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Sustainability Assessment Framework for Chemical Processes Selection under Uncertainties: A Vector-based Algorithm Coupled with Multi-Criteria Decision-Making Approaches

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Abstract: This article aims to develop a generic sustainability assessment framework for helping the stakeholders/decision-makers to prioritize chemical process alternatives under uncertainties. A comprehensive evaluation system that consists of both hard and soft criteria from the environmental, economic, social-political and technical concerns was firstly constructed in the framework, in which, different types of uncertainties with respect to the hard and soft criteria can be properly addressed by using the interval parameter and FAHP (fuzzy Analytic Hierarchy Process) method, respectively. The FDANP (fuzzy Decision Making Trial and Evaluation Laboratory-based Analytic Network Process) method, which can tackle the interdependences between the evaluation criteria, and the uncertainty among human's judgments, was employed for weighting the criteria accurately. Afterward, a novel interval vector-based algorithm was developed for rigorously prioritizing the alternative processes *via* the integration of both the absolute sustainability performance and relative sustainability balance of each chemical process under uncertainty. The proposed framework was illustrated by a case study to prioritize the sustainability of five ammonia production processes. The robustness of the assessment result was tested by conducting the sensitivity analysis; while the effectiveness and advantages of the proposed framework were demonstrated by comparing the results deprived by this framework with those determined using other MCDM (Multi-Criteria Decision-Making) approaches.

Keywords: Sustainability assessment, uncertainty, chemical process, multi-criteria decision-making, vector-based algorithm.

1. Introduction

Chemical industry plays a significant role in the development of global economy and society by providing more than 70,000 diverse products of chemicals and energies.[1] However, the enormous benefits contributed by this industry are accompanied with severe environmental and social costs, such as high energy consumption, environmental pollution, health problems and safety impacts. Therefore, it is essential to incorporate the concept of sustainability into the chemical industry for achieving its healthful development. The central philosophy of sustainability is the triple-bottom-line balance, focusing on the optimization of system's performances with respect to economic prosperity, environmental impacts, and social responsibility, simultaneously.[2] Accordingly, in the past several years, a variety of sustainability assessment and decision-making methodologies have been developed for helping the decision-makers to have a better evaluation of different chemical process alternatives. Shadiya and High[3] developed a novel impact assessment tool, i.e. "SUSTAINABILITY EVALUATOR", for assessing the sustainability of chemical processes. Tugnoli et al.[4] introduced a sustainability analysis procedure by quantitatively calculating the performance of chemical processes with respect to key criteria, offering the decision-makers a straightforward assessment of the expected sustainability results. The economy, life-cycle environmental impacts, health and safety hazard, and technical aspects were considered in the decision framework for chemical process design proposed by Sugiyama et al.,[5] which comprises four stages of process modeling and multi-objective evaluation. Othman et al.[6] proposed a systematic methodology for sustainability assessment and design by integrating hard (quantitative) criteria from economic and environmental concerns along with soft (qualitative) social criteria into design activities, in which, the AHP (Analytic Hierarchy Process) method was employed for performing the tradeoffs among the criteria system. Serna et al.[7] introduced a MCDM (Multi-Criteria Decision-Making) framework to prioritize the sustainability performance of multiple chemical processes by means of the integration of AHP and DEMATEL (Decision Making Trial and Evaluation Laboratory) technique. A sustainability prioritization framework proposed by Ren et al.[8] can be utilized for selecting the most sustainable chemical process among multiple alternatives, which incorporates the FAHP (fuzzy Analytic Hierarchy Process) method for scoring the soft criteria, the FANP (fuzzy Analytic Network Process) method for weighting the criteria, and the PROMETHEE (Preference Ranking Organization Method for Enrichment Evaluations) method for prioritizing the alternatives. According to these literatures and other relative works,[9-14] the sustainability assessment of chemical processes could be handled by using a MCDM-based framework, which prioritizes the alternatives *via* the aggregation of their performances regarding multi-criteria in terms of the weight with respect to each criterion.[15] Consequently, there would be four stages existing in the mathematical framework for sustainability assessment including establishment of criteria system, collection of alternatives' performances, determination of criteria's weights, and prioritization of alternatives' sequence. Due to the complexity and specialty of the chemical systemes, the four-stage framework for sustainability assessment of chemical processes must incorporate the following features.

Establishment of criteria system. The overall sustainability of a complex chemical system is not only decided by the conventional environmental-economic-social criteria, but also influenced by the technical and political criteria;[8, 16] meanwhile, it should be determined with the lifecycle thinking rather than only focusing on the production stage. Therefore, a comprehensive evaluation system with both hard and soft criteria from multiple concerns should be established with the lifecycle thinking.

Collection of alternatives' performances. The accuracy of the collected alternatives' performances regarding the criteria is crucial to the effectiveness of the sustainability assessment; however, different types and degrees of uncertainties associated with these data are inevitably encountered and have to be handled properly during the assessment of chemical systems.

Determination of criteria's weights. Criteria weights reflect not only the relative importance of the criteria, but also the preferences of decision-makers, implying the necessity of addressing the interdependences among the criteria and the uncertainty in human's judgments for offering an accurate weighting result.

Prioritization of alternatives' sequence. The conventional MCDM methods prioritize the alternatives *via* the aggregation of their absolute performance ratings regarding multi-criteria, failing to incorporate the relative balance among the criteria system; moreover, it is difficult for the ranking method to deal with different types and degrees of uncertainties associated with the input data. Therefore, a ranking method with the capability of aggregating the absolute ratings and relative balance of the performances regarding the criteria under uncertainties is necessary for realizing a rigorous prioritization result.

The aim of this study is to develop a novel framework that can simultaneously incorporate the aforementioned four features of sustainability assessment for prioritizing chemical processes under uncertainties. It starts from providing a comprehensive evaluation system including both hard and soft criteria from four-dimensional pillars with the lifecycle thinking; where the aleatory uncertainty and epistemic uncertainty associated with the hard and soft criteria can be appropriately handled by using the interval parameter and FAHP approach, respectively; then, the FDANP (fuzzy Decision Making Trial and Evaluation Laboratory-based Analytic Network Process) method is adopted for the weights determination with the consideration of the criteria's interdependences and subjective uncertainty; finally, an interval vector-based algorithm is developed for rigorously ranking the alternatives, which can not only fill the research gap in the conventional MCDM methods in respect of ignoring the relative sustainability balance for final ranking, but also well preserve the uncertainties from the input to the output by adopting a monolayer computation.

Besides the Introduction, this paper is organized as the follows: Section 2 presents the mathematical framework; an illustrative case is studied and discussed in Section 3; Section 4 provides the results comparison; and finally, the discussion and conclusion are offered in Section 5.

