MULTIOBJECTIVE OPTIMIZATION CONSIDERING ECONOMICS AND ENVIRONMENTAL IMPACT

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Abstract :　This paper is devoted to an application of MOOP (multi-objective optimization programming) concept to the practical field of chemical engineering for taking the trade-off between economics and pollution with appropriate analysis method. To analyze the bi-objective optimization system, non-inferior solution curve is formed in using SWOF (Summation of Weighted Objective Functions), GP (Goal Programming) and PSI (Parameter Space Investigation) methods within chemical process simulator. We can find the ideal compromise solution set based on Pareto curve. Multiobjective problem is then interpreted by sensitivity and elasticity analyses of the Pareto curve.

Keywords :　Multi-Objective Optimization Programming (MOOP), Global pollution index, Non-inferior solution curve (Pareto curve), Ideal compromise solution set, Sensitivity and elasticity analyses.

INTRODUCTION

As the interest in pollution prevention and waste reduction is heightened today, a multi-objective optimization approach considering simultaneously economics and environment is needed for designing competitive and clean chemical processes.

In the field of chemical engineering, the man-machine interactive algorithm (Umeda et al., 1980)[1] was developed for a chemical process design problem which is considered as a multi-objective optimization problem. Ciric and Huchette (1993)[2] presented the multi-objective optimization approach for the problem of process synthesis and optimization conflicted between economics and waste reduction. Finally, ε-constraint method (Luyben and Floudas, 1994)[3] within the framework of the GBD (Generalized Benders Decomposition) algorithm was used for the multi-objective MINLP (Mixed Integer Non-Linear Programming) problem concerning the interaction between design and control.

The risk-based chemical ranking and scoring in order to assess chemical toxicity and environmental fate were executed by Davis et al. (1994)[4] for hundreds chemicals which could produce an environmental pollution. This simplistic impact assessment utilizes the environment and human toxic effect data combined with exposure calculations which were based on persistence and bioaccumulation data. The WAR (WAste Reduction) algorithm (Hilaly and Sikdar, 1994)[5], by defining the pollution index of a product for a process, provides also a measure to assess the relative effect of modification on the process within chemical process simulator.

In this study, two objective functions are considered for process design and analysis. One is the global pollution index function (Φ; Impact/hr) which is introduced from potential environmental impact index (ψ_i about chemical component i ; Impact/mass). The other is the cost-benefit function with unit of $/hr. We present an algorithm that can form and handle, systematically and quickly, non-inferior solution curve for trade-off between the conflicting objectives within the chemical process simulator ProSim^{TM} which simultaneously performs the simulation of flowsheet and the optimization of design variables. Use of this algorithm is illustrated with simplified allylchloride process.

MULTI-OBJECTIVE OPTIMIZATION PROGRAMMING (MOOP)

1 Summation of Weighted **Objective Functions (SWOF)**

One of the most popular methods for multiobjective optimization is to minimize a convex combination of the objectives and thus converts the multiobjective problem to a single objective problem. For two objectives optimization problem :

$$\min_{x \in \Omega} \{ u(f_1, f_2, \alpha) = \alpha f_2 + (1-\alpha)f_1 \} \qquad \text{(UT)}$$

s. t. $\Omega = \{x : h(x)=0, g(x) \leq 0, a \leq x \leq b\}$

where, $u(f_1, f_2, \alpha)$: utility function

   f_1, f_2 : two objective functions

   α : weighting factor

   Ω : constraint set

Convex envelope of Pareto points (non-inferior solution set) can be generated by minimizing the sum of objectives for the various settings of weighting factor. Sequential Approximation Method (SAM) presented by Ciric and Huchette (1993)[2] permits to

find several Pareto points easily by choosing the weighting factor (α) by means of the slope (t_s) of previous two Pareto points. SAM is useful to quickly obtain approximate Pareto curve but it is no good to find entire Pareto points because of little difference of slopes over the several steps of SAM. In order to obtain further Pareto points, another method is therefore needed even if it is easy to apply this method into a variety of convex multi-objective problems.

2 Goal Programming (GP)

In the goal programming approach, we minimize one objective while constraining the remaining objectives to be less than the given target values (ε). This method is especially useful if the user can afford to solve just one optimization problem. Moreover, this method can be efficiently used when it is difficult to choose the weight (α) in the method of summation of weighted objective function. We can obtain the Pareto points as changing the target value of remaining objectives within the constraints.

$$\min_{x \in \Omega} f_1(x)$$

s. t. $f_i(x) \le \varepsilon_i$, (i≠1, 2≤i≤n)

$\Omega = \{x : h(x)=0, g(x) \le 0, a \le x \le b\}$

Goal programming cannot be used to effectively generate the complete Pareto set, particularly if the number of objectives is greater than two.

