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Integrated Process Design and Control: A Review of the Current State-of-the-Art and Research Challenges

Alexios-Spyridon Kyriakides, Theodoros Zarogiannis, Panos Seferlis*

Department of Mechanical Engineering, Aristotle University of Thessaloniki, P.O. Box 484, 54124 Thessaloniki, Greece
seferlis@auth.gr

In chemical and energy conversion processes, the achievable dynamic performance cannot be improved unless design limitations are waived, despite the employment of sophisticated control strategies. It is therefore, quite important to incorporate process operability as an additional criterion during process design in order to ensure the achievable of the desirable dynamic performance. The two main purposes of this survey is to concisely present, classify, and eventually assess the current state-of-art technologies towards the integration of process design and control and further outline the outstanding research challenges in the field. Ideally, the simultaneous calculation of the process and the control system design variables within a holistic framework appears as the most efficient approach. Decomposition strategies facilitate the solution of the highly complex problem. The available technologies can be classified based on their features in the decision, process and uncertainty description, and solution technique levels. Several challenges remain in utilizing engineering knowledge and hierarchical design methods in defining a reasonable design space and the smart decomposition of the resulting complex and difficult to solve optimisation problems. Heat and mass integration as well as intensified processes add to the complexity of the process system by increasing interactions and interdependencies among various process subsystems, which eventually make the integrated design and control absolutely necessary.

1. Introduction

Nowadays, a wide variety of fine chemicals are produced under stringent sustainability requirements utilizing clean and renewable energy sources. A significant research effort has been invested in order to further improve process efficiency and limit exergy losses through a process design procedure that aims to optimize economic criteria (e.g., total annualized cost). Process design procedure involves several steps. A first step would be process synthesis, where alternative flowsheet structure configurations and unit interconnections are determined. Subsequently, the calculation of the structural parameters (e.g., equipment type, geometry, and dimensions) must be performed along with the determination of the nominal operating conditions. Usually, the evaluation of alternative process flowsheets is performed within an optimisation framework that utilizes engineering knowledge and experience in order to define a meaningful design space. Within such framework performance specifications, safety regulations and environmental constrains are explicitly taken into account, whereas a representative objective function encompasses the economic impact of the process system. However, process systems operate in a continuously changing environment due to exogenous disturbances, intrinsic process uncertainties, switching between different operating conditions and so forth. In order to satisfy product and safety specifications and environmental regulations under such variable conditions, the design of an efficient automatic control system is absolutely essential to achieve an acceptable dynamic performance. The selection of the control objectives that best serve the process specifications, the definition of the input-output structure, the selection of the appropriate control algorithm and its tuning are key features of the control system design. In a sequential approach, where the major process design decisions for the process flowsheet have been determined before the design of the control system the achievable dynamic performance cannot overcome the restrictions imposed by the process structure. It is therefore important to simultaneously design process and control systems so that such burdens are lifted and superior performance is achieved under both nominal and variable operating conditions (Seferlis and Georgiadis, 2004). A schematic of the integrated process and control system design that incorporates the decisions that need to be made is shown in Figure 1.

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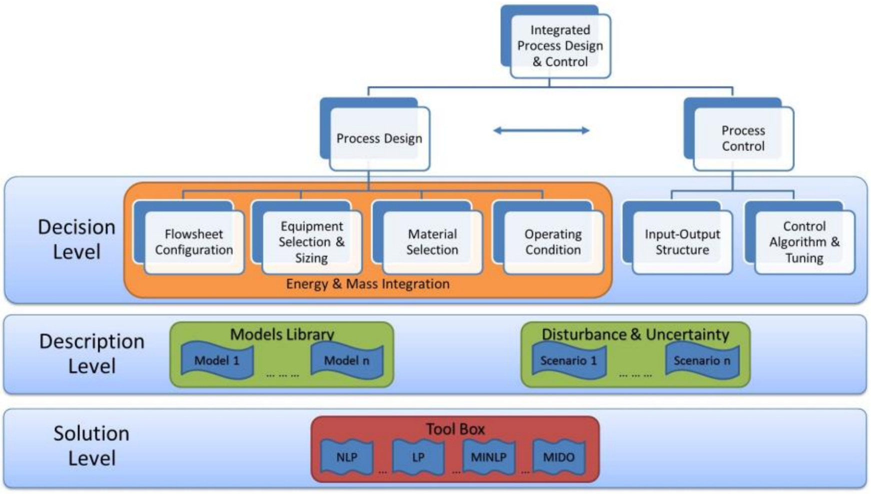

