

Application of Pareto Optimization under Uncertainty in Chemical Process Design for Sustainability

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Abstract

The development of a sustainable chemical processes aims at optimizing its economic, environmental and societal sustainability simultaneously. This can be solved as a multi-objective optimization (MOO) problem. However, in real systems, there are many uncertainties that affect the performance of a process. These include market fluctuation, changes in material properties, manufacturing variations, errors in model prediction etc. In order to generate a more robust solution, it is essential to develop a multi-objective optimization methodology including uncertainty. This would facilitate the design for sustainability.

In this paper, the authors use the Pareto optimization methodology to identify the optimal design specifications and operating conditions of chemical processes under uncertainties. The objective of this MOO problem is to maximize the overall sustainability of the process. 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 Pareto optimization, uncertainty, sustainability, multi-objective optimization

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1. Introduction

The sustainability of chemical processes can be achieved by optimizing economic, environmental and societal objectives simultaneously. This can be modeled as a multi-objective optimization (MOO) problem. Chemical processes come across uncertainties throughout process design and operation in the form of manufacturing variations, material property variations, market fluctuation, etc. Thus, in order to generate more reliable results, it is necessary to incorporate uncertainty in the MOO model.

Many researches have been conducted on solving MOO problems under uncertainty. Different approaches, such as stochastic programming, robust stochastic programming, probabilistic programming, and fuzzy programming etc. have been put forward. All these methods have their own advantages and disadvantages for optimization under uncertainty⁽¹⁻³⁾.

In this paper, an attempt has been made to develop a generic and systematic methodology in design for sustainability via systematic generation & evaluation of alternatives. This methodology utilizes the MOO method developed by Mattson and Messac⁽⁴⁾. By employing Pareto optimization methodology, this methodology aims at identifying the optimal design specifications and operating conditions for maximizing the overall sustainability of a chemical process under uncertainties. The efficacy of this methodology is demonstrated by optimizing the design of a condensate treatment unit in an ammonia plant.

This paper is organized as follows. Section 2 presents a MOO algorithm under uncertainty. A case-study from an ammonia synthesis plant is illustrated in Section 3 to demonstrate the effectiveness of this methodology while optimizing the design of a condensate treatment process. The conclusion and discussion is given in section 4.

2. Methodology for multi-objective optimization under uncertainty

Sustainability metrics proposed by the IChemE and AIChE include environmental, economic and societal metrics⁽⁵⁻⁶⁾. In this work, two dimensions of sustainability are considered, economic sustainability and environmental sustainability. The economic performance is measured in term of the profitability of a chemical process. The environmental performance of chemical process is obtained by multiplying the amount of emission with its corresponding environmental impact index (EII).

Thus, the MOO problem to optimize the economic and environmental sustainability under uncertainty can be formulated as,

$$\min. \quad f_i(x, u, \varepsilon) \quad i=1, 2, \dots, n \quad (1)$$

$$\text{s.t.} \quad h(x, u, \varepsilon) = 0$$

$$g(x, u, \varepsilon) \leq 0$$

$$x \in X, u \in U, \varepsilon \in \Xi \quad (2)$$

Where, f 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.

Since only economic and environmental objectives are optimized in the current work, it limits the value of n to 2. The impact of equality constraints is the projection of the uncertain variables on the state space with some given state variables. This implies that the required values of state variables x can be computed by a multivariate integration of the model as a function of u and ε . Hence, h will be eliminated from the above constraints.

The uncertainties affecting the performance of the process include uncertainty caused by stochastic design parameters, and uncertainty associated with the engineering design model.⁽⁷⁾ In this work, the impact of uncertainty on the performance of the process is calculated from both aspects.

The Pareto optimization methodology developed by Mattson & Messac⁽⁴⁾ for optimizing the sustainability of a process include the following steps:

Step 1: To minimize the mean values of multi-objective optimization metrics.

$$\min \bar{f}_i(x, u) \quad i=1, 2, \dots, n \quad (3)$$

where \bar{f} is the mean of f .

Step 2: To obtain standard deviations of the response variables σ_f determined by comparison of random input variables x , u and means of x (\bar{x}) and u (\bar{u}).

