ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
Volume 9, Issue 8, February 2020

A Practical Approach in the Optimization of Uncertainty for Sustainability under Constrained Conditions

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Abstract: ***In order to enhance a sustainability of a chemical process, its economic, environmental and safety objectives need to be achieved simultaneously. This can be modeled as a multi-objective optimization [M-OO] problem. Any or most of the chemical processes come across various uncertainties throughout process design and operation in the form of manufacturing variations, material property variations, market fluctuation, etc., hence, the search of the optimal sustainability enhancement strategy can be formulated as M-OO under uncertainty. The study by Messac's group developed a methodology for systematic generation & evaluation of alternatives in the design of sustainable processes. This work attempts to extend the prior research in this field by introducing M-OO under uncertainty in process design for sustainability. A multi-step optimization approach is utilized to achieve a final decision. The effectiveness of this methodology is demonstrated by means of a case study.***

Keywords: multi-objective optimization, uncertainty, sustainability, Pareto frontier.

I. INTRODUCTION

Economic, environmental and societal concerns are three integral components of sustainability [1]. In order to enhance the sustainability of chemical processes, these objectives need to be achieved simultaneously [2]. Moreover, various uncertainties occur throughout process design and operation in the form of manufacturing variations, material property variations, market fluctuation, etc., which make the task more difficult. Thus, the problem needs to be modeled as a multi-objective optimization [M-OO] problem under uncertainty.

Messac's group developed a methodology for systematic generation & evaluation of alternatives in the design of sustainable processes [3]. Our work attempts to extend the prior research in this field to develop a systematic methodology to enhance the sustainability of chemical processes.

Manuscript received: 23 January 2020
Manuscript received in revised form: 19 February 2020
Manuscript accepted: 06 March 2020
Manuscript Available online: 15 March 2020

This research of the strategy is formulated as M-OO under uncertainty, and the effect of uncertainty reflects the reliability for the optimal solution. A multi-step optimization approach is utilized in this work. The effectiveness of this methodology is demonstrated by a case study about the process condensate treatment system in an ammonia synthesis plant. The remainder of the paper is organized as follows. Section 2 includes description of the optimization objectives for sustainability enhancement. Section 3 presents a multi-objective optimization algorithm under uncertainty. Section 4 demonstrates the effectiveness of this methodology by a case study about the treatment of process condensate in an ammonia synthesis plant, and the conclusion and discussion is given in section 5.

II. OPTIMIZATION OBJECTIVES FOR SUSTAINABILITY ENHANCEMENT

Sustainability metrics proposed by the IChemE and AIChE cover environmental, economic and societal metrics [4]. In this work, as an initial attempt, only economic and environmental objectives are discussed.

A. Economic objective

Traditionally, the profitability of a process was used as the only objective to be maximized. The profit has been calculated as the difference between the income and annual cost.

$$\max f1 = In - Mc \qquad [1]$$

Where: f_1 - process profit, [$M\$\cdot year^{-1}$]., In - income from product and recycled mass and energy, [$M\$\cdot year^{-1}$]., Mc - annual cost, [$M\$\cdot year^{-1}$]. The income is expressed as:

$$In = \sum P_i E_i \qquad [2]$$

Where: E_i - rate of product and recovered by-product and energy, [$ton\cdot year^{-1}$].

Pi - price of product and energy, [$\$\cdot kg^{-1}$].

The annual cost is expressed as:

$$Mc = Rw + O_P + C_{ap} \qquad [3]$$

Where: Rw - raw material cost, [$M\$\cdot year^{-1}$]., O_p - operating cost, [$M\$\cdot year^{-1}$]. C_{ap} - annual capital cost, [$M\$\cdot year^{-1}$].

B. Environmental objective

The environmental performance of an industrial process is related to resource usage, emissions, effluents and waste[5], and can be classified into following three environmental impact factors: physical potential impacts [acidification, greenhouse enhancement, ozone depletion and photochemical oxidant depletion], human toxicity effects [air, water and soil], and eco-toxicity effects

ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
Volume 9, Issue 8, February 2020

[aquatic and terrestrial][6-8].