2. Mathematical Framework

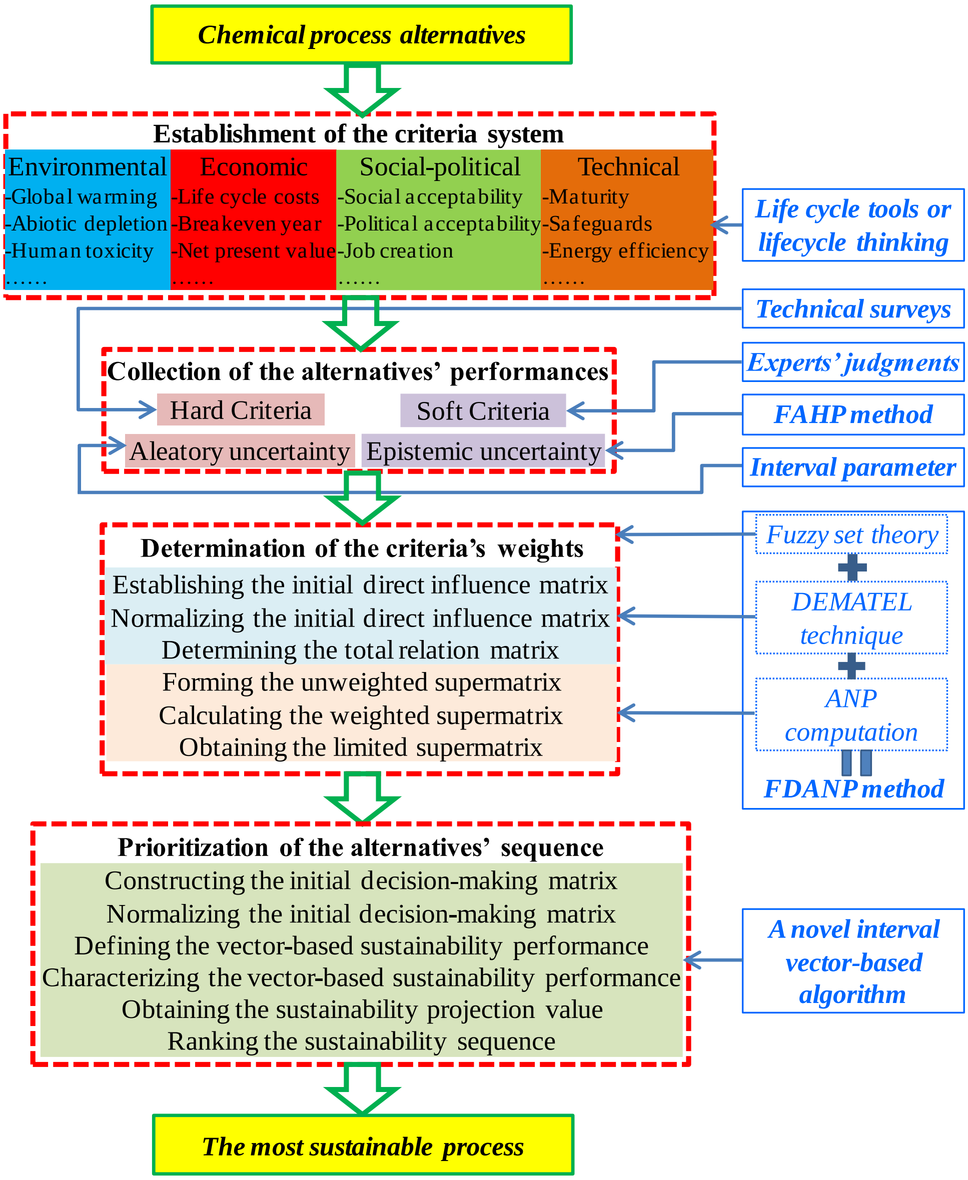

Figure 1. Framework of the sustainability assessment for chemical processes under uncertainties.

The mathematical framework of this study is summarized in Figure 1, which consists of the following four stages.

2.1 Establishment of the Criteria System

For sustainability assessment, there is a growing trend to embrace the life cycle tools to construct the evaluation system,[17, 18] including life cycle assessment for environmental criteria, life cycle costing for economic criteria, and social life cycle assessment for social criteria.[2] However, this system may not be comprehensive enough because the environmental, economic, and social performances of a chemical system could be significantly influenced by technical and political criteria.[8, 16] For instance, the criterion of "political acceptability" may include the incentives to investment, legislation on commercial and/or environmental activities, guidelines for development, taxation and other public policies,[19] which is able to directly and/or indirectly affect other criteria from the environmental, economic, social, and technical concerns.[8, 20] Therefore, a more comprehensive criteria system is suggested in this study to expand the "breadth" of the system by incorporating the technical criteria,[16,21-23] i.e. efficiency and maturity, and the political criteria,[8,16,19] i.e. political/legislative framework. Since the life cycle tools are recommended to determine the criteria from environmental, economic, and social aspects, the technical and political criteria should also be investigated using the same lifespan boundary[8] by employing the conventional life cycle assessment processes while focusing on the technical/political impacts.[23, 24] Notably, the criteria system should be created on a case-by-case basis according to specific chemical system with the actual evaluation conditions, enabling the users to select the most suitable criteria.

2.2 Collection of the alternatives' performances

Subsection 2.1 provides a comprehensive assessment system that consists of both hard and soft criteria;[6, 8] where the hard ones refer to the objective indicators that can be assessed quantitatively using real numbers, while the soft ones are subjective measures relying on the qualitative evaluation deprived from the decision-makers' knowledge and experiences. However, for a real chemical system, different types of uncertainties associated with the input data and information of the criteria are inevitably encountered and have to be considered,[13, 25] i.e. the aleatory and epistemic uncertainty. The former one refers to the inaccuracies such as variations or randomness associated with the system, which is objective and irreversible; while the epistemic uncertainty represents the incompleteness like the lack of knowledge and information on parameterization, which is subjective and reducible.[13, 25]

2.2.1 Data Collection regarding the Hard Criteria under Aleatory Uncertainty by Using Interval Parameter

The data of hard criteria can be collected from literature sources, experimental tests, system simulations, and mathematical techniques,[13] which are always available in a certain range rather than fixed numbers. For instance, it is more reasonable to estimate the capital cost of a chemical process with a range of 10.2-10.6 million US dollar (M$) than a fixed value of 10.4 M$. Typically, the interval parameter method is suitable for representing the inherent uncertainties in the quantifiable data that arise from the inaccuracies and complex nature of the chemical systems, where the range of parameter values is known while data distribution information is unavailable.[13] Hence, the interval-parameter-based method was employed to handle the aleatory uncertainty associated with the hard criteria, in which, the imprecision, variations, and randomness can be reasonably expressed and operated by using the corresponding laws as given in Table 1.

Table 1. Operational laws of interval numbers,[26] and triangular fuzzy numbers[27]

	Two interval numbers $Z_1=[Z_1^L, Z_1^U], Z_2=[Z_2^L, Z_2^U]$ where $Z_1^L \le Z_1^U,\ Z_2^L \le Z_2^U$	Two triangular fuzzy numbers: $\tilde{A}=(a^l, a^m, a^u), \tilde{B}=(b^l, b^m, b^u)$ where $a^l \le a^m \le a^u, b^l \le b^m \le b^u$
addition	$Z_1+Z_2=[Z_1^L+Z_2^L, Z_1^U+Z_2^U]$	$\tilde{A}+\tilde{B}=(a^l+b^l, a^m+b^m, a^u+b^u)$
subtraction	$Z_1-Z_2=[Z_1^L-Z_2^U, Z_1^U-Z_2^L]$	$\tilde{A}-\tilde{B}=(a^l-b^u, a^m-b^m, a^u-b^l)$
multiplication	$Z_1\times Z_2=[Z_1^L\times Z_2^L, Z_1^U\times Z_2^U]$	$\tilde{A}\otimes\tilde{B}=(a^l b^l, a^m b^m, a^u b^u)$
division	$Z_1\div Z_2=[Z_1^L/Z_2^U, Z_1^U/Z_2^L]$	$\tilde{A}\div\tilde{B}=(a^l/b^u, a^m/b^m, a^u/b^l)$
scalar	$\lambda Z_1=[\lambda Z_1^L, \lambda Z_1^U]$	$\lambda\tilde{A}=(\lambda a^l, \lambda a^m, \lambda a^u)$
power	$Z_1^f=[(Z_1^L)^f, (Z_1^U)^f]$	$\tilde{A}^f=((a^l)^f, (a^m)^f, (a^u)^f)$

2.2.2 Information Processing regarding the Soft Criteria under Epistemic Uncertainty by Using FAHP

In contrary to the hard criteria, the alternative's performance regarding an soft criterion can only be described by subjective judgments that depend on the experts' knowledge and experiences,[6, 8] e.g. the information of a process's maturity. There are usually two ways for scoring the subjective information: the pair-wise comparison method and the scaling system method.[8] Compared with the scaling system that scores the criteria by assigning scale numbers, the pair-wise comparison (especially the AHP method) is able to offer a more reliable scoring result with consistency *via* constructing pair-wise comparison matrices. However, the conventional AHP method can only provide the users with crisp numbers (1-9 scale) to express their opinions, e.g. "the performance comparison of *i*-th alternative and *j*-th alternative is 7 to 1", failing to address the uncertainty, vagueness, and imprecision of human's judgments.[28] Therefore, a FAHP method by integrating the AHP method with the fuzzy set theory to quantify experts' judgments is adopted in this study, which enables the experts to use linguistic terms rather than crisp numbers to express opinions in an easier and more humanistic way *via* the following two steps:[29, 30] 1). constructing the pair-wise comparison matrix by using linguistic terms, and then transforming it into the form of fuzzy numbers; 2) quantifying the soft criterion, and then defuzzifying it into a crisp score. The specified steps of the FAHP are offered in ***Supporting Information of Appendix A***, while a brief introduction regarding the fuzzy set theory that employs membership functions to deal with the uncertainty was introduced as follow.

