and Control. To overcome the drawback of controllability index-based optimization approach, several mixed-integer dynamic optimization-based simultaneous design and control methodologies have been proposed. These methodologies integrate the control structure selection, the controller tuning parameters with the process design problem. Traditionally, the expected total annual cost of the system is minimized subject to dynamic models, controller scheme equations, disturbance and uncertainty profiles, equality and inequality feasibility constraints.[126] The optimization variables include all design variables, set points and biases of the controllers.

The mathematical expression of the MIDO based simultaneous design and control problems is posed as follows[136] (the PID control law is chosen for manipulating the process)

$$\min_{k_p,\tau_I,\tau_D,\delta} J(dx_d(t)/dt, x_d(t), x_a(t), u(t), y(t), v, \delta, t) \tag{8}$$

Subject to

$$f_d(dx_d(t)/dt, x_d(t), x_a(t), u(t), y(t), v, t) = 0 \tag{9}$$

$$h(x_d(t), x_a(t), u(t), y(t), v, t) = 0 \tag{10}$$

$$g(dx_d(t)/dt, x_d(t), x_a(t), u(t), y(t), v, t) \leq 0 \tag{11}$$

$$f_p(dx_d(t_i)/dt, x_d(t_i), x_a(t_i), u(t_i), y(t_i), v, t_i) = 0 \tag{12}$$

$$f_0(dx_d(t_0)/dt, x_d(t_0), x_a(t_0), u(t_0), y(t_0), v, t_0) = 0 \tag{13}$$

$$\eta(x_d(t), x_a(t), u(t), y(t), v, t) = 0 \tag{14}$$

$$e_i(t) = y_{sp,i} - y_i(t), \forall i = 1, 2, \ldots, N_y \tag{15}$$

$$u_j(t) = \sum_{i=1}^{Ny} kp_{i,j}\left\{ e_i(t) + \frac{1}{\tau_{I,j}}\int_0^t e_i(t)dt + \tau_{D,j}\frac{de_i(t)}{dt} \right\}, \quad \forall j = 1, 2, \ldots, N_u \tag{16}$$

$$kp_{i,j}^L \delta_{i,j} \leq kp_{i,j} \leq kp_{i,j}^U \delta_{i,j} \tag{17}$$

$$\tau_{I,j}^L \leq \tau_{I,j} \leq \tau_{I,j}^U \tag{18}$$

$$\tau_{D,j}^L \leq \tau_{D,j} \leq \tau_{D,j}^U \tag{19}$$

$$\sum_{i=1}^{N_y} \delta_{i,j} \leq 1, \qquad \forall j = 1, 2, \ldots, N_u \tag{20}$$

$$\sum_{j=1}^{N_u} \delta_{i,j} \leq 1, \qquad \forall i = 1, 2, \ldots, N_y \tag{21}$$

$$\delta_{i,j} \in [0, 1] \tag{22}$$

where $x_d \in R^{N_d}$ and $x_a \in R^{N_a}$ are the vector of differential state and algebraic variables, $u \in R^{N_u}$ is the vector of the manipulated variables, $v \in R^{N_v}$ is the vector of disturbances acting on the plant, $y \in R^{N_y}$ is the vector of potential measurements, $\delta \in Y \equiv \{0,1\}^{N_\delta}$ comprise the binary variables for the process and the control structure; are the design variables, and $y_{sp,i}$ is the set point of the controller. The objective function J is an integral over time which is minimized subject to dynamic process model and operating constraints; f_d represents the differential equations corresponding, e.g., to mass/energy balances, h describes the algebraic equations pertaining, e.g., to thermodynamic and hydraulic relations, g and fp mean the vector of inequality and equality constraints that must be satisfied at all time during the operating time horizon, respectively, f_0 is the initial conditions of dynamic systems; η is the functional relationships between measurements, state variables and input variables, e_i represents errors between the set point of the controller and the process output, and u_j (t) is an ideal PID controller shown in the continuous time domain form k_P, τ_I, τ_D are PID controller tuning parameters. Equations 17, 20 and 21 are used to enforce the requirement of the control structure. The aim is to seek the desirable process design and the suitable control performance (v, k_P, τ_I, τ_D and δ) for minimizing the capital and operation cost.

As can be seen from the aforementioned mathematical formulation, one of the main features of the mixed-integer dynamic optimization-based methods is that process nonlinearity, process uncertainties and external time-dependent disturbances are rigorously accounted for within a single optimization framework. Hence, based on this approach, for a given set of nominal operating conditions, it is possible to identify the scenario that produces the largest process output error, the so-called worst-case scenario. Then, the simultaneous process design and control problem is solved based on the predicted worst-case scenario. A considerable amount of methodologies undertaken in the field of dynamic optimization-based simultaneous design and control and their relevant applications for different chemical processes have been proposed, as given in Table 3.

Various optimization approaches have been generally applied to this research area. In the sequel, only the most cited works are discussed later. For example, based on dynamic process models, Narraway was among the first to tackle process design/operating parameter and control structure selection simultaneously through using general mathematical programming. The problem is treated as a mixed integer dynamic optimization framework.[138] Bahri formulated a backoff-based dynamic optimization framework to address the integration of flexibility and controllability analysis for chemical processes.[84] Based on the full discretization approach, the framework is transformed to a MINLP problem. Later, the same authors proposed a two-stage procedure to treat this optimization problem, in the outer loop; a dynamic MINLP is solved to determine the process structural design, while in the inner loop, the maximum constraint violation is computed under a given set of disturbances. The main drawback of this technique is that, it cannot give a precise guide for changes in process and control system design, although it provides a quantitatively correct measure of the controllability properties.[112] Besides, this backoff framework is based on the linear models, whether it can be applied for real highly nonlinear processes needs to be further investigated. Mohideen[85] developed a basis process design framework for obtaining integrated process and control system design which are economically optimal with desirable

Table 3. Summary of Mixed-Integer Dynamic Optimization-based Simultaneous Design and Control

