Decision Making for a Sustainable Chemical Process

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ABSTRACT

Decision-making for sustainability essentially constitutes a MultiCriteria Decision Making (MCDM) problem. The real challenge relies upon properly characterizing the decision-making context at hand, and matching it to one of a wide range of available decision aiding methods. This paper briefly reviews some general MCDM topics, including optimality condition and various techniques. The different features in characterizing sustainability oriented decision-making contexts are also highlighted. A case study of a reformulated William-Otto process with two conflicting objectives is conducted. Through this chemical process design example, the authors intend to illustrate one of many possible ways to incorporate decision aiding and searching in a Multi-Objective Programming (MOP) problem.

1. INTRODUCTION

In the past two decades, sustainability has more than ever been elaborated in a wide variety of contexts, including chemical process design. However, the consensus on a core question that has to be primarily answered is still hard to establish: ***what is a sustainable chemical process?*** The answer to such a question has been problematic due to the weak grasp on three important subjects associated with sustainability: 1) broad appeal and conceptual ambiguity 2) measurements of transdisciplinary concerns; 3) incommensurability of simultaneous goals.

Agenda 21 [1], a blueprint for sustainable development agreed by the world leaders at the first “Earth Summit” in 1992, pointed out the potential solutions to this puzzle. It called for “development of indicators of sustainable development” as well as “to improve the processes of decision-making so as to achieve the progressive integration of economic, social and environmental issues.” As a consequence, various metrics and/or indicators have been developed and applied to quantify sustainability in recent years [2, 3]. However, many of today’s sustainability assessments stop at merely giving a set of numerical values, without further interpreting them or trying to make improvement.

Decision-making for sustainability, in nature, is a MultiCriteria Decision Making (MCDM) problem, in which a trade-off has to be made among multiple incommensurable goals in a preferred manner. The challenges underlying the MCDM for sustainability are twofold. On the one hand, enormous amount of multicriteria decision aiding or decision support methods exist. Most of them came from Operations Research and Management Science over the recent 20 years [4]. However, the applicability and effectiveness of each method are strongly case-specific. On the other hand, decision-making for sustainability in particular is still young and has not been sufficiently studied. Making a good sustainability-oriented decision essentially relies upon properly characterizing the decision-making context at hand, and matching it to one of a wide range of available decision aiding methods.

As far as a process design problem is concerned, the situation may get more complicated. Because designers, in many cases, not only assess and decide whether an alternative design is sustainable or not, but also they usually manage to acquire improved designs. To meet this demand, decisions need to be made consistently or favorably with respect to the course of searching for new solutions. The problems of this kind are known as multi-objective programming (MOP) or vector optimization. It should be noted that though decision aiding and searching are often applied simultaneously in a MOP problem, they are essentially independent and equally important for the 'optimal' solution to be finally reached. Various techniques have been developed for MOP problems [5, 6]. This paper presents an explorative study on how a more sustainable process design can be determined under conflicting criteria, as well as illustrates the possible variety in the pathways that may lead to a final decison.

2. MULTICRITERIA DECISION AIDING

Decision aiding has evolved into an active field of research, which set forth not only objective truths, but also subjective judgments. More importantly, decision aiding aims to bridge the two and establish a scientific basis to formulate a decision-making problem as well as provide a solving procedure to the formulated problem, in such a manner that does provide guidance to a human decision maker. Decision-making with more than one criterion has unique features and is more difficult to handle. Numerous literature has been published on these issues [4, 5, 7-10]. This section gives a brief discussion on general MCDM topics, such as the concept of Pareto optimality, different kinds of techniques and their unique characteristics.