Figure 1: Integrated process design and control procedure.

2. Motivating process example

Heat and mass integration of processes as well as process intensification generally improve greatly the efficiency and economic performance but usually results in highly complex processes where strong interactions among individual units make the control system design even more challenging and demanding, leading to plants that are difficult to control. Such an illustrative example is presented by Kyriakides et al. (2017), in which the integration of a catalytic reactor along with a membrane based separation unit are combined into an integrated membrane reactor (IMR) as shown in Figure 2a, for H_2 production via low temperature methane steam reforming (MSR). The IMR is a process where the step of production (through MSR reaction) and the step of product purification (utilizing a Pd-based membrane) are conducted simultaneously. Reactants (CH_4 and steam) are fed into the IMR, where the reforming reactions take place and at the same time H_2 is separated through the membrane that is placed on the surface of the inner tube separating the reaction from the permeation zone. Since the equilibrium is shifted towards H_2 production due to its removal from the reaction zone, a very high CH_4 conversion at relatively low temperature levels can be achieved in such a reactor. Interaction in such a process system is extremely high as a disturbance in the balance of the reforming reactions may greatly affect both the reacting and the separation tasks. Disturbances in this system are frequent as the catalytic reactions need to be thermally balanced with the outer heat source and the removed H_2 through the selective membrane.
A simple alternative design consists of a cascaded arrangement between a reactor (Figure 2b) and a membrane based separator (Figure 2c) module in series (CRM), where H_2 purification takes place only after the reaction step is completed. The reactive mixture is fed into the reactor and only after exiting the reactor module (at equilibrium composition) is fed to the membrane separator, where H_2 is separated through the membrane (inner tube). Such configuration is simpler to construct and probably involves lower investment costs than the integrated membrane reactor module. However, the manipulation of the H_2 purification conditions can be performed only after the manipulation of the reaction conditions. For example, when biogas (mainly consisted of CH_4 and CO_2) is utilized instead of pure CH_4, where its composition may deviate greatly, concentration disturbances will affect H_2 separation with a time delay at least equal to the mean residence time of the reactor. Such time delays may result in longer response periods by the control system with significant violation of the product specifications. On the other hand, the direct contact between the reactive mixture and the membrane, although it increases the complexity of the system, provides the opportunity for the simultaneous manipulation of the reaction and permeation zone operating conditions, making the system more prone to disturbances but simultaneously enabling a quicker response.
A process system such as the one described above is difficult to be designed to operate optimally under variable operating conditions unless an integrated process and control system design approach is employed. Truly, a highly intensified process may possess several advantages in terms of controllability effectiveness even though higher investment costs are associated due to the uniqueness of the process equipment and the more sophisticated control algorithms that are required to be installed. In addition to the key flowsheet configuration decisions, the equipment sizing and connectivity of the streams and in particular recycle streams offer key opportunities to assist the ability of the overall process system to cope with disturbances and uncertainty.

