A MODEL-BASED METHODOLOGY FOR SIMULTANEOUS PROCESS DESIGN AND CONTROL FOR CHEMICAL PROCESSES

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Abstract

This paper presents a new model-based methodology for integration of process design and control (IPDC) for chemical processes. The proposed systematic model-based methodology does not have difficulties in handling complex problem formulations with larger number of variables and constraints. 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 application of the methodology is highlighted through an ethylene glycol production process. The preliminary results show that the new methodology is able to find the optimum conversion of EO at the minimum operating cost and residence time by considering the operability aspects in a simple and systematic manner.

Keywords

Integration of design and control (IPDC), Model-based methodology, Decomposition method.

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. However, during the last decade, the importance of an integrated process design approach, considering operability together with the economic issues, has been widely recognized. The aim is to obtain profitable and operable process and control structures in a systematic way. The process design characteristics, the control strategies, the control structure and the controller parameters have to be selected optimally in order to minimize the total cost of the system while satisfying a number of feasibility constraints in the presence of time-varying disturbances.

More and more researchers are following the trend towards integration of process design and control (IPDC). As a result, a number of new methodologies has been developed during the last years for addressing the issues raised by IPDC problems. The challenges of the IPDC problems in a reactor-separator-recycle (RSR) system have been clearly identified and discussed by several group of researchers (Ramirez and Gani, 2007; Kiss et al., 2007).

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

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The new problem formulation based on decomposition methodology has been discussed earlier by Hamid and Gani (2007). They have also highlighted the applicability of the proposed methodology by solving simple optimization problem as a conceptual validation. The subsequent sections of this paper explain the proposed model-based methodology in general and highlighting the capabilities of Stage 1 and Stage 2 of the proposed model-based methodology through a case study involving the ethylene glycol production process.

Model-based methodology

Figure 1 shows an overview of the new IPDC methodology. The new methodology is organized in four hierarchical stages based on a decomposition of the general optimization 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.

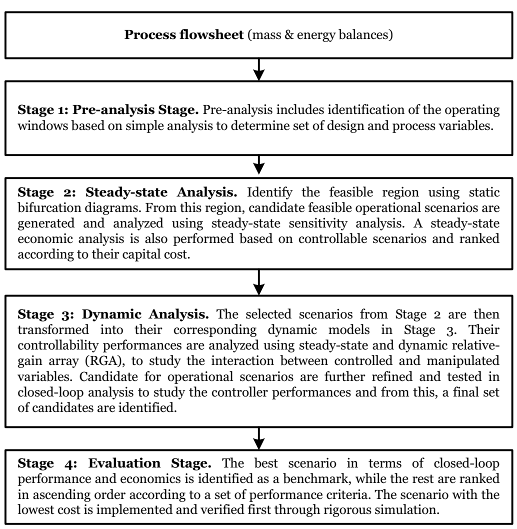

Figure 1. Overview of the new IPDC methodology

One of our main aims is to determine systematically an appropriate set of design (manipulated) and process (controlled) variables that lead to a suitable control structure design. The objective of the first stage is to determine the operating windows of the process using simple analysis. In this stage, an attainable region analysis will be performed to identify the optimum attainable of the process variables (e.g., concentration, conversion, yields, etc.). By using reverse approach, some of the design variables (e.g., flow rates, temperature, etc.) are combined together into coupled parameters (dimensionless number), and the values of these parameters will be determined to match the optimum value of the attainable process variables. From this simple analysis, we can decide the target value of the design (coupled) parameters based on desired process performance, the operational limits (process variables), and desired process behavior.

In Stage 2, the coupled parameters are dissembled with objective to determine the design variables that can match the process variables behavior and the target values of the design variables in Stage 1. If the design targets cannot be matched, new targets are defined in Stage 1 until a match is found. The matching results will determine the feasibility and operability of the process, as well as the search space for the design-process variables. In Stage 2, the overall design targets are defined and the minimum values of the design and process variables that matches this target is found. This means that all decisions that are related to the design-control structure have been made in the early stages of the design process. The process can be described in terms of the performance it will give, the values of the design variables that can achieve that performance, and the values of the process variables that will be attained by the process. From a control design point of view, these process variables will need to be controlled by manipulating the design variables, and the calculated values of process variables correspond to the setpoints for the controlled variables.

A detailed description of all four stages can be obtained from the authors.

Illustrative case study – ethylene glycol production process

This section illustrates the capability of the new model-based methodology for simultaneous process design and control through a case study involving the ethylene glycol (EG) production process.

