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This study proposes a robust optimization model to handle uncertainty during the process design stage, together with a decision-making procedure. Different robustness concepts are presented to describe the characteristic, either economic or technical, of a given variable in the model. Among economic robustness measures, partial mean of costs is analysed to address its intrinsic problem of excessive variability of performance with respect to the change of values in its parameters. To resolve it, a novel formulation of robust economic optimization is derived, providing a conceptual framework for suggesting a proper range of parameter values. Then, the model is further extended to consider technical robustness as well. Lastly, the decision-making procedure is presented using the proposed nadir vector which is computationally inexpensive and also useful in selecting a final solution. The applicability of the model was successfully demonstrated by applying it to process design examples.

Keywords: economic robustness; partial mean of costs; lower bound; technical robustness; decision-making

Nomenclature

A	Heat transfer area of the heat exchanger, m^2.
b_i	Annualized fixed cost, \$/MW.
$\mathbf{C}$	Cost vector $\{C_1, \cdots\cdots, C_N\}$.
c_1	Best-case cost by solving stochastic problem.
c_2	Possible smallest worst-case cost.
c_3	Worst-case cost by solving stochastic problem.
C_{A0}	Concentration of reactant in the product, $kmol/m^3$.
C_{A1}	Concentration of reactant in the product, $kmol/m^3$.
$\mathbf{C}^{LB}$	Lower bound of objectives.
$c_{\min}$	Minimum of expected cost.
C_p	Heat capacity of the reaction mixture, $kJ/kmol \cdot K$.
C_s	Cost of scenario s

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C_w	Heat capacity of cooling water, $kJ/kg \cdot K$.
d_j	Energy demand, MW.
d_{js}	Energy demand of scenario s, MW.
E^*	Optimum expected cost.
(E/R)	Ratio of activation energy to gas constant, K.
$\mathbf{f}$	Objective vector.
F_{0s}	Feed flow rate, $kmol/h$.
f_s^*	Minimum value of an objective function, f_s.
$f_s\ (\mathbf{x}, y_s)$	Objective function which expresses a cost under scenario s.
Fl_s	Flow rate of recycle, $kmol/h$.
Fw_s	Flow rate of cooling water, kg/h.
g_i	Operating cost, \$/MW.
i	1, I, Plant.
I	Number of plant types.
j	1, J, Operation mode.
J	Number of operation mode.
k_0	Arrehenius rate constant of reaction, h^{-1}.
n_0	Integer where $x \in R^{n_0}$.
n_1	Integer where $y_s \in R^{n_1}$.
N	Number of scenarios.
p_s	Probability of the scenario s.
Q_{HEs}	Heat exchanger load, kJ/h.
s	1, N, scenario.
t	Target value.
T_0	Temperature of feed, K.
T^1	Calculated technical robustness measure by solving Case I.
T^2	Calculated technical robustness measure by solving Case II.
T_{1s}	Reactor temperature, K.
T_{2s}	Recycle temperature, K.
T_{w1}	Inlet temperature of cooling water, K.
T_{w2}	Outlet temperature of cooling water, K.
$U_E\ (\mathbf{C})$	Utility function of expected cost.
$U_{PM}\ (\mathbf{C}, t)$	Utility function of partial mean of cost with target value, t.
$U_T\ (\mathbf{y})$	Utility function of technical robustness
$U_{WC}\ (\mathbf{C})$	Utility function of worst-case cost.
V_s	Reaction volume, m^3.
V_d	Volume of reactor (design capacity), m^3.
w	Any number between 0 and 1.
W^*	Worst case cost.
$\mathbf{x}$	Scenario independent design variables.
x_i	Total capacity assigned to plant $i \in I$.
$\mathbf{y}$	Vector of operating variables.
y_{ij}	Allocation of capacity to operation mode j from plant type i.
y_{ijs}	Allocation of capacity to operation mode j from plant type $i$of scenario s.
y_s	Operating variables corresponding to scenario s.

Greek Letters

θ_j	Duration of operation mode j, h.
Ψ	Set of feasible vectors of corresponding multi-scenario optimization problem.
Ψ^*	Set of Pareto-optimal vectors of corresponding multi-scenario optimization problem.

1. Introduction

One of the major issues in engineering design is how to handle process uncertainty such as the quality of feed streams, estimates of product demand, and values of various physical properties and parameters, which may lead to undesirable variations in process performance (Georgiadis and Pistikopoulos 1999, Bertsimas and Pachamanova 2008). Thus, it is highly necessary to study and develop a robust optimization model that can take such uncertainty into account during the process design stage. In the simplest model, one accounts for possible uncertainties using a number of scenarios. The challenge of this problem is to optimize several objectives (*e.g.* minimize the costs of the scenarios) leading to a multi-objective problem. The most common way of dealing with several objectives is to optimize the expected value of objectives, usually using a cost vector. This approach is known as the *stochastic model* (Dempster 1980) and given by the following Problem (P1):

$$\min_{\mathbf{x}, y_1, \cdots, y_N} \quad U_E(\mathbf{C})$$

$$\text{s.t.} \quad U_E(\mathbf{C}) = \sum_s p_s C_s$$

$$C_s = f(\mathbf{x}, y_s)$$

$$\mathbf{x}, y_1, \cdots, y_N \in \Psi,$$

where p_s is the probability of scenario s; $U_E(\mathbf{C})$ is the expected cost of scenarios; C_s, the cost of the scenario s estimated using a certain function $f(\mathbf{x}, y_s)$; and Ψ, the set of feasible vectors. Practically, the set of feasible vectors is often restricted to the Pareto optimal set Ψ^*. Each scenario s is constructed using different sets of control and design variables, denoted as $y_s \in R^{n_1}$ and $\mathbf{x} \in R^{n_0}$ respectively, which correspond to a certain practical realization of the operational process. The stochastic model (P1) is constructed based on the assumption that the decision maker is risk-neutral because the optimal decision depends only on the expected cost. This approach only guarantees minimizing the expected cost, the probability-weighted average of scenario costs. However, it does not guarantee that the process will perform to a certain level over all the uncertain parameters. It is thus necessary to consider some additional 'robustness measures', which are used to probe the robustness variability.