A fuzzy set, $\tilde{a}$, is in a universe of discourse, *X*, which is characterized by a membership function, $\mu_{\tilde{a}}(x)$, associating with each element *x* in *X* by a real number in the interval [0,1]. The function value represents the grade of membership of *x* in $\tilde{a}$.[27] In this study, $\tilde{a}$ is defined by using the most popular triangular fuzzy number (a^l, a^m, a^u), as illustrated in Figure 2; the corresponding operational laws can be found in Table 1.

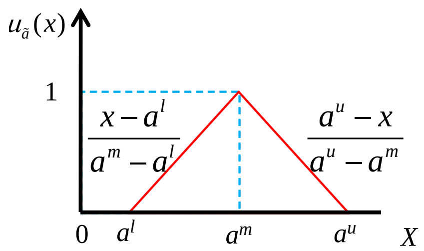

Figure 2. Schema form of the membership function with the triangular fuzzy number.[27]

2.3 Determination of the Criteria's Weights by Using FDANP

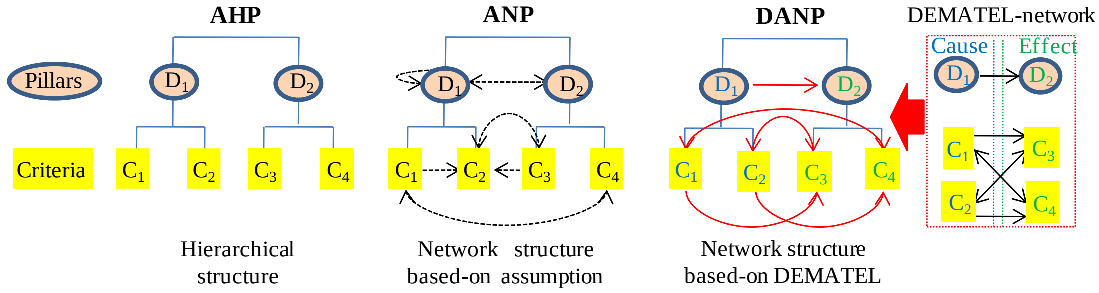

Figure 3. Structural difference among AHP, ANP, and DANP

In the decision making, the effect of each criterion on the overall sustainability of various alternatives is different, indicating that the criterion's weight is usually unequal. Although the above-mentioned FAHP method has been well practiced for the weights determination *via* the hierarchically structured assessment system (Figure 3), it ignores the interdependences among the criteria/pillars, offering unreliable weighting results for the cases that the interdependences are significant (i.e. a criterion that has more interactions with others should be assigned with a higher weight).[8, 31] Consequently, the ANP (Analytic Network Process) approach, as an improved AHP method, has been strongly suggested for weights determination with the consideration of interdependences by using a network structure characterized by interactions and feedbacks (see Figure 3). However, since the interdependences between the assessment system are assumed to be known a priori, the conventional ANP method fails to provide any guidelines on how to construct the interrelations,[32] and could offer inaccurate weighting results if the structure is ill-defined.[31] Besides, the ANP approach relies heavily on a large number of pair-wise comparison questions, which is time consuming and difficult to obtain,[33] and even nonsensical especially when the inner dependencies exist in the pillar-level.[31] Therefore, it has become extremely popular in recent years to incorporate the relationship construction technique of DEMATEL (Decision Making

Trial and Evaluation Laboratory) into the ANP method for improving the modeling capabilities and better functioning.[32] During the approach, the DEMATEL approach uses a limited number of comparisons to categorize the criteria and pillars into the cause and effect groups,[34-36] consequently, the pair-wise comparison burdens in the conventional ANP method can be relieved by using the DEMATEL-determined direct influence matrix, and the questionable network assumption in ANP can be replaced by the DEMATEL-deprived causal relationship (see Figure 3).[32] Also for addressing the uncertainty in human's judgments, the fuzzy set theory is combined with the DEMATEL-based ANP method (known as FDANP) in this work to determine the subjective weights with the following six steps:[32, 35] 1). establishing the initial direct influence matrix by using the linguistic terms, and then transforming it into the form of fuzzy numbers; 2). normalizing the initial direct influence matrix; 3). determining the fuzzy total relation matrix, where the elements in the matrix are used to draw the cause-effect relationship, and then to execute the ANP computation (steps 4-6); 4). forming the fuzzy unweighted supermatrix; 5). determining the fuzzy weighted supermatrix; 6). calculating the fuzzy limit supermatrix, and then obtaining the criteria's weights after the defuzzification (see ***Supporting Information of Appendix A*** for the specified steps of the FDANP).

2.4 Sustainability Prioritization of the Alternatives by Using an Interval Vector-based Algorithm

The sustainability prioritization of alternative processes is a typical MCDM problem, a variety of MCDM methods have been employed for ranking the chemicalrelated systems, e.g. AHP,[6] PROMETHEE,[8] Data Envelopment Analysis,[37] TOPSIS (Technique for Order of Preference by Similarity to Ideal Solution),[38] and VIKOR (VlseKriterijuska Optimizacija I Komoromisno Resenje),[39] etc. Unlike the MCDM methods that compare the alternatives only relying on the aggregation of their absolute performances regarding multi-criteria,[15] Xu et al.[14] developed an integrated approach by coupling a three-dimensional (3D) vector-based algorithm with AHP for assessing the sustainability of chemical processes, which not only determines the absolute sustainability scores, but also addresses the relative sustainability balance proposed by Moradi-Aliabadi and Huang,[40] offering a more rigorous ranking method by viewing that a real preferred process should not only focus on the absolute performance but also considerate the relative deviation of the performance from the ideal sustainable direction (Figure 4).

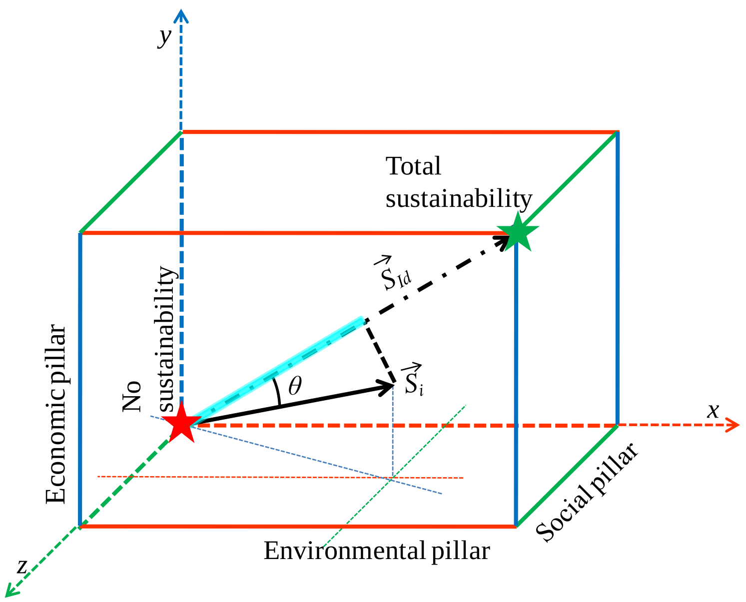

Figure 4. Principal of the 3D vector cube in previous studies[14, 40]

However, in the previous study,[14] the three pillars of environmental, economic, and social aspects were confined to a 3D cube, making it impossible to expand the evaluation system with the consideration of the technical and political criteria. Moreover, the uncertainties of data and information, the interaction among criteria, and the vagueness of decision-makers' judgments can not be tackled by the AHP-based multilayer aggregation in the previous work, indicating the necessity of enhancing the original algorithm. Therefore, an interval vector-based algorithm including 6 steps is developed in this study for the sustainability prioritization.

