



Mohd. Kamaruddin bin Abd. Hamid

Phone: +45 4525 2912
Fax: +45 4593 2906
E-mail: mka@kt.dtu.dk
WWW: <http://www.capec.kt.dtu.dk>
Supervisors: Prof. Rafiqul Gani

PhD Study
Started: July 2007
To be completed: June 2010

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) problems. 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/test a set of promising (feasible) 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 large number of variables and constraints, and its applicability is highlighted in relevant case studies.

Introduction

Traditionally, chemical process design and process control are two separate engineering problems that are 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 that will include the process design variables as optimization variables whilst, at the same time, optimizing the controller tuning parameters, is needed. The potential economic benefits of such a simultaneous approach are also investigated.

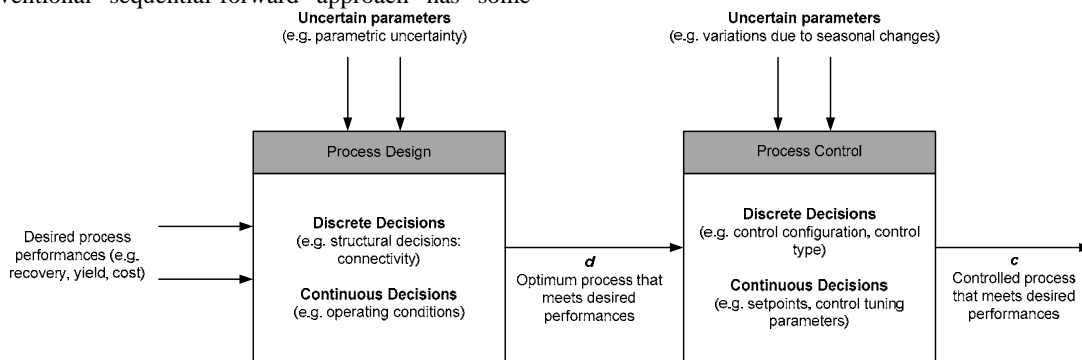


Figure 1: Conventional solution approach for process design and control problems.

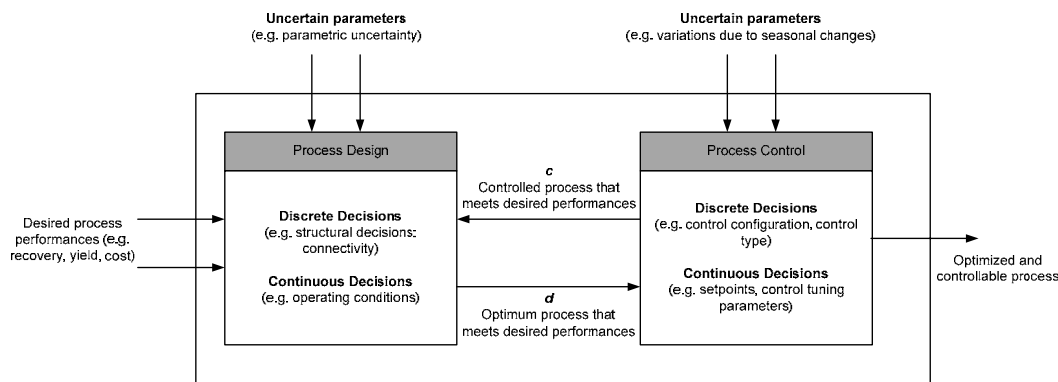


Figure 2: New approach for simultaneous solution of process design and control problems.

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 the design and control decisions simultaneously to maximize the overall process performance in the presence of the operational and model uncertainty? Or, 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 is capable of exploiting the interactions between process design and process control without having difficulties in handling complex problem formulations with large 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.