Robustness can be inferred as risk aversion from the economic and technical points of view. The nature of each variable is different, so it is important to distinguish between different robustness concepts being applied. Therefore, the current study classifies variables into three groups: (i) scenario-independent variables, (ii) scenario-dependent technical variables (*e.g.*, temperature, pressure, flow rate, and liquid holdup), and (iii) scenario-dependent monetary or economic variables (*e.g.*, cost, profit, and production yield). In the case of scenario-dependent economic variables, the robustness concept should focus on reducing comparatively high scenario costs (*i.e.*, higher than the target cost), while keeping overall average cost as low as possible. On the other hand, the robustness measures for the scenario-dependent technical variables should be considered on the basis of the requirement that the operating conditions must be insensitive to variations within certain ranges as defined by the scenarios. The robustness measures for the scenario-dependent economic variables will be referred to in this study as 'economic robustness measures' and the robustness measures for the scenario-dependent technical variables, as 'technical robustness measures'. Although the robust optimization problem considering uncertainty has been widely studied in various areas of engineering (Eppen *et al.* 1989, Wellons and Reklaitis 1989, Straub and Grossmann 1990, Shah and Pantelides 1992, Malcolm and Zenios 1994, Ruppen *et al.* 1995, Samsatli *et al.* 1998, Suh and Lee 2001, Kang *et al.* 2004, Takriti and Ahmed 2004, Li and Ierapetritou 2008) and economics (Fishburn 1977, Eppen *et al.* 1989, Wellons and Reklaitis

1989, Straub and Grossmann 1990, Ruppen *et al*. 1995, Samsatli *et al*. 1998, Suh and Lee 2001, Kang *et al*. 2004, Takriti and Ahmed 2004, Li and Ierapetritou 2008), the difference between the economic and technical variables and the associated robustness measures still remains unclear (Rao 2009). Thus, the objective of this study is to propose appropriate economic and technical robustness measures applicable to robust optimization, which are both theoretically sound and practically implementable.

The development of economic and technical robustness measures is a vigorous field of research. It has been proven that economic robust measures should be monotonic (Fishburn 1977, Eppen *et al*. 1989, Ruppen *et al*. 1995, Samsatli *et al*. 1998, Suh and Lee 2001, Kang *et al*. 2004, Takriti and Ahmed 2004, Li and Ierapetritou 2008). It has also been shown that using symmetric measures as economic robustness measures (Malcolm and Zenios 1994, Rao 2009) yields suboptimal solutions as it is directly related to reducing the variability from the mean, which itself cannot be an objective of robust optimization. In addition, Pareto optimality, one of the important criteria for solutions of multi-objective optimization, is guaranteed only for monotonic robustness measures (Suh and Lee, 2001, Kang *et al*. 2004). Unlike economic robustness, technical robustness measures have been well understood to use even functions to reduce the variation among scenarios (Eppen *et al*. 1989, Wellons and Reklaitis 1989, Straub and Grossmann 1990, Shah and Pantelides 1992, Ruppen *et al*. 1995, Samsatli *et al*. 1998, Georgiadis and Pistikopoulos 1999, Suh and Lee 2001, Takriti and Ahmed 2004, Li and Ierapetritou 2008) while economic robustness has not yet been understood clearly (Rao 2009).

A variety of economic robustness measures have been proposed for the variability control, as reviewed elsewhere (Kang *et al*. 2004, Ben-Tal and Nemirovski 2008). Suh and Lee (2001) developed the Pareto-optimal subset condition, such that worst-case cost and partial mean of costs were recommended for robust economic optimization, guaranteeing the Pareto optimality of multi-scenario problems. Worst-case cost and partial mean of costs are defined as follows.

Worst-case cost:

$$U_{WC}(\mathbf{C}) = \max\{C_s | s = 1, \cdots, N\} \tag{1}$$

Partial mean of costs:

$$U_{PM}(\mathbf{C}, t) = \sum_{s=1}^{N} p_s \max\{C_s - t, 0\} \tag{2}$$

where t is a target value to be a criterion for penalizing exceedingly high scenario costs. Although both measures have been proven to be effective for robust economic optimization, model parameters such as the tolerance of a robustness measure and a target value remain to be determined for practical application. Kang *et al*. (2004) proposed a systematic method to determine the model parameters for partial mean of costs by investigating the parameter ranges. The theoretical concepts presented in the study were illustrated with a clear graphical representation of the parameter space.

However, partial mean of costs, despite to its popular application, is difficult to use as a robustness measure in practical applications. First, it is not guaranteed that the actual expected cost of the process will be minimized, because only the mean of scenario costs above a certain target value is optimized. Second, evaluating the actual scenario probabilities and envisaging all permissible scenarios at the design stage are challenging tasks. The design of the probabilities is often based on the preference of the decision-maker and the perceived relative importance of some scenarios, which can be subjective. It probably does not require many arguments to convince one that both factors are highly uncertain. The next issue is related to the instability of the model in terms of possible variations of the probabilities; it may happen that small changes in a probability can result in significant differences in the solutions. Lastly, the choice of a proper target value can introduce some issues. For example, if the target value chosen is too large or too small, the robust partial mean problem reduces to the stochastic problem (P1) and the resulting performance varies significantly depending on the scenario actually realized without controlling variation. Therefore, one of the aims of the current study is to propose a novel formulation of robust economic optimization, which can resolve the problems associated with using partial mean of costs.

The rest of the paper is structured as follows: In Section 2, a motivating example is introduced to illustrate in detail the intrinsic problems of using partial mean of costs as a robustness measure, followed in Section 3 by the modified formulation for the theoretical investigation concerning the meaningful ranges of target values. The motivating example is then revisited in order to discuss the performance of the proposed range of target values. Subsequently, a multi-objective optimization problem is defined taking into account both economic and technical robustness and solved to generate a number of robust solutions within proposed ranges of objectives. Finally, engineering design examples are evaluated to propose a decision-making procedure for selecting a final solution amongst many different robust solutions.

2. Motivating example

Figure 1 shows the network structure of the power system capacity expansion model (Malcolm and Zenios 1994). The design capacities over a given set of plants can be selected by minimizing the capital and operating costs of the system, satisfying customer demand and physical constraints.

The mathematical formulation is given by:

$$\min_{x,y} \quad \sum_{i\in I} b_i x_i + \sum_{j\in J} \theta_j \sum_{i\in I} g_i y_{ij} \tag{3}$$

subject to

$$x_i - \sum_{j\in J} y_{ij} \geq 0 \quad \text{for all } i \in I \tag{4}$$

$$\sum_{i\in I} y_{ij} = d_j \quad \text{for all } j \in J \tag{5}$$

$$x_i \geq 0, \quad y_{ij} \geq 0 \quad \text{for all } i \in I,\ j \in J \tag{6}$$

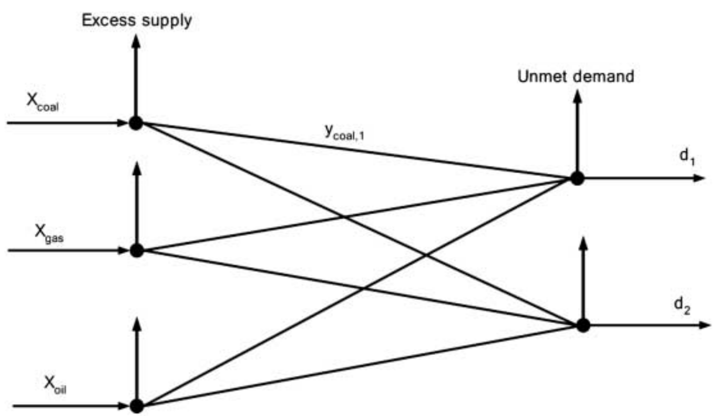

Figure 1. Network representation of a power system.

