

A Strategy for Multi-objective Optimization under Uncertainty in Chemical Process Design*

SUN Li (孙力)^{1,**} and Helen H. Lou²

¹ Department of Chemical Engineering, Dalian University of Technology, Dalian 116023, China

² Department of Chemical Engineering, Lamar University, Beaumont, Texas 77710, USA

Abstract In many circumstances, chemical process design can be formulated as a multi-objective optimization (MOO) problem. Examples include bi-objective optimization problems, where the economic objective is maximized and environmental impact is minimized simultaneously. Moreover, the random behavior in the process, property, market fluctuation, errors in model prediction and so on would affect the performance of a process. Therefore, it is essential to develop a MOO methodology under uncertainty. In this article, the authors propose a generic and systematic optimization methodology for chemical process design under uncertainty. It aims at identifying the optimal design from a number of candidates. The utility of this methodology is demonstrated by a case study based on the design of a condensate treatment unit in an ammonia plant.

Keywords multi-objective optimization, uncertainty, chemical process design

1 INTRODUCTION

A chemical process should be optimized by considering economic, environmental and societal objectives simultaneously to improve sustainability [1–3], which means that the chemical process design in practice can be formulated as a multi-objective optimization (MOO) problem.

Moreover, uncertainty is unavoidable during the optimization in the form of physical properties, product demand, environmental condition and economic cost, errors in model prediction and so on. Normally, the mean value of the uncertainty factor is used in deterministic optimization methodology. However, in reality, the value of the uncertain factor may deviate from its mean, and this may undermine the reliability of the solution from deterministic optimization. Therefore, it is essential to incorporate uncertainty in MOO to generate more reliable results.

Some researches have been conducted on MOO under uncertainty. Strategies, such as stochastic programming (SP) (SP with recourse, robust SP, probabilistic programming), fuzzy programming, and stochastic dynamic programming have been put forward. All these methods have their own advantages and disadvantages [4–6].

In this article, authors study on the basis of SP methodology, to deal with uncertain parameters, and integrating MOO deterministic algorithms to identify the optimal chemical process design from a number of alternatives. A 3-step optimization approach is proposed as a generic and systematic optimization methodology in this study. The efficacy of this methodology is demonstrated by optimizing the design of a process condensate treatment unit in an ammonia plant.

2 A STRATEGY FOR MULTI-OPTIMIZATION UNDER UNCERTAINTY

A MOO problem under uncertainty can be for-

mulated as:

$$\begin{aligned} \min \quad & f_i(x, u, \varepsilon) \quad i = 1, 2, \dots, n \\ \text{s.t.} \quad & h(x, u, \varepsilon) = 0 \\ & g(x, u, \varepsilon) \leq 0 \\ & x \in X, \quad u \in U, \quad \varepsilon \in \Xi \end{aligned} \quad (1)$$

where, f_i is the objective function. h and g are the vectors of the equality and inequality constraints. $x \in R^n$, is the n -dimensional of state vector, $u \in R^m$ is the m -dimensional decision vector, and $\varepsilon \in R^s$ is the s -dimensional uncertainty vector, respectively.

In this study, the maximization of economic and the minimization of environmental objectives are considered. Uncertainty vectors come from two sources during the design: uncertainty in the parameters, and uncertainty associated with the engineering design model [7]. In this article, the impact of uncertainties from both aspects is studied and a three-step procedure for MOO under uncertainty is proposed. The consideration of uncertainties will enhance the proposed methodology and enrich the knowledge base in design for sustainability.

First, the effects of the uncertainty parameters are considered. SP algorithms, such as two-stage SP with recourse and chance constrained programming might be utilized for the uncertain parameters [3, 8–10]. Realizations of the uncertain parameters may cause violation of certain constraints. So recourse violation of the constraints will be compensated for by introducing a penalty term in the objective function, and it is the approach of two-stage SP with recourse. In some other cases, the approach of chance constraints is utilized considering certain constraints can violate with a probability $p \in (0, 1)$, while the system is thought to satisfy the corresponding constraints. So, $P \leq p$, and P is a probability function. SP with chance constraints can be expressed in model (2), and this uncertain optimization model can be rewritten as deterministic function according to the model types.