The environmental impact of a chemical compound can be calculated in a way similar to the WAR algorithm. It is the function of chemical species emission amount and their environmental impact index [EII].

$$\min\ f_2 = \sum_{i=1}^{m} F_{uc} \times c_i \times e_i \qquad [4]$$

where: f_2 – environmental impact, [$kg \cdot year^{-1}$].
F_{uc} - mass rate of discharged fluid, [$kg \cdot year^{-1}$].
c - Concentration of discharge fluid.
e - Environmental impact index of chemical components in emission.

Environmental impact assessment [EIA] can provide guidance for different process improvement alternatives. It can be used as the preliminary evaluation to give initial solution on process optimization.

III. METHODOLOGY FOR MULTI-OBJECTIVE OPTIMIZATION UNDER UNCERTAINTY

Chemical process comes across various uncertainties throughout process design and operation in the form of manufacturing variations, material property variations, market fluctuation, etc., hence, the research of the optimal sustainability enhancement strategy can be formulated as M-OO under uncertainty.

$$\min.\quad f_i[x,u,\varepsilon] \quad i=1,2,\ldots,n \qquad [5]$$

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

$$g[x,u,\varepsilon] \le 0$$

$$x \in X,\ u \in U,\ \varepsilon \in \Xi$$

[6]

Where f is the objective function, h and g are the vectors of the equality and inequality constraints, and $x \subset R^n$, $u \subset R^m$, and $\varepsilon \subset R^S$ are vectors of state, decision, and uncertain variables, respectively.

The impact of equality constraints h is the projection of the uncertain variables to the state space, with some given u. This implies that the required values of state variables x can be computed by a multivariate integration of the model, i.e., x is a function of u and ε. So h will be eliminated from above constraints [9].

Uncertainties may change design decisions significantly. Classical methods for solving this problem under uncertainty include stochastic programming, robust stochastic programming, probabilistic [chance-constraint] programming, fuzzy programming, and stochastic programming. All these methods have their own advantages and disadvantages [10-12].

This work attempts to extend the prior research by Matton & Messac [3] in this field to apply Pareto optimization under uncertainty methodology in process design for sustainability.

In this methodology, the following steps are conducted:

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

$$\text{Min}\quad \bar{f}_i(x,u) \qquad i=1,2,\ldots,n \qquad [7]$$

Where $\bar{f}$ is the mean of f.

Step 2: To obtain standard deviations of the response variables σf 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 κσy to be [$\bar{f}$ + kσy] while considering uncertainties.

K is a positive number, corresponding to the probability of uncertainty that would happen. It also reflects the reliability for design decisions. Table 1 illustrates the relationship between k and uncertainty probability. If k = 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 k indicates lower probability of uncertainty and a more reliable decision. k=6 represents highly reliable decisions ["six-sigma" decisions] [13-14].

Step 4: To obtain the optimal solution based on the expected solution and the knowledge gained from the shifted Pareto frontiers from above steps [15].

Table 1. Relationship between k and Uncertainty Probability

K	0	0.5	1	1.5	2	3	4	4.5	5
Probability [%]	100	61.7	31.7	13.4	4.55	0.27	6.40E-05	8.00E-06	6.00E-07

IV. CASE STUDY

The Pareto optimization under uncertainty in design for sustainability methodology is applied in the treatment of process condensate in an ammonia synthesis plant.

A. *Problem statement*

Process condensate in ammonia production process [Kellogg technique] comprises of discharge from the hydrogen and nitrogen compressor as well as separators among adjacent segments. It contains ammonia, methanol, methane, urea and carbon dioxide. The condensate cannot be discharged directly due to its potential of pollution. Moreover, its direct discharge means the useful raw material such as ammonia, methanol, methane, and urea would be lost. Table 2 shows the process condensate data obtained from a plant.

Table 2. The Process Condensate Data

Concentration [ppm]					Flow rate	T	P
NH_3	CO_2	CH_3OH	Urea	CH_4	$kg \cdot h^{-1}$	°X	MPa
1612	1672	573.4	144	0.91	100000	217	3.75

ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
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B. Alternatives of treatment on process condensate

A typical technique to treat process condensate is steam stripping while natural gas, medium-pressure [MP] steam, and low-pressure [LP] steam can be mediums in stripping process condensate.

In this case study, initially five alternatives for treatment of process condensate were proposed shown in Fig.1 to Fig.5: [1]. saturated humidification by natural gas, [2]. LP steam stripping reflux, [3]. MP steam stripping, [4]. saturated humidification followed by MP steam stripping, [5]. saturated humidification followed by LP Steam stripping [16].

