Preparation of Papers for IFAC Conferences & Symposia: Integration of Process Design and Control Using Hierarchical Control Structure

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Abstract: The integration of process design and control (IPDC) has become increasingly important and received considerable academic and practitioner attention over the recent decades. Moreover, some works in the field have utilized advanced controllers into IPDC framework. Considering the fact that the hierarchical control structure which consists of local PID controllers and an advanced process control (APC) as the central controller has been used widely in industrial practice, in this paper, the two-level hierarchical control structure is taken into account within the IPDC framework for the first time. The IPDC problem using hierarchical control structure is formulated as a bi-level optimization problem, which separates the design decisions from the APC decisions and then keeps the problem size manageable. And the APC decisions are incorporated in a superstructure-based dynamic optimization formulation which considers both cost and controllability. A continuous stirred tank reactor is used to test the proposed IPDC methodology.

Keywords: process design, hierarchical control structure, bi-level optimization, integration, advanced process control

1. INTRODUCTION

Traditionally, process design and control system design are carried out sequentially (Douglas, 1988). That is, in the first step, process design is preformed that is based on steady state economic calculations; subsequently, a suitable control structure is synthesized that is generally based on heuristic rules. Therefore, the process design and controller design have been usually considered independently. Recent results of research in this field have proved that integration of process design and control (IPDC) may bring about considerable economic and operability benefits over the traditional sequential design approach. The integration of process design and control has become increasingly important and received much attention from both academic and industrial interests. A recent comprehensive review of the integration of process design and control for chemical processes can be found in Seferlis and Georgiadis (2004), Yuan et al. (2012), Sharifzadeh (2013) and Vega et al. (2014a, 2014b).

Generally, the key difficulty in the IPDC approaches for chemical processes is the computationally intensive and challenging solution procedure. Therefore, only a few works in the field of IPDC have considered incorporating advanced process control into the IPDC framework. However, more advanced control strategies need much higher computational requirements. Generally, most of the IPDC approaches using APC try to avoid the on-line solution of an optimization problem for APC. Brengel and Seider (1992) proposed firstly an approach for incorporating model predictive control (MPC) into a process design scheme. Baker and Swartz (2006) presented an IPDC approach in which the MPC optimization sub-problem is replaced by its Karush-Kuhn-Tucker (KKT) optimality conditions. In Miranda et al. (2008), two different solution methods were presented using Pontryagin's minimum principle. In Sakizlis et al. (2003, 2004), the advanced model-based predictive controllers were incorporated into the IPDC framework, in which the parametric programming technique was used to obtain the explicit state feedback control law for the designed process and remove the need for solving an optimization problem on-line. Linninger and co-workers (Malcolm et al., 2007) presented an embedded control optimization-based IPDC framework, in which linear quadratic regulator (LQR) was considered. Ricardez-Sandoval et al. (2013) provided a robust-based optimization approach to solve the IPDC problem, where MPC strategy was incorporated for optimal process design under uncertainty.

On the other hand, the hierarchical control structure consisting of lower-level conventional PID regulators and a higher-level advanced process control (APC), e.g., model predictive controller, has been widely used in modern processing plants (Qin and Badgwell, 2003). Therefore, the emphasis on incorporating the hierarchical control structure into the IPDC of chemical processes is essential for chemical engineering practice. However, to the authors' knowledge, no study about this issue has been reported in published literature.

In this study, the main contribution is that the hierarchical control structure is incorporated into the IPDC framework. In addition, in order to make the IPDC problem easier to tackle, a bi-level optimization strategy is utilized, which is an efficient and practical optimization scheme to reduce the complexity of the original IPDC optimization problem. Finally, a continuous stirred tank reactor (CSTR) example is applied to demonstrate the effectiveness of the proposed integration method.