Step 3: To shift the deterministic optimal solution by $\kappa\sigma_y$ to be $(\bar{f} + \kappa\sigma_y)$ while considering uncertainties. It needs to be explained that κ is a positive number corresponding to the probability of uncertainty that would happen. It also reflects the reliability of design decisions. Table 1 lists the relationship between κ and uncertainty probability. If $\kappa = 0$, that means the decision is deterministic, in other words, the decision is made based on the mean values of the design parameters. This decision would be unreliable in real world without considering uncertainty. In contrast, higher value of κ indicates lower probability of uncertainty and a more reliable decision. $\kappa=6$ represents highly reliable decisions ("six-sigma" decisions)⁽⁸⁾.

Step 4: To consider model uncertainty

The non-deterministic prediction of actual design response is assumed to be defined as:

$$\begin{aligned} f_i &= \alpha f_i(x, u) + \beta \\ \text{where} \\ \alpha &= \rho(x, u) \\ \beta &= \tau(x, u) \end{aligned} \quad (4)$$

Here, α and β denote the multiplicative and additive uncertainties respectively. These uncertainties can be estimated by reviewing historical accuracies of chosen modeling

approaches or by an intentional variable model-fidelity approach.

Table 1. Relationship between k and the Probability of Uncertainty

K	0.0	0.5	1	1.5	2	3	4	4.5	5
Probability (%)	100	61.7	31.7	13.4	4.55	0.27	6.4e-5	8e-6	6e-7

Step 5: To obtain the optimal solution based on the expected solution and the knowledge gained from the shifted Pareto frontiers from the above steps. Singh and Lou⁽⁹⁾ developed a methodology on hierarchical Pareto optimization for the sustainable development of industrial ecosystems⁽⁹⁻¹⁰⁾. The consideration of uncertainties in decision making/ decision analysis will enhance their proposed methodology and enrich the knowledge base in design for sustainability.

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. This 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 material such as ammonia, methanol, methane, and urea. Table 2 lists the composition and mass flow rate of process condensate obtained in the plant.

Table 2. Process Condensate Data

Concentration (ppm)					Flow rate $kg \cdot h^{-1}$	T $^{\circ}C$	P MPa
NH ₃	CO ₂	CH ₃ OH	Urea	CH ₄			
1612	1672	573.4	144	0.91	100000	217	3.75

3.1 Alternatives of treatment on process condensate

A typical technique to treat process condensate is steam stripping. Both medium-pressure (MP) steam and low-pressure (LP) steam can be used for stripping. Even natural gas can be used to separate the process condensate to reach the allowable emission concentration. Natural gas is also used as raw material in ammonia production and its flowrate is fixed based on the production throughput. However, due to the limited amount of natural gas available, it cannot be used to the full extent. In the current case study, three alternatives have been considered after pre-analysis and simulation. These alternatives are illustrated in Fig.'s 1, 2 and 3.

The first alternative (Fig. 1) utilizes MP steam for stripping process condensate. The chemical components in the condensate are stripped and transferred to the Converter I to be used as a raw material. The treated condensate from the stripping column can be used as

make-up water for boiler or can be discharged directly. In this alternative, both material and energy can be recovered from the condensate. This also results in zero emission to the environment. Hence, this is a clean process.

The second alternative utilizes saturated humidification using natural gas followed by MP steam stripping. The saturated steam leaving from the saturation column and the stripping steam from MP steam stripping column are transferred to Converter I thereby recycling all the chemicals back to be used as raw materials. The treated condensate can be recovered as boiler water or can be discharged directly. This alternative is also clean.

Alternative 3 is saturated humidification using natural gas followed by LP steam stripping. The stripping steam leaving the stripping column cannot be used in the production system directly due to its low pressure. It is condensed and recycled by the condensate separator. The condensate from the condenser is pumped and mixed with the process condensate, and separated in saturation column again. The saturated steam from the top of the saturation column is transferred to Converter I to avoid the accumulation of the chemical components. However, this treatment process cannot reduce the pollution radically. The non-condensing gas coming out of the saturation column contains small amount of chemical components which would cause environmental pollution if discharged directly into the atmosphere.