Table 1. Supply options and associated costs.

Plant types	Capital cost	Operating cost
Plant 1	200	30
Plant 2	500	10
Plant 3	380	20
Plant 4	0	200

where I denotes the set of plant types (*e.g.* hydro, coal, etc), and J is the set of operation modes (namely base and peak), b_i and g_i are the annualized fixed cost (\$/MW) and operating cost (\$/MW), respectively for plant $i \in I$. θ_j and d_j are the duration (h) and energy demand (MW), respectively at operation mode $j \in J$. Energy demand d_j (MW) is defined for operation mode $j \in J$. The variable x_i denotes the total capacity assigned to plant $i \in I$ while y_{ij} is the allocation of capacity to operation mode j from plant type i.

Four different plant types {Plant 1, Plant 2, Plant 3, Plant 4} are considered in this example. Table 1 shows annualized fixed cost (b_i) and operating cost (g_i) for each plant. Plant 1 has low capital cost but high operating cost. Plant 2 has high capital cost but low operating cost, while Plant 3 has medium capital cost and medium operating cost. Lastly Plant 4 describes external supply only used whenever necessary to meet demand in excess of the existing capacity; therefore it has zero capital cost but very high operating cost. Plant 4 implies that unmet demand is zero because demand is always satisfied, possibly via use of external supply option, if necessary.

This model is extended to consider uncertainties in demand, expressed as four scenarios over base and peak as shown in Figure 2. Then, the robust partial mean model by Suh and Lee (2001) is applied as follows:

$$\min_{x,y} \quad (U_E(\mathbf{C}), U_{PM}(\mathbf{C}, t)) \tag{7}$$

where

$$C_s = \sum_{i \in I} b_i x_i + \sum_{j \in J} \theta_j \sum_{i \in I} g_i y_{ijs} \tag{8}$$

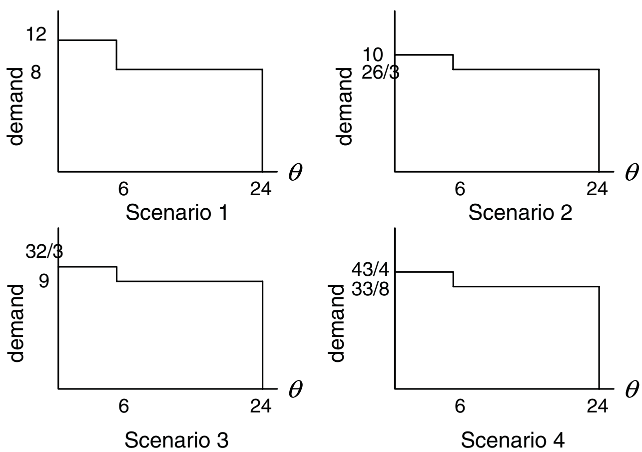

Figure 2. Cumulative load duration curves for four scenarios.

subject to

$$x_i - \sum_{j \in J} y_{ijs} \geq 0 \quad \text{for all } i \in I \text{ and } s \in N \tag{9}$$

$$\sum_{i \in I} y_{ijs} = d_{js} \quad \text{for all } j \in J \text{ and } s \in N \tag{10}$$

$$x_i \geq 0, \quad y_{ijs} \geq 0 \quad \text{for all } i \in I,\ j \in J, \text{ and } s \in N \tag{11}$$

This problem can be solved by constructing an objective of weighted sum of two objective functions as

$$\min_{x,y} wU_E(\mathbf{C}) + (1-w)U_{PM}(\mathbf{C}, t) \tag{7$'$}$$

where w varies from 0 to 1. In general, a target value, t, in Equation (7′) is determined by an expert or a system condition. In this model, the minimum of the expected cost was used as the target value, t, which is a system condition.

Figure 3 illustrates the results for the model defined by Equations (7′) and (8) to (11). In this figure, each scenario cost is plotted against expected cost as w changes from 0 to 1. The left-most points are obtained with only expected cost ($w = 0$) as an objective, resulting in stochastic problem (P1). The right-most points represent the solutions with only partial mean of costs ($w = 1$) as an objective. In other words, the left-most points are least robust solutions while the right-most points are most robust solutions.

According to Pareto optimality, scenario costs above a target value are expected to decrease with increasing expected costs as the weighting of partial mean of costs increases. It can be paraphrased that robust solutions which have small variability among scenario costs are obtained by sacrificing (*i.e.* increasing) expected cost. However, in Figure 3, the worst-case cost (scenario 3) above the target value increases from \$7695 to \$7740 with increasing expected cost from \$7395 to \$7422. Even the most robust solutions ($w = 1$) show larger variability among scenario costs than the least robust solutions ($w = 0$). This means that the partial mean of costs does not work as a robustness measure without controlling comparatively higher costs. Furthermore, in the case of

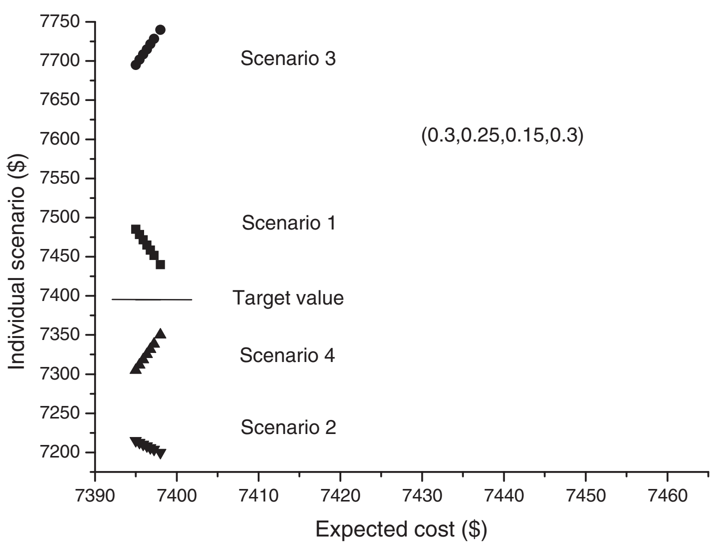

Figure 3. Individual scenario cost vs. expected costs with $p = (0.3, 0.25, 0.15, 0.3)$.

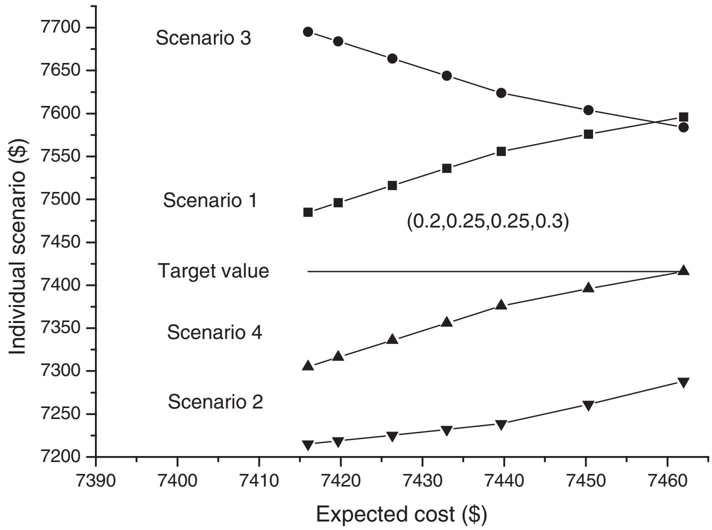

Figure 4. Individual scenario cost vs. expected costs with $p = (0.2, 0.25, 0.25, 0.3)$.