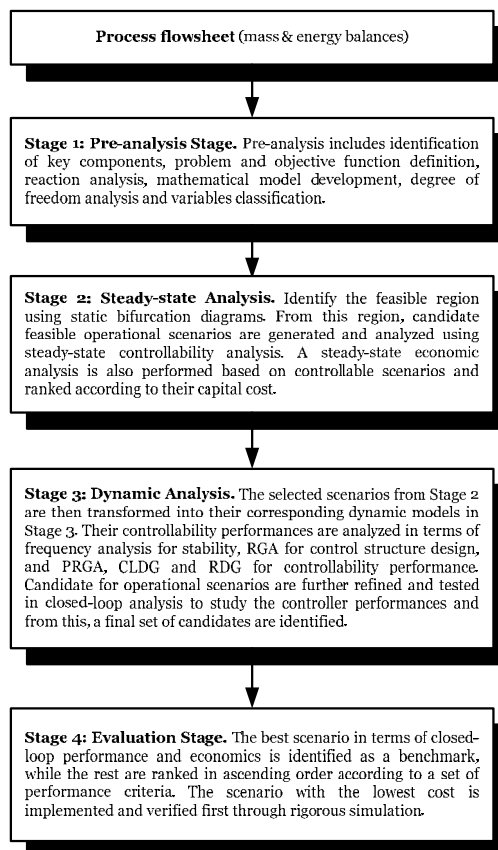


Figure 3: Overview of the new IPDC methodology.

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 that 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 Differential-Algebraic Process Model, Inequality Path Constraints, Control Scheme Equations, Process Design Equations, Feasibility of Operation, Process Variability Constraints

A general formulation for IPDC problem can be presented as:

$$\min_{w.r.t.d,x^s,u^s,x(t),u(t)} I = \Phi(d, x(t), u(t)) \quad (1)$$

s.t.

Process control constraints

$$\dot{x} = f(x(t), u(t), d, \Theta(t), t) \quad (2)$$

$$x_{\min}^d \leq x(t) \leq x_{\max}^d \quad (3)$$

$$u_{\min}^d \leq u(t) \leq u_{\max}^d \quad (4)$$

$$h^d(d, x(t), u(t), \Theta(t), t) = 0 \quad (5)$$

$$g^d(d, x(t), u(t), \Theta(t), t) \leq 0 \quad (6)$$

Process design constraints

$$f^s(d, x^s, u^s) = 0 \quad (7)$$

$$x_{\min}^s \leq x^s \leq x_{\max}^s \quad (8)$$

$$u_{\min}^s \leq u^s \leq u_{\max}^s \quad (9)$$

$$h^s(d, x^s, u^s, \Theta^s) = 0 \quad (10)$$

$$g^s(d, x^s, u^s, \Theta^s) \leq 0 \quad (11)$$

Plantwide control constraints

$$y \in \{0,1\}^{NC} \quad (12)$$

where x is the vector of state variables, u the vector of control variables, Θ 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), Φ , 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 the 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 numbers. NC represents the total number of possible plantwide control structure from controller superstructure.

The IPDC problem, which is combinatorial in nature, can be solved in many ways, but finding the optimal solution strategy is very important, especially when the constraints representing the process models are nonlinear or their number is large thereby 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 problems into subproblems that correspond 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. This is illustrated through a small MINLP problem [3], which is solved through the decomposition approach.