Step.1: Constructing the initial decision-making matrix. The collected data of the alternatives' performances (section 2.2), and the criteria's weights (section 2.3) are placed into the initial decision-making matrix as given in Eq. 1.

$$\begin{array}{ccccc} & C_1 & C_2 & \cdots & C_n \\ A_1 & [z_{11}^L, z_{11}^U] & [z_{12}^L, z_{12}^U] & \cdots & [z_{1n}^L, z_{1n}^U] \\ A_2 & [z_{21}^L, z_{21}^U] & [z_{22}^L, z_{22}^U] & \cdots & [z_{2n}^L, z_{2n}^U] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_m & [z_{m1}^L, z_{m1}^U] & [z_{m2}^L, z_{m2}^U] & \cdots & [z_{mn}^L, z_{mn}^U] \\ W & w_1 & w_2 & \cdots & w_n \end{array} \tag{1}$$

In Eq, 1, there are *m* alternatives (*A*) and *n* criteria (*C*), while $W = \left[w_1, w_2, \cdots, w_n\right]$ denotes the criteria's weights. $[z_{ij}^L, z_{ij}^U]$ is an interval number representing the performance of the *i*-th alternative with respect to the *j*-th criterion, when $z_{ij}^L = z_{ij}^U$ (*i.e.* soft criterion data), the interval number turns into a crisp value.

Step.2: Normalizing the initial decision-making matrix. Since the alternatives' performances regarding different criteria have different physical units and scales, it is prerequisite for the sustainability prioritization to normalize them into dimensionless and unitary data according to Eq. 2; which is suitable for dealing with the decision-making matrix with both crisp and interval numbers,[41] and preserving the uncertainty degrees regarding the original data very well.

$$\text{Benifit:}\left[f_{ij}^{L}, f_{ij}^{U} \right] = \left[\frac{z_{ij}^{L}}{\sqrt{\frac{1}{2}\sum_{i=1}^{m}((z_{ij}^{L})^2+(z_{ij}^{U})^2)}}, \frac{z_{ij}^{U}}{\sqrt{\frac{1}{2}\sum_{i=1}^{m}((\overline{z}_{ij}^{L})^2+(\overline{z}_{ij}^{U})^2)}} \right]$$

$$\text{Cost:}\left[f_{ij}^{L}, f_{ij}^{U} \right] = \left[\frac{1/z_{ij}^{U}}{\sqrt{\frac{1}{2}\sum_{i=1}^{m}(1/(Z_{ij}^{L})^2+1/(Z_{ij}^{U})^2)}}, \frac{1/z_{ij}^{L}}{\sqrt{\frac{1}{2}\sum_{i=1}^{m}(1/(Z_{ij}^{L})^2+1/(Z_{ij}^{U})^2)}} \right] \tag{2}$$

Step.3: Defining the interval vector-based sustainability performance. According to the previous studies,[14,40] the sustainability performance of a chemical process is depicted as a vector with the upper and lower boundary as given in Eq. 3, while the highest sustainability that a chemical process can ideally achieve is denoted as the ideal vector (Eq. 4).

$$\vec{S}_i = [\vec{S}_i^{L}, \vec{S}_i^{U}] = \left\{ \left[w_1 f_{i1}^{L}, w_1 f_{i1}^{U} \right], \left[w_2 f_{i2}^{L}, w_2 f_{i2}^{U} \right], \cdots, \left[w_n f_{in}^{L}, w_n f_{in}^{U} \right] \right\} \tag{3}$$

$$\vec{S}_{Id} = w_j f_j^{\max} = \left\{ w_1 f_1^{\max}, w_2 f_2^{\max}, \cdots, w_n f_n^{\max} \right\} \tag{4}$$

where $f_j^{\max} = \max_{i=1,2,\cdots m} \{ f_{ij}^{U} \}$.

Step.4: Characterizing the interval vector-based sustainability performance. Two interim parameters are introduced in this step for characterizing the alternatives' performance, i.e. the sustainability performance magnitude (*SM*) and the sustainability deviation angle *(SA)*.[14] During the process, the vector length from the tail to tip is defined as *SM*, representing the absolute sustainability score with respect to each alternative. Apparently, a larger score represents a better performance, while the ideal vector has the maximum magnitude.[40]

$$SM_i = [SM_i^{L}, SM_i^{U}] = \left[\left\| \vec{S}_i^{L} \right\|, \left\| \vec{S}_i^{U} \right\| \right] = \left[\sqrt{\sum_{j=1}^{n} (w_j f_{ij}^{L})^2}, \sqrt{\sum_{j=1}^{n} (w_j f_{ij}^{U})^2} \right] \tag{5}$$

$$SM_{Id} = \left\| \vec{S}_{Id} \right\| = \sqrt{\sum_{j=1}^{n} (w_j f_j^{\max})^2} \tag{6}$$

As for the parameter of *SA*, since the ideal vector represents the totally balanced sustainability performance regarding the whole criteria system, the corresponding vector of any investigated process that does not follow the direction of the ideal vector indicates a deviation of its sustainability performance from the ideal balanced direction.[40] Here, the cosine of *SA* (cos(*SA*)) is used to quantify the deviation from the ideal direction as given in Eq. 7; while the ideal vector indicates the totally balanced direction (Eq. 8). Apparently, the higher the value of cos(SA_i), the less the deviation between the *i*-th alternative and the ideal one, implying a more sustainable scenario.

$$\begin{aligned}
\cos(SA_i) &= \left[\cos(SA_i^L), \cos(SA_i^U)\right] = \left[\min\left\{\left(\frac{\vec{S}_i^L \cdot \vec{S}_{Id}}{SM_i^L SM_{Id}}\right), \left(\frac{\vec{S}_i^U \cdot \vec{S}_{Id}}{SM_i^U SM_{Id}}\right)\right\}, \max\left\{\left(\frac{\vec{S}_i^L \cdot \vec{S}_{Id}}{SM_i^L SM_{Id}}\right), \left(\frac{\vec{S}_i^U \cdot \vec{S}_{Id}}{SM_i^U SM_{Id}}\right)\right\}\right] \\
&= \left[\min\left\{\left(\frac{\sum_{j=1}^{n}(w_j^2 f_{ij}^L f_j^{\max})}{\sqrt{\sum_{j=1}^{n}(w_j f_{ij}^L)^2} \times \sqrt{\sum_{j=1}^{n}(w_j f_j^{\max})^2}}\right), \left(\frac{\sum_{j=1}^{n}(w_j^2 f_{ij}^U f_j^{\max})}{\sqrt{\sum_{j=1}^{n}(w_j f_{ij}^U)^2} \times \sqrt{\sum_{j=1}^{n}(w_j f_j^{\max})^2}}\right)\right\},\right. \\
&\quad \left. \max\left\{\left(\frac{\sum_{j=1}^{n}(w_j^2 f_{ij}^L f_j^{\max})}{\sqrt{\sum_{j=1}^{n}(w_j f_{ij}^L)^2} \times \sqrt{\sum_{j=1}^{n}(w_j f_j^{\max})^2}}\right), \left(\frac{\sum_{j=1}^{n}(w_j^2 f_{ij}^U f_j^{\max})}{\sqrt{\sum_{j=1}^{n}(w_j f_{ij}^U)^2} \times \sqrt{\sum_{j=1}^{n}(w_j f_j^{\max})^2}}\right)\right\}\right]
\end{aligned} \tag{7}$$

$$\cos(SA_{Id}) = \left(\frac{\vec{S}_{Id} \cdot \vec{S}_{Id}}{SM_{Id} SM_{Id}}\right) = \left(\frac{\sum_{j=1}^{n}(w_j f_j^{\max})^2}{\left(\sqrt{\sum_{j=1}^{n}(w_j f_j^{\max})^2}\right)^2}\right) = 1 \tag{8}$$

Step.5: Obtaining the sustainability projection value. Theoretically, the ultimate sustainability assessment of a process should considerate both the absolute sustainability score and the relative sustainability balance, resulting in a parameter of sustainability projection (*SP*) that incorporates both of the sustainability magnitude and angle by calculating the normalized projection of the investigated vector on the ideal one (Eq. 9). Apparently, the normalized sustainability projection value of the ideal vector on itself should be 1 (see Eq. 10), implying the totally ideal scenario.[14]

$$SP_i = \left[SP_i^L, SP_i^U \right] = \left[\frac{SM_i^L \times \cos(SA_i^L)}{\sqrt{\sum_{j=1}^{n} (w_j f_j^{\max})^2}}, \frac{SM_i^U \times \cos(SA_i^U)}{\sqrt{\sum_{j=1}^{n} (w_j f_j^{\max})^2}} \right] \tag{9}$$

$$SP_{Id} = \frac{SM_{Id} \times \cos(SA_{Id})}{\sqrt{\sum_{j=1}^{n} (w_j f_j^{\max})^2}} = \frac{\sqrt{\sum_{j=1}^{n} (w_j f_j^{\max})^2} \times 1}{\sqrt{\sum_{j=1}^{n} (w_j f_j^{\max})^2}} = 1 \tag{10}$$

