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Multi-objective design space exploration under uncertainty

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Abstract

In this work, we propose a new technique for efficiently exploring a multi-objective design space to find non-dominated solutions in the presence of uncertainty. Our approach uses a two-stage optimization technique. In the first-stage, the design problem is represented by a multi-objective optimization problem considering the performances associated with design parameters. In the second stage, the design problem is expressed as a single objective optimization problem taking into account the operating performances of the process under uncertainty. We propose a new hybrid algorithm to efficiently explore a multi-objective design space. Our algorithm combines the advantage of both gradient-based and non-gradient-based optimization algorithm. A genetic algorithm (GA) is used to handle the multi-objective optimization problem in the first stage. In comparison, the sequential quadratic programming (SQP) method with problem decomposition is applied to solve the sub-problems in the second stage. Our proposed technique can improve the speed of computation and reduce computational time. The proposed methodology is implemented by integrating in-house software with commercial software. We illustrate the applicability of the proposed methodology in a case study.

Keywords: Multi-objective optimization, Process design, Environmental impact, Uncertainty

1. Introduction

Chemical process usually involves significant uncertainty during its design and operation. The uncertainties may result in a great loss of process performances. Thus, the potential effect of the uncertainties on process decisions regarding process design and operations is an important issue and constitutes a challenging problem.

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)

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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 feasible operation region. In this direction, the designers make a decision on the 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 through a two-stage stochastic programming approach (Acevedo and Pistikopoulos, 1998). 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 (Kheawhom and Hirao, 2004).

The purpose of this paper is to introduce a new hybrid algorithm for efficiently exploring a multi-objective design space. Our algorithm combines the advantage of both gradient-based and non-gradient-based optimization algorithm. A genetic algorithm (GA) is used to handle the multi-objective optimization problem in the first stage. In comparison, the gradient-based optimization algorithm is applied to solve the sub-problems in the second stage. We illustrate the applicability of the proposed algorithm in a case study, synthesis of closed-loop membrane-based toluene recovery process. This case study was firstly studied by Kheawhom and Hirao (2004). Our proposed technique can improve the speed of computation and reduce computational time by up to 65%.

2. Multi-objective Optimization under Uncertainty

The primary attributes of a design 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 performances of a chemical process consist of two parts. The first part is associated with design variables, or process configuration, which cannot be altered 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 design problem is expressed as:

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

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.

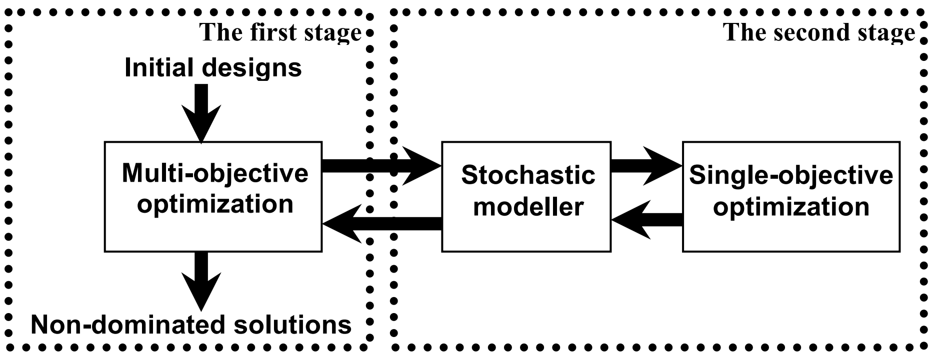

Figure 1. The graphical representation of multi-objective optimization under uncertainty.

The graphical representation of multi-objective optimization under uncertainty is shown in Figure 1. Once the vector of design variables is selected at the first stage, the optimal vector of control variables is obtained from the second stage by optimizing the run-time performance of the process. Therefore, the evaluation of each alternative in the first stage requires the solution of the second stage.

A key difficulty in this type of problem is in dealing with an uncertainty space that is huge and very computational expensive.

3. The Proposed Algorithm

Our algorithm combines the advantage of both gradient-based and probabilistic-based optimization algorithm. A multi-objective genetic algorithm

(MOGA) is used to handle the multi-objective optimization problem in the first stage. In comparison, the sequential quadratic programming (SQP) method is applied to solve the sub-problems in the second stage. The MOGA provides some important advantages in solving multi-objective optimization problem over other optimization algorithms. The population of solutions carried in a MOGA can be directed to converge along the non-dominated set in a single run by the fact that MOGA works with a population of solutions. In contrast, SQP method requires the computation of gradient information. Moreover, it requires special treatment in the case that a design space contains discontinuities. But the advantage of SQP lies on speed of the algorithm.

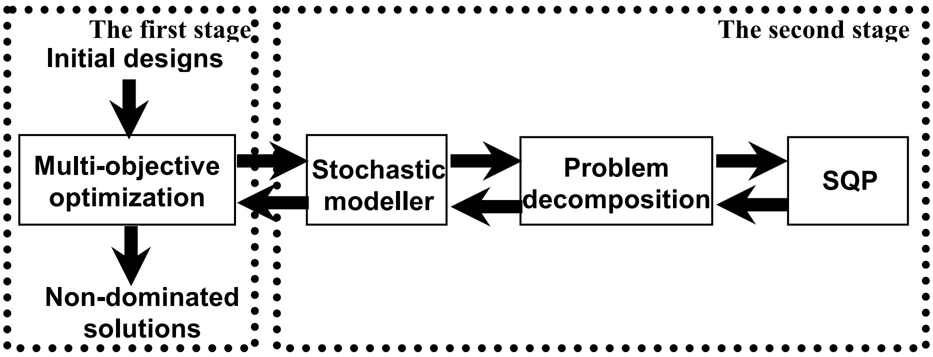

Figure 2. The graphical representation of the proposed algorithm.