2.1 Pareto Optimality

Vilfredo Pareto, an Italian economist, first formally proposed a solution in early 1900s to the contradiction in judging optimality with respect to multiple incommensurable criteria. The optimality condition that he developed was later named Pareto optimality, which is defined as: *A decision vector $\boldsymbol{x}^* \epsilon D$ (or an objective vector $\boldsymbol{f}^* \epsilon O$) is Pareto optimal if there does not exist another decision vector $\boldsymbol{x} \epsilon D$ (or an objective vector $\boldsymbol{f} \epsilon O$) such that $f_i(\boldsymbol{x}) \leq f_i(\boldsymbol{x}^*)$ (or $f_i \leq f_i^*$) for all $i=1,\ldots.,n$ and $f_j(\boldsymbol{x}) < f_j(\boldsymbol{x}^*)$ (or $f_j < f_j^*$) for at least one index j.*

Pareto optimality has different names, such as noninferiority, nondominance, efficiency, and Paretian efficiency. This concept stands at the heart of many MCDM techniques. It is easier to understand with visualizations as shown in Figure 1.

Pareto optimality reflects a relative relationship among a specific group of solutions. This relationship may vary when different individuals are considered. In most cases, there are lots of or an infinite number of Pareto optimal solutions, whose relative goodness can not be distinguished if criteria are treated equal. However, in a practical sense, a pool of Pareto optimal solutions usually need to be further decided to reach one single "best" solution.

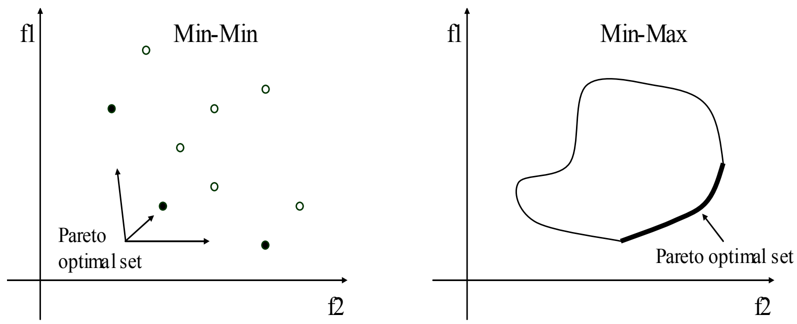


Figure 1. Visualizations of Pareto optimality

2.2 Method Classification

MCDM methods can be classified in a variety of ways. Readers can refer to [5, 11] for a complete discussion. Nevertheless, any classification emphasizes the difference in handling either criteria preference or alternative solutions.

A widely recognized classification presented in [12] differentiates MCDM methods in terms of the timing of preference articulation. "A priori" and "a posteriori" methods require the preference to be elicited before and after the solution process, respectively, while progressive articulation is used in "interactive" methods. Other criteria-based partition may be focused on examining what (rank, order, or score) and how (normative or descriptive) preference is articulated.

Methods of MCDM are sometimes split into two types, depending on the property of the solution space. One is Multiple Attribute Decision Making (MADM), which deals with picking the most desired solution from an explicit list of finite alternatives. The other class usually has a continuous domain of infinite number of solutions that are often defined implicitly by a mathematical programming problem. This class is named as Multiple Objective Decision Making (MODM) for distinction. Moreover, individuals in the solution space could be evaluated in different ways, such as pairwise comparison, threshold elimination, etc.

2.3 MCDM Techniques

Method selection has become increasingly challenging, as more MCDM techniques are available. The author of [13] called it as "meta MCDM." In order to exhibit the main streams of MCDM practice, three selected schools of methods are introduced here without intention to be comprehensive.

Analytic Hierarchy Process (AHP)- AHP, whose origin can be traced back to 1970s, is a MCDM tool that may have the most widespread use worldwide [14]. The success of AHP can be explained by its three primary functions: 1) hierarchical structuring of complexity; 2) ratio scale measurement derived from pairwise comparison; and 3) synthesis of priorities [14-16]. The simplicity and robustness of AHP have led to a wide range of applications, varying from planning, selection, resource allocation, conflict resolution, design and technologies, etc [17,18]. AHP is especially suited for MADM problems with large number of criteria and alternatives.

