A Case Study of Multi-Objective Optimization under Uncertainty in Process Design for Sustainability

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Abstract

In order to design a sustainable chemical process, its economic, environmental and societal objectives need to be achieved simultaneously. This can be formulated as a multi-objective optimization (M-OO) problem. A chemical process comes across various uncertainties throughout process design and operation in the form of manufacturing variations, material property variations, market fluctuation, etc. Hence, M-OO under uncertainty techniques need to be deployed to search the optimal strategy for sustainability enhancement.

Gani's group developed a methodology for systematic generation and 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 the final decision. The effectiveness of this methodology is demonstrated by means of a case study.

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

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1. 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 affect the chemical process throughout process design and operation in the form of manufacturing variations, material property variations, market fluctuation, etc., which make the task more difficult. Thus, we need to solve this multi-objective optimization (M-OO) problem under uncertainty in order to identify the most sustainable process design solution.

Gani's group developed a methodology for systematic generation and evaluation of alternatives to design sustainable processes[3]. Our work attempts to extend the prior research in this field to develop a systematic methodology to identify the most sustainable chemical process from a number of alternatives. The utility of this methodology is demonstrated by optimizing the design of a condensate treatment unit in an ammonia 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 on the treatment of process condensate in an ammonia synthesis plant, and the conclusion and discussion is given in section 5.

2. Design Objectives

Sustainability metrics proposed by the IChemE and AIChE cover environmental, economic and societal aspects of sustainability[1,4]. In this work, as an initial attempt, only economic and environmental objectives are considered.

2.1 Economic objective

Traditionally, while optimizing a process, only the profitability of the process was used as the objective to be maximized. In this work, the profit is defined as the difference between the income and annual cost.

$$max \quad f_1 = In - Mc \tag{1}$$

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:

$$In = \sum P_i E_i \tag{2}$$

where: E_i – production rate of product, recovered by-product and energy, (10^6 units$\cdot$ $year^{-1}$).

Pi - price of product and energy, ($\$ \cdot unit^{-1}$).

The annual cost is expressed as:

$$Mc=Rw+O_P+C_{ap} \quad (3)$$

where: Rw - raw material cost, ($M\$ \cdot year^{-1}$).

O_p - operating cost, ($M\$ \cdot year^{-1}$).

C_{ap} - annual capital cost, ($M\$ \cdot year^{-1}$).

2.2 Environmental objective

The environmental performance of an industrial process is related to resource usage, emissions, effluents and waste[5]. These can be classified into three environmental impact categories: physical potential impacts (acidification, greenhouse enhancement, ozone depletion and photochemical oxidant depletion), human toxicity effects (air, water and soil), and eco-toxicity effects (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 defined as a function of the amount of chemical species being dischareged and its corresponding environmental impact index(EII). Thus the environmental objective, which is to be minimized, can be defined as,

$$\min f_2 = \sum_{i=1}^{m} F_{uc} \times c_i \times e_i \quad (4)$$

where□f_2 – environmental impact, ($kg \cdot year^{-1}$).

F_{uc} - mass flow rate of discharged fluid, ($kg \cdot year^{-1}$).

c_i - mass fraction of chemical species i in discharge fluid.

e_i - Environmental impact index of chemical component i in discharge fluid

m – total number of chemical species present in the discharge fluid

3. Methodology for Multi-Objective Optimization under Uncertainty

A Chemical process comes across various uncertainties throughout the phase of design and operation. These uncertainties include manufacturing variations, material property variations, market fluctuation, etc. Hence, the search for the optimal design and operational strategy for sustainability can be formulated using techniques of M-OO under uncertainty.

$$\min. \quad f_i(x,u,\varepsilon) \quad i=1,2,\ldots,n \quad (5)$$

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

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

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

(6)

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

The impact of equality constraints h is the projection of the uncertain variables in the state space, given some decision variables 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 can be eliminated from the above constraints[9].

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

This work is based on the prior research done by Matton and Messac[13] and applies Pareto optimization under uncertainty methodology to process design for sustainability. The optimization steps in this methodology are discussed below:

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

$$\min \quad \bar{f}_i(x,u) \qquad i=1,2,\cdots,n \tag{7}$$

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 ($\bar{f}$ + kσ_y) while considering uncertainties. It needs to be explained that k is a positive number that corresponds to the probability of uncertainty that would happen. It also reflects the reliability for design decisions. Table 1 illustrates the relationship between k and probability of uncertainty. 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) [14].

Table 1. Relationship between k and Uncertainty Probability

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 4: 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[15] developed a methodology on hierarchical Pareto optimization for the sustainable

development of industrial ecosystems.[15] The consideration of uncertainties in decision making/ decision analysis will enhance their proposed methodology and enrich the knowledge base in design for sustainability.