Prescreening and multi-objective optimization are conducted to identify which alternative is most desirable from both economic and environmental point of view. In this work, Aspen simulation was used to do the initial analysis.

Natural gas is as a raw material in ammonia production. Its flow rate is fixed based on the production throughput. Alternative [1] can be used to separate the wastewater in a saturation column, and most of chemical components can transfer from the liquid phase to the gas stream. But the treated condensate could not reach the allowable emission concentration due to the limited amount of natural gas available. Thus alternative [1] could not satisfy the separation requirement.

Alternative [2] is also called reflux stripping. According to the simulation results, the treated condensate from the LP stripping column can be used as make-up water for boiler or discharged directly. The stripping 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 emitted in air as it contains ammonia, methanol, methane, and carbon dioxide. Thus, it is condensed and flow back to the stripping column to recover these useful components. The non-condensing emission gas from the condenser is discharged in the atmosphere directly, but the trace ammonia, methanol, and carbon dioxide in it would have negative environmental impacts.

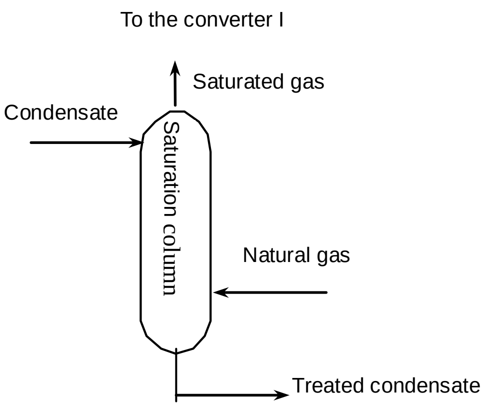

Fig. 1 Saturated Humidification by Natural Gas

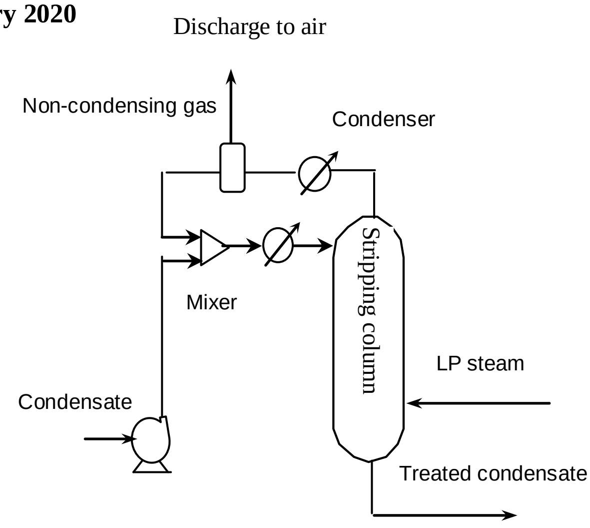

Fig. 2 LP Steam Stripping

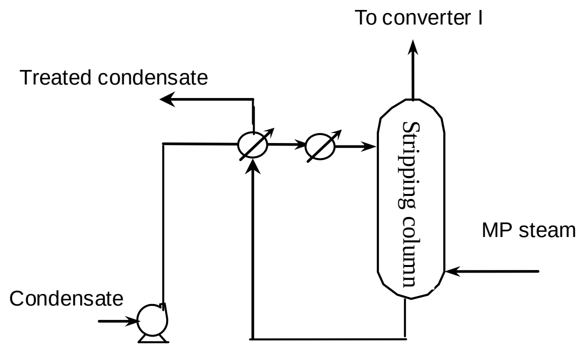

Fig .3 MP Steam Stripping

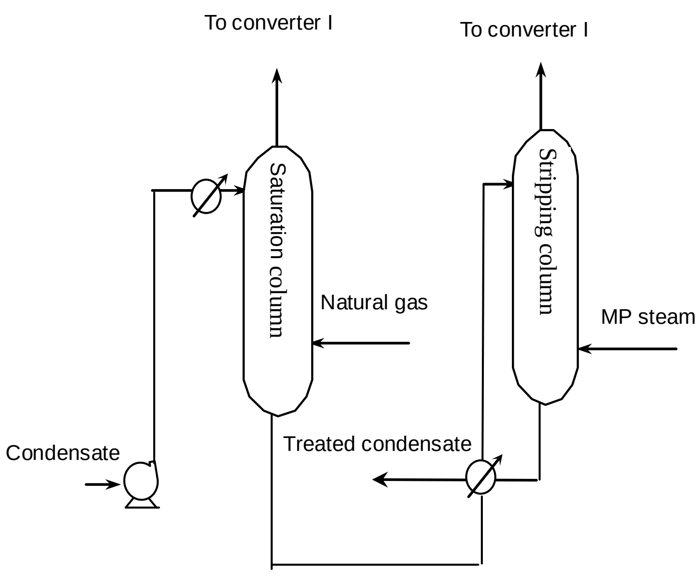

Fig. 4 Saturated Humidification Followed by MP Steam Stripping

ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
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Thus both alternatives [1] and [2] are rejected for future consideration. The other three alternatives can satisfy the separation requirement for stripped process condensate. The saturated gas leaving from the saturation column and the stripping steam from MP steam stripping column are transferred to the converter I as raw material, and the treated condensate can be discharged, or reused as boiler supply water.

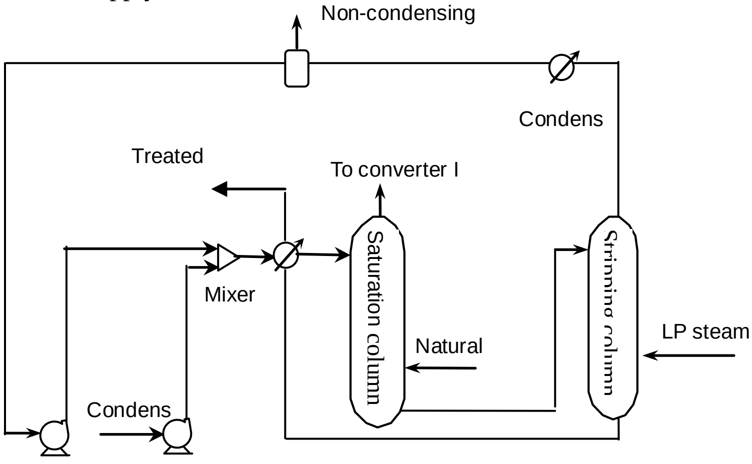

Fig. 5 Saturated Humidification Followed by LP Steam Stripping

C. Decision variables