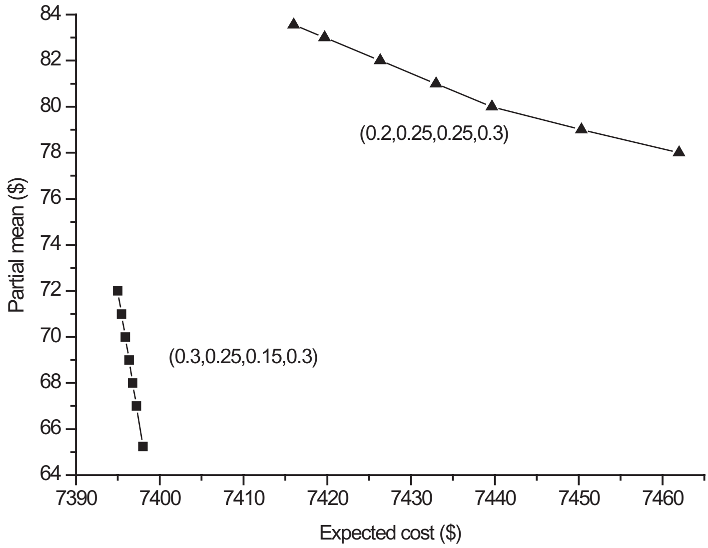

Figure 5. Pareto curves between expected cost and partial mean of cost.

a small change in the probability set to (0.2, 0.25, 0.25, 0.3), the optimization results in completely different solutions as described in Figure 4. A comparison between Figure 3 and 4 demonstrates that even the most robust solutions can be quite different in the same system with respect to a change in the set of probability although they are expected to be similar. This difference can be also observed from Pareto curves between expected cost and partial mean of costs in Figure 5. These results clearly illustrate the problems associated with using the partial mean of costs as an economic robustness measure. There can be a couple of reasons for this excessive performance variability. One is the fact that the partial mean of costs is not a Lipschitzian function of probability (Miettinen 1999). The other is that using uncertain information such as a target value or probability contributes to this variability.

Therefore, this study proposes a modified formulation of robust partial mean model, to resolve the issues with partial mean of costs and provide a theoretical ground for selecting a desirable target value.

3. Modified formulation

In this section, a novel formulation for robust economic optimization is proposed. The objectives of robust partial mean model (Equation (7)) can be reformulated as follows:

$$\min_{\mathbf{x}, y_1, \cdots, y_N} (\max\{C_1 - t, 0\}, \cdots, \max\{C_N - t, 0\}, U_E(\mathbf{C})) \tag{12}$$

This formulation with $N + 1$ objectives guarantees Pareto optimality (Kang *et al.* 2004). The first N objectives are robustness measures to penalize scenario costs above a target value, t. It should be noted that these robustness measures are independent of probabilities, implying that the potential issues originating from using probability can be avoided. Since the first N objectives have the same characteristic, they are investigated separately as an initial step, and only then expected cost, $U_E(\mathbf{C})$, is considered. For the feasible treatment of these first N objectives, an appropriate ordering is introduced below.

3.1. *Ordering objectives*

To deal with multiple objectives in Equation (12), an ordering relation applicable to comparing the order of objective vectors is defined as follows:

DEFINITION 1 *Two N-vectors $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$ have an order denoted by $\leq_t$*

$$\mathbf{C}^{(1)} \leq_t \mathbf{C}^{(2)} \tag{13}$$

if

$$\max\left\{C_s^{(1)} - t, 0\right\} \leq \max\left\{C_s^{(2)} - t, 0\right\} \tag{14}$$

for all $s = 1, \ldots, N$.

The ordering relation $\leq_t$ is monotonic in the sense that in general, $\mathbf{C}^{(1)} \leq \mathbf{C}^{(2)}$ implies $\mathbf{C}^{(1)} \leq_t \mathbf{C}^{(2)}$. As a consequence, $\leq_t$ is a pre-order – it is reflexive and transitive, but not necessarily anti-symmetric (Just and Weese 1995). In this relation $\leq_t$, if $C_s^{(1)}$ and $C_s^{(2)}$ are less than the given target value, $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$ pairs may be treated as if they are indifferent to each other although one is strictly larger than the other. To avoid this undesirable insensitivity, $U_E(\mathbf{C})$, the last entry in Equation (12), is included in the objectives. Note that $U_E(\mathbf{C})$ is strictly monotonic with respect to t leading to the following definition.

DEFINITION 2 *Two N-vectors $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$ have an order $\mathbf{C}^{(1)} \leq_{(t,U_E)} \mathbf{C}^{(2)}$ if $\mathbf{C}^{(1)} \leq_t \mathbf{C}^{(2)}$ and $U_E(\mathbf{C}^{(1)}) \leq U_E(\mathbf{C}^{(2)})$.*

The ordering relation $\leq_{(t,U_E)}$ is still a pre-order, but it is strictly monotonic (Kang et al. 2004) so that $\mathbf{C}_1$ is strictly preferred to $\mathbf{C}_2$ if $\mathbf{C}_1 < \mathbf{C}_2$.

Now, the definitions mentioned above define a lower bound among the first N objectives in Equation (12).

DEFINITION 3

$$\mathbf{C}^{LB} = \textit{Lower bound} \quad \textit{if}\, \mathbf{C}^{LB} \leq_t \mathbf{C}\, \textit{for all}\, \mathbf{C} \in (\Psi^*, t) \tag{15}$$

It is observed that a lower bound is not unique because every Pareto optimal solution can be a lower bound of a certain target value. However, another objective, expected cost, is a strictly monotonic function of a target value which can be effective in ordering multiple solutions. Depending on a target value, the existence or multiplicity of lower bounds is decided, affecting robust solutions. If t is chosen too small so that it is not larger than any entries of $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$, Equation (13) reduces to $\mathbf{C}_1 \leq \mathbf{C}_2$. This means there is no lower bound and the robust optimization formulation becomes the original multi-objective problem. On the other hand, if t is chosen too large so that it is not less than any entries of $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(2)}$, Equation (13) reduces to $\mathbf{C}^{(1)} = \mathbf{C}^{(2)}$. Since all the robustness measures in Equation (12) become zero, the robust optimization formulation reduces to the stochastic problem (P1). Only with proper target values, the robustness measures can be effective for robust optimization. In the following section, the meaningful ranges of target values are discussed in detail.

