MULTI-OBJECTIVE OPTIMIZATION APPROACH FOR ROBUST DESIGN UNDER UNCERTAINTY

Soorathep Kheawhom* and Masahiko Hirao
Department of Chemical System Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Abstract

This paper presents a new strategy for synthesizing an appropriate process with multi-objective under uncertainty. The uncertainty is classified depending on its sources and mathematical model structure as deterministic or stochastic. The proposed methodology is a two-layer algorithm. In the outer layer, the synthesis problem is represented by a multi-objective optimization problem considering the performances associated with design parameters. In the inner layer, the problem is expressed as a single-objective optimization problem taking in to account the operating performances in the presence of uncertainty. The formulated design problem is solved to construct a trade-off set. A set of feasible solution is then selected through analyzing the constructed trade-off set. The proposed methodology is implemented by integrating in-house software with commercial software tools. We illustrate the applicability of the proposed methodology in a designing of an ethanol dehydration process. Two main technological schemes, azeotropic distillation and pervaporation distillation hybrid processes, and a newly developed reverse osmosis membrane process are investigated to compare their economic, environmental performances under uncertainty. The developed methodology can select solutions with minimal environmental impacts and adequate flexibility at a desired economic performance.

Keywords

Multi-objective optimization, Robust process design, Environmental impact, Uncertainty, Ethanol dehydration.

Introduction

Chemical process typically involves significant uncertainty and variations during its design and operation due to either external (e.g. price variations) or internal sources (e.g. model uncertainties). While the representation of uncertainty is an important issue, the potential effect of variability on process decisions regarding process design and operations constitutes another challenging problem, because these uncertainties may result in a great loss of process performances. Therefore, more flexible and robust process has received increasing attention in the design and operation of chemical processes.

The process design under uncertainty is complicated, and the required information is usually missing or unknown in the design stage. Normally, in actual process design and simulation operations, the associated uncertainty is covered using safety factors, which can increase costs and investment without a quantitative measure of the avoided risk.

There are several developed methodologies that can be applied to address the problem of process design under uncertainty. Three main directions can be broadly distinguished: (1) flexibility analysis (Pistikopoulos and Grossmann, 1988), (2) deterministic approach (Paules and Floudas, 1992) and (3) probabilistic approach (Straub and Grossmann, 1993).

Flexibility analysis has also evolved as a tool for designing under uncertainty. It provides a measure of the size of the region of feasible operation. In this direction, the designers make a decision on the structure and configuration of the process in the above level first, and flexibility issues are considered thereafter in a late stage of the process design.

In the deterministic approach, the description of uncertainty is provided either by specific bounds or via a finite number of fixed parameter values. Consequently, the original optimization problem is transformed to a deterministic approximation. Thus, the solution obtained this way is not so accurate. In addition, a model configuration uncertainty cannot be handled.

In the probabilistic approach, uncertainty is described by probability distribution functions. Consequently, the original optimization problem is transformed to the two-stage stochastic programming. The basic idea is based on selecting an optimal vector of the design variables in the first stage while seeking operational feasibility in the second stage. This technique offers a reasonable accuracy. Unfortunately, the computational burden of this approach is extreme.

Recently, the studies on the process design under uncertainty are based on the probabilistic approach (Acevedo and Pistikopoulos, 1998; Ostrovosky et al., 1997). Optimal design under uncertainty is usually formulated by maximizing the expected value of profit over all range of uncertain parameters subject to feasibility of the process constraints.

Generally, a real problem of process design involves more than one objective such as economic and environmental performances. This results in requiring of solving and analyzing a multi-objective optimization problem. Recently, many studies on the process design and synthesis have been focused on the application of a multi-objective optimization problem (Steffens et al., 1999; Kheawhom and Hirao, 2002). But only a few studies have been on the development of methodologies for simultaneous considering a number of objectives under uncertainty.

The purpose of this paper is to introduce a new systematic framework for designing a chemical process with multi-objective under uncertainty. The developed method uses uncertainty classification and two-stage stochastic optimization techniques. Further, the proposed methodology provides a way of designing what is likely to be the most promising solution that are environmental friendly and robust over the specified range of uncertainty with adequate economic performance.

Design Methodology

The primary attributes of a synthesis problem are classified according to the following quantities: state variables, design variables, control variables, deterministic uncertainties and stochastic uncertainties. The deterministic uncertainty is usually described by either specific bounds or a finite number of fixed parameter values. In comparison, the stochastic uncertainty is typically expressed in terms of probability distribution functions. The distribution type of each stochastic uncertain parameter is selected by considering characteristics of that uncertain parameter.

The stochastic and deterministic uncertainties are inherently handled using a stochastic modeler. A sampling unit is used to generate representative samples from the defined probability distributions.