Author	Key Features	Applications	Controller
Mohideen[86,87,111]	Mixed integer stochastic optimal control formulation; Multi-period decomposition approach	Ternary distillation column	PI
Bahri[85]	Back-off minimization to capture the uncertainty	Two series CSTRs	PI
Bansal[112,128]	Applied Mohideen's framework in a rigorous distillation model	Binary distillation; double-effect distillation systems	PI
Ross[129,130]	The simplification involves fixing the integer decisions pertaining to the existing process and control structure	high-purity industrial distillation system	PI IMC
Kookos[131]	Infinite-dimensional, stochastic, mixed integer dynamic optimization;	Evaporator system; Binary distillation; Reactor-Separator	Multivariable PI
Bansal[113]	Developed a novel, multi component, mixed integer dynamic optimization algorithm	Distillation column	PI
Bansal[114]	Proposed a new MIDO algorithm without the solution of an intermediate adjoint problem	Binary distillation	PI
Sakizlis[132]	Presented a novel method for integrating advanced controller in a simultaneous design and control	Binary distillation; Evaporator system	Parametric controllers
Asteasuain[133]	Used gPROMS/gOPT to solve MIDO	Semi-batch polymerization reactor	PI
Panjwani[134]	Used a high fidelity dynamic model to predict the behavior under varying disturbances	Reactive distillation	PI
Asteasuain[135]	Implemented a multi objective optimization to minimize the cost	Styrene polymerization reactor	Multivariable PI
Asteasuain[136]	Performed a simultaneous design and control under uncertainty for optimal grade transition operation	polymerization reactor	Multivariable PI; Ratio controller
Flores-Tlacuahuac[90]	Non convex formulation, Big-M formulation, and GDP based MINLP	Two series CSTRs	PI
Flores-Tlacuahuac[96]	Full discretization approach; MINLP was solved by a full nonconvex optimization formulation	polymerization reactor	PI
Lopez-Negrete[95]	Full discretization approach; Relaxed versions based decomposition approach	Binary distillation	PI
Paramasivan[137]	Full discretization approach; Formulate MIDO to determine the optimal control structure and controller parameters	Reactive distillation	PID
Khajuria[138]	Incorporating the highly nonlinear and dynamics nature into dynamic optimization framework	Pressure Swing Adsorption Systems	PI

dynamic performance in the presence of parametric uncertainties and process disturbances. Based on a dynamic mathematical model, the problem is formulated as a mixed integer stochastic optimal control problem which is then solved by an iterative decomposition approach whose detailed steps can be found in Ref. [85]. With process and control model simplifications,[139] the framework was applied for a single and a double-effect distillation system, respectively. With fixed discrete decisions and simplifications in the treatment of uncertainties, the framework was also applied for a rigorously modeled multicomponent mixed-integer distillation column,[112] a double-effect system[140] and an industrial two-column system.[128,129]

Combining the benefits of the control vector parameterization and orthogonal collocation on finite elements approach, Mohideen[141] proposed an alternative approach to solve MIDO problems arising from simultaneous design and control. A schematic of the prototype software implementation of this framework is shown in Figure 4. In the primal problem of this methodology, the differential-algebraic model equations are substituted by discrete-time implicit equations resulting from the integration of the system by an implicit Runge-Kutta method. Efficient adjoint-based arguments are used to calculate the reduced gradients and the dynamic optimization is only carried out over the reduced space of the control variables.[142] The dual information that is used to construct the master problem is directly available from the adjoint variables of the primal problem (thus, the intermediate adjoint problem is avoided). This methodology has been further applied to high-purity industrial distillation systems by Ross.[128,129]

Based on a variant-2 of the generalized benders decomposition (v2-GBD) methodology for MINLP problem, a new procedure without the computation of the dual variables and intermediate adjoint information for tackling MIDO was presented[113] to reduce the computation burden. The master problem of this framework has a much simpler form compared to algorithms where adjoint variables are required. Additionally, this new algorithm is independent of the type of method used for solving the dynamic optimization primal problem. To demonstrate its computational merit and efficiency, this novel algorithm was applied for a binary distillation column. Since this approach is based on v2-GBD, it is only guaranteed to converge to the global optimum under convexity conditions for the primal problem with binary variables appearing linearly and separably.[143]

As the advanced control schemes involve solving an online optimization problem which leads to a sharp increase in the complexity of the design framework, the implementation of advanced model-based control algorithm in simultaneous design and control framework has largely been ignored. From Table 3, it is worth highlighting that very limited work has been done toward incorporating advanced control techniques into the simultaneous framework. Most of these mixed-integer

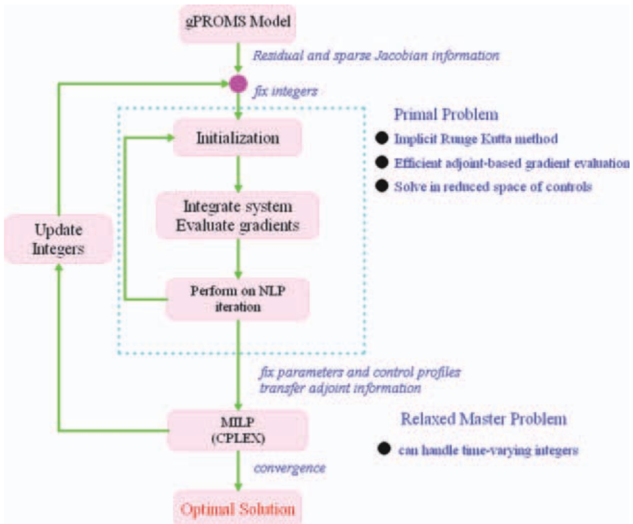

Figure 4. Prototype software implementation for the simultaneous design and control.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