3 Parameter Space Investigation (PSI)

The PSI method is aimed at solving low-dimensional design problem in engineering field that are highly nonlinear and even nonsmooth. It is essentially a random sampling procedure, which involves the following steps :

(a) Sampling points on a uniform grid in the space of the decision variables constrained only by finite bounds.

(b) Evaluating the objectives and constraints (nonlinear inequalities) at each point.

(c) Discarding the points not satisfying the inequality constraints.

(d) Ordering the objective vectors and retaining the non-inferior points.

After one such a run, the designer sets goals on the objectives and tries to find objective vectors that satisfy them. If no such objective vector is found, either the goals are relaxed or more points are sampled and the process repeated (Steuer and Sun,1995)[6].

4 Ideal compromise solution set

Based on equation (UT), we suppose that (f_1^L, f_2^U) and (f_1^U, f_2^L) are solution sets in objective space when minimized respectively over the constraints set Ω. The point (f_1^L, f_2^L) can be defined in the objective space as the utopia point. Once a non-inferior solution curve is generated, we can directly convert to normalized non-inferior solution curve with each optimum points in the normalized objective space ($\hat{f}_1 - \hat{f}_2$).

An ideal mathematical compromise solution set can be obtained by determining Pareto solution set which is closest to the utopia point. This requires the distance between the utopia point and the non-inferior solution curve should be at a minimum. This distance, δ_p, depends on the particular norm p selected as follows :

$$\delta_p = ((\hat{f}_1)^p + (\hat{f}_2)^p)^{1/p}$$

$$1 \le p \le \infty$$

At norm p=1, weighting factor (α) is equal to 0.5 since the slope of Pareto curve ($d\hat{f_2}/d\hat{f_1}$ = $-(1-\alpha)/\alpha$) = -1. The minimum distance of δ_p at norm p=∞ lies in a point of $\hat{f_1}=\hat{f_2}$. In consequence, the ideal compromise solution set can be found on Pareto curve between norms p=1 and p=∞ in case of continuous convex Pareto curve. It is worth emphasizing that the solutions with the norm p=1 and p=∞ will provide lower and upper bounds of the ideal compromise solutions, respectively.

5 Sensitivity and elasticity analyses of Pareto curve

In our study considering the cost-benefit function (f_2) and the pollution function (f_1), sensitivity analysis of Pareto curve is defined as response of normalized utility function with respect to marginal cost ($\partial f_2/\partial f_1$) at each optimum point:

$$\hat{u}(\hat{f_1}, \hat{f_2}, \alpha) = (1-\alpha)\hat{f_1} + \alpha\hat{f_2} \tag{NUT}$$

$$\hat{f_2} = -\left(\frac{1-\alpha}{\alpha}\right)\hat{f_1} + \frac{\hat{u}}{\alpha},$$

so that,

$$\left[\frac{\partial \hat{f_2}}{\partial \hat{f_1}}\right]_{\hat{u}} = -\left(\frac{1-\alpha}{\alpha}\right)$$

and then, the normalized sensitivity is converted into marginal cost ($/Impact) for real scale of sensitivity.

$$\frac{\partial f_2}{\partial f_1} = \gamma\left(\frac{\partial \hat{f_2}}{\partial \hat{f_1}}\right) = -\gamma\left(\frac{1-\alpha}{\alpha}\right)$$

where,

$$\gamma = \left(\frac{f_2^U - f_2^L}{f_1^U - f_1^L}\right).$$

γ is a characteristic value ($/Impact) in a given process.

In the field of economics, elasticity using logarithmic derivatives for the productivity analysis can be defined as follows :

$$\frac{\partial \ln f_2}{\partial \ln f_1} = \frac{(\partial f_2 / f_2)}{(\partial f_1 / f_1)} = \frac{(\partial f_2 / \partial f_1)}{(f_2 / f_1)} = \frac{(\text{marginal cost})}{(\text{mean cost})}$$

This elasticity is denoted by the normalized functions and the normalized sensitivity :

$$\frac{\partial \ln f_2}{\partial \ln f_1} = \gamma\left(\frac{\partial \hat{f_2}}{\partial \hat{f_1}}\right)\left[\frac{(f_1^U - f_1^L)\hat{f_1} + f_1^L}{(f_2^U - f_2^L)\hat{f_2} + f_2^L}\right]$$

This may indicate a relative increasing or decreasing rate between two variables with dimensionless unity.

