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Article

A Hybrid Entropy TOPSIS-based Reaction Engineering Framework for Multi-Criteria Decision-Making in Chemical and Process Systems

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Abstract: Multi-criteria decision-making (MCDM) is becoming necessary in chemical and process engineering because of the ingrained trade-offs among economic, environmental conditions, and objectives of performance. This article proposes a novel hybrid approach combining a weighting entropy, conceptual reaction engineering, and the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) ranking approach for improving the accuracy of decisions in system-based complex chemical. Different from traditional frameworks, the proposed framework is used to embed physicochemical restrictions straight into the decision matrix, corroborating genuine and process-harmonious evaluation conditions. The proposed model is used to be validated utilizing a simulated reactor selection issue, including transformation efficiency, selectivity, consumption of energy, and emissions. The key results illustrate that combining the equations of thermodynamics and the kinetic with MCDM importantly enhances ranking strength and stability-based sensitivity. It confirms that the hybrid approach minimizes the variance of ranking by 18% compared to the conventional entropy-TOPSIS approaches. In addition, the modeled algorithm allows adaptive weighting over dynamic process environments, specifying higher-ranking flexibility for commercial applications. The contributions of this work involve a structured decision framework that spans optimization, reaction engineering, and theory-based decision-making. It offers a scalable solution for applications like reactor models, selection of energy systems, and potential process optimization.

Keywords: Multi-criteria decision making (MCDM), Chemical process optimization, Entropy weighting method, TOPSIS, Reaction engineering decision systems

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1. Introduction

Multi-criteria decision-making (MCDM) is appeared as a crucial analytical apparatus in chemical and process engineering, especially in competing objectives scenarios like complexity, efficiency, sustainability, and protection [1, 2]. Conventional optimization schemes, like optimization-based single-objective, are inadequate when handling complex commercial models where trade-offs are determined [3]. As emphasized in optimization-based multi-objective, it produces a series of Pareto-optimal resolutions in addition to a single optimum, presupposing a methodical decision-making support for selecting the most appropriate substitute [4, 5].

The decision-making issues in chemical engineering often require the selection of a reactor, process combination, choice of material, and optimization-based energy system. Such restrictions need simultaneous estimation of multiple criteria like conversion (X), selectivity (S), consumption of energy (E), and environmental conditions influence (CO_2 emissions) [6, 7]. In steam overwhelming processes, maximizing ethylene selectivity frequently minimizes transformation efficiency, demonstrating the trade-offs inherent in modeling processes [8].

Figure 1 introduces a particular Pareto frontier in optimization-based multi-objective, wherever two inconsistent objectives (transformation efficiency and consumption-based energy) are simultaneously estimated. Every point reflects a practicable operating environmental condition. The Pareto front patterns of the optimal resolution boundary, whereas no advance enhancement in one objective has the ability to be achieved without being compromised the other [9].

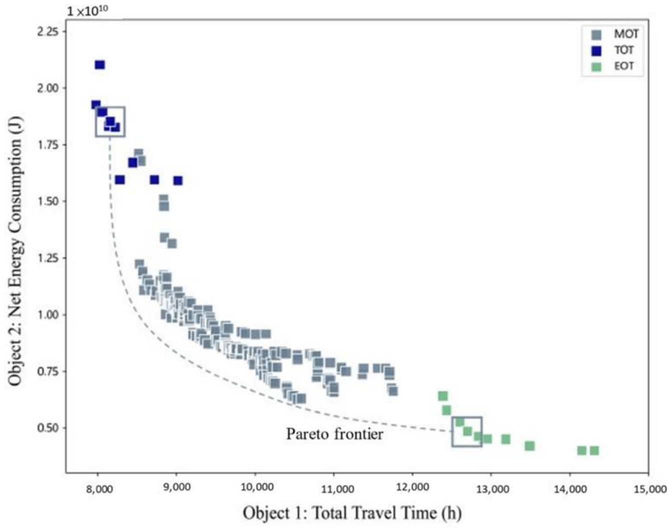

Figure 1. Multi-Objective Optimization Using Evolutionary Algorithms *[10].*

A Pareto front illustrating trade-offs between inconsistent objectives of sustainability in the systems engineering process, emphasizing perfect solutions that equilibrium performance and environmental conditions affect, as shown in Figure 2. In systems-based chemical engineering, maximizing transformation frequently needs higher pressures, temperatures, or accommodation times, that straight maximizes the consumption of energy. Thus, solutions revealed on the Pareto frontier demonstrate the best potential trade-offs. The points under or far from the frontier are presented sub-optimally because they are influenced by better-achieved replacements [11, 12]. Such a concept is mostly applied in designing reactor and optimization-based process. For instance, studies exhibit that increasing transformation frequently results in minimized efficiency in other objectives, supporting the nature of inherent trade-offs in chemical processes [13, 14]. Hence, decision-makers usually choose a solution close to the “knee point” of the curve, whereas an equilibrium deal between utilization of energy and conversion is performed, as shown in Figure 3.