Normally, there are two types of decision variables in engineering: operating/equipment variables, which affect objectives distinctly; Boolean variables, which represent existence or absence of process unit operation or a stream. In this work, there are no Boolean variables. Condensate inlet temperature [*T*] and MP/LP steam flow rate [*F*] have significant influence on the separation, and they are considered as decision variables. *T* is controlled in the range of 100-245℃. *F* is in the range of 8000-35000 $kg{\cdot}h^{-1}$. Other operating or equipment parameters are considered fixed during optimization. Inlet temperature/flow rate of natural gas is 217℃ /22000 $kg{\cdot}h^{-1}$. The number of plates required in saturation column /stripping column is 15 /15.

D. Objective functions and constraints

There are two optimization objectives in this work. They are economy maximum and environmental impact minimization as discussed in part 2.

It is difficult to express the relationship between the decision variables [*F, T]* and the economic and environmental performance. In this research, firstly, Aspen Plus is used to simulate the proposed design, then regression models are utilized to correlate the decision variables-objectives relationship based on the Aspen Plus simulation results. Parameters used in environment and profit optimization are listed in Table 3-4. Note these monetary values are based on information from a foreign plant, and they are not being the same price as the US. In this work, environmental impact index [EII] e_i in eq. [4] to expresses the environmental objective is calculated by a short-cut approach for simplification, which to calculate the "relative" stress caused by each chemicals rather than the "absolute" value of the environment impacts.

The absolute values of the environment impacts were retrieved from the U.S. EPA's TRACI data base [17-18]. In order to calculate the relative impact factor for a given compound in a mixed stream, firstly all the impact factors for each category [e.g. acidification, eutrophication, human health noncancer, etc.] are listed, and then the relative value of each factor for these chemicals in particular category is calculated. For example, both methane and carbon dioxide contribute to "Global Warming" and have an impact factor of 23 and 1 respectively. In order to calculate the relative impact factor, the two are added and divided each factor by the sum. This short cut provides a rough idea of the impact a chemical can cause relative to other chemicals. The calculated EII reflect relative impact for a given chemical relative to other chemicals in a mixed stream. Table 5-6 are the calculation on EII in air and water.