Step.6: Ranking the sustainability sequence. By conducting the interval vector-based analysis technique, the ultimate sustainability performance of each alternative is obtained as interval numbers, implying that the uncertainties are involved in the results. Generally, two approaches can be used for comparing the interval numbers: the determinacy method[42] and the possibility measure.[26,43] The determinacy method utilizes the score, accuracy and certainty functions to rank the interval numbers; while the possibility measure prioritizes the interval numbers in the form of uncertain implication rules, and has been proved to be a more reasonable way to coincide with the increasing complexity in real decision issues.[26, 43] Hence, for comparing the sustainability of any two alternatives like $SP_i = [SP_i^L, SP_i^U]$ and $SP_j = [SP_j^L, SP_j^U]$, the parameter of possibility degree (PD_{ij}) can be calculated *via* the possibility approach in Eq. 11 to demonstrate the occurrence probability of the uncertainty event that the *i*-th alternative is superior to *j*-th alternative.[43, 44]

$$PD_{ij} = \max\{1 - \max(\frac{SP_j^U - SP_i^L}{SP_j^U - SP_j^L + SP_i^U - SP_i^L}, 0), 0\} \tag{11}$$

Subsequently, a possibility degree matrix (*PD*) involving *m* alternatives can be obtained in Eq. 12.

$$PD = \begin{bmatrix} PD_{11} & PD_{12} & \cdots & PD_{1m} \\ PD_{21} & PD_{22} & \cdots & PD_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ PD_{m1} & PD_{m2} & \cdots & PD_{mm} \end{bmatrix} \tag{12}$$

where $PD_{ij} + PD_{ji} = 1$, and $PD_{ii} = 0.5$. Then, the elements in each row of the possibility degree matrix are summarized according to Eq. 13,[44] the obtained priority value (PV_i) regarding the *i*-th alternative is then used to rank the alternatives with a higher value indicating a better sustainability.

$$PV_i = \frac{\sum_{j=1}^{m} PD_{ij} + 0.5\text{m-1}}{m(m-1)} \tag{13}$$

In Eq. 13, *m* represents the number of alternatives.

In summary, the conversion or perversion of uncertain data/information among the whole mathematical framework can be clarified as follows: the FAHP (***2.2.2***) and FDANP (***2.3***) methods were correspondingly used to generate the soft data and criteria's weights with deterministic values, where the epistemic uncertainty of human's judgments in both of the two procedures can be addressed instantly by using the fuzzy set theory. The aleatory uncertainty in the hard data that arises from the inaccuracies and complex nature of the chemical systems is represented by the interval parameter (***2.2.1***), and then preserved thoroughly untill the end of sustainability prioritization (***2.4***). While the prioritization (***2.4***) integrates the weight and data for each criterion into a unique synthesizing score by resorting to a novel vector-based additive aggregation, which is characterized by well preserving the uncertainty degrees of the original data and the monolayer of the interval-based multiplication, offering a easy but rigorous way for sustainability assessment under uncertainties.

3. Case Study

In order to illustrate the developed framework, the sustainability of five ammonia production processes including two mature routes, i.e. steam methane reforming (SMR) and coal gasification (CG), and three promising electrolysis-based pathways, i.e. hydropower-electrolysis (HE), nuclear high temperature-electrolysis (NE), and biomass gasification-electrolysis (BE), were assessed in this study. In the SMR and CG processes, hydrogen is produced by the steam reforming of natural gas or coal gasification, and used as the feedstock for the Haber-Bosch (HB) unit to synthesize ammonia.[45] As for the three electrolysis routes, the hydrogen generated from the hydropower-electrolysis, nuclear high temperature-electrolysis, and biomass gasification-electrolysis, respectively, and the nitrogen that is deprived from the cryogenic air separation (CAS) are input to the HB process for ammonia production.[21] The schematic diagram of the five alternative processes are depicted in Figure 5 according to the works of Bicer et al.[21, 45]

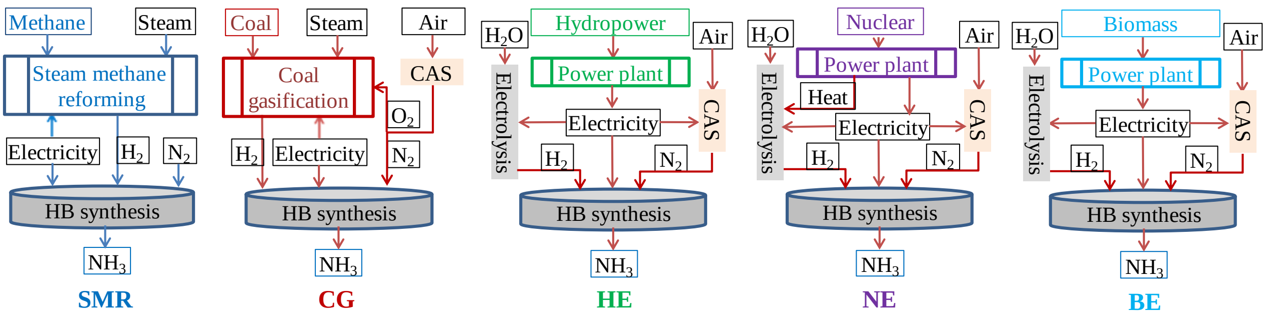

Figure 5. Schematic diagrams of the five alternative processes.

Establishment of criteria System

A comprehensive evaluation system that involves ten criteria from environmental impacts (En includes $C_{1\text{-}3}$), economic prosperity (Ec includes $C_{4\text{-}5}$), social-political concerns (SP include $C_{6\text{-}7}$), and technical performance (Te includes $C_{8\text{-}10}$) is established in Table 2.

Table 2. Evaluation system for the sustainability assessment of ammonia production processes

pillars	Criteria	abbreviation	Type	Reference
	global warming	C_1	hard(cost)	[21]
En	abiotic depletion	C_2	hard(cost)	[21]
	human toxicity	C_3	hard(cost)	[21]
Ec	life cycle costs	C_4	hard(cost)	[18]
	contribution to GDP	C_5	soft(benefit)	[46]
SP	social acceptability	C_6	soft(benefit)	[46]
	political acceptability	C_7	soft(benefit)	[8]
	Maturity	C_8	soft(benefit)	[28]
Te	safeguards	C_9	soft(benefit)	[28]
	energy efficiency	C_{10}	hard(benefit)	[21]

Collection of alternatives' performances regarding each criterion

In Table 2, the hard and soft criteria should be collected by technical surveys and expert's descriptions, respectively, in which the corresponding uncertainty is handled by the interval parameter or FAHP method. Notably, for ensuring the equality of comparison, the collected data are based on the per unit output of each criterion.

The data with respect to the five hard criteria, namely global warming (C_1), abiotic depletion (C_2), human toxicity (C_3), life cycle costs (C_4), and energy efficiency (C_{10}) are interval numbers that are derived from the literatures[21, 45, 47, 48] by altering the original data with ±10% derivations as the aleatory uncertainty (Table 3).

Table 3. Data collected for the hard criteria

	C_1 kg CO_2 eq	C_2 10^{-2}kg Sb eq	C_3 kg1,4-DB eq	C_4 10^3\$/(t-NH_3/day)	C_{10} %
SMR	[1.680, 2.054]	[1.705, 2.083]	[0.643, 0.785]	[272, 332]	[35.9, 43.9]
CG	[2.820, 3.446]	[0.240, 0.294]	[0.065, 0.079]	[514, 628]	[38.8, 47.4]
HE	[0.347, 0.424]	[0.253, 0.309]	[0.113, 0.138]	[1126, 1376]	[38.4, 47.0]
NE	[0.758, 0.926]	[0.580, 0.708]	[0.861, 1.053]	[475, 581]	[21.4, 26.2]
BE	[0.769, 0.939]	[0.251, 0.307]	[0.068, 0.083]	[446, 545]	[13.9, 16.9]

For scoring the information regarding the five soft criteria, i.e. contribution to GDP (C_5), social acceptability (C_6), political acceptability (C_7), maturity (C_8), and safeguards (C_9), three representative experts that are denoted as $DM_{1\text{-}3}$ are participated in the decision-making process for contributing their insightful judgments on the alternatives' performances regarding each soft criterion by using the linguistic terms, which were then converted into the corresponding quantified results (Table 4) by using the FAHP method. The linguistic-based pair-wise comparison matrices can be found in ***Supporting Information of Appendix B***.