IMPLEMENTATION OF MOOP ALGORITHM IN PROCESS SIMULATOR

1 Global pollution index (Φ)

Global pollution index by unit time (Φ, Imp/hr) about a chemical process can be produced by incorporating with the potential environmental impact index (ψ_i) and global pollution balance equation (Mallick et al., 1996)[7]. Input impact (I_{in}^{raw}) is calculated with the previous environmental impact index, (ψ_i)$_{previous}$, produced by preceding process, with unit of Imp/kg-feed i :

$$\Phi = \sum_j\sum_i O_j x_{i,j} \psi_i + \sum_j\sum_i I_j y_{i,j} (\psi_i)_{previous} + \sum_j\sum_i E_j z_{i,j} \psi_i \tag{GPI}$$

where, O_j : flowrate of output stream j except product streams (kg/hr)

I_j : flowrate of input stream j (kg/hr)

E_j : flowrate of fugitive emission stream j (kg/hr)

$x_{i,j}$: weight fraction of chemical i in the output stream j

$y_{i,j}$: weight fraction of pollution chemical i generated by input stream j

$z_{i,j}$: weight fraction of chemical i in the fugitive emission stream j

The global pollution index (Φ) is used as objective function of pollution (f_1) in our study. However, we do not take account of the input impact of raw material within the pollution function because of the absence of general data about $(\psi_i)_{previous}$.

2 MOOP Module in process simulator

Approach of MOOP can be obtained by substituting the module MOOP for the module Optimization in process simulator. Fig. 1 shows MOOP algorithm using SQP (Successive Quadratic Programming) solver. Objective functions are first normalized by SWOF method with the weighting factors of α=0.0 and α=1.0. Then SWOF method with SAM (Sequential Approximate Method) is performed to search abridged Pareto curve. According to the target value of GP method, further points of Pareto are found within the interesting zone of the objective function to obtain entire Pareto curve. If nonconvex part of Pareto curve is detected, we can try to find nonconvex Pareto points in changing decision variables around nonconvex part, using PSI method. Finally, one can take trade-off between the conflicting objectives, understand the process characteristics and determine new operating conditions through the Pareto curve analysis using ideal compromise solution set, sensitivity and elasticity of Pareto curve.
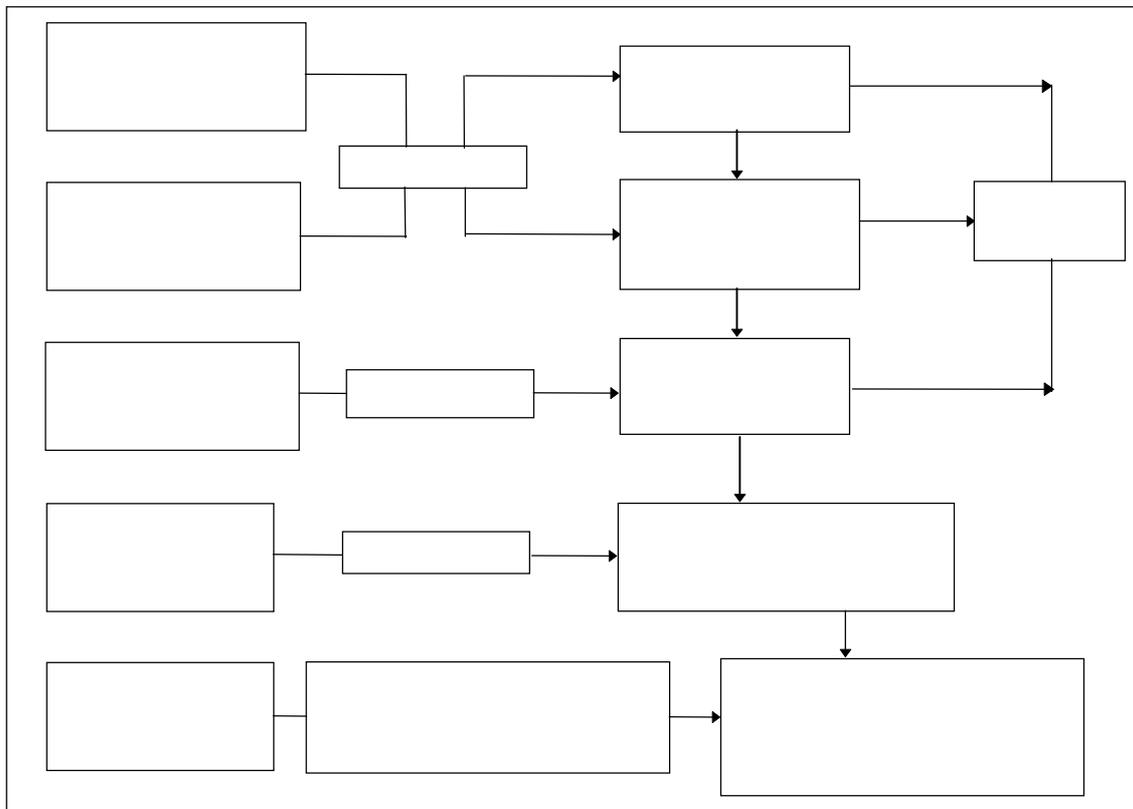