Description of the ethylene glycol production process

In this case study, the production of ethylene glycol (EG), as shown in Figure 2, from ethylene oxide (EO) and water (W) is a non-equimolar, irreversible reaction and can be represented as follows:

$$C_2H_4O(EO) + H_2O(W) \rightarrow C_2H_6O_2(EG) \quad (1)$$

The rate model is

$$r = kC_{EO}C_W \quad (2)$$

The rate constant is expressed in Eq. (3) and nominal operating point is tabulated in Table 1 below , taken from Kahrs and Marquardt (2007).

$$k = 5.238\exp\left(30.163 - 10583/T\right)\ \mathrm{h}^{-1},\ T(\mathrm{K}) \quad (3)$$

As shown in Figure 2, the reactants EO and W are fed to a reactor, where they react to form ethylene glycol. The unreacted reactants from the reactor are separated from the product in a separator and recycled to the reactor. Since the reactants EO and W are lighter than the product EG, the flowsheet involves one separator and one recycle.

Table 1. Nominal operating point of the ethylene glycol process

Variable	Value	Description
$T_{reactor}$ (K)	295	Reactor temperature
$V_{reactor}$ (m^3)	288.9	Liquid hold-up of the reactor

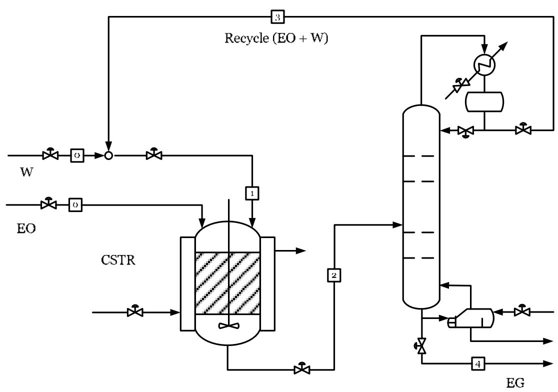

Figure 2. Flowsheet of the ethylene glycol process

Stage 1: Pre-analysis. The objective of this stage is to determine the operating windows of the process using simple analysis. In this article, only a summary of steps involved with Stage 1 is presented. More details of the Stage 1 algorithm can be obtained from the authors.

Can we design a process that can obtain an optimum conversion of EO at the minimum operating cost and residence time by considering the operability aspects?

First of all, we need identify the attainable conversion for this process. In order to do that, the attainable region analysis was carried out and the conversion of EO with respect to residence time is plotted as shown in Figure 3.

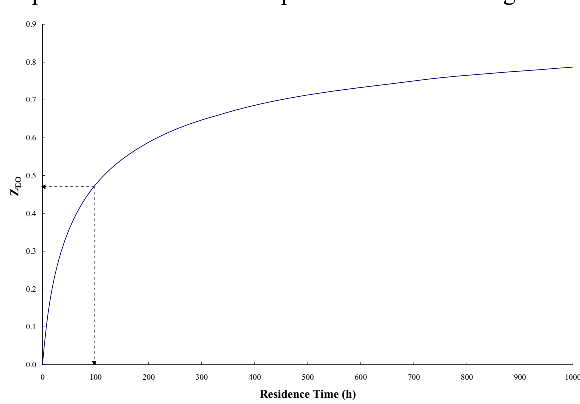

Figure 3. Conversion of EO as function of residence time

From this figure, there are lots of possibilities of finding the optimal solution. To reduce the search space, we limit the attainable conversion region to 100 hours only with maximum conversion of 0.476.

The model that describing the process is represented by Eq. (4). By using the reverse approach, we can decide the target value of the design (coupled) parameters, the Damköhler number (D_a) and the recycle flow rate (f_1) that can match the optimum attainable conversion.

$$D_a = \frac{(f_1+1)}{z_{EO,2}} \frac{1}{(f_1 - f_{W,0}) - (f_1+1)z_{EO,2}} \tag{4}$$

where

$$D_a = \frac{kV}{F_{EO,0}} C_{EO,0}$$

Eq. (4) is a nonlinear algebraic equation in terms of concentration of EO ($z_{EO,2}$) as the unknown variable. Given the nature of this reactive process with respect to the nonlinearity in the reaction rate combined with the effect of the recycle, the possibility of encountering multiple steady states was investigated. In this respect, the existence of bifurcation points, which relate the locus where only one solution can be obtained and also establishes the limiting operation conditions was examined. The conversion of key component x_{EO} is shown in Figure 4. For given value of recycle flow rate, f_1, the critical D_a^{cr}, and critical concentration of EO, z_{EO}^{cr}, respectively are:

$$D_a^{cr} \geq \frac{4(f_1+1)^2}{(f_1 - f_{W,0})^2} \tag{5}$$

$$z_{EO}^{cr} \geq \frac{(f_1 - f_{W,0})}{2(f_1+1)} \tag{6}$$

In addition, by rearranging Eq. (5), the critical recycle flow rate where state multiplicity can be found at a given feed flow rate ratio, $f_{W,0}$ and D_a can be expressed as:

$$f_1^{cr} \geq \frac{2 + f_{w,0} \cdot \sqrt{D_a}}{\sqrt{D_a} - 2}, \quad \text{for } D_a > 4 \tag{7}$$