2. METHODOLOGY

2.1 Problem Description

The IPDC considers simultaneously steady-state design and dynamic control into one optimization step in order to obtain an economically optimal plant, with the best process structure, dimensioning and operating conditions together with control structures and controller parameters in the presence of external perturbations and uncertainties in the process parameters. The problem of the integration of process design and control can be conceptually posed as follows (Pistikopoulos and Sakizlis, 2002):

minimize Expected Total Annualized Cost

subject to

Differential-Algebraic Process Model

Inequality Path Constraints

Control Scheme Equations

Process Design Equations

Feasibility of Operation (over time)

Process Variability Constraints

It is shown that the IPDC problem is a mixed integer dynamic optimization (MIDO) problem, which is an extremely challenging problem to the existing mathematical programming techniques.

2.2 IPDC Formulation Using Hierarchical Control Structure

In modern processing plants, the APC controller is part of a multi-level hierarchy of control functions. The PID controllers at the lowest layer reject disturbances, and the APC controller is deployed in major process units to supervise several regulatory PID controllers. APC strategy combined PID cascade control structure can obtain excellent set-point tracking performance and robustness under various process constraints. In our work, the designed processes and PID control closed loops are treated as generalized object and controlled by APC. Then, the complicated IPDC using hierarchical control structure is formulated as a tractable bi-level optimization problem. At one level, where APC decisions are not made and instead incorporated for each candidate design, the design decisions such as equipment sizes that govern the dynamic performance are searched by dynamic optimal design. At another level, the dynamic process performance is evaluated using an optimal APC controller for each design candidate. Fig. 1 depicts the proposed solution framework for IPDC using hierarchical control structure.

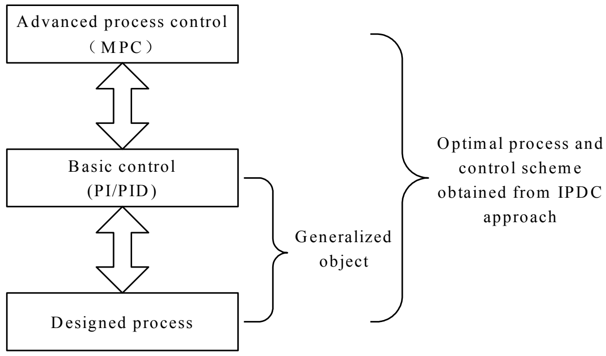

Fig. 1 IPDC framework using hierarchical control structure

Hence, this new problem can be formulated a bi-level optimization framework as follows:

$$
\begin{aligned}
&\min_{\mathbf{d},\mathbf{x}(t),\mathbf{u}(t),\mathbf{X}_p} \psi(\mathbf{d},\mathbf{X}_p) + \int_{t=0}^{t_f} \phi(\mathbf{d},\mathbf{X}_p,\mathbf{x}(t),\mathbf{u}(t))dt \\
&\text{s.t.} \\
&\quad f(\dot{\mathbf{x}}(t),\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t),\mathbf{d},\mathbf{X}_p) = 0 \\
&\quad h(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t),\mathbf{d},\mathbf{X}_p) = 0 \\
&\quad g(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t),\mathbf{d},\mathbf{X}_p) \le 0 \\
&\quad \min_{\mathbf{d}_c} \int_{t=0}^{t_f} \phi(\mathbf{d}_c,(t),\mathbf{u}(t))dt \\
&\quad \text{s.t.} \\
&\quad\quad f(\dot{\mathbf{x}}(t),\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t)) = 0 \\
&\quad\quad h(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t)) = 0
\end{aligned} \tag{1}
$$

where ψ is the function of capital cost; ϕ is the function of operation cost; $\mathbf{x}(t)$ is the vector of state variables; $\mathbf{z}(t)$ is the vector of algebraic variables; $\mathbf{u}(t)$ is the vector of manipulated variables; $\mathbf{d}$ and $\mathbf{X}_p$ are the vector of design variables and integer variables defining process topology, respectively; $\mathbf{d}_c$ is the vector of controller parameters; f and h are the vector function of the differential equations and algebraic equations of the process, respectively; g is the vector function of the inequality constraints of the process.

As showed in (1), one level problem is to minimize the total annualized cost (comprising capital cost and operating cost) and another level objective is to obtain optimal APC decisions.