Reference Point- The name of "reference point" is adopted here to refer to a school of MCDM methods, in which solutions are evaluated in terms of its "closeness" to an identified reference point. The classical goal programming [19], compromise programming [20] and the so-called "reference point" approach developed by International Institute for Applied Systems Analysis (IIASA) [21] fall into this class. The methods, though differing in mechanisms of defining the "goal" and the "closeness", have been applied in numerous MOP projects.

Multiattribute Utility Theory (MAUT)- MAUT is one most traditional approach for MCDM, which borrowed utility concept from economics [22]. This method assumes the existence of utility functions for each concerned attribute. The mutual independence of the preferences between two utility functions is checked using conditions derived from lotteries. The final decision is made based on the composite utility of solutions with an identified utility decomposition technique. The application of MAUT is often limited to decision problem with a reduced number of attributes and discrete feasible solutions.

3. MCDM FOR SUSTAINABILITY

The context of a decision-making involves every aspect of information that specifically describes the situation in which the decision is made. Enormous factors need to be taken into consideration to fully characterize a decision-making context, such as decision agents, criteria, alternatives, and how they relate to each other. Although decision-making contexts are heavily case-dependent, there are some recently discovered common features that have made sustainability-oriented decision making a bit more difficult compared with general MCDM contexts.

First of all, criteria may be ill-defined. Many sustainability-related questions remain open and their underlying issues are not sufficiently understood. Therefore, there are cases where recognition of certain criteria is incomplete so that the target sustainability concerns are not represented properly.

Second, societal valuation of sustainability criteria is somewhat young, which leads to a very dynamic judgment of the relative significance among multiple sustainability criteria. In this sense, uncertainty and arbitrariness associated with sustainability preference articulation are high.

Third, the primary hindrance for evaluating alternatives is the scarcity of adequate information and available data. As a consequence, alternative evaluation often ends up with "a mixture of quantitative and qualitative, precise and imprecise, subjective and objective data" [23].

Fourth, sustainability calls for equity not only within but also between generations. To this end, various stakeholders with controversial interests are often present as multiple decision makers. How all these different interests can be taken care of in the course of decision making, and how the stakeholders with similar or diametrically opposed interests can be treated differently constitute another challenge.

4. CHEMICAL PROCESS DESIGN EXAMPLE

The Williams-Otto (WO) plant first developed in [24] has been widely studied in chemical engineering literature. Different researchers have applied various single objective optimization techniques under slightly different problem formulations. More information can be found in [25-35]. In this study, a new bi-objective WO problem was formulated, which pursues an improved operating condition with respect to two conflicting criteria. The preference was not elicited until the searching process is accomplished in such a manner that the obtained solutions are non-dominated to each other. The final solution was then decided from a finite number of non-dominated alternatives using Analytic Hierarchy Process (AHP).

4.1 Problem Formulation

Appendix A has a detailed description of the WO process. The re-formulated model based on [25] is shown below. This new model has two objectives: maximizing return on investment (ROI) and minimize waste, 11 bounded variables and 8 equality constraints. The "optimal" solution in [25] is adopted as design condition. The 11 variables, including 10 flowrates and reactor temperature, are allowed to vary within the -5%~+5% range around the design condition. The reactor volume is fixed at 60 ft^3.

$$Max.\quad f_1 = 0.000056\,[50.04F_D + (2207.52)(4762) - 168F_A - 252F_B - 2.22F_R - 180000]$$

$$Min.\quad f_2 = F_G$$

subject to:

$$h_1 = F_{RP} - 0.1F_{RE} - 4762$$

$$h_2 = \frac{F_D F_{RE}}{(F_R - F_G - F_P)} - (2)(2.5962*10^{12})(e^{-15000/T})(\frac{50F_{RB}F_{RC}V}{F_R^2})$$