4. Case Study

The Pareto optimization under uncertainty developed to design for sustainabile processes is applied to a process condensate treatment unit in an ammonia synthesis plant.

4.1. Problems statement

Process condensate in an ammonia production process (Kellogg process) 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 would cause loss of useful raw material such as ammonia, methanol, methane, and urea. Table 2 shows the process condensate data obtained from a plant.

Table 2. Process Condensate Data

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

4.2. Process Alternatives

A typical technique to treat process condensate is steam stripping. Natural gas, medium-pressure (MP) steam, or low-pressure (LP) steam can be used for stripping the process condensate. In this case study, initially five alternatives for treatment of process condensate were proposed as shown in Fig.1 to Fig.5. Figure 1 illustrates saturated humidification by natural gas, Fig. 2 shows LP steam stripping reflux, Fig 3. shows condensate stripping technique using only MP steam, schematic in Fig. 4 uses saturated humidification followed by MP steam stripping and the schematic in Fig. 5 uses saturated humidification followed by LP Steam stripping[16].

Pre-screening 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 for the initial analysis.

Natural gas is one of the raw materials used in ammonia production. In this case study, the flowrate of natural gas is fixed based on the production throughput. Alternative (1) uses natural gas to strip the condensate in the saturation column. Here most of the chemical components are transferred from liquid phase to gas phase. Still, the treated condensate does 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 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. Thus, it is condensed and sent back to the stripping column to recover these useful components. The non-condensing emission gas from the condenser, which has trace amounts of ammonia, methanol, and carbon dioxide, is discharged to the atmosphere directly, thereby causing negative environmental impact.

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 the saturation column and the stripping steam from MP steam stripping column are transferred to the converter I to be used as raw material. The treated condensate is either discharged, or reused as boiler supply water.