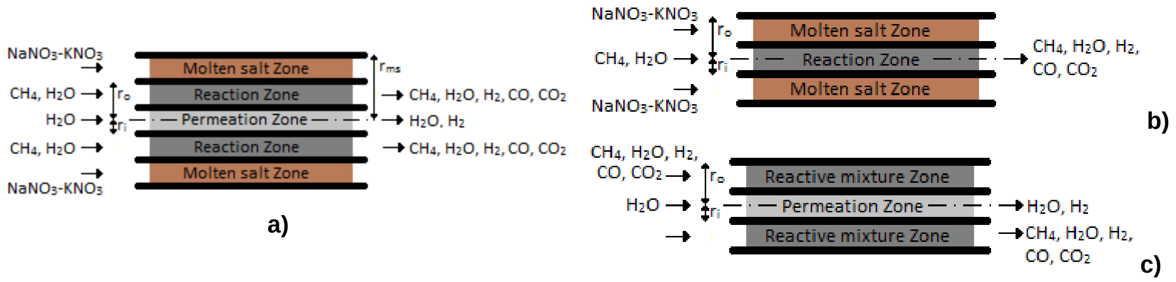

Figure 2: a) Integrated membrane reactor module geometry (IMR flowsheet) and Cascaded b) reactor and c) membrane module geometry (CRM flowsheet).

3. Integration of process design and control technologies

A large variety of methods are proposed in the literature that address the simultaneous process and control system design utilizing various sets of comprehensive criteria, that aim to take into account the underlying interactions among the design decisions. Such criteria, that would consider the ability of the process to achieve a desirable dynamic performance, usually incorporate properties like feasibility, flexibility, controllability and operability. Feasibility is the ability of ensuring feasible steady-state operation, meaning satisfying the operational inequality constraints (e.g., operational limits, product specifications, safety regulations) for a chosen control action when design variables and uncertain parameters are given (Swaney and Grossmann, 1985). Flexibility, as described by Swaney and Grossmann (1985), is the ability of ensuring feasible steady-state and dynamic operation over a variety of operating conditions. Controllability, among different definitions that can be found in literature, most commonly is considered as an inherited characteristic of the system indicating the existence of the system's (process and control system) ability to achieve the desired performance despite the presence of disturbances and uncertainties using available inputs and measurements (Skogestad and Postlethwaite 1996). Operability, which includes all the aforementioned features, describes the capability of the process (given the available set of external inputs) on satisfying the desired steady-state and dynamic conditions under the presence of uncertainties and anticipated disturbances, without violating any performance process constraints.

3.1 Problem formulation

The conceptual formulation of the problem of integration of design control in its most general form can be expressed as a mixed-integer dynamic optimisation (MIDO) problem. As shown in Eq(1), the optimisation problem that involves the maximization of a performance index is subject to the differential and algebraic equations of the process, the inequality constraints that define the feasible region and possibly the flexibility space and the controller differential and algebraic equations.

$$
\begin{aligned}
&\text{Max (Performance Index)} \\
\text{s.t.:}\quad &\text{Process Physical Model (Differential and Algebraic Equations, Inequality Constraints)} \\
&\text{Controller Relations (Differential and Algebraic Equations)}
\end{aligned}
\qquad (1)
$$

The decision variables of the problem in Eq(1) are the integer variables associated with flowsheet configuration, equipment and material selection and control system input-output structure as well as the continuous process and controller variables associated with the sizing of the selected equipment, the operating conditions and the tuning of the selected control algorithm.