The performances of a chemical process consist of two parts. The first part is associated with design variables, or process configuration, which cannot be changed during operation. Thus, the performances associated with design variables are independent of operating condition or operating policy. The second one is a performance associated with control variables, or operating condition. This value depends on operating condition, and it varies under the effect of process uncertainties. The synthesis problem is expressed as:

$$\min_{D}[FP_i + \overline{OP}_i]$$
$$\overline{OP}_i = \sum_{j=1}^{n} \omega_j \overline{OP}^{o}_{i,j} \tag{1}$$
$$OP^{o}_{i} \in \{OP_i \mid \min_{Z} OP_r\}$$

Where, D is a vector of design variables. Z is a vector of control variables. ω denotes a weight factor of each period. FP and OP represent a performance associated with design and control variables, respectively.

By considering the synthesis problem, a design strategy consists of two layers. The vector of process performances of each design alternatives is evaluated at the vector of optimal control variables, where this point is usually the company's best economic interest.

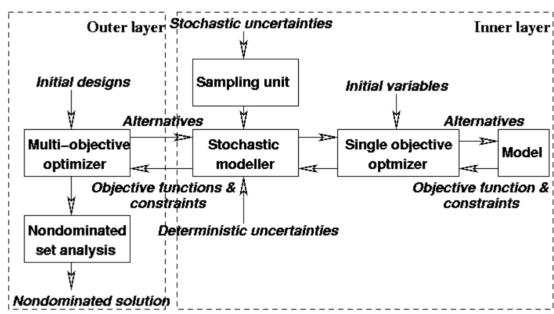

Figure 1. The schematic representation of the developed algorithm

The proposed algorithm is shown in Fig. 1. Once the vector of design variables is selected at the outer layer, the optimal vector of control variables is obtained from the inner layer by optimizing the run-time performance of the process. In the outer layer, the synthesis problem is represented by a multi-objective optimization problem (MOP), which requires a trade-off among objectives. The problem of this layer takes into account the performances associated with design parameters. By contrast, the problem of the inner layer is expressed as a single-objective optimization problem (SOP).

The outer layer is connected with the inner layer via the stochastic modeler. The information related to the vector of design variables is passed from the MOP optimizer to the stochastic modeler. A set of the inner layer problems is then formulated by the stochastic modeler.

Each inner layer problem is solved in the SOP optimizer, and the vector of process performances at the vector of optimal control variables is transmitted back to the stochastic modeler. In the stochastic modeler, the effects of uncertainties are analyzed using statistical techniques.

A genetic algorithm (GA) is implemented in the SOP optimizer. An advantage of GA over other optimization algorithms is that derivatives of the objective function are not essential. This fact ensures that GA may be readily exploited on potential surfaces containing discontinuities without any special treatments. Further, the algorithm exploited in the MOP optimizer is a multi-objective genetic algorithm (MOGA). The MOGA provides some important advantages in solving MOP. The population of solutions carried in a GA can be directed to converge along the trade-off set in a single run by the fact that GA works with a population of solutions.

The constructed non-dominated set requires trade-off among the objectives to select the most promising solution. The methodology used here is adapted from the methodology proposed by Kheawhom and Hirao (2002).

Objective Functions

Economic Performance

The economic performance can be represented by a summation of fixed costs and operating costs and the subtraction of product revenues. The fixed cost must be discounted by the life spans of the units.

Environmental Performance

The Sustainable Process Index (SPI) (Krotscheck and Narodoslawsky M., 1996) is designed to deal with various environmental objectives simultaneously. The basic concept of the SPI is to calculate the area required to sustainingly embed a process into an environment. All mass flows that the process either extracts from or emits to the environment must not influence the environment in such a way that brings natural evolution into danger.

Case Study

Recently, the use of biomass-derived ethanol as an alternative energy source is receiving increasing attention. Ethanol is produced from a fermentation process. However, the concentration of ethanol from the fermentation process is not high enough to use as an alternate fuel. Thus, the ethanol dehydration process is necessary.

In our case study, the problem description is to design an ethanol dehydration process that can efficiently operate in two periods with equal probability. Each period involves two deterministic uncertainties, as shown in Table 1. The mass fraction of ethanol in the product stream must be over 0.96. All distributions of stochastic uncertainty were assumed to follow a normal distribution with a standard deviation ratio = 2×10^{-6}.

Table 1. Deterministic uncertain parameters

Period	Flowrate	Mass fraction
1	100 kgmol/hr	0.1
2	110 kgmol/hr	0.14

A complete separation of water-ethanol mixture is quite difficult and cannot be achieved by a simple distillation because of the formation of an azeotrope. The traditional way of separating ethanol from water is by an azeotropic distillation process. However, the energy consumption of azeotropic distillation process is high. The ethanol produced this way is too expensive. Therefore, a hybrid pervaporation distillation process was introduced to reduce the cost of producing ethanol. The other possible option consuming very low amount of energy are pervaporation and reverse osmosis membrane processes (Nakao, 1994). Table 2 shows the amount of energy required in each ethanol dehydration process.