dynamic optimization-based simultaneous design and control approaches utilize conventional PI(D) controllers that usually feature a single-input-single-out (SISO) structure and do not explicitly handle process specifications such as environmental, safety and operational constraints.[131] Kookos and Perkins amalgamated multivariable PI controller with the simultaneous process and control design framework.[130] PI and multivariable PI controllers are relatively easy to tune, but the latter one has marginally superior performance compared to conventional SISO PI controllers. Loeblein and Perkins merged the online optimization-based MPC controllers with fluid catalytic cracking unit design.[144,145] Swartz and coworkers[146,147] proposed a systematic framework for applying the control Q-parameterization into the design and control problem. Although the aforementioned approaches solved the resulting multilevel process design optimization problems by making significant simplifications in the MPC controller structure, these works are indicative of the potential of MPC schemes to improve the process economics and controllability.[35] In light of the parametric controller is capable of eliminating the online optimization, Sakizlis presented a novel method for integrating advanced explicit parametric model-based controller into a simultaneous design and control framework. The methodology was employed for a binary distillation column and an evaporator system, respectively, to highlight its virtue.[35,131] Also the author compared alternative designs generated from traditional sequential design approach with those from mixed-integer dynamic optimization-based simultaneous approach to demonstrate clearly the benefits of pursing a simultaneous approach in process and control design. The study reveals that the total cost obtained from the simultaneous design approach is cheaper than that found by a state-of-the-art sequential design approach. Since the parametric controller contains a feed-forward element to compensate for the external disturbance effect, the methodology that exploits the aforementioned advanced controller allows the chemical plant to operate closer to the constraint limit. Meanwhile, the introduction of the parametric controller to the design framework enables the direct accommodation of the stability performance criteria in the controller synthesis stage.[131]

The foregoing mixed integer dynamic optimization-based simultaneous design and control frameworks were mainly developed within the center of process systems engineering at the Imperial College London, UK. Based on the control vector parameterization, these approaches only discretize the control variables and integrate the DAE model at each iteration of the optimization process. In their work, they successfully achieved the design and control issues for relatively simple chemical processes via simple SISO PI controllers or parametric controllers successfully. Through the application of these methods into binary distillation column, high-purity industrial distillation system, evaporator system, advantages of optimization-based simultaneous framework including higher profitability, more effective to deal with constraints, better control performance have been highlighted. However, the sequential (control vector parameterization) based approaches might be at a disadvantage as it can not evaluate transitions where one (or all) of the steady states is (are) unstable.

As the decision of controller parameters generally requires treatment of unstable dynamic responses and other undesirable inherent process properties, simultaneous design formulations are essential to avoid convergence failures of the DAE model and to obtain robust performance of the optimization algorithm. For instance, Biegler and Flores-Tlacuahuac proposed a framework for tackling the simultaneous process control and design problem of polymerization reactors during dynamic grade transition operation.[95] The formulation of the MIDO aims to compute optimal steady states for grade production, design parameters, dynamic grade transition trajectories among the designed grades, the best control structure subject to minimum transition times, and the controller tuning parameters. Their framework is based on the orthogonal collocation on finite elements approach where both the state and control variables are discretized. This result in a MINLP which is solved using a full-space nonconvex optimization formulation. Moreover, a novel decomposition strategy is used, and the virtue of this decomposition approach is to converge simpler versions of the MIDO problem and use the previous optimal solutions to attempt the solution of complex MIDO problem versions. The aforementioned methods were successfully applied for methyl methacrylate polymerization reactor and high-impact polystyrene polymerization reactor. Lopz-Negrete extended the above method to a binary distillation column carrying out the separation of the methanol-water system to find the optimal feed tray location, optimal operating steady states, and the optimal open-loop trajectory between them.[94] It is important to note that solving MIDO problems for highly nonlinear systems by the full discretization approach requires careful initialization. This may be the main reason for proposing the above decomposition solving strategy. However, in the aforementioned studies, model/process uncertainties are not taken into account. In order to extend the proposed simultaneous design and control framework to a larger and plantwide chemical process and to keep CPU time to a reasonable level, an efficient decomposition strategy for seeking good initialization needs to be further investigated, as the use of proper initialization strategy is crucial to solve large-scale MINLPs.

Although the mixed-integer dynamic optimization based methodologies outlined earlier solve the simultaneous design and control problem with realistic scenarios and on the basis of rigorous nonlinear dynamic models, the application of the aforementioned simultaneous frameworks for many realistic chemical processes feature highly nonlinear behavior around optimal design regions will generate a strong nonlinear optimization formulation. The computational complexity associated with the resulting nonlinear dynamic optimization problems is a key obstacle of these methods. Especially, the resulting MINLP problem arising from the full discretization method for dynamic optimization has special characteristics including relatively few integer variables and large NLP problems. Hence, the MINLP strategy needs to handle NLPs that are often large and difficult to solve. Consequently, the huge computational times involved make these strategies impractical for solving industrial problems. On the other hand, the controller tuning parameters obtained from the aforementioned MIDO based simultaneous design methods could potentially result in a closed-loop unstable process, only Mohideen[110] and Sakizlis[148] explicitly considered the system stability when investigating the simultaneous design and control problem. Hence, further investigation of incorporating stability analysis into the simultaneous framework should also be carried out.

Robust-based optimization approach

In the anterior works including controllability index-based optimization approach and mixed-integer dynamic optimization based approach, the process design and control costs are incorporated into the objective function which are traditionally treated as the function of design variables. Mixed-integer dynamic optimization-based approaches use the nonlinear dynamic models directly and may usually result in difficult and often intractable problems. The commonality between most of these methods is that they consider the process/model uncertainty as the range of the design or operating variables, and do not deal with the issue of control robustness explicitly.

In light of the aforementined questions, a new use of a robust control and simpler optimization approach, where the nonlinear dynamic system is approximated by a first-order plus time delay linear one with model uncertainty has been presented.[149,150] Compared with the mixed-integer dynamic optimization based approach, where they obtained the worst scenarios through incorporating the full nonlinear dynamic models into the optimization problems, the principal idea of the robust control based approach is that they seek the worst scenarios via tools borrowed from robust control theory. As the function of the design variable is integrated into the objective function together with the capital and operating costs, one of the main novelties in this methodology is that the cost of variability in controlled variables and model error under model uncertainty has been quantified explicitly. The robust performance criteria including a robust stability term and a performance term related to the closed-loop variability in the controlled variables is used as a constraint in the optimization framework to assure that the system is stable in face of uncertainties. The mathematical formulation can be obtained from Ref. [150].