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** To whom correspondence should be addressed. E-mail: bonnia@dlut.edu.cn

$$\begin{aligned}
\min. \quad & f_i(x, u, \varepsilon) \quad i = 1, 2, \dots, n \\
\text{s.t.} \quad & h(x, u, \varepsilon) = 0 \\
& g(x, u, \varepsilon_j) \leq 0 \\
& P(g(x, u, \varepsilon_k) \geq 0) \leq p \\
& j + k = s \\
& x \in X, \quad u \in U, \quad \varepsilon \in \Xi, \quad p \in (0, 1)
\end{aligned} \quad (2)$$

Second, the inherit uncertainty in the model is investigated. The optimization model is formulated based on simulation results and certain parameters were obtained from the best estimation from plant operation, and these would cause some model prediction error unavoidably. In this study, the uncertainty associated with the engineering design model is proposed by adding the multiplicative uncertainty α and additive uncertainty β to the optimization model [7], and these uncertainties can be estimated by reviewing historical accuracies of chosen modeling approaches or by an intentional variable model-fidelity approach.

$$\min \quad \alpha f_i + \beta \quad i = 1, 2, \dots, n \quad (3)$$

Third, the optimal solution is identified by considering the tradeoffs. Usually, there is more than one feasible solution for MOO with competitive and ambivalent objectives, so, a Pareto frontier is obtained from the above-mentioned two steps. It is necessary to evaluate the tradeoff and to obtain the optimal solution based on the expected solution and the knowledge gained from the Pareto frontiers [11].

3 CASE STUDY

Process condensate in an ammonia production process (using Kellogg's technique) comprises of discharge from the hydrogen and nitrogen compressor, as well as separators in adjacent segments. The discharge contains ammonia, methanol, methane, urea and carbon dioxide. The condensate in discharge cannot be disposed directly due to its harmful environmental impacts. Moreover, it would also lead to loss of useful raw materials, such as ammonia, methanol, methane and urea. Table 1 lists the composition and mass flow rate of process condensate obtained in the plant.

Table 1 Process condensate data

Concentration $\times 10^6 / \text{kg} \cdot \text{L}^{-1}$					Flow rate $/\text{kg} \cdot \text{h}^{-1}$	$T/^\circ\text{C}$	p/MPa
NH_3	CO_2	CH_3OH	Urea	CH_4			
1612	1672	573.4	144	0.91	100000	217	3.75

3.1 Process analysis

A typical technique to treat process condensate is steam stripping. Natural gas, medium-pressure (MP) steam, and low-pressure (LP) steam can be used for stripping the process condensate. Pre-analysis and Aspen simulation are conducted to compare the different designs.

Natural gas is one of the raw materials used in ammonia production, and its flow rate is fixed based

on the production throughput. Simulation results indicate that the treated condensate after stripping by only the natural gas does not reach the allowable emission concentration due to the limited amount of natural gas available, so it cannot be used as the only media for the separation.

Neither can LP steam accomplish the separation task all by itself. If LP steam is used for stripping the process condensate, the effluent steam from the top of the column can neither be transferred to the production operation unit (converter I) directly due to its low pressure and low temperature, nor be emitted in air as it contains ammonia, methanol, methane and carbon dioxide. Even though the effluent steam can be condensed and sent back to the stripping column to recover these useful components, the non-condensing emission gas from the condenser with trace amounts of ammonia, methanol and carbon dioxide would cause negative environmental impact if it is discharged to the atmosphere directly. Thereby, LP steam stripping only is not sufficient to satisfy the environmental regulations.

After pre-analysis, three designs are proposed to be optimized [12]. Design 1 is MP steam stripping, design 2 is saturated humidification followed by MP steam stripping, and design 3 is saturated humidification followed by LP Steam stripping. The schematic flowsheet of these three designs are shown in Figs. 1–3.