3.2. *Range of target values*

Target values play an important role in deciding the existence or multiplicity of lower bounds. Since the modified formulation in the previous section is derived based on the definition of partial mean of costs, the meaningful ranges of partial mean of costs with target values proposed by Kang *et al*. (2004) are employed to decide a proper target value (Figure 6). ABC curve in Figure 6 is generated by solving the robust partial mean model and changing either a target value or tolerance of partial mean of costs within the range of partial mean of costs. Kang, *et al*. (2004) proved that target values and tolerance of partial mean of costs inside ABC curve guarantee Pareto optimality. In this curve, c_1 and c_3 are the smallest and largest scenario costs, respectively, obtained by solving the stochastic problem (P1). The smallest possible value of worst-case cost, c_2, can be obtained by minimizing worst-case cost (Equation (1)) as an objective; $c_{\min}$ is the minimum expected cost obtained by solving the stochastic problem (P1). If the target value is greater than c_3, a lower bound exists for every t, indicating that a lower bound does not act as a robustness measure. In this case, all of the first N objectives in Equation (12) are always equal to zero resulting in the stochastic problem (P1). On the contrary, if t is smaller than c_1, there is no lower bound. If t is smaller than c_2 but, greater than c_1, neither worst-case cost nor expected cost is better than

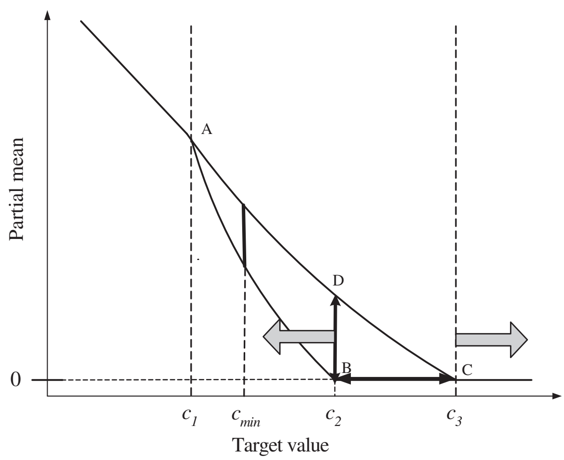

Figure 6. Meaningful ranges of target values.

solutions obtained with t between c_2 and c_3. Therefore, values of t between c_2 and c_3 could be appropriate candidates to offer effective lower bounds among first N objectives in Equation (12).

Then, robust solutions could be attained in two ways: (i) BC direction—increasing t from c_2 to c_3 with zero tolerance of robustness measures; and (ii) BD direction—fixing t at c_2 with changing the tolerance of robustness measures. Either changing t or tolerance has the same effect as changing the weight of robustness measures among objectives. It is not easy to conclude which direction would be more desirable for obtaining robust solutions. This issue will be further discussed in the next section with an example.

3.3. *Revisiting the motivating example*

The power system capacity expansion model (Malcolm and Zenios 1994) is revisited to verify the meaningful range of a target value proposed in the previous section. Figure 7 shows the robust optimization results obtained with two different probability sets with changing a target value from c_2 to c_3. In both cases, the expected cost increases from \$7440 to \$7476 and from \$7480.5 to \$7500, respectively, while the worst-case cost (scenario 3) decreases from \$7695 to \$7590. A comparison between Figure 3 and 7 indicates that the proposed range of a target value is very effective to achieve economic robustness; Figure 7 shows smaller variability among scenario costs as the expected cost increases. With a target value between c_2 and c_3, the same scenario costs are obtained regardless of the difference in the set of probabilities. In addition, increasing expected cost does not greatly affect the robustness of solutions within this range of a target value. The sensitivity of expected cost to the change in a target value is 34% ($p = 0.3, 0.25, 0.15, 0.3$) and 18.6% ($p = 0.25, 0.15, 0.3, 0.3$), respectively.

As mentioned in Section 3.2, two possible directions (BC and BD) can be considered between c_2 and c_3 (Figure 6) to attain robust solutions. When the model is extended to technical robustness, these two directions should be evaluated to decide which direction is more desirable for economic robustness. In the BC direction, the robustness measures are always zero, so the optimization problem reduces to the robust worst-case model (Kang *et al.* 2004). That is, the comparison between two directions presents the comparison between worst-case cost and partial mean of costs. Between them, worst-case cost may be more suitably applied together with technical robustness measures for the following reasons. Firstly, since partial mean of costs only penalizes the mean

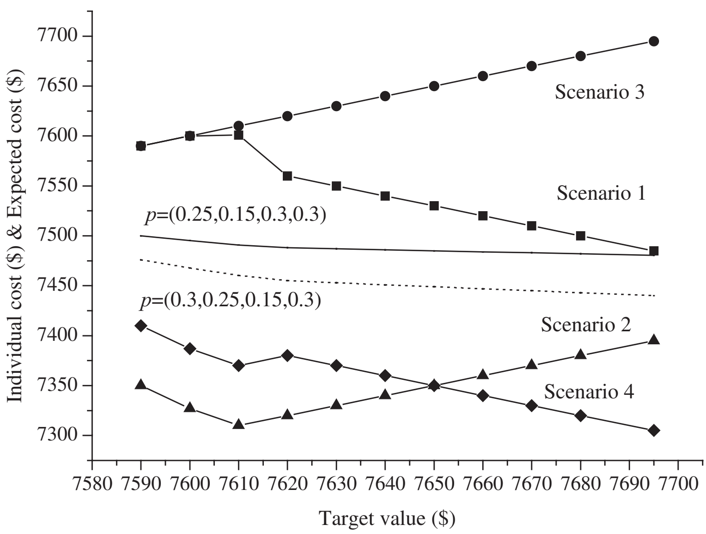

Figure 7. Robust solutions with target values.

of scenario costs above a target value, the worst-case cost may increase in some range although robustness increases (*i.e.*, the expected cost increases). Secondly, partial mean of costs is not a Lipschitzian function of probability (Miettinen 1999), even with the proposed target values. This may cause a difficulty in controlling variability among scenarios. Lastly, when considering technical robustness, there can be many technical robustness measures depending on the number of scenario-dependent technical variables. Therefore, using a simpler economic robustness measure, worst-case cost, may give more allowance to consider technical robustness than partial mean of costs. If partial mean of costs is used, two probability-based objectives, partial mean of costs and expected cost, would leave little chance for technical robustness measures to control variability among scenario-dependent technical variables.

In the next section, a comprehensive robust optimization model is addressed whose objectives consist of expected cost, worst-case cost as an economic robustness measure, and technical robustness measures.