The proposed method comprises an inner-loop optimization and a main outer optimization problem, the purpose of the inner-loop optimization is to maximize the variability costs. The main outer optimization minimizes the capital and operating cost. Through implementing two types of controllers, i.e., IMC and MPC, the proposed simultaneous design and control framework was applied for a relative simple depropanizer distillation to demonstrate its traits.[150] The main shortcoming of this methodology is that it only considers the particular disturbance profile such as sinusoidal disturbances at one given frequency. Therefore, the proposed approach does not guarantee that the resulting design can be capable of handling other external perturbations and uncertainties in the process/model parameters. In order to circumvent this limitation, subsequently, Ricardez-Sandoval and coworkers proposed several methodologies for simultaneous design and control of chemical process.[151–156]

Quadratic Lyapunov Function-based Approach. This work utilizes an uncertain nominal linear state-space model with model parameters varied within identified ranges to represent the closed-loop nonlinear dynamic behavior of the system.[151] In this framework, the robust models obtained from identification of the closed-loop process nonlinear dynamic models are used to check the robust stability and to predict bounds on the worst deviations in process variables in response to external disturbances based on a quadratic Lyapunov function.

The formulated optimization problem corresponds to a nonlinear constrained optimization problem. This approach is applied for a mixing tank process, and the results are also compared with that from Mohideen's mixed-integer dynamic optimization-based approach,[85] the comparison between these two methodologies shows that the presented approach is an order of magnitude faster than the mixed-integer dynamic optimization based simultaneous approach.

There are several issues of this method that should be noted. First, the nonlinear process model equations and control algorithm equations do not appear explicitly within the mathematical formulation. Second, in this approach, the process variables follow a normal distribution function, the process parameter uncertainties and external disturbances have a uniform probability. Third, the challenging task of solving computationally intensive dynamic optimization problems is avoided via the application of the ''robust'' criteria, however, the design may be conservative. Fourth, the robust variability index that is used to assess process variability and process feasibility only provides a bound on the output error's variance.

Singular Structured Value-based Approach. In this revised approach, a technique based on the structured singular value analysis is adapted to seek the critical time-dependent profile in the disturbance variables producing the largest variability of the output variables. A robust finite impulse response (FIR) model between the disturbance and the output variable to evaluate the worst-case scenario is generated based on the robust model. Similarly, this methodology also uses the quadratic Lyapunov function to ensure process asymptotic stability. In this framework, as the LMI equation is incorporated into the optimization constraints, it is necessary to identify a robust model around the nominal operating point to evaluate the process stability at each iteration step, which will be computationally expensive for large-scale systems.

In order to avoid the aforementioned disadvantage, based on the previous framework, a new methodology is then presented,[153] two preliminary tests to determine whether a nominal operating state is stable or not are carried out. A discrete closed-loop linear impulse response model with uncertainty is used to describe the transient behavior of the nonlinear closed-loop process around a nominal steady state to avoid identification of an uncertain state-space model.

The quadratic Lyapunov function based robust stability criterion is used to test the system's stability only when the two preliminary tests are not satisfied. On the other hand, the quadratic Lyapunov function-based robust stability test is also applied for the optimal solution to assure that the final design is stable. The application of the proposed method on the Tennessee Eastman process has demonstrated its efficiency and practical values.

Hybrid Worst-Case Approach. The research work presented earlier used the analytical bound based worst-case approach to calculate the bounds on the output variability and related variables constraints. In light of the conservatism resulting from the use of analytical bounds, a new hybrid worst-case combining the analytical calculation of the worst-case disturbance and dynamic simulations based simultaneous design and control approach for large-scale systems has been developed.[154,155] The differences between this framework and the ones above are as follows (1) structured singular value norm calculation is utilized to recognize the critical realizations in the disturbance variables and the worst value in the uncertain process parameters, and (2) dynamic simulations using the first principle closed-loop dynamic models are carried out to find the maximal variability in outputs and constraints of related variables. The hybrid worst-case approach was tested on the isothermal liquid storage tank process and the Tennessee Eastman process, respectively, and compared with the structured singular value-based approach. The hybrid worst-case approach requires more computations to obtain less conservative designs. Note, however, the hybrid worst-case approach is also carried out to investigate the influence of the redesign of the Tennessee Eastman process units on the optimization outcomes.

Through the application of the aforementioned robust-based optimization approaches for different chemical processes which are subject to external disturbances and process parametric uncertainties, and the comparison with the mixed-integer dynamic optimization-based methods, the results illustrate that the greatest advantage of the robust index-based methodology is probably its less computational burden as the problem is formulated as a nonlinear constrained optimization with nonlinear dynamic behavior represented by a nominal linear model with uncertainties. Hence, this methodology is computationally efficient and is a practical tool that can be used in the simultaneous design and control of large-scale processes.

However, several unsolved problems should be outlined. First, as previously mentioned, the resulting design, which depends on the differences between the uncertain model and the actual nonlinear process dynamics, would tend to be conservative. Model parameters with large uncertainty descriptions will produce more conservatism in the resulting design. Second, the overall nonlinear constrained optimization problem is nonconvex, different starting points will result in different design and control solutions, so process knowledge is required to guess suitable initial values of optimization variables. Third, the framework assumes that the process flow sheet and the control structure have been fixed *a priori*; fourth, when the robust index based approach is applied for the more complex chemical processes with higher degree of nonlinearity described by large sets of ordinary differential equations; higher-order models will be required for stability test. Last, only the conventional PI controllers have been implemented (and tested) into the simultaneous design and control framework.