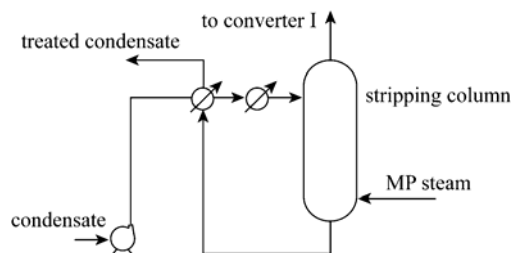


Figure 1 MP steam stripping

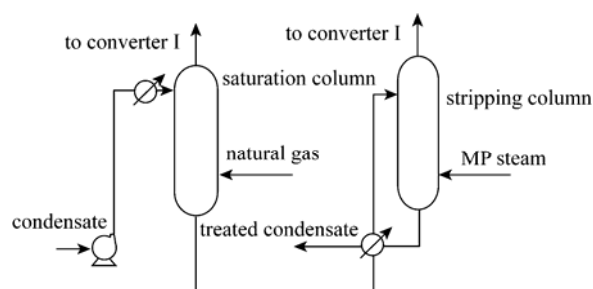


Figure 2 Saturated humidification followed by MP steam stripping

These scenarios can satisfy the separation quality requirement for stripped process condensate. The treated condensate is either discharged, or reused as boiler supply water. The saturated gas leaving the saturation column and the stripping steam from MP steam stripping column are transferred to the converter I as raw material. Note that in design 3, the non-condensing emission gas from the condenser has trace amounts of ammonia, methanol and carbon dioxide. If it is discharged to the atmosphere directly, it may cause negative environmental impact.

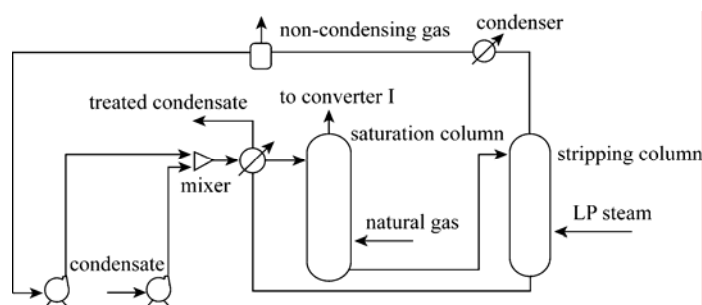


Figure 3 Saturated humidification followed by LP steam stripping

3.2 Decision variables and uncertainty variables

Condensate inlet temperature (T) and MP/LP steam flow rate (F) are considered as decision variables which have significant influence on separation. The value of inlet temperature ranges from 100°C to 245°C and that of steam flow rate is from 8000 kg·h⁻¹ to 35000 kg·h⁻¹. Other operating or equipment parameters are considered fixed during optimization. The inlet temperature/flow rate of natural gas is 217°C/22000 kg·h⁻¹. The number of plates required in the saturation column, as well as the stripping column is 15.

In this case study, the effect of price fluctuation of LP/MP steam on the performance of the process is investigated, and the price of LP/MP steam is considered as the uncertainty variable (expressed in price per heat load). It is assumed that there is 40% of probability that the price of steam would be 6.90 dollars·MJ⁻¹ and 60% of probability of the price being 8.28 dollars·MJ⁻¹.

3.3 Problem formulation

There are two optimization objectives in this study: profit maximization and environmental impact minimization. The profitability of the process to be maximized is defined as the difference between the income and annualized cost. The environmental impact can be calculated in a way similar to the WAR algorithm. It is a function of the amount of chemical species being discharged and its corresponding environmental impact index (EII) [13]. In this study, EII is a normalized value using a short-cut approach, which calculates the “relative” stress caused by each chemical species present in a discharge stream rather than the “absolute” value of their environmental impact. The absolute value of the environmental impact caused by each chemical was retrieved from the U.S. EPA’s TRACI data base [14–17]. Table 2 illustrates the normalized value of EII of those chemicals in air and water.

Table 2 Normalized value of environmental impact index

Media	NH ₃	CH ₃ OH	CH ₄	CO ₂
water	0.6677	0.3323	0	0
air	2.9668	0.0332	0.9583	0.0417

It is difficult to express the relationship between the decision variables and objectives. Therefore the

proposed design is simulated using ASPEN Plus first. Then the regression models are correlated using the data from plant and the simulation results of the proposed design scenarios. The parameters used in this optimization are listed in Tables 3 and 4.