Fig. 1. MOOP algorithm in process simulator.

CASE STUDY – SIMPLIFIED ALLYLCHLORIDE PROCESS

The fundamental illustration is based on allylchloride process (Biegler and Hughes, 1983)[8] that is simplified by a separation unit instead of complex separation parts after reactor. Global pollution function by unit time (equation (GPI); Φ or f_1) is calculated only for byproduct of effluent stream from separation unit. The environmental impact index (ψ_i) is normalized by dividing with ($\mu+2\sigma$) and we use relative values based on propylene (C_3H_6) for global pollution function. The objective function of profit (f_2) is simply expressed by yield of product with the price of 131.5942 \$/kmol (Chemical Market Reporter, October 1998) with two decision variables (Reaction temperature and Cl_2 feedrate). The impact of fugitive emission is ignored. After mixing of feed and recycle streams, molar ration (η) of C_3H_6 to Cl_2 should be between 2.0 and 12.0. Propylene feedrate (F_{C3H6}) is fixed at 45.359 kmol/hr. For convenience, we set the profit function (f_2) be negative to minimize it.

Fig. 2 shows 11 Pareto points, which are found by using MOOP algorithm suggested in this study, with the fitting line of Pareto points in the normalized objective space. Ideal compromise solution set on the Pareto curve is located between points A and B, that is, non-inferior solutions from norm p=1 to norm p=∞.

The characteristic value (γ, \$/Imp) calculated in this process :

$$\gamma = \left(\frac{f_2^U - f_2^L}{f_1^U - f_1^L} \right) = (3467.76\text{-}3282.71)/(119.31\text{-}93.33) = 7.123$$

It is noteworthy that γ is the cost value (=7.123 \$) corresponding to such a pollution impact that one kmol of propylene (C_3H_6) can generate in this process. With the characteristic value, the sensitivity curve ($\hat{\underline{u}}$ vs. $\partial f_2/\partial f_1$) and the elasticity curve ($\hat{\underline{u}}$ vs. $\partial \ln f_2/\partial \ln f_1$) can be analytically drived from this fitting Pareto curve as shown in Figs. 3 and 4.
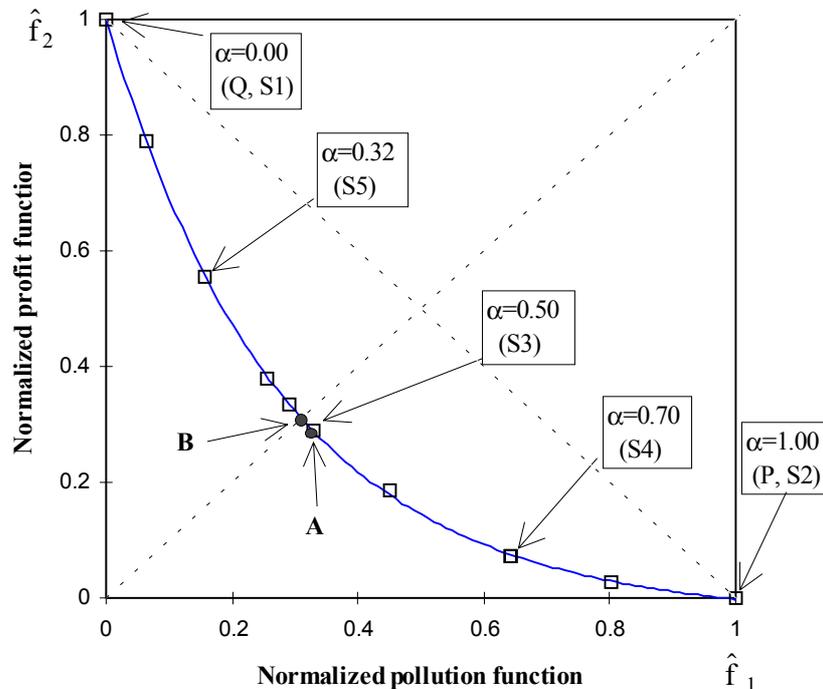
Fig. 2. Pareto points ($\square$) and fitting line of Pareto points (—) in normalized objective space.