Table 3. List of Relative Substances and Energy Price

	H_2O	NH_3	CH_3OH	Natural	Heat energy
Price	0.125	312.5	250	160	6.25
	[$\$\cdot ton^{-1}$]	[$\$\cdot ton^{-1}$]	[$\$\cdot ton^{-1}$]	[$\$\cdot ton^{-1}$]	[$\$\times 10^{-6} kCal^{-1}$]

Table 4. List of Capital Cost

	Saturation column	LP-stripping column	MP-stripping column
Capital Cost（$\$\cdot y^{-1}$）	2.25×10^4	1.88×10^4	2.63×10^4

Table 5 and Table 6 are shown in Appendix

Constraints for this problem are expressed as environment regulations posed on the ammonia and methanol in the treated water and emission gas. i.e., $C_{o4} \leq 10$ *mg/l*, $C_{o5} \leq 15$ *mg/l*.

E. Uncertainty

Uncertainty normally is due to the random behavior in the process, property, or market, etc. In this case study, the effect of the fluctuation of LP/MP steam on the design choice is investigated.

F. Solution on the optimization under uncertainty

The optimization methodology given in part 3 is utilized in this work.

Firstly, Genetic Algorithms [GA] [19-20] is utilized to identify the Pareto frontier that can maximize the economic objective and minimize the environmental objective value simultaneously in deterministic case.

The Pareto frontier for every design alternative is shown in Fig. 6, where every point on the Pareto frontier reflects a non-dominant solution regarding both the economic and environmental objectives.

From the Pareto frontiers in Fig.6, it is known that the alternative [3] provides the lowest value of profit and high environmental impact compared to other two design

ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
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alternatives, so it will not be considered any further. It is also found that alternative [4] can yield the highest possible profit and low environmental impact, so it is the optimal candidate in deterministic optimization.

Note the Pareto frontier of alternative[5] is in fact not vertical, and a zoomed view of this curve is provided in Fig. 7.

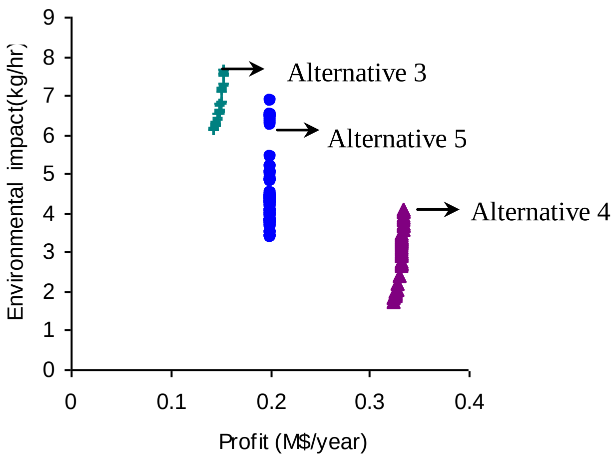

Fig. 6 Pareto Frontiers in Deterministic Optimization

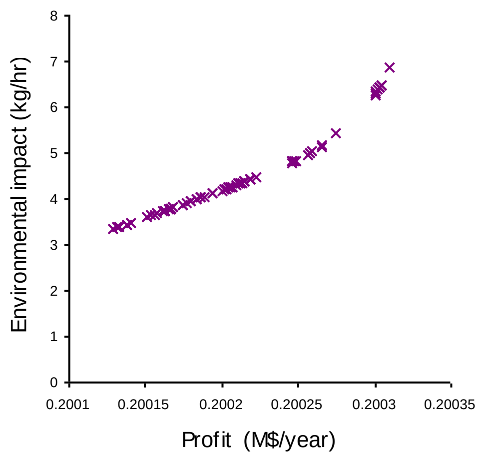

Fig. 7 Pareto Frontier of Alternative 5 in Deterministic Optimization

Secondly, In this case, the price of MP/LP steam[expressed by price of heat load, $/[106 Cal]] is thought as uncertainty variable. and the variation of the price is in normally distributed. The expected value is 6.25$[106 Cal]-1, and the standard deviation is assumed as 1.25$[106 Cal]-1.

The effect of parameter uncertainty on Pareto frontiers is expressed as kσ_y, and k reflects the probability of parameter uncertainty on optimal objective deviation. In this work, two levels of the probability P=31.74% and P=13.4% for uncertainty are calculated, corresponding to k=1.5 and k=3 respectively.