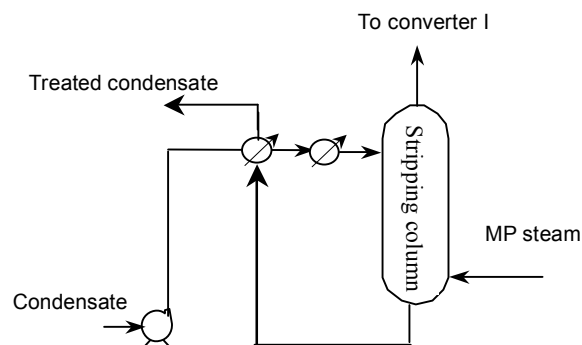


Figure 1. MP Steam Stripping

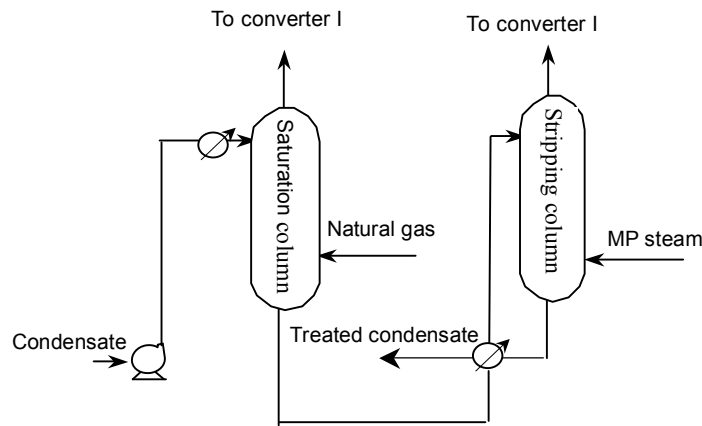


Figure 2. Saturated Humidification followed by MP Steam Stripping

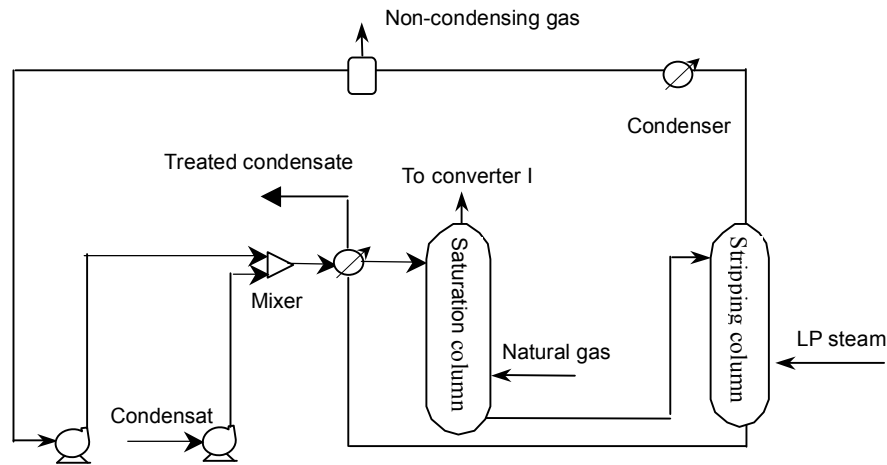


Figure 3. Saturated Humidification followed by LP Steam Stripping

3.2 Formulation of optimization problem under uncertainty

In this work, two objectives have been optimized: maximization of economic benefits while minimizing environmental impacts.

Two decision variables identified are condensate inlet temperature (T) and MP/LP steam flow rate (F). The value of inlet temperature ranges from 100°C to 245°C and that of steam flow rate is from 8000 kg/hr to 35000 kg/hr . The remaining operating or equipment parameters are assumed to remain fixed during optimization. The inlet temperature and flow rate of natural gas is 217°C and 22000 kg/hr respectively. The number of plates required in saturation column as well as the stripping column is 15.

A regression model is developed to model the relationship between the decision variables and the objective function using the simulation results of the proposed design scheme. This model is used as the basis of the optimization. The parameters used for formulating the environmental and economic objectives are listed in Tables 3 - 6.

The environmental impact index (EII) used to express the environmental objective is calculated by a short cut approach⁽¹⁰⁾. The “relative” stress caused by each chemical is calculated rather than the “absolute” value of the environmental impact caused by each chemical. This impact data was retrieved from the U.S. EPA's TRACI data base⁽¹¹⁻¹²⁾.