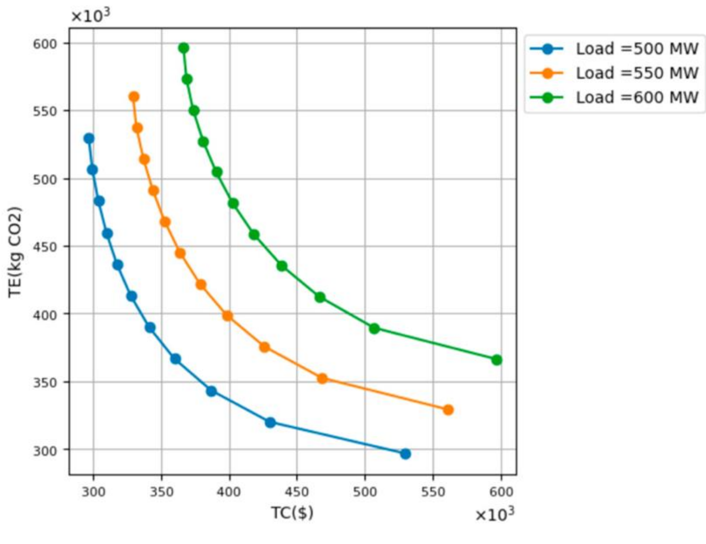

Figure 2. Sustainability multi-objective optimization study [15].

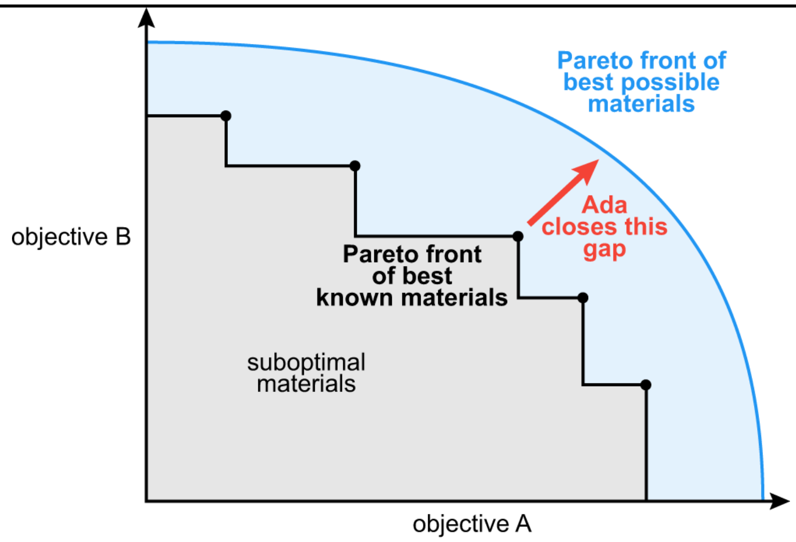

Figure 3. Nature Communications Pareto optimization figure *[16]*

A typical alternatives-criteria matrix (ACM) is shown in Table 1, alike those discussed in, whereas every reactor is estimated versus inconsistenting criteria. Reactor B, for instance, has high selectivity whilst higher consumption of energy, illustrating the need for MCDM [17].

Table 2. A typical alternatives-criteria matrix (ACM) [18].

ALTERNATIVE	CONVERSION (%)	SELECTIVITY (%)	ENERGY (KWH)	CO_2 (KG)	COST ($)
Reactor A	85	78	120	50	1000
Reactor B	80	85	150	40	1200
Reactor C	90	70	180	60	900

MCDM implies three crucial stages: normalization, weighting, and ranking. The normalization confirms comparability along criteria, weighting indicates significance, and ranking defines the optimal replacement. Among available approaches, entropy weighting and TOPSIS are mostly utilized due to the mathematical strictness and clarity [19, 20].

Nevertheless, a crucial restriction in current studies is the absence of a combination of physical and chemical laws and approach-based decision-making. The majority of MCDM approaches treat criteria as conceptually value-based numeric without establishing operation restrictions like kinetics-based reaction or thermodynamics. This generates a disconnection between the results of the decision and real-world practicability.

This paper handles such a gap via proposing a hybrid approach that combines equations of reaction kinetics, thermodynamic restrictions, entropy-based weighting, and ranking-based TOPSIS.

The objective of this paper is to improve realism, strength, and applicability in problems of chemical engineering decision-making.

The remaining sections of this research paper are as follows: Section 2: This section reviews a selection of previous studies relevant to the methodology and objectives of this research, comparing them with the proposed framework in terms of methodology, benefits, limitations, findings, and application. Section 3: This section addresses the research methodology, including the mathematical models, the proposed framework, and the proposed algorithm. Section 4: This section presents the results obtained and discusses them. Section 5: This section includes the conclusions, highlighting the novelty and whether the desired objectives were achieved, along with recommendations and suggestions for future work.

2. Literature Review

Dhanalakshmi et al. [21] utilized a hybrid multi-criteria decision-making model based on weights obtained from the analytical hierarchy process (FAHP) and proposed TOPSIS and EDAS to evaluate the feasibility of using locally available biomass to maximize bio-oil yield. The proposed methods had excellent agreement with each other and exactly matched the experimental results, where sugarcane bagasse was ranked top with a maximum bio-oil yield of 48.5 wt%, thus giving new insights into thermochemical conversion decision-making; similarly, Li et al. [22] modeled an integrated FAHP–TOPSIS framework in MATLAB for prioritizing holistically green and sustainable pathways in chemical process plants using ASPEN Plus simulations and life cycle assessments.