In Table 4, new operating conditions from MOOP are compared with the nominal points of decision variables, minimum point of pollution function ($\alpha=0.0$) and traditional operating condition at the optimum point of profit function ($\alpha=1.0$).
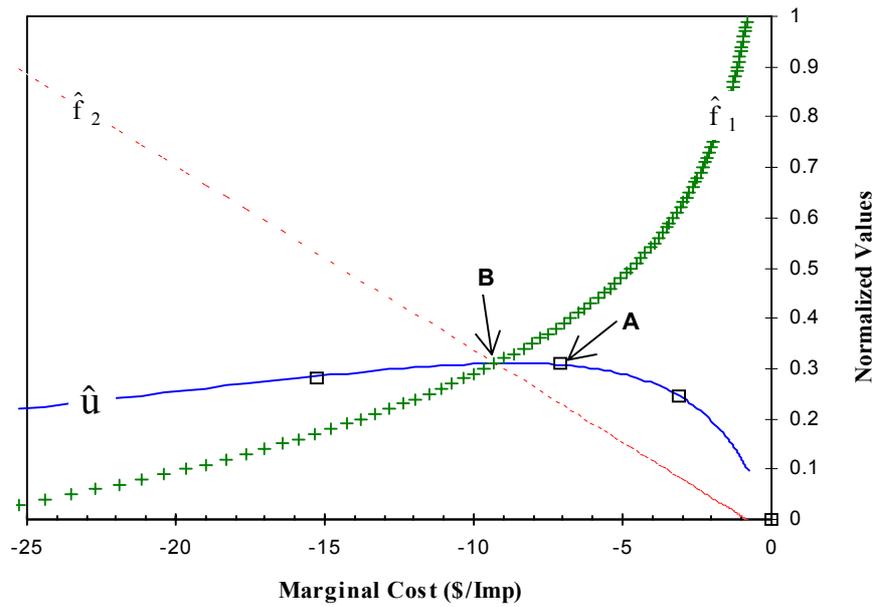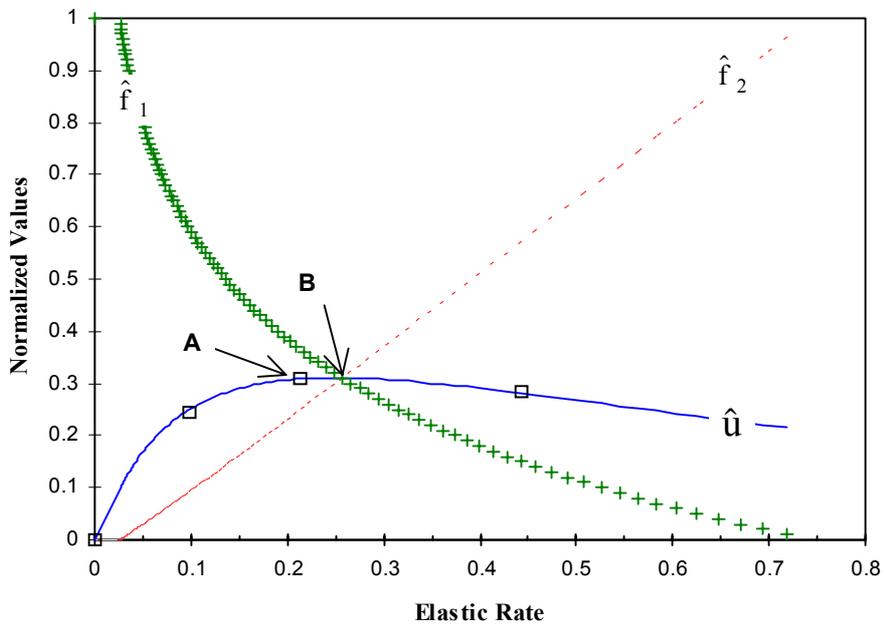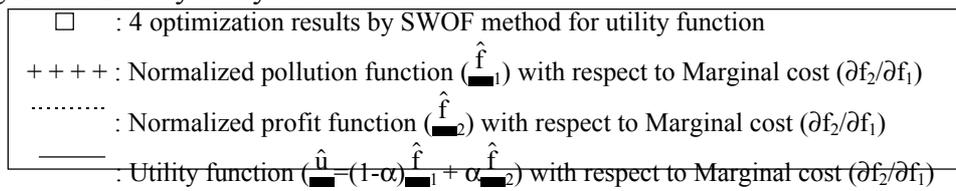
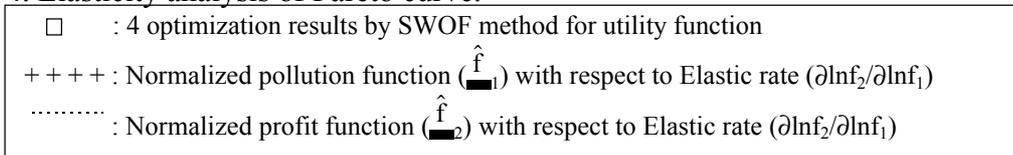Fig. 3. Sensitivity analysis of Pareto curve.