The environment regulations posed on the ammonia ($C_{\text{ammonia}} \leq 10 \text{ mg/l}$) and methanol ($C_{\text{methanol}} \leq 15 \text{ mg/l}$) concentration in treated water and emission gas are used as constraints for this optimization model. The price fluctuation of LP/MP steam is considered as a parameter uncertainty in the following work.

Table 3. Price Data

	H ₂ O	NH ₃	CH ₃ OH	Natural Gas	Steam
Price	0.125 (\$/ton)	312.5 (\$/ton)	250 (\$/ton)	160 (\$/ton)	6.25 (\$/MMkCal)

Table 4. List of Capital Cost

	Saturation column	LP-stripping column	MP-stripping column
Capital Cost (\$/yr)	2.25×10^4	1.88×10^4	2.63×10^4

Table 5. Normalized Value of Environment Impact Index (Media: Air)

Category	Acidification		Global Warming		Eutrophication		Human Health Non-Cancer		EII
	Factor	Norm. Factor	Factor	Norm. Factor	Factor	Norm. Factor	Factor	Norm. Factor	
NH ₃	95.485	1.0000	0	0.0000	0.1186	1.0000	3.1826	0.9668	2.9668
CH ₃ OH	0	0.0000	0	0.0000	0	0.0000	0.1093	0.0332	0.0332
CH ₄	0	0.0000	23	0.9583	0	0.0000	0	0.0000	0.9583
CO ₂	0	0.0000	1	0.0417	0	0.0000	0	0.0000	0.0417
Σ	95.485		24		0.1186		3.2919		

Table 6. Normalized Value of Environment Impact Index (Media: Water)

Category	Acidification		Global Warming		Eutrophication		Human Health Non-Cancer		EII
	Factor	Norm. Factor	Factor	Norm. Factor	Factor	Norm. Factor	Factor	Norm. Factor	
NH ₃	0	0	0	0	0	0	0.0590	0.6677	0.6677
CH ₃ OH	0	0	0	0	0	0	0.0294	0.3323	0.3323
CH ₄	0	0	0	0	0	0	0	0	0
CO ₂	0	0	0	0	0	0	0	0	0
Σ							0.0883		

3.3 Application of Pareto Optimization under Uncertainty

The optimization methodology discussed in section 2 has been utilized to optimize this case study. First, the mean values of objectives are calculated by using Genetic Algorithms⁽¹³⁻¹⁴⁾ to identify the Pareto frontier for every alternative shown in Fig. 4. Through these calculations, it was found that alternative (1) provides the lowest value of profit and higher environmental impact compared to other two design alternatives, so it is not considered for future optimization. Alternative (2) can yield the highest possible profit and relatively low environmental impact. So it is considered as the optimal candidate in deterministic optimization. In a magnified view of the Pareto frontier of alternative (3), it is observed that it is a curve and not vertical.

Secondly, the price of MP/LP steam is treated as uncertain variable in this case. The variation in the price expressed by price of heat load (\$/MMkcal) follows a normal distribution where the expected value is \$6.25/MMkcal, and the standard deviation is assumed as \$1.25/ MMkcal. The probability (P) of price variation is assumed to be 13.4%.

As a result of this, the Pareto frontiers are shifted according to $f = \bar{f} + k\sigma_y$, where k is equal to 1.5. The comparison of results between deterministic and parameter uncertainty optimization are shown in Fig. 5.

It is obvious that the profit decreases with increase in the price of MP/LP steam. As a consequence of variation of MP/LP steam price, the Pareto frontiers shift to the left but the environmental objective remains unaffected.

Next, the model uncertainty is incorporated by selecting suitable α and β values. In this work, it is assumed that the model uncertainty worsens the performance of the chemical process by reducing the profit and increasing the environmental impact. The values chosen for α and β are:

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

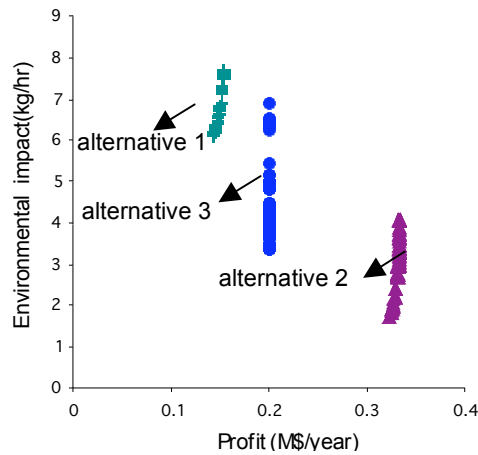


Figure 4. Pareto Frontiers in Deterministic Optimization

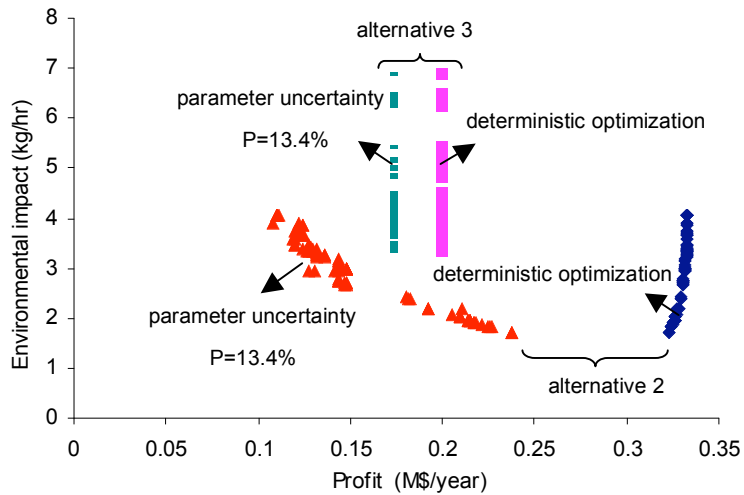


Figure 5. Effect of Parameter Uncertainty on Optimization

Figure 6 illustrate the effect of model uncertainty on optimization. Figure 7 presents a comparison of the optimal results for both parameter and model uncertainty. As can be seen in Fig. 7, the shifts of Pareto frontiers are different when considering both parameter and model uncertainties. Part A in the shift Pareto frontier for alternative (2) is better in terms of both economic and environmental objectives, but part B for alternative (2) is not optimal compared to that of alternative (3). In other words, some optimal solutions in alternative (3) have better process profit compared to part B of alternative (2), however, their environmental performance is similar. These results are different from the results obtained for deterministic optimization as well as that incorporating only parametric uncertainty.

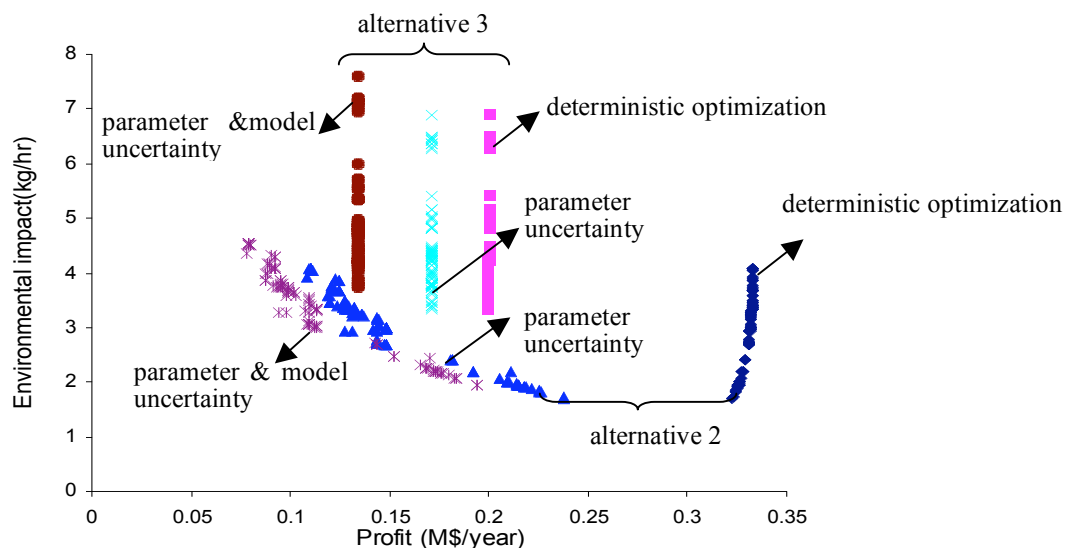


Fig. 6 Effect of Model Uncertainty on Optimization Result

4. Discussion and summary

- 1) Sustainability of a chemical process shall be enhanced by improving the triple-bottom line simultaneously.
- 2) Uncertainties should be taken into consideration during optimization, which can change the optimization result.
- 3) Pareto optimization methodology under uncertainty can be used for identifying the most sustainable solution from different design alternatives.