Table 4. Information scored for the soft criteria

	C_5	C_6	C_7	C_8	C_9
SMR	0.171	0.206	0.260	0.220	0.218
CG	0.183	0.185	0.227	0.220	0.194
HE	0.235	0.252	0.171	0.189	0.286

NE	0.277	0.122	0.183	0.189	0.118
BE	0.134	0.235	0.160	0.180	0.183

Weights determination regarding the interrelated criteria

The FDANP method was applied to determine the weights of the interrelated criteria, where a rigorous network structure of the criteria system is the prerequisite for obtaining a reliable weighting result. In this case study, the linguistic judgments regarding the relationships among the criteria that are contributed by the three experts were firstly used for constructing the network structure (Figure 6) according to the DEMATEL technique in the FDANP method. According to the result in Figure 6, the three technical criteria (C_8-C_{10}) and the criterion of life cycle costs (C_4) from the economic concerns with positive values of $(r_i - s_i)$, should be regarded as key drivers (cause group) for enhancing other criteria (effect group) including another economic indicator (C_5) and all the environmental (C_1-C_3) and social-political (C_6, C_7) criteria; and the technical pillar might be the root that affects other categorized sustainability concerns, approving that the technical criteria will obviously effect other criteria from the environmental, economic, and social-political concerns.

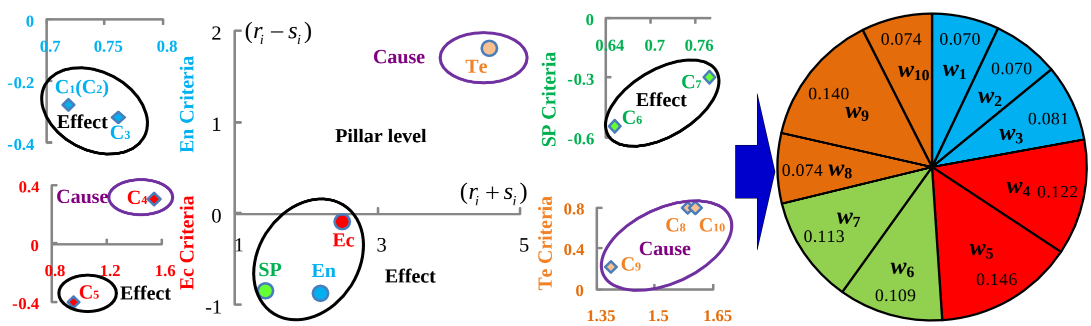

Figure 6. Relationship among the assessment system, weighting results regarding the criteria.

Note: r_i is the total direct and indirect effects of criterion i on the other criteria, s_i is the total direct and indirect effects that the i-th criterion receives from the other criteria.

Based-on the network structure, the ANP computations in the FDANP approach were conducted to generate the unweighted supermatrix, weighted supermatrix, and limited supermatrix orderly, which can significantly eliminate the burdensome (a total number of 44) comparison matrices in the conventional ANP approach. Consequently, the weights (w_i) regarding the interacted criteria can be obtained as crisp values (see Figure 6) after defuzzifying the limited supermatrix. According to the weighting results in Figure 6, the criteria of contribution to GDP (C_5), safeguard (C_9), life cycle costs (C_4), and political acceptability (C_7) are the top four important criteria for the overall sustainability, implying the necessity of incorporating the technical and political criteria into the evaluation system. The detailed computations of the FDANP method were specified in ***Supporting Information of Appendix B***.

Sustainability sequence of the alternative processes

By integrating the database in Tables 3-4 and the weights in Figure 6, the initial decision-making matrix is constructed (see ***Table S16 in Supporting Information***). Notably, this matrix is mixed with both interval numbers and crisp values. By using Eq. 2, cost criteria C_1-C_4, and benefit criteria C_5-C_{10} were normalized, generating the normalized decision-making matrix as given in Table 5, in which, the crisp values regarding the soft criteria data were represented by the interval numbers.

Table 5. Normalized decision-making matrix

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}
SMR	[0.152,0.186]	[0.073,0.089]	[0.060,0.073]	[0.627,0.767]	[0.370,0.370]	[0.450,0.450]	[0.571,0.571]	[0.491,0.491]	[0.471,0.471]	[0.485,0.560]
CG	[0.091,0.111]	[0.516,0.631]	[0.594,0.727]	[0.332,0.406]	[0.397,0.397]	[0.404,0.404]	[0.499,0.499]	[0.491,0.491]	[0.418,0.418]	[0.495,0.605]
HE	[0.739,0.903]	[0.490,0.599]	[0.342,0.419]	[0.151,0.185]	[0.511,0.511]	[0.549,0.549]	[0.375,0.375]	[0.422,0.422]	[0.618,0.618]	[0.491,0.600]
NE	[0.210,0.313]	[0.214,0.262]	[0.045,0.055]	[0.359,0.439]	[0.600,0.600]	[0.266,0.266]	[0.402,0.402]	[0.422,0.422]	[0.255,0.255]	[0.273,0.334]

BE	[0.333,0.407]	[0.494,0.604]	[0.571,0.698]	[0.383,0.468]	[0.291,0.291]	[0.512,0.512]	[0.351,0.351]	[0.402,0.402]	[0.396,0.396]	[0.177,0.216]
W	0.070	0.070	0.081	0.122	0.146	0.109	0.113	0.074	0.140	0.074

Based-on the dataset in Table 5, the vector functions with respect to the five alternatives and the ideal one can be presented (see ***Table S17 in Supporting Information***) according to Eqs. 3 and 4. Then, by running the interval vector-based algorithm, the values of *SM* and cos(*SA*) can be calculated by using Eqs. 5-6, and Eqs. 7-8, respectively; both of them were then incorporated into the sustainability projection value (*SP*) according to the formulas 9-10. Here, the obtained results regarding each parameter in the interval vector-based algorithm are given in Table 6.

Table 6. Parameters for the interval vector-based algorithm

	SM	cos*(SA)*	*SP*
SMR	[0.150, 0.161]	[0.912, 0.913]	[0.648, 0.697]
CG	[0.141, 0.152]	[0.943, 0.944]	[0.631, 0.682]
HE	[0.160, 0.170]	[0.925, 0.935]	[0.703, 0.752]
NE	[0.126, 0.132]	[0.900, 0.918]	[0.539, 0.576]
BE	[0.129, 0.141]	[0.962, 0.964]	[0.590, 0.643]
Ideal	0.211	1	1

Subsequently, the probability matrix could be generated by running Eqs. 11-12. Taking PD_{12} as an example, it can be calculated to represent that the probability of $[SP_1^L, SP_1^U]$ (SMR) is greater than $[SP_2^L, SP_2^U]$ (CG):

$$\begin{aligned} PD_{12} &= \max\{1-\max(\frac{SP_2^U - SP_1^L}{SP_2^U - SP_2^L + SP_1^U - SP_1^L},0),0\} \\ &= \max\{1-\max(\frac{0.682-0.648}{0.682-0.631+0.697-0.648},0),0\} = 0.660 \end{aligned} \tag{14}$$

The value of PD_{12} implies that the possibility degree that the SMR process is superior to the CG pathway is 66.0%, denoted as $\text{SMR} \underset{(0.660)}{\succ} \text{CG}$. In the same way, all the possibility degrees in the probability matrix can be determined as given in Eq. 15, offering detailed comparison result with respects to each pair of alternatives, and then realizing the ranking values of the five alternatives according to Eq. 13.

$$PD = \begin{array}{c} \text{SMR} \\ \text{CG} \\ \text{HE} \\ \text{NE} \\ \text{BE} \end{array} \begin{bmatrix} 0.500 & 0.660 & 0.000 & 1.000 & 1.000 \\ 0.340 & 0.500 & 0.000 & 1.000 & 0.880 \\ 1.000 & 1.000 & 0.500 & 1.000 & 1.000 \\ 0.000 & 0.000 & 0.000 & 0.500 & 0.000 \\ 0.000 & 0.120 & 0.000 & 1.000 & 0.500 \end{bmatrix} \overset{\text{Eq.13}}{\Rightarrow} \begin{cases} PV(\text{SMR})=0.233 \\ PV(\text{CG})=0.211 \\ PV(\text{HE})=0.300 \\ PV(\text{NE})=0.100 \\ PV(\text{BE})=0.156 \end{cases} \tag{15}$$