The new formulation separates the design and APC control problems by utilizing bi-level programming, which keeps the IPDC problem size manageable and reduces the computational complexity. Additionally, the PID control decisions are embedded into the generalized object. It is clear that APC decisions are not included at the level of design decisions and process dynamic performance is assessed by solving the process dynamic problems rigorously at the other level. As a result, the superstructure-based formulation considers simultaneously both controllability and economy. Moreover, the closed-loop dynamic performance of candidate design can be assessed by using the optimal APC.

In order to reduce the computational load and eliminate the online control optimization, linear quadratic regulator is used in our study.

Assumed that the linearized state-space model around the operating point can be obtained from nonlinear system dynamics for different candidate designs as follows:

$$\dot{\tilde{x}}_p(t) = A_p \tilde{x}_p(t) + B_p \tilde{u}_p(t) \tag{2}$$

$$\tilde{y}_p(t) = C_p \tilde{x}_p(t) \tag{3}$$

PI controllers are used as low-level controllers.

$$\tilde{u}_p(t) = u_{p,0} + K_p(e + \frac{1}{T_i}\int edt) \tag{4}$$

$$e = \tilde{u}_{sp}(t) - \tilde{y}_p(t) \tag{5}$$

Thus, the generalized state-space model can be defined as follows:

$$\dot{\tilde{x}}(t) = A\tilde{x}(t) + B\tilde{u}_{sp}(t) \tag{6}$$

$$\tilde{y}(t) = C\tilde{x}(t) \tag{7}$$

where $\tilde{x}(t) = \begin{bmatrix} \tilde{x}_p(t) \\ \tilde{x}_q(t) \end{bmatrix}$; $\tilde{x}_q(t) = \int edt$; $\tilde{u}_{sp}$ is the outputs of LQR;

$A = \begin{bmatrix} A_p \text{ - } B_p K_p C_p & \frac{B_p K_p}{T_i} \\ -C_p & 0 \end{bmatrix}$; $B = \begin{bmatrix} B_p K_p \\ 1 \end{bmatrix}$; $C = \begin{bmatrix} C_p & 0 \end{bmatrix}$.

Then, the LQR problem can be mathematically defined as follows:

$$\begin{aligned} & \min \frac{1}{2}\int (\tilde{x}(t)^T Q\tilde{x}(t) + \int (\tilde{u}_{sp}(t)^T Q\tilde{u}_{sp}(t)) \\ & \text{s.t.} \\ & \dot{\tilde{x}}(t) = A\tilde{x}(t) + B\tilde{u}_{sp}(t) \end{aligned} \tag{8}$$

An explicit control law can be derived by solving the above LQR problem.

It should be noted the PID controller parameters are included in the generalized object and updated at each iteration step.

Based on these developments, the proposed bi-level optimization framework for the solution of IPDC using hierarchical control structure involves the following steps

Step 0 (initialization). Set the initial guess of design parameters, e.g., equipment sizes, process structure.

Step 1. Linearize process dynamic model and obtained PI controller parameters with economically tuned controllers or Ziegler–Nichols tuning rule. Then, fix the process design obtained from last iteration and obtain the generalized state-space model. Finally, optimal LQR control law can be obtained subsequently. In this step, the dynamic performance is evaluated for given design decisions.

Step 2. Incorporate the obtained LQR control decisions into a superstructure-based process design optimization problem. And then obtain the resulting optimal decision variables by dynamic optimization.

Step 3. If the stopping criterion ($\left\|\mathbf{d}^k - \mathbf{d}^{k-1}\right\| \le \varepsilon$) is satisfied then stop and the optimal solution has been obtained. Else, go to Step 1.

In the next section, a case study of chemical processes will be used to illustrate the application of the proposed method.

3. CASE STUDY

In this section, the methodology proposed in the previous section is applied for the integration of process design and control of a CSTR. Fig. 2 presents the process flow-sheet for the case study.