Constructive Nonlinear Dynamics-based Approach. Early applications of sensitivity, singularity and numerical bifurcation analysis were aimed at obtaining a deep understanding of the qualitative nonlinear dynamics of chemical process systems in general.[3,26,157–160] Until now, most of the numerical bifurcation-based methods have focused on analysis rather than addressing the synthesis problem of chemical process.[161] In light of this situation, Marquardt and co-workers presented a novel approach based on constructive nonlinear dynamics, which extends and applies ideas from nonlinear dynamics to address synthesis of chemical process.[162–169] The proposed design framework allows the formulation of a steady-state optimization problem that employs constraints on the asymptotic process behavior rigorously into account. Compared to previous numerical bifurcation-based methods, constructive nonlinear dynamics allows a quantitative tradeoff between the various constraints in the problem such as process feasibility, stability and dynamic performance. All constraints are integrated as nonlinear boundaries in the space of process parameters (e.g., process and controller design parameters, uncontrolled inputs, or model parameters), the so-called critical manifolds,[162] which separate regions of desirable process behavior from regions of undesirable process behavior. Therefore, the distance of an operating point to a boundary is interpreted as a physically meaningful measure of parametric robustness of the design with desired process behavior. The framework has been successfully applied for process design,[164,165] robust controller tuning,[170,171] simultaneous design and control.[172–175]

When the constructive nonlinear dynamics based approach is applied to the optimization-based simultaneous design and control problem, the mathematical formulation and its detailed solving algorithms and steps can be found elsewhere.[172,174] Grosch applied this framework for the solution of a simultaneous design and control case study for a continuous MSMPR crystallization process focusing on the analysis of the interaction between the economic and dynamic performance constraints under uncertainties in both design and model parameters.[172] The case study shows that a proper tradeoff between different measures for economic and robust dynamic performance is essential to obtain meaningful results for integrated design and control problems.[173] Recently, Gerhard derived two new types of critical manifolds that separate regions with qualitatively different system behavior based on the transient system behavior and the corresponding normal vectors.[167,173] Through incorporating these new constraints into the optimization problem, they applied the constructive nonlinear dynamics-based approach to the simultaneous robust design and control design of the Tennessee Eastman process to investigate the transient behavior under fast disturbances and uncertain model parameters.

Through application of the constructive nonlinear dynamics-based approach into the crystallization process and Tennessee Eastman process, it has been demonstrated that this methodology has potential to tackle more complex and realistic scenarios. However, in its present form, this method requires *a priori* knowledge of the dynamics of parametric uncertainty. Similar to the hybrid worst-case approach, the constructive nonlinear dynamics-based approach assumes that the process flow sheet and the control structure have been fixed *a priori*. Besides, only the PI controller is carried out and implemented into the framework to manipulate the process.

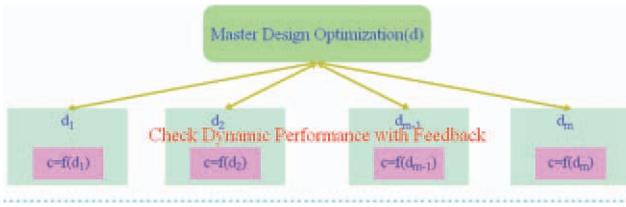

Figure 5. Framework for the embedded control optimization-based approach.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Embedded control optimization approach

An extensive body of literature in the simultaneous design and control for chemical processes has been published. It is noteworthy that the simultaneous search for flow sheet decisions, design/operating variables, optimal control structure and controller parameters alongside process design exceeds the capabilities of the most existing optimization algorithms.[176] In the mixed-integer dynamic optimization based approaches, integer decisions for flow sheet configuration and each possible pairing between manipulated and controlled variables causes a combinatorial explosion of design alternatives and introduces discontinuities in the search space. In order to reduce the combinatorial complexity of simultaneous design and control, a framework based on embedded control optimization has been proposed.[176–180]

This embedded control optimization-based formulation separates design decisions from control decisions to keep the problem size manageable. The whole framework is decomposed into two subproblems. The first subproblem also called master level seeks optimal design decisions that maximize performance under uncertainties, and the main design parameters that govern the dynamic process performance are obtained using stochastic design optimization. The second subproblem performs rigorous dynamic flexibility tests based on design decisions obtained previously by fixing a particular control strategy alongside its tuning parameters. This problem is formulated as a deterministic optimization problem.

This approach allows reduction of the combinatorial complexity of the simultaneous design and control problem by separating the design decisions from the control decisions as shown in Figure 5. It can be seen that for every decision, the embedded control problem is solved with the help of dynamically adaptive control optimization operating under uncertain conditions.

The objective of the embedded control optimization-based simultaneous design framework includes the expected operating cost and capital cost; the conservation laws, the selected control algorithm; the safety, equipment and production requirements are included in the optimization framework as constraints. Malcolm gave the detailed solving steps for the aforementioned optimization problems.[176]

Iterations between the first subproblem and the second one will be needed before achieving an optimal and flexible design. As presented earlier, the framework is based on simpler adaptive state-space models (replacing the full nonlinear system equations) and a linear quadratic regulator is used to compute the best control action to minimize a cost function. The state-space model is identified in every step of the discretized time horizon through the sequential least-squares method[174] or the moving horizon estimation.[178,180]

The proposed methodology has been successfully applied on polymerization reactors, plant-wide process including a reactor and a distillation column, and isomerization process flow sheet, respectively. Compared with the mixed-integer dynamic optimization based approaches, from a computational point of view, the embedded control optimization approach may be attractive and offers better practicality options for solving industrial problems, although the design may result in suboptimal design solutions. Since this approach is implemented based on simple state-space identification that is executed in every step of the discretized time horizon, its applicability for highly nonlinear processes may be limited. In order to improve the quality of identification, more advanced identification algorithms may be used. However, these advanced algorithms are computationally expensive and will deteriorate the performance of the proposed approach. Hence, a tradeoff between accuracy and performance of algorithms needs to be considered.

In order to reduce the complexity of the embedded control optimization-based simultaneous design and control problem, Patel introduced an optimal control (modified linear quadratic regulator (mLQR)) for achieving simultaneous design and control in a practical manner.[181] The principal idea of this framework is to utilize an optimal controller to evaluate the best achievable control performance for each candidate design during the process synthesis stage. Subsequently, the evaluation of the detailed and complete closed-loop process dynamics is meshed with a superstructure-based process design algorithm. In this approach, the simultaneous design and control is formulated as a bilevel optimization problem, which is then solved through a two-stage sequential, feasible path method that keeps the problem size manageable. The whole framework includes a main optimization step dealing with design variables and an inner dynamic optimization for handling control (dynamic) variables. In the inner dynamic optimization, the objective is to minimize the integral of squared deviations from the set points, while the main optimization problem, based on the results from the inner dynamic optimization, the product quality and other relevant constraints, generates a new candidate through adjusting the design variables. This is repeated between the inner dynamic optimization and the main optimization until a feasible design with suitable profitability and dynamic performance is achieved. However, the mLQR formulation is not allowed to consider the inequality constraints in the dynamic optimization framework. As the mLQR formulation is based on the linearized model, its applicability for highly nonlinear processes is limited as the linearized model can not represent the highly nonlinear chemical process correctly.