Table 2. Energy required in each ethanol dehydration process

Process	Energy
Azeotropic distillation	9.96 MJ/kg
Hybrid pervaporation distillation	5.35 MJ/kg
Pervaporation membrane	5.32 MJ/kg
Reverse osmosis membrane	7.17 kJ/kg

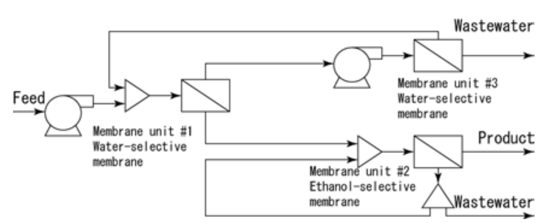

Figure 2. The reverse osmosis membrane process

On the basis of the energy consumption, the reverse osmosis membrane process is the most attractive option, and it is selected to be further studied. Figure 2 shows the flow-sheet of the reverse osmosis membrane process. The design variables are the membrane area, permeability and selectivity. The control variables are the pressure of both sides of the membrane and recycle ratio. Figure 3 shows the trade-off set in the normalized form. The most economically attractive solution may not necessarily be environmentally attractive. Hence, a trade-off between economic and environmental objectives is required to ensure a satisfactory design. Alternatives C can be selected as the most attractive alternative. Table 3 shows the configuration of alternative C. The expected economic (profit) and environmental (SPI) performances of alternative C were 170,000 \$/yr and $8.5x10^7$ m^2/yr, respectively.

Table 3. A configuration of the most promising solution

Parameter	Value
Membrane unit #1	
Area	106 m^2
Ethanol permeability	0.0015 kgmol/ m^2s
Water permeability	$3x10^{-6}$ kgmol/m2s
Membrane unit #2	
Area	46.9 m^2
Ethanol permeability	$7.5x10^{-5}$ kgmol/ m^2s
Water permeability	$1.5x10^{-6}$ kgmol/ m^2s
Membrane unit #3	
Area	72.36 m^2
Ethanol permeability	0.0015 kgmol/ m^2s
Water permeability	$3x10^{-6}$ kgmol/m2s

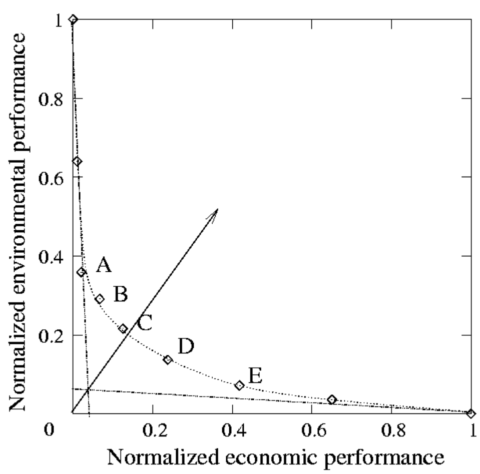

Figure 3. The trade-off set between economic and environmental performances

Conclusions

We proposed the framework for designing a chemical process with multi-objective under uncertainty. We introduced the use of uncertainty classification and two-stage stochastic programming formulation to handle the uncertainty and to analyze the effect of variability on decisions related to process performances. The applicability of the proposed framework has been described and demonstrated in a case study of synthesis of an ethanol dehydration process. The proposed methodology was implemented by integrating in-house software with commercial software tools.

References

Acevedo, J., Pistikopoulos, E. N. (1998). Stochastic optimization based algorithms for process synthesis and design under uncertainty. *Computers and Chemical Engineering*, *22*, 647.

Kheawhom, S., Hirao, M. (2002). Decision support tools for process design and selection. *Computers and Chemical Engineering*, *26*, 747.

Krotscheck, C., Narodoslawsky M. (1996). The Sustainable Process Index. A new dimension in ecological evaluation. *Ecological Engineering*, *6*, 241.

Nakao, S. (1994). Optimization of membrane process for concentrating alcohol solution. *Membrane*, *19*, 344.

Ostrovosky, G., Volin, Y. M., Senyavin, N. M. (1997). An approach to solving a two-stage optimization problem under uncertainty, *Computers and Chemical Engineering*, *21*, 317.

Paules, G. E., Floudas, C. A. (1992). Stochastic programming in process synthesis: a two-stage model with MINLP recourse for multiperiod heat-integrated distillation sequences. *Computers and Chemical Engineering*, *16*, 189.

Pistikopoulos, E. N., Grossmann, I. E. (1988). Stochastic optimization of flexibility in retrofit design of linear systems. *Computers and Chemical Engineering*, *12*, 1215.

Steffens, M. A., Fraga, E. S., Bogle, I. D. L. (1999). Multi-criteria process synthesis for generating sustainable and economic bio-process. *Computers and Chemical Engineering*, *23*, 1455.

Straub, D. A., Grossmann, I. E. (1993). Design optimization of stochastic flexibility. *Computers and Chemical Engineering*, *17*, 339.