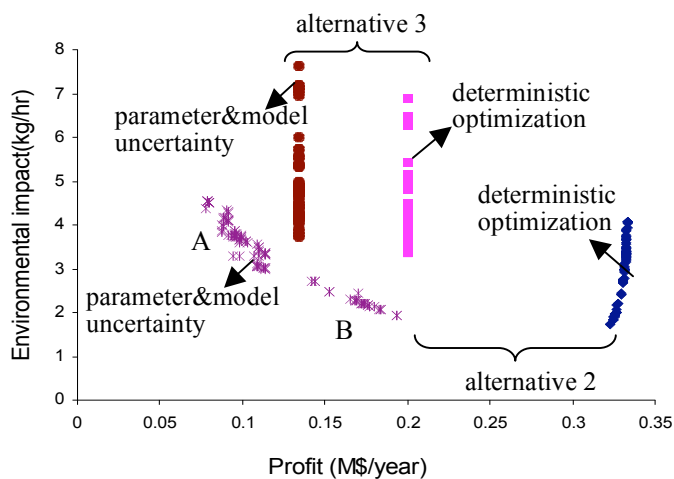


Fig. 7 Optimization under Uncertainty

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References

1. Wendt, M., P. Li, and G. Wozny, "Nonlinear-constraint Process Optimization under Uncertainty," *Ind. Eng. Chem. Res.*, 41, 3621-3629, 2002.
2. Cheng, L., E. Subrahmanian, and A. W. Westerberg, "Design and Planning under Uncertainty: Issues on Problem Formulation and Solution," *Computers and Chemical Engineering*, 27, 781-801, 2003.
3. Sahinidis, N. V., "Optimization under Uncertainty: State-of-the-Art and Opportunities," *Computers and Chemical Engineering*, 28, 971-983, 2004.
4. Mattson, C. A. and A. Messac, "Pareto Frontier Based concept Selection under Uncertainty with Visualization," *Springer – Special Issue on Multidisciplinary Design Optimization*, Invited (refereed) Paper, *OPTE: Optimization and Engineering*, 6, 85-115, 2005.
5. Sikdar, S., "Sustainable Development and Sustainability Metrics," *AIChE J.*, 49, 1928-1932, 2003.
6. AIChE Center for Waste Reduction and Technology (CWRT), *Collaborative Projects Focus Area: Sustainable Development*, AIChE, New York, NY, 2000.
7. Alexandrov, N. M., R. M. Lewis, C. R. Gumbert, L. L. Green, and P. A. Newman, "2000a: Optimization with Variable-Fidelity Models Applied to Wing Design," *Proceedings of the 38th AIAA Aerospace Sciences Meeting and Exhibit*, AIAA Paper 2000-0841, Reno, NV, USA, Jan 10-13, 2000.
8. Patterson, A., P. Bonissone, and M. Pavese, "Six Sigma Applied throughout the Lifecycle of an Automated Decision System," *Qual. Reliab. Engg. Int.*, 21:275-292, 2005.
9. Singh, A. and H. H. Lou, "Hierarchical Pareto Optimization for the Sustainable Development of Industrial Ecosystems," *Ind. Eng. Chem. Res.*, 46, 3265-3279, 2006.
10. Li, S., Singh A., and H. H. Lou., "A Case Study of Multi-Objective Optimization under Uncertainty for Sustainability," *AIChE Annual National Meeting*, San Francisco, CA, November 12-17, 2006.
11. Bare, J. C., G. A. Norris, D. W. Pennington, and T. McKone, "TRACI, the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts," *Journal of Industrial Ecology*, 6(3-4), 49-78, 2002.
12. National Risk Management Research Laboratory (NRMRL), USEPA, http://epa.gov/ORD/NRMRL/std/sab/iam_traci.htm.
13. Davis, L., *Handbook of Genetic Algorithms*, International Thomson Computer Press, 1996.
14. Gen, M. and R. Cheng, *Genetic Algorithms and Engineering Design*, Wiley-Interscience, USA, 1997