4. Robust optimization model for process design problems

4.1. *Robust optimization formulation*

The robust process design model is formulated with three kinds of objectives, expected cost, an economic robustness measure, and technical robustness measures as follows:

$$\min_{\mathbf{x}, y_1, \cdots, y_N} (U_E(\mathbf{C}), U_{WC}(\mathbf{C}), U_T(\mathbf{y}))$$

subject to

$$\mathbf{x}, y_1, \cdots, y_N \in \Psi.$$

The feasible region of solutions using three objectives can be described as Figure 8. The number of technical robustness measures depends on the number of scenario-dependent technical variables considered. As discussed in the previous section, worst-case cost is utilized as an economic robustness measure. In this context, it appears to be desirable to use the half interval as a technical robustness measure for the following reasons:

(i) it is an even function (a requirement for technical robustness);
(ii) its concept is consistent with worst-case cost, because it controls worst cases in both directions; and
(iii) linearity is maintained. The half interval is defined as follows:

$$U_T(\mathbf{y}) = \frac{1}{2}(\max_s \mathbf{y} - \min_s \mathbf{y}) \tag{16}$$

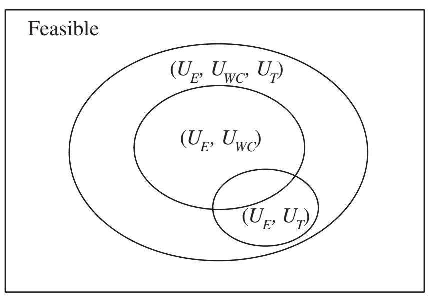

Figure 8. Feasible regions of robust solutions using robustness measures.

4.2. *Generating robust alternatives*

A number of methods for solving multi-objective linear problems have been suggested based on finding Pareto optimal extreme points (Evans and Steuer 1973, Yu and Zeleny 1975, Gal 1977, Isermann and Steuer 1988, Ecker *et al.* 1980, Solanki *et al.* 1993). However, the number of extreme points increases exponentially as the number of variables and constraints increases. This also means that the number of Pareto optimal extreme points, which is the subset of the set of extreme points, increases exponentially resulting in heavy computational load. From the viewpoint of decision-making, generating a large number of solutions does not appear to be attractive in any practical sense. Therefore, one of the aims of the present study is to determine the range of the Pareto optimal set in an efficient manner while avoiding heavy computations.

The lower bounds of the Pareto optimal set, the components of an ideal objective vector (Miettinen 1999), are obtained easily by minimizing each objective, such as expected cost, an economic robustness measure, and technical robustness measures, individually subject to the constraints. The ideal objective vector is used as the reference points to scale the objective vector, together with the upper bound of Pareto optimal set. This is the application of the method of global criterion (Miettinen 1999), which is commonly utilized for making decisions. The upper bounds of the Pareto optimal set, the components of a nadir objective vector, are much more difficult to obtain (Miettinen 1999). As the size of a problem increases, obtaining an exact nadir vector increases computational load significantly. In the current study, the efficient formulation originates from using a rough estimate of the nadir vector rather than the exact nadir vector itself. The proposed nadir vector is attained by solving a bi-objective problem with expected cost and an economic robustness measure in a lexicographic method (Miettinen 1999). The expected cost and the economic robustness measure are chosen because they use the same monetary unit. In the lexicographic method, the decision-maker must arrange the objective functions according to their absolute importance described in Figure 9. The detailed procedure in this study is as follows:

Case I. When the expected cost has priority

$$\text{Solve } \min_{\mathbf{x}, y_1, \cdots, y_N} \quad U_E(\mathbf{C})$$
$$\text{Subject to } \mathbf{x}, y_1, \cdots, y_N \in \Psi$$

Let the optimum objective value of the above problem be denoted by E^*. Then,

$$\text{Solve } \min_{\mathbf{x}, \mathbf{y}} \quad U_{WC}(\mathbf{C})$$
$$\text{Subject to } U_E(\mathbf{C}) \leq E^*, \mathbf{x}, y_1, \cdots, y_N \in \Psi$$

The technical robustness measure, T^1, is calculated.

Case II. When the economic robustness has priority

$$\text{Solve } \min_{\mathbf{x}, y_1, \cdots, y_N} \quad U_{WC}(\mathbf{C})$$
$$\text{Subject to } \mathbf{x}, y_1, \cdots, y_N \in \Psi$$

Let the optimum objective value of the above problem be denoted by W^*. Then,

$$\text{Solve } \min_{\mathbf{x}, y_1, \cdots, y_N} \quad U_E(\mathbf{C})$$
$$\text{Subject to } U_{WC}(\mathbf{C}) \leq W^*, \mathbf{x}, y_1, \cdots, y_N \in \Psi$$

Then, a technical robustness measure, T^2, is calculated.

The larger of the values, T^1 and T^2, is taken as the nadir objective value of the technical robustness measure because, in most cases, the value of technical robustness increases or decreases monotonically between T^1 and T^2. The nadir objective value of the economic robustness measure is decided from solving Case I, while the one for expected cost is obtained from solving Case II. In this way, one needs four single-objective optimizations to find the proposed approximate nadir vector, while the determination of the exact nadir vector requires six single-objective optimizations. If there are n technical robustness measures, then, the exact nadir vector will be achievable after $2n + 4$ consecutive solutions of single objective sub-problems given in Figure 9. In contrast to it, the proposed nadir vector is obtained only after four solutions of single objective sub-problems given in Case I and Case II (Section 4.2) regardless of n. Furthermore, calculating the exact nadir vector requires of deciding the priority among several technical robustness measures, which is often tricky. This can be also avoided by using the proposed nadir vector.

Revisiting the power system capacity expansion model, the ranges of objectives are obtained as follows:

$$7440 \leq U_E(\mathbf{C}) \leq 7476$$
$$7590 \leq U_{WC}(\mathbf{C}) \leq 7695$$
$$0.125 \leq U_T(\mathbf{y}) \leq 0.4167$$

After obtaining the range for each objective, the robust set of Pareto optimal solutions is calculated by changing the priority among objectives, and altering the tolerance of the objective values within the obtained ranges. Figure 10 shows the robust Pareto optimal solutions resulted according to

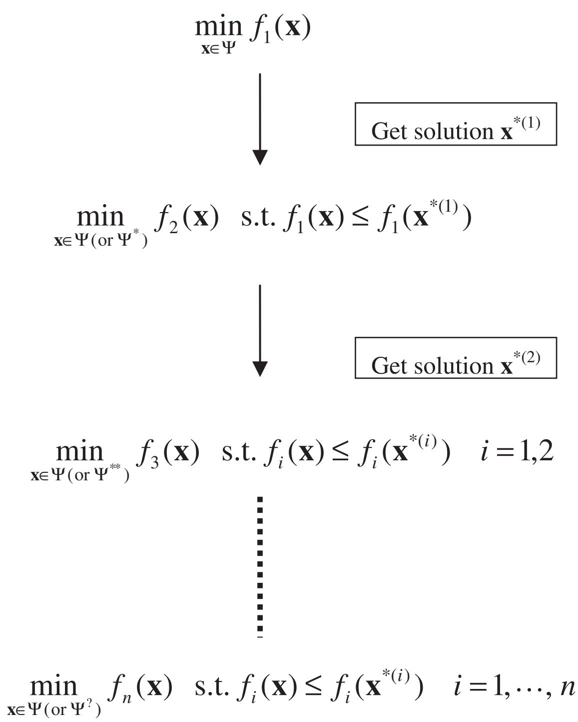

Figure 9. Lexicographic method.