Thirdly, due to uncertainty, the Pareto frontiers are shifted from the deterministic non-dominant solutions to the new one [$\bar{f}$ + kσ_y]. The shifted Pareto frontiers are shown in Fig. 8.

It is obvious that the variation of MP/LP steam price would change the process profit but not the environmental objective. With the rise of the price of MP/LP steam, the operating cost would increase, so the profit decreases correspondingly. The Pareto frontiers would be shifted to the left.

It is observed from Fig. 8 that the shifts of Pareto frontiers are different while considering uncertainties for alternative [4] and [5]. The profit of the process in alternative [4] decreases greater than that in alternative [5]. When k=3, most points on the shifted Pareto frontier in alternative[5] has higher value of profit compared to that in alternative[4], even though some points in alternative[4] have higher environmental impact. So the optimal design choice can be either [4] or [5]. The uncertainty has changed the process decision-making. It is not same as the results from deterministic optimization.

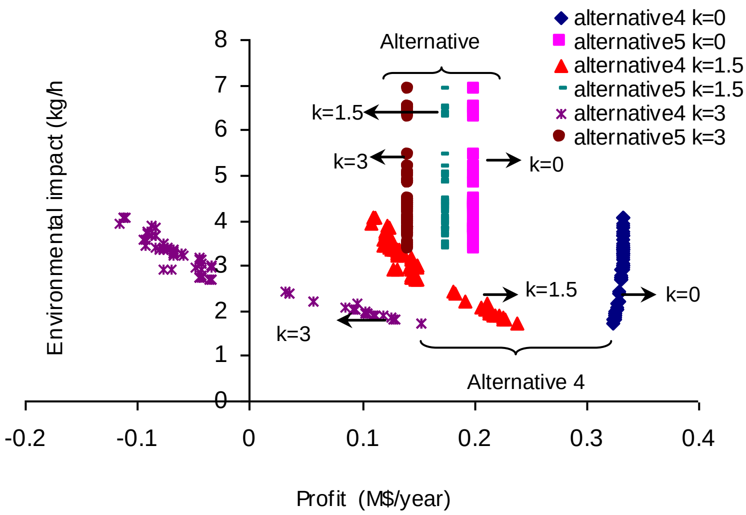

Fig.8 Effect of Uncertainty on Pareto Frontiers

V. DISCUSSION AND SUMMARY

1] It is clear that consideration of uncertainty may change the designer's choice.

2] Sustainability of the chemical process shall be enhanced mainly by improving the triple-bottom line simultaneously. A multi-objective decision-making framework will be needed to evaluate different design alternatives.

3] The consideration of uncertainty may change the designer's choice. Uncertainties are unavoidable in real world, and the designer shall take uncertainties into consideration in order to avoid or minimize the potential risks.

4] In the case study, only the variation of steam price is considered, and the environment impact is not affected by the price change. Nevertheless, if other uncertainties of the

ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
Volume 9, Issue 8, February 2020

process are considered, the environment performance maybe changed as well.

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ISSN: 2277-3754
ISO 9001:2008 Certified
International Journal of Engineering and Innovative Technology [IJEIT]
Volume 9, Issue 8, February 2020

APPENDIX

Table 5. Calculation on Environment Impact Index in Air

Category	Acidification		Global Warming		Eutrophication		Human Health Non-Cancer		EII
	Factor	Normalized Factor	Factor	Normalized Factor	Factor	Normalized Factor	Factor	Normalized Factor	
NH_3	95.485	1	0	0	0.1186	1	3.1826	0.967	2.9668
CH_3OH	0	0	0	0	0	0	0.1093	0.033	0.0332
CH_4	0	0	23	0.96	0	0	0	0	0.9583
CO_2	0	0	1	0.04	0	0	0	0	0.0417
Σ	95.485		24		0.1186		3.2919		

Table 6. Calculation on Environment Impact Index in Water

Category	Acidification		Global Warming		Eutrophication		Human Health Non-Cancer		EII
	Factor	Normalized Factor	Factor	Normalized Factor	Factor	Normalized Factor	Factor	Normalized Factor	
NH_3							0.059	0.6677	0.668
CH_3OH							0.029	0.0332	0.033
CH_4							0	0	0
CO_2							0	0	0
Σ							0.088		