$$h_3 = [(2.5962*10^{12})(e^{-15000/T})(F_{RB}F_{RC}) - (0.5)(9.6283*10^{15})(e^{-20000/T})(F_{RC}F_{RP})](\frac{50V}{F_R^2}) - F_D(\frac{F_{RP}-F_P}{F_R-F_G-F_P}) - F_P$$

$$h_4 = F_A - (5.9755*10^9)(e^{-20000/T})(F_{RA}F_{RB})(\frac{50V}{F_R^2}) - F_D(\frac{F_{RA}}{F_R-F_G-F_P})$$

$$h_5 = F_B - [(5.9755*10^9)(e^{-20000/T})(F_{RA}F_{RB}) + (2.5962*10^{12})(e^{-15000/T})(F_{RB}F_{RC})](\frac{50V}{F_R^2}) - F_D(\frac{F_{RB}}{F_R-F_G-F_P})$$

$$h_6 = [(2)(5.9755*10^9)(e^{-20000/T})(F_{RA}F_{RB}) - (2)(2.5962*10^{12})(e^{-15000/T})(F_{RB}F_{RC}) - (9.6283*10^{15})(e^{-20000/T})(F_{RC}F_{RP})](\frac{50V}{F_R^2}) - F_D(\frac{F_{RC}}{F_R-F_G-F_P})$$

$$h_7 = (1.5)(9.6283*10^{15})(e^{-20000/T})(F_{RC}F_{RP})(\frac{50V}{F_R^2}) - F_G$$

$$h_8 = F_{RA} + F_{RB} + F_{RC} + F_{RE} + F_G + F_{RP} - F_R$$

		Design condition	Lower bound	Upper bound
F_A	(lb/hr)	13546	12869	14223
F_B	(lb/hr)	31523	29947	33099
F_D	(lb/hr)	36697	34862	38532
F_G	(lb/hr)	3609	3429	3789
F_{RA}	(lb/hr)	18187	17278	19096
F_{RB}	(lb/hr)	60915	57869	63961
F_{RC}	(lb/hr)	3331	3164	3498
F_{RE}	(lb/hr)	60542	57515	63569
F_R	(lb/hr)	157391	149522	165261
F_{RP}	(lb/hr)	10817	10276	11358
T	(^{o}R)	656	623	689
f_1	(%)	89.58		
f_2	(lb/hr)	3609		
Ω		250.82		

The objective values at the design condition are 89.58% and 3609 lb/hr, respectively. Though there is no inequality constraint in this model, the total constraint violation Ω is calculated with the formula:

$$\Omega = \sum_{i=1}^{nh} \Omega^h{}_i + \sum_{j=1}^{ng} \Omega^g{}_j = \sum_{i=1}^{nh} |h_i| + \sum_{j=1}^{ng} \max(0,g)_j$$

, where h_i is equality constraint and g_j is inequality constraint in the equal-or-less-than form.

The design condition has the Ω value of 250.82, which indicates that this condition is not strictly feasible. However, loosening equality constraints to a certain degree is necessary to make many constrained problems solvable. Therefore, Ω=250.82 is applied in this study as a threshold for constraint satisfaction. In other words, only the solutions with a total constraint violation equal-or-less-than 250.82 are thought feasible.

4.2 Multi-Objective Evolutionary Algorithm (MOEA)

The unique population-based and heuristics-based characteristics of Evolutionary Algorithms (EA) made it particularly suited for solving multi-objective problems. References [36-38] provide good overviews of EAs and MOEAs. In this study, a revised real-coded Strength Pareto Evolutionary Algorithm 2 (SPEA2) along with a novel constraint handling technique is applied.

Constraint Handling- Optimization with a large number of nonlinear equality constraints is the toughest kind. The constraint handling became particularly difficult in this problem, mainly due to: 1) high dimensionality; 2) large searching spacing; 3) many nonlinear equality constraints; 4) rare and unpredictably distributed feasible solutions.