Table 3 Price data

Item	Price
H ₂ O	0.125 dollars·t ⁻¹
NH ₃	312.5 dollars·t ⁻¹
CH ₃ OH	250 dollars·t ⁻¹
natural gas	160 dollars·t ⁻¹

Table 4 Annualized capital cost

Item	Annual capital cost/dollars
saturation column	2.25×10 ⁴
LP-stripping column	1.88×10 ⁴
MP-stripping column	2.63×10 ⁴

Constraints in this optimization reflect the environmental regulations posed on the allowable amounts of ammonia and methanol in the treated water and emission gas, *i.e.* $c_{\text{ammonia}} \leq 10 \text{ mg} \cdot \text{L}^{-1}$, $c_{\text{methanol}} \leq 15 \text{ mg} \cdot \text{L}^{-1}$.

3.4 Optimization under uncertainty

In this case study, the price of LP/MP steam is considered as a stochastic design parameter. The effect of the uncertainty is expressed in Eq. (4), and they are formulated in the constraints of the optimization.

$$P(p = 6.90 \text{ dollars} \cdot \text{MJ}^{-1}) = 0.4$$

$$P(p = 8.28 \text{ dollars} \cdot \text{MJ}^{-1}) = 0.6 \quad (4)$$

To solve the optimization problem under uncertainty, the objective function is rewritten as a deterministic function by incorporating the probability constraints into the objective function.

The model uncertainty is reflected in α and β values. In this study, it is assumed that the model uncertainty worsens the performance of the chemical process by reducing the profit and increasing the environmental impact. Best on experience, the values for α and β are chosen as:

$$\alpha = [0.9, 1.1], \quad \beta = [0.02, 0.05].$$

Genetic algorithm (GA) [18–20] can be used to solve multi-objective optimization problems, and is utilized in this case study to identify the Pareto frontier for each design scenario, where every point on the Pareto frontier reflects a non-dominant solution for both economic and environmental performance. Fig. 4 shows the Pareto frontiers for each scenario while considering uncertain parameters and model uncertainty, respectively. Fig. 5 illustrates the comparison of results in both deterministic optimization and optimization under uncertainty.

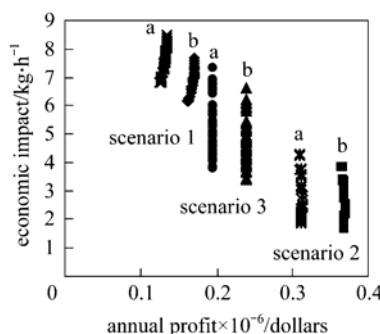


Figure 4 Effect of parameter uncertainty and model uncertainty on Pareto frontiers

a—optimization considering both uncertain parameters and model; b—optimization only considering uncertain parameters

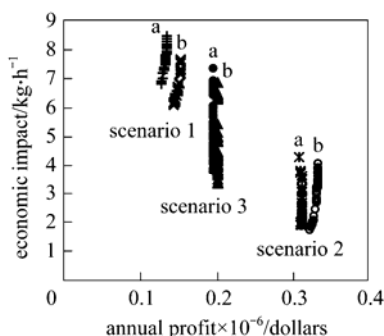


Figure 5 Comparison of deterministic optimization and optimization under uncertainty on Pareto frontiers

a—optimization under uncertainty; b—deterministic optimization

It is clearly known that the consideration of uncertainty would change the process profit and the environmental objective, and shift the Pareto frontiers to the left. From Fig. 5, it can be seen that the shifts of Pareto frontiers are different for the three designs. The profit of design 1 decreases more drastically than that of the others. Points on the Pareto frontier for scenario 2 have higher value of profit compared to that of other two scenarios, even though some points for scenario 2 have higher environmental impact. Thus, the optimal design choice could be scenario 2.

4 CONCLUSIONS

In this study, a strategy for multi-objective optimization under uncertainty in chemical process design is presented. It is clear from the results that consideration of uncertainty may generate more reliable results, and avoid or minimize the potential risks.

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