Black-box optimization approach

Several frameworks have been presented for addressing the solution of simultaneous design and control, which can be formulated as a mixed-integer nonlinear programming (MINLP) problem. Subsequently, these problems can be solved by outer approximation methods, the general benders decomposition method or Branch and Bound algorithms. As these methodologies either need to solve relaxed problems or solve a sequence of nonlinear problems with fixed-integer values, also the MINLP is frequently nonconvex, local optimization techniques usually fail to locate the global solution. Therefore, several stochastic methods have been adopted to solve the optimization problems arising from the optimization based simultaneous design and control,[182–188] where the integer and the continuous variables are treated simultaneously through the stochastic intelligence algorithms, such as particle swarm optimization, genetic algorithm and tabu search-based algorithm that do not require transformation of the original problem.

For example, Banga et al. presented a hybrid solution strategy based on the tabu search algorithm, and employed a sequential quadratic programming to treat the MINLP problem arising from the simultaneous design and control for a wastewater treatment plant.[184] Then, they proposed the use of a global optimization algorithm based on an extension of the ant colony optimization metaheuristic to address the simultaneous design and control of the Tennessee Eastman process in an efficient and robust way.[185] Recently, Lu presented a particle swarm optimization-based method that combines the fuzzy modeling/control and the particle swarm optimization to solve simultaneous design and control problems.[188] The proposed method decomposes the whole problem into two optimization loops, the inner loop named embedded control optimization, and outer loop called master design optimization. In the inner loop, a linear matrix inequality is utilized to solve the fuzzy-modeling based controller design problem. In the outer loop, a particle swarm optimization is carried out to tackle the process design problem. Obviously, the proposed framework has incorporated the merits of both fuzzy modeling/control and particle swarm optimization methods, and has the ability to solve the complex nonlinear problem.

Although the aforementioned black-box optimization methods have a capability to reduce the combinatorial complexity, when applied these methods for the simultaneous design and control for highly nonlinearity chemical processes, it should be noticed that compared with the deterministic algorithms, black-box optimization approaches lack of any theoretical background without any guarantee of optimality.

Integration plant-wide process design and control

Simultaneous plant-wide process design and control is defined as the development of a plant-wide process by considering both steady-state economics and dynamic operability at all stages of flow sheet synthesis. There is no guarantee that a process flow sheet that has been developed to optimize some steady-state economic objectives will provide excellent plant-wide dynamic performance. Typically, heuristics based approach is used for tackling the integration of a complex plant-wide process design and control including process flow sheet synthesis, control structure selection and controller parameter tuning. Luyben gave a detailed review on the simultaneous plant-wide process design and control.[189] Two excellent surveys on the plant-wide process control design were issued by Skogestad[190] and Stephanopoulos.[191]

Recently, a decomposition-based optimization approach is proposed to tackle the integration of process design and controller design for reactor-separator-recycle process.[192] The main merit of this proposed solving strategy is, based on the reverse approach and thermodynamic-process insights, to decompose the whole framework into four sequential hierarchical subproblems (1) preanalysis, (2) design analysis, (3) controller design analysis, and (4) find selection and verification.[193] Based on the solution of the decomposed set of four sequential hierarchical subproblems, large number of infeasible solutions within the search space are identified and eliminated. Hence, it is able to yield a final subproblem that is significantly smaller. The detailed algorithm for solving the above problems is found elsewhere.[193,194] There are two points that need to be clarified: First, the resulting final optimal design and control scheme cannot be guaranteed feasibility under parameter/model uncertainties and external disturbances; second, this work does not explicitly consider the closed-loop stability and, consequently, the final design could be unstable.

To the author's knowledge, existing optimization-based simultaneous design and control methodologies address problems mainly at the level of single-unit operations, although the robust-based approach and embedded control optimization-based approach deal the plant-wide processes including a reactor and a distillation column, TE process and isomerization flow sheet process successfully, however, this framework for simultaneous design and control assume that the process flow sheet and the control structure have been fixed *a priori*, as well as the feed and process specifications.

Summary

Historically, initial research in the optimal design for chemical processes mainly concentrated on the development of the process design and control system design as the sequential procedures. During the last 15 years, great efforts have been carried out to provide optimization based methodologies for dealing with process design and control simultaneously, where the process design characteristics, flow sheet configurations, control strategies, control structures and controller's tuning parameters have been selected optimally in order to achieve suitable profitability and good dynamic performance under the amounts of feasibility constraints, parameter/model uncertainties and external disturbances. Powerful methods and tools are being developed in the field of optimization-based simultaneous design and control for chemical processes. They are general enough to be transferred to other application domains, thereby providing a common interface among often separated research communities. Previous research works have demonstrated that optimization based simultaneous design and control approach may result in numerous economic and operability benefits over the traditional sequential design approach.[195] From the earlier discussions, the optimization-based simultaneous design and control methods can be segregated into: controllability index-based optimization approach; mixed-integer dynamic optimization based approach; robust based optimization approach; embedded control optimization-based approach; decomposition based approach and intelligence-based approach, and the main intellectual merits of these methods are summarized as Table 4.