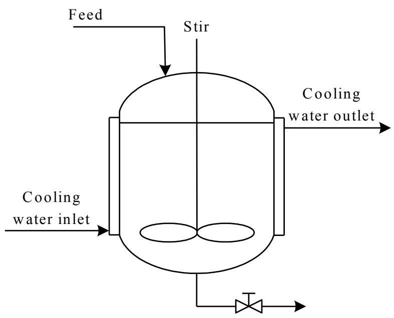

Fig. 2. Flowsheet for the CSTR process

An exothermic, irreversible reaction, of the type A→B, which transforms reactant A into product B takes place in the continuous stirred tank reactor. The CSTR dynamic model is a set of nonlinear ordinary differential equations obtained from dynamic material and energy balances as follows:

$$\frac{dC_A}{dt} = (\frac{F}{V_R})C_{A,0} - (\frac{F}{V_R})C_A - C_A k_0 e^{-\frac{E}{RT_R}} \tag{9}$$

$$\begin{aligned} \frac{dT_R}{dt} = & (\frac{F}{V_R})T_0 - (\frac{F}{V_R})T_R - \frac{\Delta H_R C_A k_0}{\rho_R C_{PR}} e^{-\frac{E}{RT_R}} \\ & - \frac{U_R A_R}{\rho_R V C_{PR}}(T_R - T_J) \end{aligned} \tag{10}$$

$$\frac{dT_J}{dt} = (\frac{F_J}{V_J})(T_{J,0} - T_J) + \frac{U_R A_R}{\rho_J V_J C_{PJ}}(T_R - T_J) \tag{11}$$

where C_A is the concentration of reactant; F is the process flow rate; V is the CSTR volume; $C_{A,0}$ is the feed concentration; k_0 is the reaction rate constant; E/R is the activation energy term; T_R and T_J are the reactor and jacket temperatures, respectively; T_0 is the feed temperature; ΔH_R is the reaction enthalpy; U_R is the heat-transfer coefficient; A_R is the reactor heat-transfer area; C_{PJ} and C_{PR} are the heat capacity of water and the reaction mixture, respectively; ρ_R and ρ_J are the liquid density of the reaction mixture and water, respectively; F_J is the inlet flow rate of cooling water; $T_{J,0}$ is the inlet temperature of cooling water; V_J is the jacket volume. The detail of the CSTR model parameter values used in this work is given elsewhere (Seferlis and Georgiadis, 2004).

The (9-11) based on mass and energy balances constitute the fundamental process model equations. The following restrictions are considered in the design formulation:

$$V_R = \frac{\pi}{4} D_R^2 L_R \,, \quad A_R = \pi D_R L_R \tag{12}$$

$$L_R = 2D_R \,, \quad V_J = 0.25 V_R \tag{13}$$

$$1 \le D_R \le 6 \,, \ 0 \le C_A \le 800.9 \,, \ 300 \le T_R \le 333.15 \tag{14}$$

where L_R and D_R are reactor height and diameter, respectively.

Assuming that there is a time varying sinusoidal disturbance in the coolant inlet temperature around an uncertain mean value:

$$T_{J,0} = 294 + 5\sin 2t \tag{15}$$

A PI controller has been considered to control this process. The controlled variable is the reactor temperature; the manipulated variable is the flow rate of cooling water that is adjusted to maintain the reactor temperature at the desired level and to get a minimum of 95% conversion.

Here, the objective for the CSTR case study is to minimize the capital and operation cost, and the closed-loop variance that is able to satisfy the product specification, while maintaining the feasible operation of the reactive process against the external disturbance. The process design variables include the reactor geometry, reactor temperature set point, feed flow, coolant flow. The control system design includes the tuning parameters of the PI controller.

The objective function is to minimize the sum of the annualized capital and operating costs. The objective functions are respectively given by

$$\min_{D_R, F_J, T_R, T_J, C_A} J = c_1 r D_R^{1.066} H_R^{0.802} + c_2 \int_0^{t_f} F_J \, dt \tag{16}$$

The objective is to find the economically optimal reactor volume and nominal steady-state operating conditions (reactant and cooling rate) such that feasible operation is maintained for the coolant inlet temperature disturbance. The problem is solved as a dynamic optimization problem.