$$\min 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \quad (v1)$$

subject to

$$x_1^2 + y_1 - 1.25 = 0 \quad (v2)$$

$$x_2^{1.5} + 1.5y_2 - 3 = 0 \quad (v3)$$

$$x_1 + y_1 - 1.6 \leq 0 \quad (v4)$$

$$1.333x_2 + y_2 - 3 \leq 0 \quad (v5)$$

$$x_1, x_2 \geq 0 \quad (v6)$$

$$y_1 y_2 - 1 = 0 \quad (v7)$$

$$-y_1 - y_2 + y_3 \leq 0 \quad (v8)$$

$$y_1, y_2, y_3 = \{0,1\} \quad (v9)$$

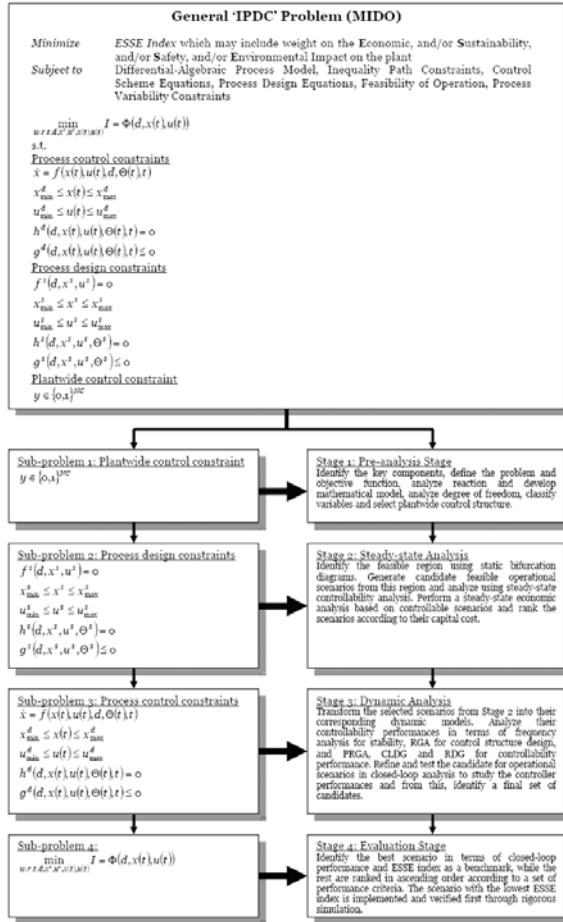


Figure 4: Decomposition methodology.

The above MINLP problem is decomposed using the proposed decomposition methodology as shown in the Figure 5. Since this is an 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 have been obtained by other method in [3], is

$$(y_1, y_2, y_3, x_1, x_2, f_{obj}) = (1,1,1, 0.5000, 1.3103, 7.9311)$$

Table 1: Solution of NLP Problems

candidate	x_1	x_2	f_{obj}
(1,1,1)	0.5000	1.3103	7.9311
(1,1,0)	0.5000	1.3103	8.4311

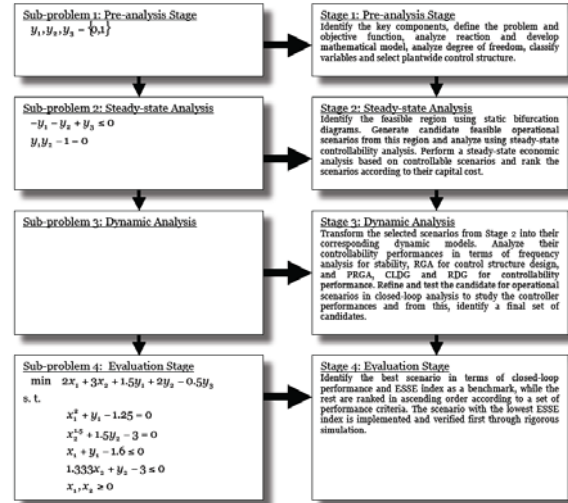


Figure 5: Decomposition methodology of small MINLP example problem.

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 (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 through a simple conceptual example. The result shows that the new methodology is able to find the same solution reported by others. Current and future work is involved with the further development of IPDC and illustrate its application through case studies involving reactor-separator-recycle systems.

Acknowledgement

The author acknowledges the financial support of the Ministry of Higher Education (MoHE) of Malaysia and Universiti Teknologi Malaysia (UTM).

References

1. A. Malcom, J. Polan, L. Zhang, B. A. Ogunnaike, A. A. Lingger. Integrating systems design and control using dynamic flexibility analysis. *AIChE Journal*, 53(8) (2007) 2048-2061.
2. P. Seferlis, M. C. Georgiadis. *The integration of process design and control*. Amsterdam: Elsevier B. V., 2004.
3. A. T. Karunanithi, L. E. K. Achenie, R. Gani. A new decomposition based CAMD methodology for the design of optimal solvents and solvent mixtures. *Industrial & Engineering Chemistry Research*, 44(13) (2005), 4785-4797