□	: 4 optimization results by SWOF method for utility function
+ + + +	: Normalized pollution function ($\hat{f}_1$) with respect to Marginal cost ($\partial f_2/\partial f_1$)
· · · · · · ·	: Normalized profit function ($\hat{f}_2$) with respect to Marginal cost ($\partial f_2/\partial f_1$)
———	: Utility function ($\hat{u}=(1-\alpha)\hat{f}_1 + \alpha\hat{f}_2$) with respect to Marginal cost ($\partial f_2/\partial f_1$)

Fig. 4. Elasticity analysis of Pareto curve.

□	: 4 optimization results by SWOF method for utility function
+ + + +	: Normalized pollution function ($\hat{f}_1$) with respect to Elastic rate ($\partial \ln f_2/\partial \ln f_1$)
· · · · · · ·	: Normalized profit function ($\hat{f}_2$) with respect to Elastic rate ($\partial \ln f_2/\partial \ln f_1$)

_____ : Utility function ($\hat{u}=(1-\alpha)\hat{f}_1 + \alpha\hat{f}_2$) with respect to Elastic rate ($\partial \ln f_2/\partial \ln f_1$)

The optimum value at norm p=∞ is obtained by GP method with target value = 0.31035 of normalized pollution function ($\hat{f_1}$). It is pointed out that new operating conditions between the ideal compromise solution points (norm p=1 and norm p=∞) are an advanced level for the decision maker to simultaneously satisfy an increase of the profit and a reduction of pollution.

Table 1. New operating conditions by MOOP in simplified allylchloride process.

	Decision Variables	Lower Value	Upper value	Nominal Value	Optimum value			
					Pollution function (f_1) at point Q	Profit function (f_2) at point P	Norm p=1 (α=0.5) At point A	Norm p=∞ (α=0.4518) at point B
1	Reaction Temp. (T_R, K)	650.0	750.0	690.0	650.0	698.8	684.0	683.0
2	Flowrate Cl_2 (F_{Cl2}, kmol/hr)	40.0	60.0	41.0	40.0	43.37	40.08	40.00
Objective function Values (f_1 and f_2)		f_1(Imp/hr)	106.88	93.33	119.31	101.93	101.38
		f_2($/hr)	-3442.35	-3282.71	-3467.76	-3414.00	-3409.98

CONCLUSION

The result of NLP is one optimization point, while MOOP gives a set of optimization results (Pareto curve). Therefore, it is necessary to choose one compromise point among the many optimum points. At least one objective must be sacrificed to enhance the other one objective because Pareto curve is unfortunately non-inferior solution points.

In this study, our MOOP algorithm, which consists of the mixed using of SWOF, GP, and PSI after pre-level of normalization and then post-level of Pareto curve analysis, is performed in the problem of economics-environment with the example of the chemical process. The ideal compromise solutions between norm p=1 and p=∞ on the Pareto curve are thought as a mild condition for satisfying two objectives. Using sensitivity and elasticity analyses of Pareto curve, MOOP approach gives a decision information to take a trade-off between economics and pollution.

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