The optimal CSTR design, operating conditions and controller parameters and associated costs are shown in Table 1. In addition, the results are compared with that obtained using the sequential strategy with optimal tuned controllers. The CSTR system resulting from the integrated approach using hierarchical control structure has lower total cost. The sequential design was tested in the existence of the sinusoidal cooling water inlet temperature. This was solved as a dynamic optimization problem where the controller parameters and set-point of the PI controller were searched to minimize the sum of the constraint violations. After the dynamic feasibility was tested, the optimal tuning parameters, set-point and bias of the PI controller were obtained to minimize the total annualized cost of the system. The 1st column of Table 1 represents the sequential design result. As opposed to this sequential procedure, the integrated approach extracts a better economic advantage (Column 2 Table 1). Note that the integrated approach has higher the operating cost, but the difference is small. In fact, the cost of cooling water can be negligible compared to that of the reactor in this case.

Table 1. Comparison of Optimal CSTR obtained from sequential and integrated method

Variable	Sequential approach	Integrated approach
D_R (m)	4.15	4.11
T_{R_setpoint} (K)	332.86	332.99
K_c	−5	−10.10
T_i	100	49
Capital cost ($/yr)	4.388e4	4.299e4
Operating cost ($/yr)	1.781e3	1.787e3
Total cost ($/yr)	4.566e4	4.478e4

Figs. 3-4 show the dynamic profiles of the controlled variables for both the sequential and the integrated approaches proposed. The result clearly shows that better dynamic performance has been achieved within constraint boundary using the proposed approach. Meanwhile, the integrated approach gives tighter the reactant concentration control with a closer to the constraint boundary of 800.9 mol/m^3.

4. CONCLUSIONS

In this work, from the applications point of view, the hierarchical control structure has been taken into account within the IPDC framework. The key for solving the resulting IPDC problem is to utilize an efficient bi-level optimization strategy that separates the design decisions from the APC decisions and then keeps the problem size manageable. The case study illustrated to show suitability of our methodology. However, in this paper, uncertainties in the process parameters and multi-input multi-output processes are not considered. In future, more complex chemical processes under uncertainty will be examined.

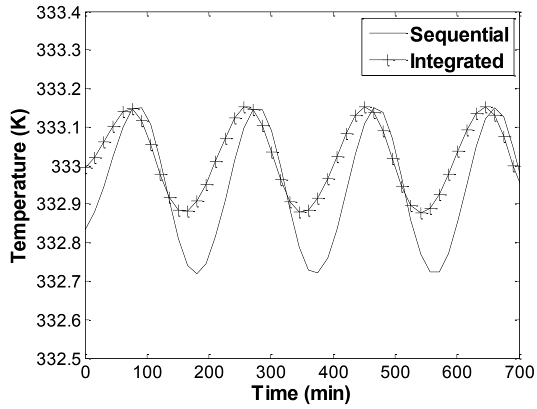

Fig. 3. Comparison of the reactive temperature using sequential and integrated design/control strategies.

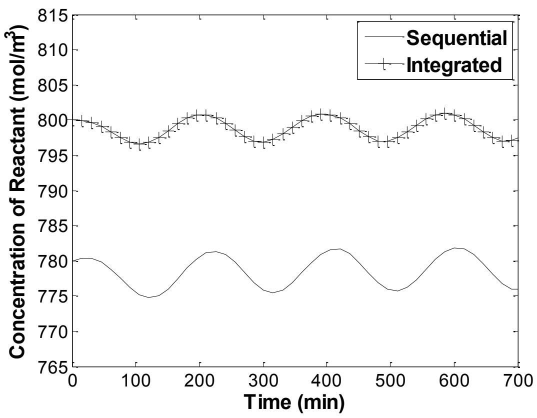

Fig. 4. Comparison of the concentration of reactant using sequential and integrated design/control strategies.

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