[39-41] give good discussions on various constraint handling techniques for EAs. The constraints in this study were handled following an "infeasible path" strategy through introducing the total magnitude of constraint violation Ω as an additional objective. As a result, solutions are evaluated with respect to three independent criteria: f1, f2, and Ω to determine their Pareto dominance.

This extra objective is used to direct the searching towards feasible regions. As the feasibility criterion has been set as satisfying a threshold: $\Omega<=250.82$, the third objective Ω needs to be treated differently as the other two that tend to pursue extreme values. Hence, in terms of Ω only, the following heuristics were applied:

- If at least one of the individuals A and B are infeasible (either Ω_A or $\Omega_B >250.82$), the one with a lower Ω is better.
- If the individual A and B are both feasible (both Ω_A and $\Omega_B <=250.82$), they tie regardless of their Ω values.

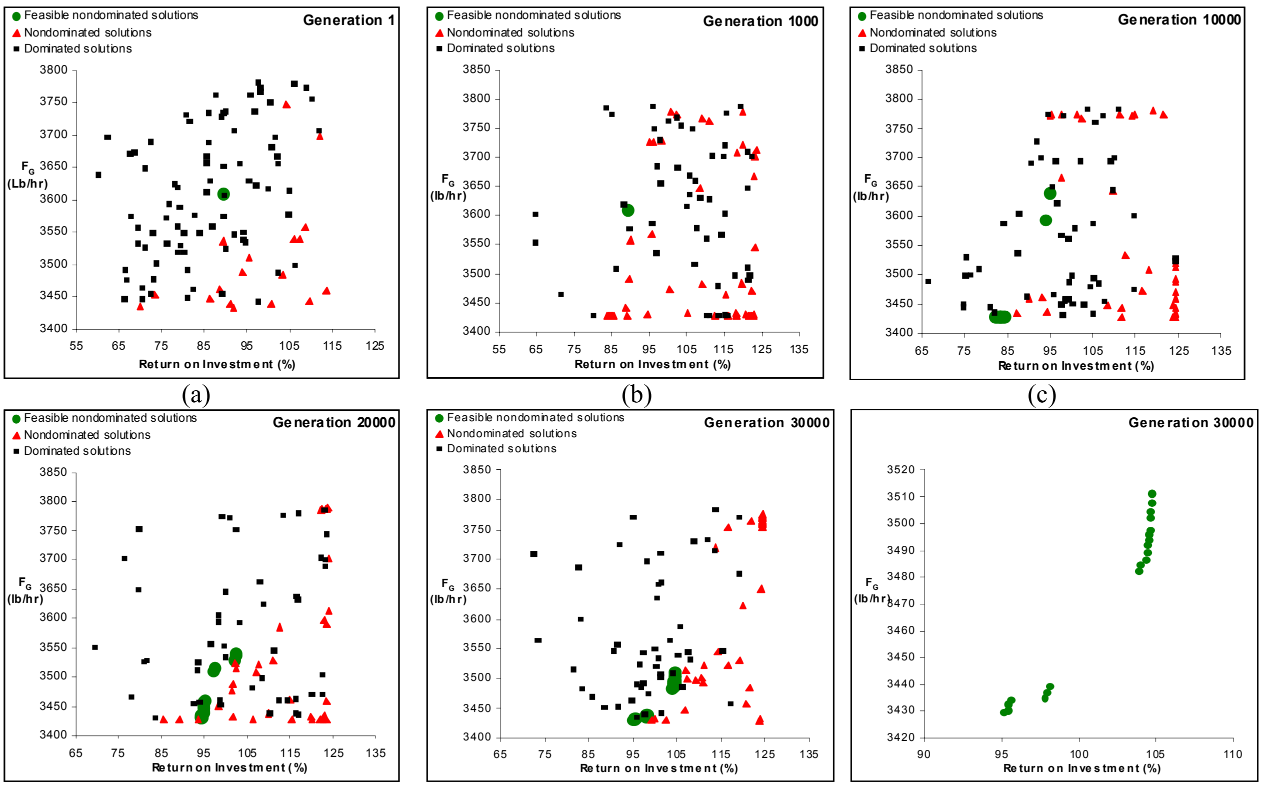
Real-Coded Representation- Binary coded representation has dominated the EA research and applications, because EAs were initially inspired by natural evolution and devised to mimic operations on chromosomes and genes. However, real-coded representation has inherent advantages for tackling optimization with variables in continuous domains. More importantly, it has been proved that EAs' effectiveness does not stem from using bit strings [42].