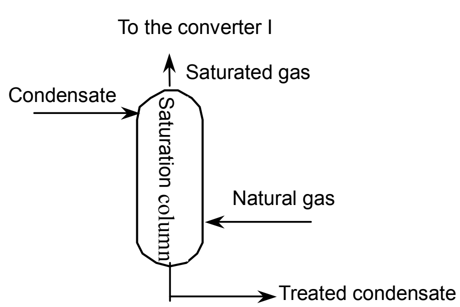

Fig. 1. Saturated Humidification by Natural Gas

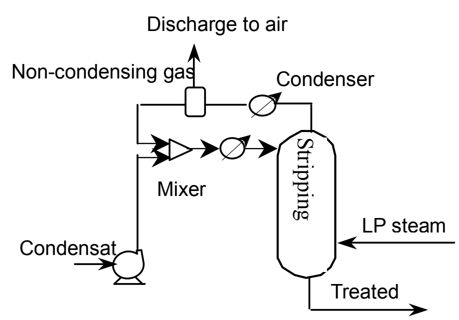

Fig. 2. LP Steam Stripping

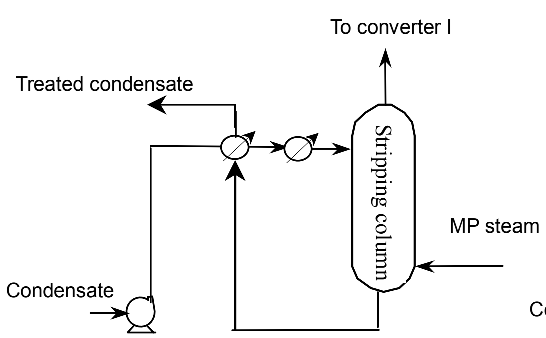

Fig. 3. MP Steam Stripping

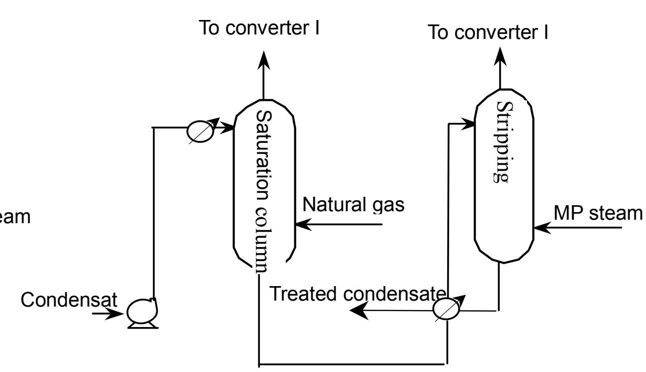

Fig. 4. Saturated Humidification followed by MP Steam Stripping

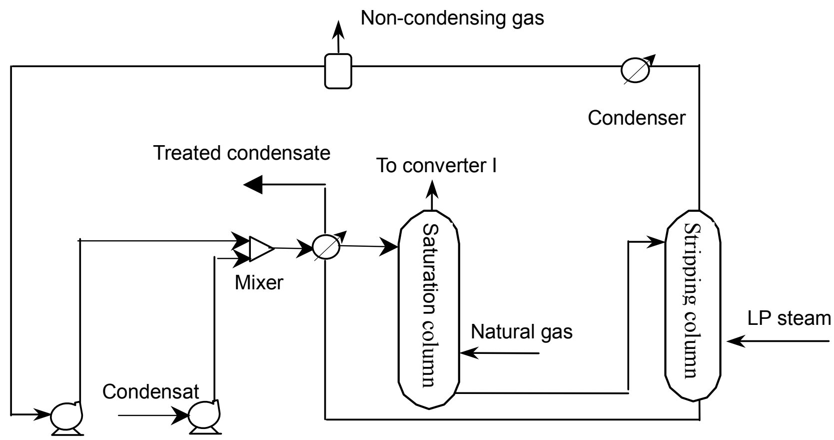

Fig. 5. Saturated Humidification followed by LP Steam Stripping

4.3. Decision variables

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

4.4. Objective functions and constraints

As discussed in part 2, there are two optimization objectives in this work: profit maximization and environmental impact minimization. It is difficult to express the relationship between the decision variables (*F, T*) and the economic and environmental performance. Therefore, the proposed design is simulated using ASPEN Plus firstly. Then, using these results regression models are developed to correlate the relationship between the decision variables and the economic and environmental performance. The parameters used in this optimization are listed in Tables 3 and 4. Note that since these monetary values are based on the information from a foreign plant, they may not reflect the prices in US.

In this work, the environmental impact index (EII) e_i in Eq.(4) is calculated 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 [6,17]. 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 non-cancer, etc.) are identified, 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, each factor is divided by the sum of all the factors. This short cut approach provides a rough idea of the impact a chemical can cause relative to other chemicals. The EII value reflects the "relative" impact of a given chemical relative to other chemicals used in or discharged from these target processes. Tables 5 and 6 illustrate the calculation of EII of process chemicals in air and water. This short-cut method can be conveniently used in evaluating the environmental performance of process alternatives.

Table 3. Price Data

	H_2O	NH_3	CH_3OH	Natural Gas	Steam
Price	0.125 ($\$\cdot ton^{-1}$)	312.5 ($\$\cdot ton^{-1}$)	250 ($\$\cdot ton^{-1}$)	160 ($\$\cdot ton^{-1}$)	6.25 ($\$.MMkCal^{-1}$)

Table 4. Annualized Capital Cost

	Saturation column	LP-stripping column	MP-stripping column
Capital Cost ($\$\cdot yr^{--1}$□	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	95.4850	1.0000	0.0000	0.0000	0.1186	1.0000	3.1826	0.9668	2.9668
CH3OH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1093	0.0332	0.0332
CH4	0.0000	0.0000	23.0000	0.9583	0.0000	0.0000	0.0000	0.0000	0.9583
CO2	0.0000	0.0000	1.0000	0.0417	0.0000	0.0000	0.0000	0.0000	0.0417
Σ	95.4850		24.0000		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	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0590	0.6677	0.6677
CH3OH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0294	0.3323	0.3323
CH4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Σ							0.0883		

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. $C_{ammonia} \leq 10\ mg \cdot l^{-1}$, $C_{methanol} \leq 15\ mg \cdot l^{-1}$.

4.5. Pareto Optimization under Uncertainty

Normally, uncertainty is caused due to the random behavior in the process, property, or market, etc. In this case study, the effect of price fluctuation of LP/MP steam on the performance of the process is investigated in terms of sustainability using Pareto optimization methodology given in part 3.

First, Genetic Algorithm (GA)[18-19] is utilized to identify the Pareto frontier that can maximize the economic objective and minimize the environmental objective value simultaneously in a deterministic case. The Pareto frontier for each design alternative is shown in Fig. 6, where every point on the Pareto frontier reflects a non-dominant solution for both economic and environmental objectives.

In the Pareto frontiers in Fig. 6, it is observed that alternative (3) provides the lowest value of profit and highest environmental impact compared to other two design alternatives Thus, it is not considered for further analysis. It is also observed that alternative (4) can yield the highest possible profit and lowest environmental impact, so it is the optimal candidate in deterministic optimization. Note that the Pareto frontier of alternative (5) is, in fact, not vertical, as can be seen in a magnified view of this curve provided in Fig. 7.