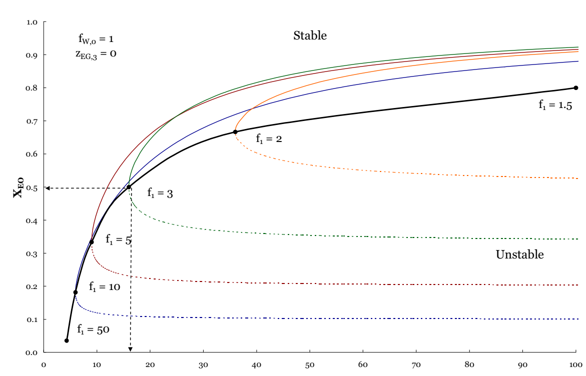

Figure 4. Conversion of EO as function of D_a number

Higher recycle flow rate shift the critical point points to lower conversion and lower the D_a values, and therefore enlarge the region of feasible steady state and the range of achievable conversions. The range of D_a and f_1 that can satisfy the optimum attainable conversion as shown in Figure 4 are $D_a < 16$ and $f_1 > 3$, respectively.

Next, coupled parameters are dissembled with objective to determine the design variables that can match the process variables behavior and the target values of the design parameters defined in Stage 1

Stage 2: Steady-state analysis. A brief overview of the Stage 2 algorithm is given below:

Step 2.1: Steady-state feasibility analysis. Using the identified optimum attainable conversion of EO for the system, a more detailed model with respect to the important design-operational variables was developed by decoupling the coupled parameter (such as D_a).

The steady state model for Stage 2 is given by:

$$\frac{kV}{f_{EO}} = \frac{(f_1 + f_{EO})}{z_{EO,2}} \frac{1}{(f_1 - f_{W,0})(1 - z_{EG,3}) - (f_1 + f_{EO})z_{EO,2}} \quad (8)$$

The new model (Eq. 8) represents a set of nonlinear algebraic equations where parameters such as recovery of product ($z_{EG,3}$) is considered. Eq. (8) is solved implicitly for $z_{W,2}$, $z_{EG,2}$ and x_{EO}, and explicitly for the z_{EO} given the kinetic constant at certain temperature, parameters defining the D_a and the inlet feed ratio of W, $f_{W,0}$.

Step 2.2: **Feasible scenario candidates.** Nominal operating points in Table 1 with inlet feed ratio $f_{EO,0} = 1$ will give the value of $D_a \approx 5$, which is near the value of D_a^{cr}. Designing the system in a stable region but close to the turning point (D_a^{cr}) could cause serious operability problems due to high sensitivity around the fold (Kiss et al., 2007). Therefore, we need to avoid those problems, but how? How many options do we have to avoid those problems since this is existing system with its nominal operating points (constant volume and temperature)? Assuming that we have those options, what is the optimum achievable conversion of EO, x_{EO} that we can achieve with minimum of cost? Are those options sensitive to the changes in the inlet feed ratio, $f_{EO,0}$ (disturbance)? To answer those questions, we need to identify the feasible scenario candidates that can fulfill all the performances and the constraints.

Let's take $D_a \approx 5.5$ as a first candidate that is slightly close to the nominal D_a. Since the existing system has a constant volume, the possible design variables that we can determine to get desired value of D_a is the inlet feed ratio, $f_{EO,0}$. From Eq. (7), the critical recycle flow rate with given value of D_a and $f_{W,0} = 1$ is $f_1^{cr} \geq 13.6$. With that critical recycle flow, the maximum achievable conversion x_{EO} is 0.15 and the range of inlet feed ratio, $f_{EO,0}$ that the process can accommodate is $0 < f_{EO,0} \leq 0.9$. Next, analysis was carried out for the other candidates with value of D_a equal to 7, 10 and 15, respectively, and the results are shown in Table 2.

As shown in Table 2, candidate with smaller D_a required large recycle flow rate, f_1. Taking large recycle flow rate is not operably and economically feasible because of the high sensitivity (snowball effect) and operating cost, but it is less sensitive with variation of $f_{EO,0}$ and has lower conversion x_{EO}. On the other hand, taking D_a at higher value will have higher conversion and lower recycle rate (no snowball effect and low cost), but more sensitive to the variation of $f_{EO,0}$. Therefore, the design of a reliable control structure needs to consider these operational limits.

Table 2. Feasible scenario candidates

Cand-date	D_a	$f_{W,0}$	f_1 *min*	x_{EO} *max*	$f_{EO,0}$
1	5.5	1	13.6	0.15	$0 < f_{EO,0} < 0.9$
2	7	1	8.2	0.23	$0 < f_{EO,0} < 0.7$
3	10	1	5.4	0.33	$0 < f_{EO,0} < 0.5$
4	15	1	4.1	0.41	$0 < f_{EO,0} < 0.35$

Conclusions and Future Work

In conclusion, the results derived from the model-based analysis were useful not only to identify operational constraints and limiting conditions, but also to determine the appropriate control structure needed in order to maintain operational targets such as conversion with minimum cost. Future works will involve with further development of the new methodology into the next stage and illustrate its application through more complex case studies of the reactor-separator-recycle systems.

Acknowledgments

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

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