Mohideen et al. (1996) introduced a MIDO framework to simultaneously design and control dynamic systems in the presence of process uncertainty and disturbances. The optimisation was performed through an iterative decomposition technique that separated the problem into the solution of a multi-period design and control problem followed by the solution of a dynamic feasibility problem. Matrix norms were also used to account for process stability in the presence of uncertainty and disturbances. Luyben and Floudas (1994) proposed a similar problem formulation which combined process synthesis, design and control. The proposed procedure was consisted of four steps, where process synthesis was addressed through the search within a set of flowsheet superstructures that included several possible design alternatives. Then the superstructures were translated into mathematical models and the multi objective optimisation problem was solved using a generalized Benders decomposition (GBD) algorithm and finally the best compromise solution was obtained. Narraway and Perkins (1993) have proposed a method based on the minimization of the economic penalties associated with the back-off from active constraints. The importance of this contribution was the incorporation of economic goals into the problem definition. In most cases economic objectives are fulfilled on the intersection of the constraints but uncertainties and disturbances tend to violate these constraints. Therefore, the operating point should be moved within the feasible region away from the constraints intersections to enable feasible operation at the presence of disturbances. The back-off method was also extended to time domain controller design by considering decentralized (Heath et al.,2000) and centralized (Kookos and Perkins, 2003) PI controllers. The performance index is usually formulated in such way that takes into account the annualized process capital cost (based on steady state economics) and the operational cost. The effect of the dynamic performance was expressed by the variability cost (Ricardez-Sandoval et. al, 2008) which reflects to the possible losses during dynamic transitions by applying a penalty for economic losses due to non-optimum or not-on-specs performance usually expressed in terms of aggregate or average deviations. Sharifzadeh (2013) reported that the incorporation of the controllability measures into the process design as a multi-objective optimisation was helpful in obtaining design of superior control performance.

3.2 Decision Level

The first key aspect of differentiation of the proposed approaches is related to the extent of decisions that are included in the integrated design procedure of Figure 1. For example, the process synthesis step that also involves equipment and material selection is not usually incorporated due to the high combinatorial complexity it introduces. Similarly, the control algorithm is selected a priori based on guidelines that are derived from the nature of the process system and the facilitation of the calculations. However, the controller tuning parameters have been part of the optimisation problem (Mohideen et al., 1996). Recent challenges involve the incorporation of heat integration within the process and control system design framework, taking into account the flexibility and structural controllability in a heat exchanger network as presented by Hafizab et al. (2016). Patraşcu et al. (2017) dealt with the process dynamics utilizing an effective control structure of a proposed heat integrated design of a heat pump assisted extractive distillation process. An attempt in the field of the simultaneous material selection and process design has been described by Papadopoulos et al. (2017). They have developed a systematic methodology addressing the integrated computer-aided molecular and process design (CAMPD) under variability by considering a static operability analysis without however considering explicitly the process dynamics or the control system.

3.3 Description Level

The selection of the appropriate process model and the characterization of the process uncertainties and disturbances are two features that distinguish the proposed integrated design techniques. While the most accurate approach would be to utilize a non-linear dynamic process model, a comparative increase in computational effort is inevitable. Most methodologies utilize linear dynamic or non-linear steady-state models if the degree of nonlinearity in the actual process is moderate. Hamid et al. (2010) presented a systematic model-based methodology for the integration of process design and controller design. The primal problem is decomposed into four sub-problems, namely: pre-analysis, design analysis, controller design analysis and final selection and verification. An extended version of this methodology on binary element reactive distillation processes is presented by Mansouri et al. (2016). Similarly, the selection of the type of the control algorithm to be implemented and the technique used for the pairing of manipulated and controlled variables in the case of decentralized controllers, can significantly affect the complexity of the mathematical model and its solution. Conventional PID controllers in multi-loop schemes (Ricardez Sandoval et. al, 2008) or perfect control, where controlled variables are kept constant with manipulated variables adjusted accordingly (Kookos and Perkins, 2003) are usually implemented. In some cases, advanced model-based control schemes, like model predictive control (Sanchez-Sanchez and Ricardez-Sandoval, 2013) improved the achieved process economics and controllability. A comparison between the utilization of PI and MPC control scheme is performed under an integrated procedure by Sanchez-Sanchez and Ricardez-Sandoval (2013) and Gutierrez et al. (2014). The main drawback when advanced control schemes are used is that solving a dynamic optimisation problem requires an increased computational effort.

