Integration of Modeling, Design and Control for Efficient Operation of Chemical Processes

Abstract
The purpose of this study is to develop a model-based methodology for integration of process design and control (IPDC) problem. The new methodology is organized in four hierarchical stages based on a decomposition of the general optimization problem. The objective of each stage is to define the search space and enumerate a set of promising candidates. In each subsequent stage, the search space is reduced until in the final stage only a small number of candidates need to be evaluated. Therefore, while the problem complexity increases with every subsequent stage, the dimension and size of the problem is reduced. The proposed methodology does not have difficulties in handling complex problem formulations with larger number of variables and constraints, and its applicability is highlighted in solving simple optimization problem.

Introduction
Traditionally, chemical process design and process control are two engineering problems that performed independently, with little or no feedback between each other. Figure 1 shows a schematic representation of the two problems. That is, first the process is designed to achieve an optimum objective based on a fully specified nominal case. Only after the process has been designed the operability aspects are taken into account. These might include the control system design and the safety, reliability and the flexibility of the design. Chemical processes therefore tend to be highly constrained with few degrees of freedom left for process control purposes. This conventional sequential-forward approach has some inherent limitations such as dynamic constraint violations, process overdesign or under performance and does not guarantee robust performance [1]. In practice, process design is often tackled by chemical and process engineers, while process control is often done by control and instrumentation engineers.

To overcome the limitations encompassed by the conventional approach, a simultaneous approach for exploiting interactions between process design and process control is needed that will include the process design variables as optimization variables whilst, at the same time, optimizing the controller tuning parameters. The potential economic benefits of such a simultaneous approach are also investigated.

Figure 1: Conventional solution approach for process design and control problems.
Figure 2: New approach for simultaneous solution of process design and control problems.

Figure 2 illustrates the simultaneous approach for process design and process control. Using this approach, both process design and control will share the same variable(s) in their decisions.

One important question needs to be answered here. Can we optimize design and control decisions simultaneously to maximize the overall process performance in the presence of the operational and model uncertainty? Or in the simple words, can chemical and process engineers sit down together with control and instrumentation engineers to make simultaneous decisions to guarantee robust performance of the new processes.

The challenges of the integration of process design and control (IPDC) were clearly identified and discussed by several group of researchers [2]. The subsequent section will explain the objective of the entire study. A new problem formulation based on decomposition methodology will be presented in Methodology section. Conceptual Validation section will highlight the applicability of the proposed methodology in solving simple optimization problem. This article closes with conclusions and suggestion for future work.

Specific Objective
The aim of this study is to develop a systematic model-based methodology that capable to exploit interactions between process design and process control without having difficulties in handling complex problem formulations with larger number of variables and constraints.

In general, the solution of this IPDC problem will require the determination of:
- the optimal process design, in terms of structural decisions and connectivity (discrete decisions), and the operating parameters/conditions such as reactor volume, column length, etc. (continuous decisions); and
- the optimal control scheme design, in terms of the control configuration, control type, etc. (discrete decisions), and the tuning parameters for the given control structure (continuous decisions).

Methodology
Figure 3 shows an overview of the new IPDC methodology. The new methodology is organized in four hierarchical stages based on a decomposition of the general IPDC problem into four subproblems: (1) pre-analysis stage, (2) steady-state analysis stage, (3) dynamic analysis stage, and (4) evaluation stage. The objective of each stage is to define the search space and enumerate (and/or generate) a set of promising candidates. In each subsequent stage, the search space is reduced until in the final stage only a small number of candidates need to be evaluated. Therefore, while the problem complexity increases with every subsequent stage, the dimension and size of the problem is reduced.

Figure 3: Overview of the new IPDC methodology.
Problem formulation

The general IPDC problem is treated as a mixed-integer dynamic optimization (MIDO) problem where control-related dynamic properties are considered simultaneously with ESSE Index which is index of performance which may include weight on the Economic, and/or Sustainability, and/or Safety, and/or Environmental Impact on the plant in order to design a cost effective, sustainable, and highly controllable process. It can be conceptually posed as follows:

Minimize $ESSE$ Index which may include weight on the Economic, and/or Sustainability, and/or Safety, and/or Environmental Impact on the plant

Subject to

Process control constraints

$$
\begin{align*}
\dot{x} &= f(x(t), u(t), d(t), \Theta(t), t) \\
\dot{x}_m^d &\leq x(t) \leq \dot{x}_m^d \\
u_m^d &\leq u(t) \leq u_m^d \\
h^d(d(x(t), u(t), \Theta(t), t)) &= 0 \\
g^d(d(x(t), u(t), \Theta(t), t)) &\leq 0
\end{align*}
$$

Process design constraints

$$
\begin{align*}
f^s(d, x_s^d, u_s^d) &= 0 \\
x_m^s &\leq x_s^d \leq x_m^s \\
u_m^s &\leq u_s^d \leq u_m^s \\
h^s(d, x_s^d, u_s^d, \Theta_s^d) &= 0 \\
g^s(d, x_s^d, u_s^d, \Theta_s^d) &\leq 0
\end{align*}
$$

Plantwide control structure

$$
y \in \{0,1\}^{NC}
$$

where $x$ is the vector of state variables, $u$ the vector of control variables, $\Theta$ the vector of disturbances, and $d$ is the vector of design variables. Superscripts $d$ and $s$ denote dynamic and steady-state of relevant variables, respectively.