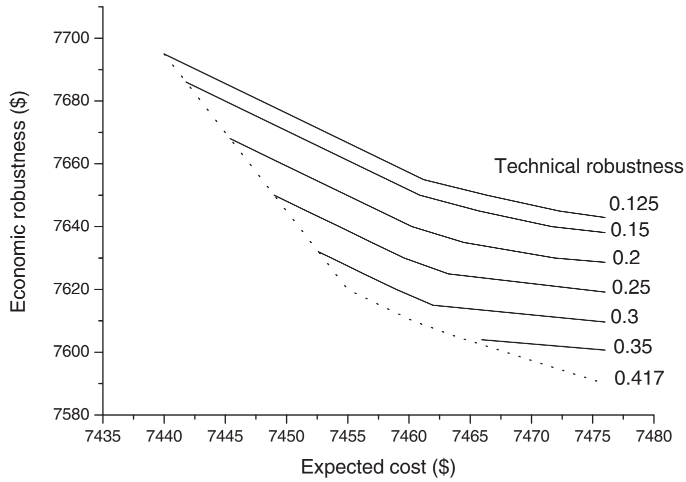

Figure 10. Robust Pareto optimal solutions.

technical robustness. There are several ways to express robust solutions in two-dimensional space. In this figure, the economic robustness measure and expected cost are taken for each axis based on the fact that they use the same monetary unit.

4.3. *Decision making procedure*

In principle, any robust solution obtained from this multi-objective problem is equally acceptable because it satisfies Pareto optimality. However, sometimes it is important to decide a best desirable solution, called a final solution. In this study, the method of global criterion applies under the assumption that there is no specific requirement from decision-makers (Miettinen 1999). This also implies that a Pareto optimal solution whose ideal objective value is located nearer the feasible objective region receives more importance (Miettinen 1999).

In the power system capacity expansion model, the range of each objective is different. Thus, rescaling the objectives using ideal and nadir objective vectors is required as follows:

$$\frac{f_s(x, y) - f_s^*}{f_s^{nad} - f_s^*} \tag{17}$$

In this example, normalization is calculated for each objective as follows:

$$\frac{U_E(\mathbf{C}) - 7440}{7476 - 7440}, \quad \frac{U_{WC}(\mathbf{C}) - 7590}{7695 - 7590}, \quad \frac{U_T(\mathbf{y}) - 0.125}{0.4167 - 0.125}$$

After normalizing objectives, the range of each objective becomes [0, 1]. Then, the final solution is proposed as the point which has the shortest distance from the ideal objective vector. For the distance, L^2-norm is used as follows.

Definition 4 *A vector norm defined for a vector*

$$\mathbf{x} = \begin{vmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{vmatrix} \text{ with complex entries by } |\mathbf{x}|_2 = \sqrt{\sum_{r=1}^{n} |x_r|^2} \tag{18}$$

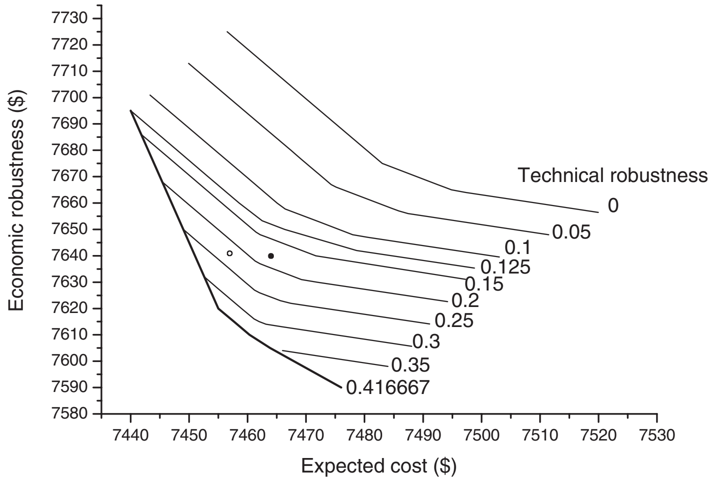

Figure 11. Comparison according to nadir vectors.

Now, the optimization problem for decision making is constructed as follows:

$$\min_{\mathbf{x},\mathbf{y}} \sqrt{\left|\frac{U_E(\mathbf{C})-7440}{7476-7440}\right|^2+\left|\frac{U_W(\mathbf{C})-7590}{7695-7590}\right|^2+\left|\frac{U_T(\mathbf{y})-0.125}{0.416667-0.125}\right|^2}$$

$$\text{subject to} \quad \mathbf{x},\mathbf{y}\in\Psi. \tag{P4}$$

Then, the final solution of (U_E, U_W, U_T) is (7457.1, 7640.9, 0.246). In this problem, the final solution with the exact nadir vector is (7464, 7640.9, 0.173). Figure 11 shows these two final solutions—the hollow point represents the final solution obtained using the proposed nadir and the filled point shows the final solution obtained using the exact nadir vector. Both final solutions are located in close proximity. Although the proposed nadir vector is smaller than the exact nadir vector, it does not appear to have a significant effect for selecting the proper final solution, because all three objectives are reduced simultaneously to some degree. Therefore, this result demonstrates that the proposed nadir vector is practically useful for deciding a desirable final solution with less computational load than the exact nadir vector.

4.4. *A reactor and heat exchanger system*

Another typical process design is presented here. It is a nonlinear problem consisting of a reactor and a heat exchanger (Figure 12), where a first order exothermic reaction $A \rightarrow B$ takes place (Grossmann *et al.* 1983). The goal is to determine the optimal design (reactor volume, V, and area of the heat exchanger, A, for a minimum of 80% conversion under the presence of parameter uncertainty. The uncertain parameters are two input streams: (i) the feed flow rate F_0 and (ii) the temperature of the feed stream T_0. The values are shown in Table 2. The deterministic parameter values are given in Table 3. The objective function is the total annual plant cost, including annualized fixed cost and operating cost. The mathematical formulation of the problem is addressed in the Appendix. The objective function can be expressed as follows:

$$C_s = (691.2Vd^{0.7} + 873.6A^{0.6}) + (1.76Fw_s + 7.056Fl_s) \quad s \in N \tag{19}$$

The problem is formulated as a multi-objective problem consisting of five scenarios with the probabilities: 0.3, 0.2, 0.2, 0.15, and 0.15, respectively. Economic robustness is applied to the cost

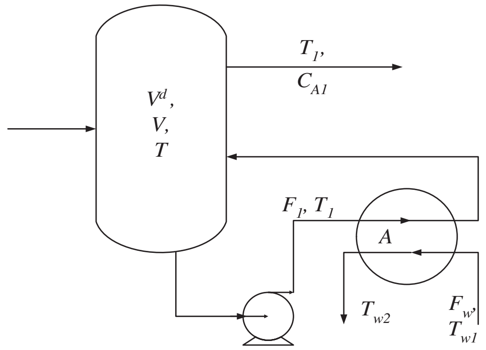

Figure 12. Flowsheet of a reactor–heat exchanger system.