From Table 4, it can be easily noted that only "robust-based" approach and embedded control optimization-based approach investigate the stability characteristic of the final optimal design, but they do not consider the flow sheet structure or control configuration decisions in the optimization framework. Although mixed-integer dynamic optimization-based approach can integrate the flow sheet structure and control structure decision in a single optimization framework, and may even guarantee global optimality (through use of the full nonlinear dynamic models), it does require significantly more computational effort, especially for highly nonlinear chemical processes. It should be pointed out that

Table 4. Summary of Different Optimization-based Simultaneous Design and Control Approach

Methodologies	Model type	Stability analysis	Flow-sheet structure	Performance indices	Controller type	Control structure
Controllability index based optimization approach	Linear	No	Yes	RGA;CN ISE	PI MPC	Yes
Mixed integer dynamic optimization based approach	Nonlinear	No	Yes	ISE Worst-case disturbance	PI MPC	Yes
Robust based approach	Linear	Yes	No	Worst deviations	PI MPC	No
Embedded control optimization based approach	Linear	Yes	No	Dynamic flexibility	PI	No
Black box optimization approach	Nonlinear	No	Yes	ISE	PI	Yes

Note: RGA=Relative Gain Array; CN=Condition Number; ISE=Integral Squared Error

till now, only a few works in the field of optimization-based simultaneous design and control utilize advanced controllers such as Q-parameterization controller,[146,147,196] parametric controller[131,148] and model predictive controller[59,197–201] to manipulate the process. There are various techniques for evaluating the dynamic performance, from Table 4, it can be easily found that different control performance indices such as RGA, ISE and worst-case disturbance are used to formulate the optimization problem for simultaneous design and control. Hence, the obtained results may change significantly when different control performance indices are utilized.

Challenges and Future Directions

The strength of the field of optimization-based simultaneous design and control is the close bidirectional interaction between methodological developments and advances in applications as illustrated in Figure 6.

Significant progress has been achieved in the field of optimization-based simultaneous design and control for chemical processes over the last several decades. Many strategies and their relevant solving algorithms have been presented to tackle their application in different chemical processes. As can be shown in Figure 6, research related to application domains provides new solutions to pressing problems in these areas and also generates new approaches. For example, theoretical algorithms and frameworks that can be transferred to other application domains as well as challenges to fundamental research. The complexity of the dynamic interaction between theoretical frameworks and applications will be beyond what can currently be handled with available methods. There is a strong need for new methodological and engineering approaches that ensure efficient, predicable, safe and secure behavior of large-scale highly nonlinear systems. The existing research work addresses a large number of novel unexplored avenues in the field of optimization-based simultaneous design and control that aim to bridge the gap between academia and industry, and substantially meet the real industrial needs. Some of these research potentials and future developments are listed briefly as follows.

Embedding the advanced controller into the simultaneous design and control framework

Incorporating control decisions into the optimization-based simultaneous framework are recognized as essential for assembling a profitable operation. Advanced control offers huge benefits for a more economic, safer and ecologically more benign operation of potentially unsafe or unstable chemical process. Hence, advanced controllers such as predictive control are widely used today in the chemical industry, especially for the control of multivariable systems with constraints. The use of advanced control is especially attractive since once multivariable controllers are used the control structure selection step may not be necessary. Implementing the advanced controller into the simultaneous design and control framework is of great practical value as it can improve the process profitability and process dynamic performance.

Considering process flowsheet topology structure, stability analysis in the simultaneous framework

To the best of authors' knowledge, currently, there is no simultaneous design and control methodology available that simultaneously considering flow sheet configuration selection and operating point optimization with guaranteeing robust stability under disturbances and parametric/model uncertainties. Our recent work demonstrates that certain chemical process with highly nonlinearity will show undesirable characteristics (including open-loop unstable and nonminimum-phase behavior[30]), which would adversely affect the process dynamic performance over the entire operating region under the fixed flow sheet,[202] i.e., chemical process will exhibit different internal characteristics under different fixed flow sheets.[203] Therefore, it is important to include the process flow sheet topology structure decision and stability aspects within the optimization-based simultaneous design and control framework. The inclusion of the flow sheet topology structure and stability within the optimization is expected to provide a more economically attractive, energy efficient design with desirable dynamic performance characteristics such as flexibility, controllability, robustness and safety.

Application of optimization-based simultaneous framework into novel, highly nonideal, realistic industrial and more complex process

Till now, existing simultaneous design and control methodologies have only been applied for relatively small and complex processes such as distillation columns, reactor-separator systems, and waster-water treatment process, in order to further bridge the gap between the theoretical development and industrial development requirements, and substantially, the application of optimization-based simultaneous design and control frameworks for highly nonideal and realistic industrial plant-wide process should be given more emphasis.

In addition, aiming at transcending the boundaries of the classical chemical processes where the optimization-based simultaneous design and control strategies are only applied. Future studies should focus on extending the application of these frameworks to novel processes involving complex