Therefore, the final priority (*SP*) with the possibility degree regarding the five alternatives can be concluded in Eq. 16, indicating that the hydropower-electrolysis process has the highest sustainability, followed by two mature pathways of SMR, CG, and two promising processes of BE, NE in a descending order. Moreover, in order to illustrate the effects of *SM* and cos(*SA*) on the final ranking (*SP*), analyses with respect to these two parameters were also conducted by running the probability measure (Eqs. 11-13), and the calculated priority sequences regarding *SM* and cos(*SA*) with the possibility degrees were given in Eqs. 17 and 18, respectively.

$$SP:\ \text{HE} \underset{(1.000)}{\succ} \text{SMR} \underset{(0.660)}{\succ} \text{CG} \underset{(0.880)}{\succ} \text{BE} \underset{(1.000)}{\succ} \text{NE} \tag{16}$$

$$SM:\text{HE} \underset{(0.958)}{\succ} \text{SMR} \underset{(0.885)}{\succ} \text{CG} \underset{(1.000)}{\succ} \text{BE} \underset{(0.829)}{\succ} \text{NE} \tag{17}$$

$$\cos(SA):\ \text{BE} \underset{(1.000)}{\succ} \text{CG} \underset{(1.000)}{\succ} \text{HE} \underset{(1.000)}{\succ} \text{SMR} \underset{(0.698)}{\succ} \text{NE} \tag{18}$$

Here, a larger *SM*/cos(*SA*) score indicates that the corresponding alternative is more sustainable. Apparently, the *SM*-based and the *SP*-based priorities are the same, implying that the absolute sustainability performance plays a role of cornerstone in the final sustainability ranking. However, the gap of $\text{SMR} \underset{(0.660)}{\succ} \text{CG}$ in *SP* has been narrowed for given that the process of CG has a significant advantage over SMR in the sustainability deviation angle, highlighting that a satisfactory process should balance the environmental, economic, social-political, and technical performance, simultaneously.

4. **Results Comparison**

To test the robustness of the assessment result, as well as to demonstrate the effectiveness and advantages of the developed framework, three analysis items were conducted in this section, i.e. (1). sensitivity analysis regarding criteria's weights for testing the robustness of the prioritization results, (2). embedment of the FAHP-based weights for clarifying the significance of considering the criteria's interrelationship, (3). comparison with the existing MCDM methods for approving the effectiveness of the original study and reflecting its advantage.

4.1 Sensitivity Analysis

In the proposed framework, the criteria's weights were contributed by experts' subjective descriptions, which might be changed when different experts with varied knowledge backgrounds are involved. For testing the robustness of the prioritization result, a sensitivity analysis was conducted to probe into the weights' influence on the final ranking of the five alternatives by gradually changing one criterion's weight while fixing the weights portions of the other nine criteria. Taking case 1 for C_1 as an example, the weight of C_1 has decreased or increased 30%, 60%, 90% compared with its original weight w_1 with the change being denoted as δw_1; while the weights of other nine criteria are proportionally modified based-on their original relative importance. By using Eq.

19 for the normalization, the new weights in case 1 are employed to run the interval vector-based algorithm, and the prioritization results of 10 cases regarding each criterion are exhibited in Figure 7.

$$w_1' = \frac{w_1 + \delta w_1}{1+\delta w_1};\ w_j' = \frac{w_j}{1+\delta w_1},\ j = 2,3,\cdots,10 \tag{19}$$

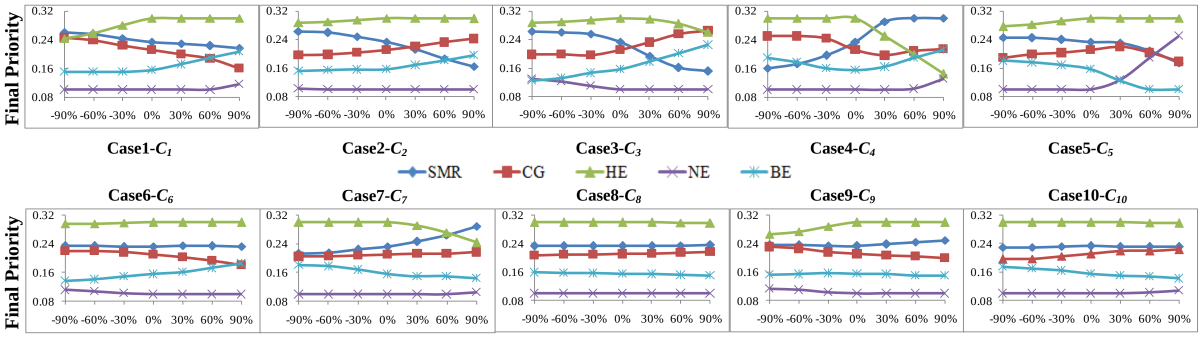

Figure 7. Sensitivity analysis results for the weights fluctuation of each criterion

It can be observed that the alternative HE remains the best choice for almost all the weights-change situations, except for the massive incensement in the weights of C_4 and C_7, where the best choice is replaced by the process of SMR. Accordingly, it can be concluded that the proposed mathematical framework is effective to identify the most sustainable chemical process among various alternatives. However, the values of the final priority are sensitive to the weights of criteria, implying that it is a critical step toward a reliable assessment result to determine the criteria's relative importance in an accurate way.

4.2 Weights Comparison between FAHP and FDANP

The necessity of considering the interrelationship among the criteria system was demonstrated by comparing the weights that were deprived from the FDANP technique with those determined using the FAHP method, as shown in Figure 8. Notably, the same three experts were asked to construct the pair-wise comparison matrices for FAHP analysis (see ***Supporting Information of Appendix B***), which has been stated in subsection 2.2.2.

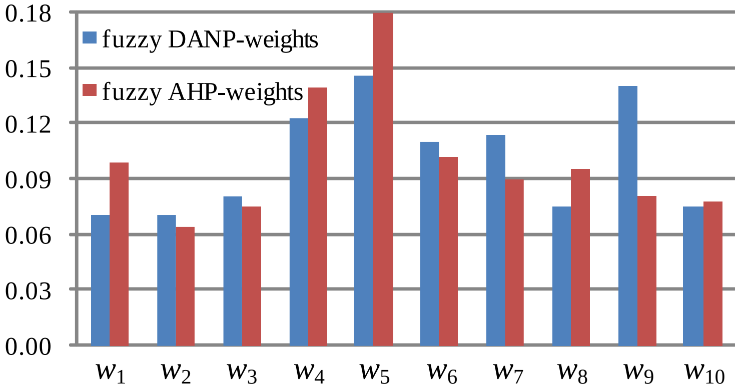

Figure 8. Comparison of the FDANP-weights and the FAHP-weights

Apparently, the weights deprived from the FDANP and FAHP approaches are different, for instance, the relative importance of Safeguard (C_9) is quite underrated by the FAHP method, where only the direct effect of C_9 on people's preferences to the process alternatives is considered, while the indirect effects of C_9 contributed by the interactions among criteria are totally ignored. To take one step forward by employing the FAHP-weights for prioritizing the five alternatives *via* the same procedures as stated in section 2.4, the ranking result can be generated as $\underset{(1.000)}{\mathrm{HE} \succ} \mathrm{SMR} \underset{(0.868)}{\succ} \mathrm{NE} \underset{(0.581)}{\succ} \mathrm{CG} \underset{(0.644)}{\succ} \mathrm{BE}$. The least choice of NE in the original rank has been promoted as the third best decision in the sequence based-on the FAHP-weights. However, this result is considered to be unreasonable as NE still faces many severe problems especially regarding the social-political and technical concerns, and this unfavorable perception with respect to NE can be found in the literatures.[17, 49, 50]

Therefore, the importance for considering the relationships among the assessment system has been demonstrated indirectly, which implies the necessity and advantage regarding the utilization of the FDANP weighting method.