The proposed algorithm is shown in Figure 2. The first stage is connected with the second stage 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 second stage subproblems is then formulated by the stochastic modeler. A sampling technique is employed to sample the stochastic uncertainties. In the second stage, the subproblems formulated by stochastic modeler are decomposed into a number of subsubproblems. A design space in each subsubproblem now contains no discontinuity so that the SQP method can be readily exploited. Each subsubproblem is solved in the SQP 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. Therefore, expected performances of each design under uncertainty are obtained.

4. Case Study

Table 1. Deterministic uncertain parameters for the case study.

Period	Flow rate (kgmol/h)	Toluene concentration (vol%)
1	3000	3
2	2800	2.8
3	2600	2.6
4	2400	2.4
5	2200	2.2

The algorithm described above was applied to a case study in designing of a closed-loop membrane-based toluene recovery process. This case study was firstly studied by Kheawhom and Hirao (2004). The problem description is to synthesize a process that can efficiently operate in five periods with equal probability as shown in Table 1. Distribution of stochastic uncertainties were assumed to follow a normal distribution with a standard deviation = 2 x 10^{-6}. Four configuration: single stage, two-stage enriching, two-stage stripping, and two-stage enriching with pre-membrane stage of membrane-based toluene recovery process were investigated.

The economic performance is quantified by mapping each design into flow rates and process equipment specifications. The flow rates are converted to revenues and operating costs. Fixed costs are estimated by the factorial estimating method (Gerrard, 2000). This method is based on historical knowledge of the relative cost of various purchases and activities. The main plant items are listed and sized. The purchased cost is then obtained and multiplied by installation factors to give a total erected cost. The economic performance is represented by total annualized cost (TAC).

In this study, the environmental performance is represented by the sustainable process index (SPI) which is developed by Krotscheck and Narodoslasky (1996).

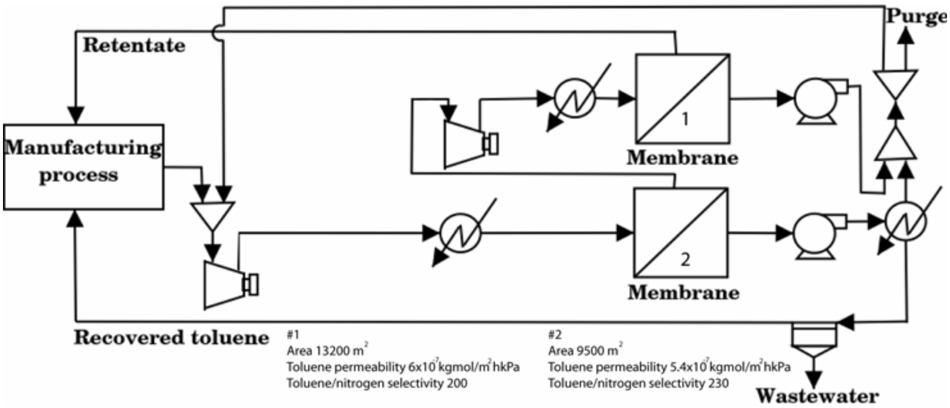

Figure 3. The promising solution (two-stage stripping process).

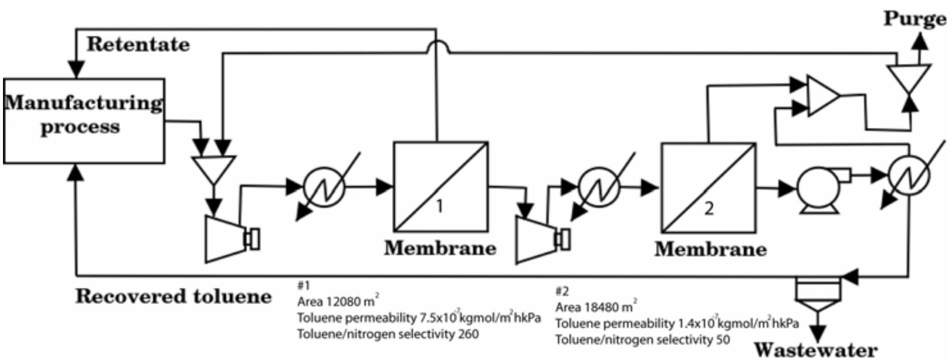

Figure 4. The promising solution (two-stage enriching process).

There are two promising solutions in this case. One alternative (alternative A) is a two-stage stripping process, while the other one (alternative B) is a two-stage enriching process as shown in Figure 3 and 4, respectively. The total amount of discharged toluene in purge stream of alternative A is higher than the amount of toluene discharged from alternative B resulting in a higher environmental load. However, alternative A requires a smaller total membrane area. Thus, alternative A is more economic attractive than alternative B.

This case study was solved on a Pentium III 1GHz machine with 256 MB RAM. Kheawhom and Hirao (2004) had solved this problem using GA in both the first and second stage. Their technique requires 330 hrs of computational time. In comparison, our proposed algorithm took 112 hrs of computation, which reduced the computational time by up to 65%.

5. Conclusions

This article presents a new hybrid algorithm for efficiently exploring a multi-objective design space. Our algorithm combines the advantage of both gradient-based and non-gradient-based optimization algorithm. A genetic algorithm (GA) is used to handle the multi-objective optimization problem in the first stage. In comparison, the gradient-based optimization algorithm is applied to solve the sub-problems in the second stage. Our proposed technique can improve the speed of computation and reduce computational time by up to 65%.

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