Vectors of floating point numbers are applied to represent solutions in the searching space. For example, a solution in the decision space of the WO model mentioned above is represented by an 11-dimensional real vector that contains the value of eleven corresponding decision variables. Real coding requires disparate genetic operators from those applied in binary-coded EAs, especially crossover and mutation. The BLX-α crossover and random mutation are applied in this study. More details regarding these two operators can be found in [42, 43, 44].

Revised SPEA2- [45] has more information on SPEA2. The algorithmic details on the adapted SPEA2 method applied in this study are summarized in Appendix B. The revisions were performed to make the algorithm more effective for this particular problem.

Significant differences are noted in the revised algorithm. First of all, though density is still managed to range between 0~0.5, it is calculated from ranking the average distance to all non-dominated individuals in the current population. Second, the size of archive (set of elites) is not fixed. It varies with the number of non-dominated solutions within pre-specified bounds. Third, tournament selection is performed on entire population, instead of only on archive. Consequently, every individual has a chance to reproduce, but the probability is associated with its fitness.

Searching Results- Figure 2(a)~(e) illustrate the snapshots of the 100 solutions distributed in the space of the two objectives at different generations. Figure 2(f) shows a closer view of the 19 feasible and nondominated solutions that are found after 30,000 generations. The decision variable values are listed in Table 1. These 19 final solutions are feasible Pareto optimal solutions, which need to be further determined for a single 'best' solution.



(d) (e) (f)

Figure 2. Solution distribution at different generations

4.3 Decision Making with AHP

The final decision now needs to be made from a finite list of alternatives. The famous AHP software Expert Choice v.11 was applied to assist this MADM. Observation reveals that some of the 19 alternatives in Table 1 are fairly close. Also, the trial version software downloaded from www.expertchoice.com has restrictions on the scale of the problems to be solved. Therefore, the final solution is determined from a subset containing five selected alternatives as summarized in Table 2.

Table 1. The 19 feasible nondominated solutions after 30,000 generations

	1	2	3	4	5	6	7	8	9	10	11	19	
F_A	13467	13463	13464	13455	13393	13393	13386	13231	13225	13224	13201	13223	lb/hr
F_B	31078	31063	31056	31048	30907	30892	30877	30474	30470	30448	30435	30431	lb/hr
F_D	36197	36191	36178	36164	36018	36009	35988	35502	35483	35483	35483	35483	lb/hr
F_G	3429	3430	3432	3434	3435	3437	3439	3482	3484	3486	3511	3497	lb/hr
F_R	18328	18329	18329	18328	18328	18328	18328	18325	18325	18325	18325	18325	lb/hr
F_R	60394	60369	60369	60360	60351	60353	60355	60262	60262	60262	60262	60262	lb/hr
F_R	3361	3361	3362	3362	3367	3367	3370	3368	3369	3369	3369	3369	lb/hr
F_R	61053	61063	61065	61065	61051	61072	61064	61122	61121	61121	61121	61121	lb/hr
F_R	157424	157419	157424	154722	157419	157419	157421	157459	157459	157459	157459	157459	lb/hr
F_R	10861	10863	10865	10866	10866	10866	10866	10874	10875	10874	10873	10874	lb/hr
T	656	656	656	656	656	655	655	655	655	655	655	655	^oR
f_1	**95.14**	95.43	95.49	**95.63**	97.81	**98.00**	98.21	**103.98**	104.37	104.37	**104.77**	104.61	%
f_2	**3429.49**	3430	3432.44	**3433.98**	3434.82	**3436.90**	3439.17	**3482.21**	3486.44	3486.44	**3510.92**	3497.28	lb/hr
Ω	246.47	242.69	244.45	250.81	249.46	245.79	244.86	249.72	250.20	250.34	245.19	248.98	