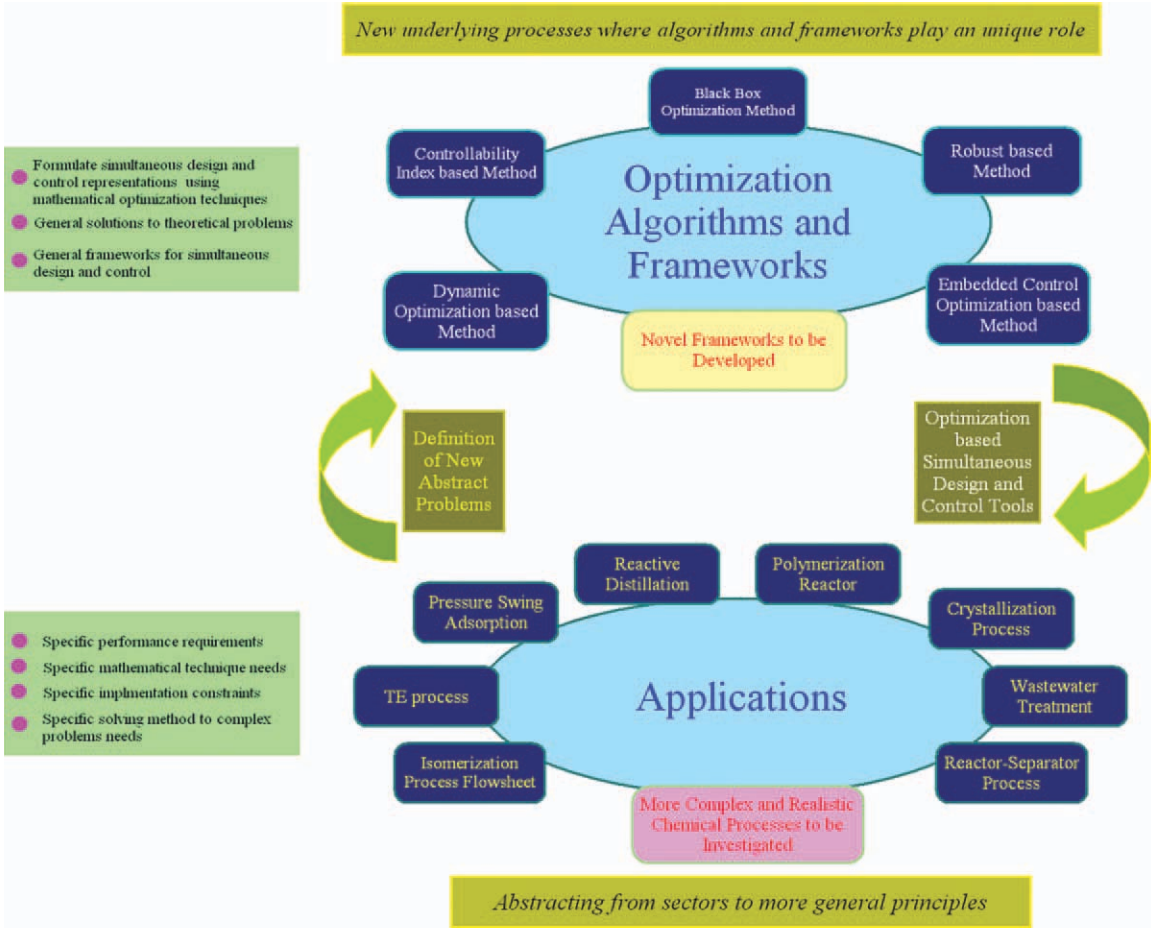

Figure 6. Bidirectional interaction between methodological developments and advances in applications.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

chemical processing systems, biochemical production processes, biological/biomedical systems, hybrid energy systems, pharmaceuticals manufacturing processes, and microscale chemical processes, the importance of which has grown rapidly.[204,205] Recently, Gani and coworkers implemented the decomposition-based approach into the simultaneous design and control for a bioethanol production process,[206] which can provide the basis for future developments in this area.

Rigorous, robust and efficient global mixed-integer nonlinear programming algorithm for simultaneous design and control

When the mixed-integer dynamic optimization-based simultaneous design and control frameworks are applied to the complex chemical process, the resulting large-scale and stochastic MINLP problem is presently quite difficult to handle, hence, the efficient numerical solution of these problems needs to be further studied.

In practice, models of MIDO or MINLP generating from optimization-based simultaneous design and control framework are merely approximate descriptions of the real chemical process and are subject to uncertainties and disturbances performance. Most of the methods listed in this survey article can only guarantee convergence to the suboptimal solution of the underlying optimization problems, which may result in serious economic and environmental consequences, and may also result in unsafe operating conditions, when implemented on realistic chemical process. It is widely known that the main encumbrance of the application of optimization-based simultaneous design frameworks for large-scale chemical processes is that computational complexity requires a huge computational effort.

Hence, in order to prevent the generation of economically undesirable designs under uncertainties and to make the application of simultaneous design framework for the aforementioned novel, complex and realistic industrial processes successfully, the need for the theoretical and algorithmic development of new rigorous, robust and efficient global optimization methods for MINLPs under uncertainty becomes extremely important. Recent a steady-state process optimization strategy[207] provides well understood significance and importance to establish guaranteed robust stability, guaranteed convergence to a desired state of nonlinear chemical process under parametric uncertainties, and it supports an excellent start point for looking into this challenge topic.

Developing software tools for optimization-based simultaneous design and control

Despite significant achievements and numerous success records in the field of optimization-based simultaneous design and control for chemical processes, the successful realistic industrial applications are rare. The foremost justification for the developed methodologies not penetrating industrial practice is largely due to a lack of commercial software which packages the optimization-based simultaneous design and control strategies into computer tools that are easily accessible to the industrial practitioner. Evidently, the main driver for industrial applications of optimization-based simultaneous design methods is not only the mere existence of the academic solving technologies, but also the availability of these techniques in robust software tools.

As much as possible the developed methodology should be implemented into a systematic computer-aided framework to develop a user-friendly software tools which may boost the potential of optimization-based simultaneous design methods for industrial applicability and acceptance significantly. To this end, Hamid's software named ICAS-IPDC[208] may set a good example for future software development.

Conclusions

Optimization-based simultaneous design and control has two facets: research in basic principles, theories and tools, and research related to specific application domains. The strength of the optimization-based simultaneous design and control is the interplay between these two sides. Over the last 3 decades, this field has seen huge advances, leveraging technology improvements in mathematical formulation and theoretical solution framework with breakthroughs in the application to different kinds of chemical processes.

A comprehensive review of the state-of-the-art of optimization based simultaneous design and control for chemical processes has been given in this review article. The shortcomings of traditional sequential design approaches have shown the necessity and significance of the optimization-based simultaneous design and control for chemical processes. The review indicates that the various optimizations-based simultaneous design and control studies can be classified under five different themes depending on their solution approach: controllability index-based optimization approach, mixed-integer dynamic optimization-based approach, robust theory based approach, embedded control optimization-based approach, decomposition-based approach and intelligence based approach. These different classes have been illustrated and discussed in detail pointing out their advantages and drawbacks. Finally, motivated by the record of success in the application of existing methodologies to chemical process design and control, numerous new unexplored avenues in this field is briefly discussed including new domain applications such as polymerization, reactive distillation, crystallization, wastewater treatment among others. These suggestions aim to bridge the gap between developments from academia and industry requirements have been discussed briefly.

It is hoped this article will stimulate future academic researchers and industrial practitioners with the research in developing fundamental theory, optimization-based frameworks and commercial computational tools for process design and process control design simultaneously. Even though significant achievements have been made in the field of optimization-based simultaneous design and control, robust and efficient global optimization algorithms for solving the complex large-scale optimization problems under uncertainties and relevant realistic chemical process and manufacturing system applications are still unsolved issues.

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