Another feature related to the decomposition of the proposed framework is the way that these frameworks deal with the uncertainty of several model parameters and the disturbances that are taken into account. Ricardez-Sandoval et al. (2008) attempted to implement uncertainty in the process model parameters, in which linearized dynamic process models are utilized. Even though, the process configuration as well as the control algorithm was specified a priori, the optimisation framework was formulated in such way that different process models (e.g., finite impulse response) and alternative control algorithms could be used. In addition, stochastic approaches, such as worst-case variability (Ricardez-Sandoval et al., 2012), were implemented in order to study the behaviour of the system to the time dependent disturbance profile that produced the largest variability in the system. The flowsheet synthesis and control structure selection was then performed using Monte Carlo sampling techniques to characterize the worst-case variability scenario. An approach of analysing the sensitivity of the system dynamics through eigenvalue and transmission zeros tracking with respect to variations in operating conditions, design changes and disturbances was presented by Seferlis (2010).

3.4 Solution Level

A third key feature of the proposed approaches is related to the chosen solution procedure of the decomposed procedure. The main categories can be identified towards this direction, with the first category assess controllability analysis (e.g. RGA and condition number) during the design of the process and utilizing it as a decision criterion for the identification of a more meaningful and tractable design space. Furthermore, the formulation of the objective function can distinguish one approach from another, where indices that measure controllability (like interaction and error metrics) are used. Such methods, although consider the dynamic performance of the system, use arbitrarily selected weights in the multi-objective function to scale controllability and capital or/and operational cost that are usually not equivalent to the effect on actual economics of the process. A back-off methodology was presented by Rafiei-Shishavan et al. (2017) where power series expansions is employed in order to represent the cost function and the constraints of the optimisation problem. Malcom et al. (2007) presented a procedure that finds the optimal trade-offs between design and control decisions, based on a two-stage decomposed problem that is reduced on terms of size and complexity by utilizing a state-space model. Fuentes-Cortes et al. (2016) presented a multi-objective mixed-integer nonlinear optimisation approach for the optimal design and control of combined cooling, heat and power systems. Nordin et al. (2015) presented a methodology where sustainability criteria are taken into account leading to cost efficient and controllable designs, in a constrained optimisation problem, decomposed in six sequential hierarchical sub-problems.

The second category is consisted of methods that incorporate simultaneous process design and control system design aspects into a single holistic model-based optimisation problem and employ a successive execution of steps for the determination of the optimal solution. To deal with the large computational effort, Bansal et al. (2000) applied dual information and GBD algorithm, whereas full discretization of the dynamic system based on orthogonal collocation was also applied. Sakizlis et al. (2003) and Khajuria and Pistikopoulos (2011) incorporated the concept of parametric programming and extended this method by including multi-parametric model predictive controllers.

4. Conclusions - Challenges

Generally, a truly generalized approach that incorporates every aspect of the integrated process and control system design would require the solution of an extremely complex problem where the computational burden would become cumbersome. In order to obtain a meaningful and realizable solution the integrated problem is required to be decomposed into successive and interacting stages where the decision criteria are applied gradually using models and uncertainty characterization techniques of various resolution in order to simplify the calculations but without compromising the validity of the results. Based on the resulting sub-problem an appropriate solution procedure is employed.

Obviously, significant effort should be invested in defining a reasonable design space for the process system. General engineering knowledge, process design heuristics, and hierarchical decomposition of the design decision procedure should be utilized to ensure that the design space encompasses the best performing solutions but efficiently eliminates options of definite inferior performance. Similarly, in the design of the control system, even though controllability is basically considered as an inherent property of the process, the selection of the control algorithm and its employment in the process system plays a significant role. Basically, the control system would enable a more compact process system by transferring process variability from the economically important process variables (e.g., product quality) to the less important variables (e.g., auxiliary utilities). The interaction of the control algorithm with the achieved process design is still quite unexplored. The identification of the optimal model reduction that would allow an accurate process and control system representation but with the least computational effort is a task that requires to become more systematic.

The explicit inclusion of the control system performance in the design of heat and mass integrated process system has started to attract the attention of the research community. Moreover, the integration of materials selection in process and control system design is a new challenge with very few contributions that attempt to investigate the effect of catalysts, reactants, solvents and working media in the overall closed loop system performance, appears as one of the new fields with great challenges to be addressed.

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