Table 2. Five alternatives to be decided with respect to two criteria

	A# 1	A# 2	A# 3	A# 4	A# 5	
C#1: Return on Investment	95.14	95.63	98.00	103.98	104.77	%
C#2: Waste discharged	3429.49	3433.98	3436.90	3482.21	3510.92	lb/hr

The hierarchic composition is constructed as shown in Figure 3. The parameters applied in pairwise comparison of five alternatives and two criteria are shown in Table 3(a)~(c), respectively. The return on investment is preferred by a moderate degree over waste discharged. The alternative priority of 1~9 scale is calculated via uniformly dividing the range between the minimum and maximum values of two objectives.

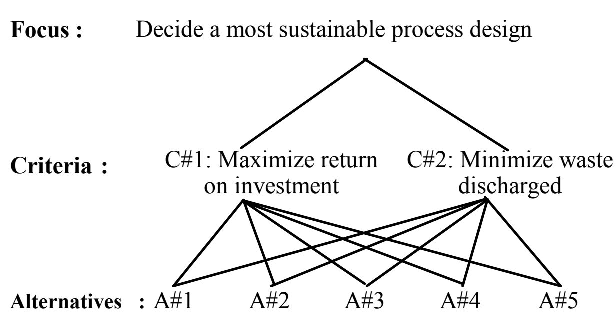


Figure 3. Hierarchic composition of MADM for a sustainable WO process

Table 3. Pairwise comparisons

(a)

Pairwise comparison of alternatives with respect to return on investment

	A#1	A#2	A#3	A#4	A#5
A#1	1	2	4	8	9
A#2	1/2	1	2	8	8
A#3	1/4	1/2	1	6	6
A#4	1/8	1/8	1/6	1	2
A#5	1/9	1/8	1/6	1/2	1

(b)

Pairwise comparison of alternatives with respect to waste discharged

	A#1	A#2	A#3	A#4	A#5
A#1	1	2	2	6	9
A#2	1/2	1	2	6	8
A#3	1/2	1/2	1	6	8
A#4	1/6	1/6	1/6	1	4
A#5	1/9	1/8	1/8	1/4	1

(c)

	C#1	C#2
C#1	1	2
C#2	1/2	1

Table 4. Calculation results using Expert Choice

	Priority with respect to C#1	Priority with respect to C#2	Overall priority
A#1	0.022	0.147	16.9
A#2	0.032	0.11	14.2
A#3	0.057	0.084	14.1
A#4	0.219	0.024	24.3
A#5	0.294	0.011	**30.5**

The results from Expert Choice are shown in Table 4, which clearly shows that the alternative #5 is the "best" solution under the given preference configuration.

5. CONCLUSIONS

Growing demand for handy and robust MCDM techniques has emerged in sustainability related areas to help decision makers to structure and solve problems. Past experience has revealed that there is no normative decision aiding method that is without critics, though many techniques have been pretty mature and produced appealing success stories. On the other hand, people's understanding on sustainability is at an early stage. Along with knowledge progress, decision-making contexts for sustainability may get more flexible and dynamic in the coming years. In this sense, more efforts need to be put into the both modeling sustainability and specializing MCDM, in order to tackle real-world decision-making problems in such a way that is more case-specific and effective.

APPENDIX A Process Description of the Williams-Otto process

Figure 4. illustrates a simplified Process Flow Diagram (PFD) of the Williams-Otto process. The plant under consideration manufactures a chemical P at a capacity of 40 million pounds per years. The plant is operated 8000 hours per year. The process consists of a continueously-stirred tank reactor (CSTR), a heat exchanger, a decanter, and a distillation column in series. A portion of the bottom product of the distillation column is recycled to the CSTR.