In the objective function (Eq. 1), $\Phi$, represents the ESSE Index which may include weight on the Economic, and/or Sustainability, and/or Safety, and/or Environmental Impact on the plant related to dynamic properties. The system dynamics is described by a set of differential equations given in Eq. 2. Eqs. 3 - 4 are, respectively, the dynamic bounds on system and control variables. In Eqs. 5 - 6, signify possible dynamic equality and inequality constraints, respectively.

The steady-state system is described by a function given in Eq. 7. The steady-state bounds on system and control variables are represented in Eqs. 8 - 9, respectively. In Eqs. 10 - 11, the possible steady-state equality and inequality constraints are expressed, respectively.

In Eq. 12, plantwide control structure selection is considered using binary number. $NC$ represents the total number of possible plantwide control structure from controller superstructure.

In IPDC problem, which is combinatorial in nature, can be solved in many ways, but finding the solution is very important, especially when the constraints representing the process models are nonlinear or their number is large causing difficulties in convergence and computational efficiency. Due to the large number of constraints involved, the feasible region can be very small compared to the search space. All of the feasible solutions to the problem may lie in that relatively small portion of the search space. The ability to solve such problems depends on the ability to identify and avoid the infeasible portion of the search space. One way to this is by decomposing the problem into subproblems, which are relatively easy to solve.

In Figure 4, we present a decomposition methodology of general IPDC problem into subproblems that correspondence to their subsequent stages of the new model-based IPDC methodology. In this way, the solution of the decomposed set of subproblems is equivalent to that of the original general IPDC problem. The advantage is a more flexible solution approach together with relatively easy to solve subproblems and a solvable final optimization subproblem no matter how complex the problem formulations are.

**Conceptual Validation**

The solution through the proposed decomposition methodology is illustrated with the help of an analytical example. The objective here is to highlight the applicability of the decomposed methodology to solve a simple optimization problem. The example is a small MINLP problem, have been illustrated in [3], which is solved through the decomposition approach.

$$
\begin{align*}
\min & \quad 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \\
\text{subject to} & \\
x_1^2 + y_1 - 1.25 &= 0 \\
x_2^{1.5} + 1.5y_2 - 3 &= 0 \\
x_1 + y_1 - 1.6 &\leq 0 \\
1-333x_2 + y_2 - 3 &\leq 0 \\
x_1, x_2 &\geq 0 \\
y_1, y_2 - 1 &= 0 \\
-y_1 - y_2 + y_3 &\leq 0 \\
y_1, y_2, y_3 &\in \{0,1\}
\end{align*}
$$
The above MINLP problem is decomposed using a proposed decomposition methodology and shown in Figure 5. Since this is MINLP problem, then it is only decomposed into 3 stages where the Stage 3 of dynamic analysis is skipped since there are no dynamic constraints involved.

The MINLP problem is reduced to an NLP problem for each set of candidates selected from Stage 2. For the selected feasible solutions, the NLP problems are solved using ICAS MoT, and the solution having the minimum objective function value is the optimal solution for the MINLP problem. The solutions are given in Table 1. The smallest objective function value is 7.9311, corresponding to (1,1,1). Therefore, the optimal solution for the MINLP problem using decomposed methodology, which could also been obtained by other method in [3], is

\[ y_1, y_2, y_3, x_1, x_2, f_{obj} = (1, 1, 1, 0.5, 0.000, 1.3103, 7.9311) \]

Table 1: Solution of NLP Problems

<table>
<thead>
<tr>
<th>candidate</th>
<th>( x_1 )</th>
<th>( x_2 )</th>
<th>( f_{obj} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,1,1)</td>
<td>0.5000</td>
<td>1.3103</td>
<td>7.9311</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>0.5000</td>
<td>1.3103</td>
<td>8.4311</td>
</tr>
</tbody>
</table>

Conclusions and Future Work

This article presents a new model-based methodology for solving simultaneous process design and process control problems. The methodology is organized in four hierarchical stages based on a decomposition of the general optimization problem into four sub-problems: (1) pre-analysis stage, (2) steady-state analysis stage, (3) dynamic analysis stage, and (4) evaluation stage. The objective of each stage is to define the search space and enumerate (or and/or generate) a set of promising candidates. In each subsequent stage, the search space is reduced until in the final stage only a small number of candidates need to be evaluated. Therefore, while the problem complexity increases with every subsequent stage, the dimension and size of the problem is reduced. The applicability of this methodology was highlighted in solving simple optimization problem. The result shows that the new methodology is able to find the same solution reported by others. In the future, this new methodology will be implemented in solving more complex IPDC problem involving reactor-separator-recycle system.

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References