Table 2. Uncertain parameters for a reactor–heat exchanger system.

	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
$T_0(K)$	333	336.77	329.23	339.34	326.66
$F_0(kmol/h)$	45	48.77	41.23	51.34	38.66

Table 3. Parameters for a reactor–heat exchanger system.

$T_{w1}(K)$	300	$C_{A0}(kmol/m^3)$	32.04
$k_0(h^{-1})$	12	$-\Delta H(kJ/kmol)$	23260
$Ua(kJ/m^2 \cdot h \cdot K)$	1635.34	$Cp(kJ/kmol \cdot K)$	167.4
$E/R(K)$	555.6	$C_{pw}(kJ/kmol \cdot K)$	75.4

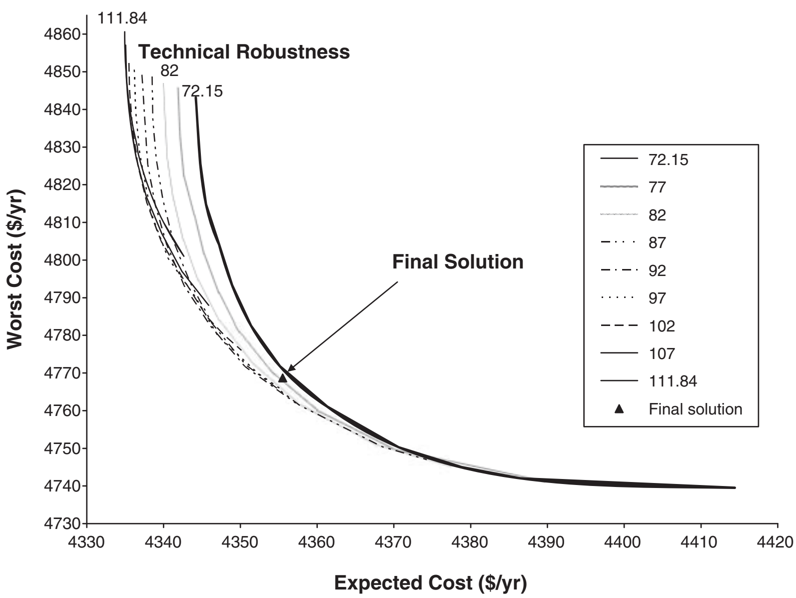

Figure 13. Robust Pareto optimal solutions.

of each scenario and technical robustness is applied to the flow rate of cooling water. By solving Case I and Case II, the ranges of the objectives are obtained as follows:

$$4334.9 \leq U_E(\mathbf{C}) \leq 4739.5$$
$$4739.5 \leq U_{WC}(\mathbf{C}) \leq 4860.1$$
$$72.15 \leq U_T(\mathbf{y}) \leq 111.84$$

The ranges of robust solutions are described in Figure 13.

For obtaining a final solution, the problem is solved resulting in the final solution of $(U_E, U_W, U_T) = (4355.5, 4768.7, 74.9)$.

5. Conclusion

This study presents a comprehensive robust optimization model for process design problems based on a scenario-based approach, in conjunction with a decision-making procedure. Depending on the variable type (either scenario-dependent economic or technical), different robustness concepts can be introduced, considering economic and technical robustness measures as monotonic and even functions, respectively. A novel formulation of robust economic optimization was then proposed, supported by the theoretical analysis to deal with many objectives using the concept of pre-ordering. Importantly, the lower bound defined by ordering objectives provided a conceptual framework for suggesting a proper range of desirable target values in partial mean of costs. Two possible directions in this range presented worst-case cost and partial mean of costs, respectively.

Then, the robust optimization model was proposed with three kinds of objectives – expected cost, an economic robustness measure, and technical robustness measures. Of a number of robust Pareto solutions, the best solution candidate could be identified by minimizing the distance between the ideal objective vector and the objective vector after normalization. This decision-making procedure was proposed including the efficient calculation of the nadir vector, upper bound of the objective vector. Applying the proposed model to process design examples successfully demonstrated the applicability of the proposed model and the decision making procedure.

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Appendix

The mathematical formulation of the reactor–heat exchanger system can be formulated as follows:

(1) Reactor—Material balance

$$F_{0s}\frac{C_{A0}-C_{A1_s}}{C_{A0}} = V_s k_0 \exp\left(-\frac{E}{RT_{1_s}}\right) C_{A1_s} \quad s \in S \tag{A1}$$

(2) Reactor—Heat balance

$$(-\Delta H)F_{0_s}\frac{C_{A0}-C_{A1_s}}{C_{A0}} = F_0 C_p (T_{1_s} - T_{0_s}) + Q_{HE_s} \quad s \in S \tag{A2}$$

(3) Heat exchanger—Heat balance

$$Q_{HE_s} = Fl_s C_p (T_{1_s} - T_{2_s}) \quad s \in S \tag{A3}$$

$$Q_{HE_s} = Fw_s C_{pw} (T_{w2_s} - T_{w_1}) \quad s \in S \tag{A4}$$

(4) Heat exchanger—Design equation

$$Q_{HE_s} = AUa(\Delta T_{\ln_s}) \quad s \in S \tag{A5}$$

$$\Delta T_{\ln_s} = \frac{(T_{1_s} - T_{w2_s}) - (T_{2_s} - T_{w1})}{\ln\left\{\frac{T_{1_s} - T_{w2_s}}{T_{2_s} - T_{w1}}\right\}} \quad s \in S \tag{A6}$$

(5) Specific inequalities

$$V^d \geq 0 \tag{A7}$$

$$A \geq 0 \tag{A8}$$

$$V_s \geq 0 \quad s \in S \tag{A9}$$

$$V^d - V_s \geq 0 \quad s \in S \tag{A10}$$

$$Fw_s \geq 0 \quad s \in S \tag{A11}$$

$$Fl_s \geq 0 \quad s \in S \tag{A12}$$

$$\frac{C_{A0} - C_{A1_s}}{C_{A0}} \geq 0.8 \quad s \in S \tag{A13}$$

$$311 \leq T_{1_s} \leq 389 \quad s \in S \tag{A14}$$

$$311 \leq T_{2_s} \leq 389 \quad s \in S \tag{A15}$$

$$301 \leq T_{w2_s} \leq 355 \quad s \in S \tag{A16}$$

$$T_{1_s} - T_{2_s} \geq 0 \quad s \in S \tag{A17}$$

$$T_{w2_s} - T_{w1} \geq 0 \quad s \in S \tag{A18}$$

$$T_{1_s} - T_{w2_s} \geq 11.1 \quad s \in S \tag{A19}$$

$$T_{2_s} - T_{w1} \geq 11.1 \quad s \in S \tag{A20}$$