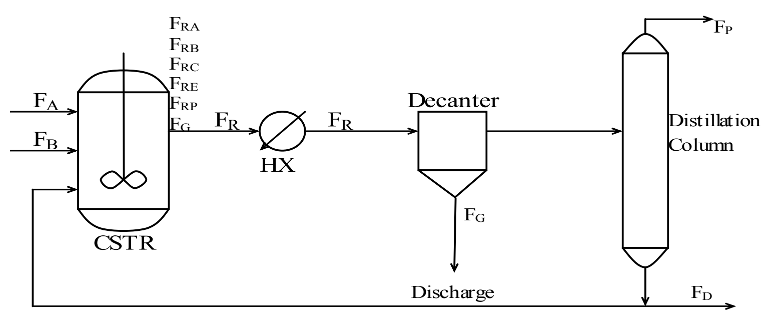


Figure 4. Williams-Otto process diagram

Three second-order irreversible reactions are involved:

$$A + B \xrightarrow{K_1} C$$
$$C + B \xrightarrow{K_2} P + E$$
$$P + C \xrightarrow{K_3} G$$

C and E are intermediates that have no sale value but can be used as plant fuel. G is assumed to be a discharged waste, which will cause negative environmental effects. The reaction coefficients can be expressed in the Arrhenius form:

$$k_i = A_i \exp(-B_i / T)$$

The values of A and B are listed in Table 5.

Table 5. Parameters for reaction coefficients

i	A_i (hr) (weight fraction)	B_i (°R)
1	5.9755×10^{9}	12000
2	2.5962×10^{12}	15000
3	9.6283×10^{15}	20000

Interested reader may refer to [1, 2, 7] for parameter values and more background information.

APPENDIX B Pseudo-Code of the Revised SPEA2

{ } contains the content of the subroutine immediately above.
!! is followed by documentations.
Italic fonts are subroutine names

```
CALL initialization                    !! Randomly generate initial population
DO
   CALL objectives                     !! Calculate objective functions f1 and f2
   CALL constraints                    !! Calculate constraints h (and g)
   CALL augmented_objectives           !! Calculate Ω and combine with f1 and f2
   CALL fitness_assignment
      {CALL strength                   !! s(i) = number of individual it dominates
      CALL raw_fitness                 !! r(i) = sum of the strength of its dominator
      CALL density                     !! d(i) = 0.5*(rank(i)/p)
         !! p: total population; rank(i): rank of average distance to non-dominated population
      CALL fitness                     !! fitness(i) = r(i) + d(i)
      }
   CALL fitness_ascent_ranking         !! Arrange the population in the ascent order of fitness values
   CALL elite                          !! Determine elites in the current population
      { DO j = 1 , p
       IF (fitness(i) > 1) THEN        !! First accept all the individuals with less-than-1 fitness
          p_elite = j - 1              !! p_elite: number of elites
       END IF
       END DO
       IF (p_elite > = p/3) THEN
          p_elite = p/3
       ELSE IF (p_elite < = p/6) THEN
          p_elite = p/6
       END IF
       }      !! if less-than-1-fitness individuals are too many or too rare, use pre-specified elite size.
IF (gen >= n_gen) EXIT                 !! Termination criteria
   CALL variation
      {DO
         CALL tournament-selection     !! Perform tournament selection on the whole population
         DO
            CALL tournament-selection
```

```
            IF (champion1 /= champion2) EXIT        !! Two parents have to be distinct
            END DO
            CALL crossover                          !! Crossover is always invoked
            IF (rannum < mutation_rate) THEN        !! Mutation is invoked at a specified rate
               CALL mutation
            END IF
         IF (n_new > p-p_elite) EXIT               !! Stop variation after all the non-elite positions are filled
         END DO
       }
   gen=gen+1
END DO
```

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