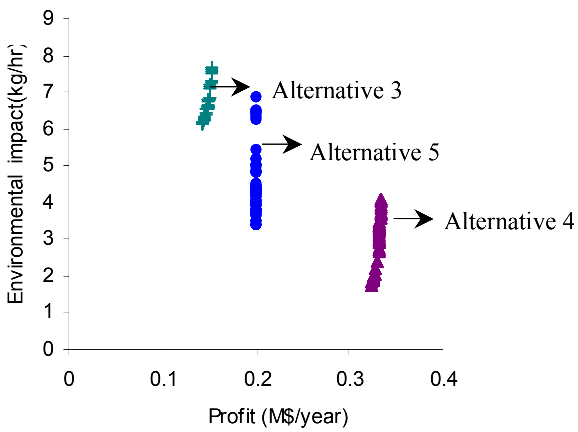

Fig. 6. Pareto Frontiers in Deterministic Optimization

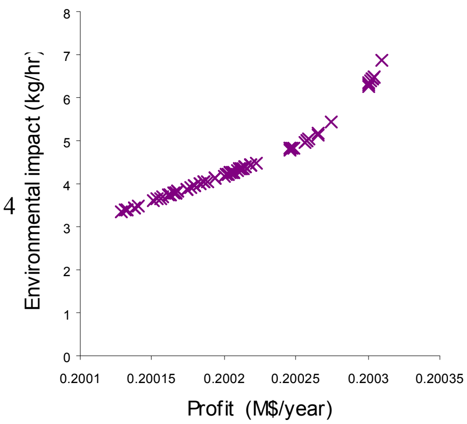

Fig. 7. Pareto Frontier of Alternative 5 in Deterministic Optimization

In the second step, the fluctuation in the price of MP/LP steam (expressed in price per heat load, ($\cdot$MMkCal^{-1}) is considered. It is assumed that the variation of the price follows a normal distribution, with the expected value of \$6.25 MMkCal^{-1}, and standard deviation of \$1.25 MMkCal^{-1}.

The effect of parameter uncertainty on Pareto frontiers is expressed as kσ_y, where k reflects the probability of parameter uncertainty on the optimal objective deviation. In this work, two levels of probability for uncertainty are calculated, i.e., k=1.5 and k=3 respectively.

Next, the shifted Pareto frontiers are plotted, as illustrated in Fig. 8. Due to uncertainty, the Pareto frontiers shift from the deterministic non-dominant solutions to the new solution ($\bar{f}$ + kσ_y).

It is obvious that the variation of MP/LP steam price would change the process profit but not the environmental objective. As the price of MP/LP steam increases, the operating cost also increases which consequently decreases the profit, thereby shifting the Pareto frontiers to the left.

The shifts of Pareto frontiers in Fig. 8 are different for alternative(4) and (5). The decrease in the total profit for alternative(4) is higher than that for alternative(5). When k=3, most points on the shifted Pareto frontier for alternative(5) have higher value of profit compared to that of alternative(4), even though some points in alternative(4) have higher environmental impact. Thus, the optimal design choice could be either alternative (4) or (5). It is clear that the consideration of uncertainty has changed the optimal solution significantly from the solution for deterministic optimization.

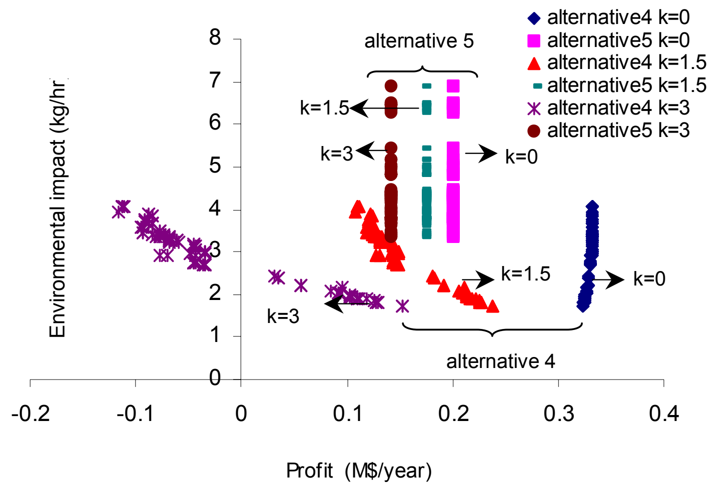

Fig.8. Effect of Uncertainty on Pareto Frontiers

5. Discussion and Summary

Sustainability of chemical processes can be enhanced significantly by optimizing the triple-bottom line simultaneously. A multi-objective decision- methodology under uncertainty is required to evaluate different design alternatives. It is clear from the results presented in previous sections that consideration of uncertainty may change the designer's choice, and avoid or minimize the potential risks.

In this preliminary study, only the variation of steam price is considered which has significant effect on economic performance of the process but does not affect the environmental impacts. Nevertheless, if other uncertainties affecting the process are considered, the environmental performance may change as well.

Acknowledgement

This work is in-part supported by the National Science Foundation under Grant CTS-0407494, the Texas Advanced Technology Program under Grant No. 003581-0044-2003 and the Gulf Coast Hazardous Substance Research Center.

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