4.3 Priorities Comparison between Interval Vector-based Algorithm and Representative MCDM Methodologies

To verify the effectiveness of vector-based ranking algorithm in the proposed framework, three representative MCDM methodologies with different ranking logics, i.e., SAW (Simple Additive Weighting), PROMETHEE method, and TOPSIS method, were utilized for the alternatives prioritization based-on the dataset in Table 5. Among the three MCDM methodologies, SAW might be the simplest method, which determines the rank by a weighted sum of the performance ratings of each alternative regarding all criteria;[51] PROMETHEE is the most practiced outranking technique, in which, pair-wise comparisons are performed between the alternatives to determine their outranking relationships with other alternative;[52] TOPSIS, as the most popular compromise ranking technique, follows the idea that the desirable alternative has lower distance from the ideal solution and higher distance from the nadir solution.[53] Notably, the three existing MCDM methodologies were conducted in the same interval conditions for offering the final sustainability score of each alternative as shown in Table 7, the detailed operation rules for each technique can be found in the works of Hajkowicz and Higgins,[51] Qu et al.,[52] and Jahanshahloo et al.,[53] respectively. In Table 7, the final scores [t^L, t^U] determined by different methods are 1). compared by using Spearman's rank correlation coefficients (ρ) (Eqs. 20-22);[54] and 2). employed to rank the alternative processes by running Eqs. 11-13. The obtained results were given in the last two rows of Table 7, respectively.

$$\bar{t}_i^{L(U)} = (t_i^{L(U)} - \underset{i=1,2\cdots,m}{t^L_{\min}}) / (\underset{i=1,2\cdots,m}{t^U_{\max}} - \underset{i=1,2\cdots,m}{t^L_{\min}}) \tag{20}$$

$$\rho(\alpha|\beta) = 1 - \frac{6\sum_{i=1}^{m} d_i(\alpha|\beta)}{m(m^2-1)} = 1 - \frac{6\sum_{i=1}^{m}[(\bar{t}_i^L(\alpha) - \bar{t}_i^L(\beta))^2 + (\bar{t}_i^U(\alpha) - \bar{t}_i^U(\beta))^2]}{m(m^2-1)} \tag{21}$$

$$\rho(\alpha) = \frac{\sum_{\beta\ (\beta\neq\alpha)}^{R} \rho(\alpha|\beta)}{R-1} \tag{22}$$

where m(=5) and R(=4) is the number of the alternative processes and that of the ranking methods, respectively; Eq. 20 is to standardize the scores; $\rho(\alpha|\beta)$ in Eq. 21 is the similarity between the ranking methods α and β, and $d_i(\alpha|\beta)$ is the difference between the standardized scores regarding the i-th alternative process that deprived from the two methods; Eq. 22 offers the result of the coefficient regarding each method.

Table 7. Sustainability sequence results offered by different methods

		Vector-based	SAW	PROMETHEE,	TOPSIS
score $[t^L, t^U]$	SMR	[0.648, 0.697]	[0.402, 0.431]	[-0.034, 0.029]	[0.423, 0.528]
	CG	[0.631, 0.682]	[0.421, 0.459]	[-0.007, 0.062]	[0.482, 0.500]
	HE	[0.703, 0.752]	[0.463, 0.501]	[0.045, 0.113]	[0.526, 0.563]
	NE	[0.539, 0.576]	[0.336, 0.359]	[-0.118, -0.059]	[0.364, 0.365]
	BE	[0.590, 0.643]	[0.387, 0.424]	[-0.050, 0.018]	[0.477, 0.482]
ρ		0.994	0.996	0.995	0.990
rank		HE $\succ$ SMR $\succ$ CG $\succ$ BE $\succ$ NE	HE $\succ$ CG $\succ$ SMR $\succ$ BE $\succ$ NE	HE $\succ$ CG $\succ$ SMR $\succ$ BE $\succ$ NE	HE $\succ$ CG $\succ$ SMR $\succ$ BE $\succ$ NE

The values of the coefficients (ρ) show that there is a very strong correlation between the score outputs of the vector-based algorithm and the conventional MCDM methods ($\rho = 1$ means a complete agreement)[54], demonstrating that the proposed method can offer a similar final sustainability score as these MCDM methods. However, the rank deprived from the vector-based algorithm is slightly different from those determined by the MCDM (SAW, PROMETHEE, and TOPSIS) methods, where the priority order between SMR and CG is reversed. This reversion is understandable, because as stated in the Case study, the possibility degree for $\mathrm{SMR} \succ \mathrm{CG}$ is calculated as $PD_{12} = 66.0\%$, implying that the difference between the priority of the two processes is relatively small. More importantly, this difference could be attributed to the fact that the relative sustainability balance among the criteria system is innovatively incorporated into the final scores, which influences the final ranking of the alternative processes. Since it is well favored to balance the performances among multiple concerns by the nature of the sustainability,[14, 42] one can draw the conclusion that a more comprehensive and reliable sustainability sequence can be determined by integrating the absolute ratings and relative balance of each alternative's performances regarding multi-criteria; while the proposed vector-based algorithm with sound logic and easy-operation can shed new light on the sustainability assessment.

5. Discussion and Conclusion

A novel mathematical framework of sustainability assessment for chemical process alternatives under uncertainties is proposed in this paper, which could efficiently select the most sustainable scenario in real-world issues by combining MCDM methods with a novel interval vector-based algorithm within a comprehensive evaluation system. The framework includes four stages: establishment of criteria system, collection of alternatives' performances, determination of criteria's weights and prioritization of alternatives' sequence. The advantages and contributions regarding this framework are as below:

- A comprehensive evaluation system is offered by integrating the criteria from the environmental, economic, social-political, and technical pillars, in which, the involved criteria can be investigated with the lifecycle thinking.
- Different types and degrees of uncertainties with respect to both the hard and soft criteria can be properly handled by using the interval parameter and the FAHP method, respectively.
- The criteria's weights can be reliably determined by adopting the FDANP approach, which can not only tackle the interdependencies and interactions among the criteria system, but also address the vagueness and uncertainty existing in human's judgments.
- A rigorous sustainability prioritization of the alternative processes under uncertainties can be obtained by developing a novel interval vector-based algorithm, which is characterized by well preserving the uncertainty degrees of the original data and the monolayer of the interval-based multiplication, offering an easy but rigorous way to handle different types of uncertainties during the prioritization. More importantly, by integrating the absolute ratings and the relative balance of each alternative's performances regarding multi-criteria, the algorithm is more suitable than the conventional MCDM methods for prioritizing the sustainability of the chemical processes.

The proposed framework was illustrated by a case study of the sustainability assessment of five ammonia production processes, and the deprived results demonstrated that this framework is feasible to identify the most sustainable scenario among multiple alternatives. Moreover, the robustness of the assessment result was tested *via* the sensitivity analysis; the necessity of adopting the FDANP method for the weights determination was verified by comparing with the FAHP weighting method, while the effectiveness and advantage of the interval vector-based algorithm for the alternatives' prioritization were approved by the comparison with three representative MCDM methods.

Although this framework provides a sustainability assessment methodology for chemical processes under uncertainties, some existing limitations need to be improved in the future studies. (1) This framework directly adopts the interval calculation to handle the random events associated with the hard criteria, this aleatory uncertainty could be expressed more explicitly in further work by combining with specific distribution and/or Monte Carlo simulation. (2) This study does not specify the methodology for determining the classical fields that divide the sustainability into different levels such as pillar-, criteria-, and sub-criteria, further efforts should focus on enabling the framework to conduct the sustainability assessment hierarchically.

Supporting Information

Appendix A. Detailed steps regarding the mathematical methodologies (A1. Steps for the FAHP method, A2. Steps for the FDANP method); **Appendix B**. Detailed computations regarding the case study (B1. FAHP for Scoring the Soft Criteria, B2. FDANP for weighting the Criteria, B3. Information of the Interval Vector-based

Algorithm, B4. FAHP for Weighting the Criteria)

This information is available free of charge via the Internet at http://pubs.acs.org/.

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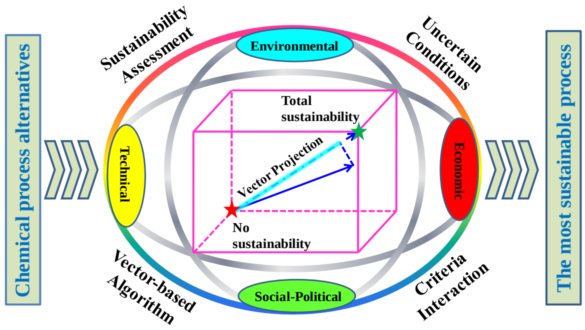

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