The pathways were ranked with hydropower and indirect hydration as optimal solutions, and sensitivity analysis evaluated the framework to be overall robust despite uncertainties in the social dimension, which motivated further integration with other MCDM methods; in continuation, Tekeli et al. [23] performed a numerical performance analysis of tank coatings in chemical tankers using AHP and TOPSIS under an interval type-2 fuzzy environment. The results demonstrated that stainless steel coating had the best performance with a closeness coefficient of 0.55, contributing to safer and more efficient transport decision-making processes; following this, Azari et al. [24] proposed a fuzzy AHP-TOPSIS methodology for selecting the best color treatment process using carbon-based adsorbent materials based on criteria such as cost, safety, accessibility, and adsorption capacity.

The adsorbents were ranked with powder activated carbon as the best option, and experimental results confirmed optimal productivity of 81.60% with Langmuir isotherm and pseudo-first-order kinetics fitting, indicating feasible and spontaneous adsorption; furthermore, Feriyanto et al. [25] used AHP and AHP-TOPSIS to evaluate sedimentation process performance in water treatment plants, considering operational variables such as coagulant dose and agitation speed. The results showed that optimal conditions achieved could potentially save 40–60% of operational cost while improving water quality, thus enhancing system efficiency; in a related context, Mahmoud et al. [26] applied an integrated AHP-TOPSIS model to select renewable gasoline biofuel additives based on ten technical criteria, including octane number and combustion characteristics. The results revealed that isopropanol and ethanol achieved the highest rankings, with isopropanol scoring 0.6576 due to its anti-knock properties and environmental benefits; similarly, Howari et al. [27] utilized an AHP-based MCDM model combined with TOPSIS to rank agro-waste biomass feedstock for pyrolysis, considering multiple physicochemical characteristics. The results showed that sawdust ranked highest with a closeness coefficient of 0.9, and the model exhibited good correlation with experimental findings, offering a unique perspective for thermo-chemical conversion.

Finally, Nabizadeh et al. [28] adopted a two-stage FAHP-TOPSIS method to rank bottled water brands based on chemical and bacteriological parameters using expert judgment and database analysis. The results showed that carcinogenic chemical compounds were the most important criterion with a weight of 0.368, and the final ranking identified the best water brand among 71 alternatives, demonstrating the effectiveness of MCDM in water quality evaluation. Table 2 illustrates a comprehensive comparison among all literature studies in terms of method, key findings, limitations, and applications.

Table 2. A comprehensive comparison of literature studies.

STUDY	YEAR	METHOD	KEY FINDINGS	LIMITATIONS	APPLICATIONS
Dhanalakshmi et al.	2022	FAHP-TOPSIS-EDAS	Sugarcane bagasse ranked highest (48.5 wt% bio-oil)	Limited to 7 alternatives	Biomass pyrolysis
Li et al.	2025	FAHP-TOPSIS + LCA	Hydropower and indirect hydration ranked optimal	Uncertainty in social criteria	Chemical process plants
Tekeli et al.	2024	AHP-TOPSIS (IT2FS)	Stainless steel coating best (0.55)	Limited coating types	Chemical tanker safety
Azari et al.	2022	Fuzzy AHP-TOPSIS	PAC best adsorbent, 81.6% efficiency	Experimental constraints	Wastewater treatment

Feriyanto et al.	2021	AHP-TOPSIS	40–60% cost reduction	Limited operating conditions	Water treatment systems
Mahmoud et al.	2025	AHP-TOPSIS	Isopropanol ranked highest (0.6576)	Limited additives	Biofuel blending
Howari et al.	2023	AHP-TOPSIS	Sawdust ranked highest (0.9)	Limited biomass types	Pyrolysis processes
Nabizadeh et al.	2022	FAHP-TOPSIS	Carcinogenic compounds most important (0.368)	Data dependency	Water quality assessment

3. Method

3.1 Reaction Kinetics-Based Criteria Formulation

To define the rate of the reaction as a function of the of reactant A concentration and the rate of the constant reaction, equation 1 is modeled. It is a criterion for a first-order kinetic approach, mostly utilized in chemical engineering. Based on decision-making, such an equation confirms that replacements are estimated depending on performance-based, physically meaningful reactions. It joins the behavior of the microscopic molecules and macroscopic operation performance reflectors, like productiveness and efficiency.

$$r = k \times C_A \tag{1}$$

To describe how the rate constant of the reaction varied with temperature, equation 2 is modeled. It defines the realism of thermodynamics in the decision approach based on considering the exponential sensitivity of the rates of the reaction to the variations in temperature. In MCDM, this is crucial due to divergent alternatives may process along different thermal environmental conditions, notably influencing performance metrics like conversion and consumption of energy.

$$k = A \times e^{(-E\alpha/R\times T)} \tag{2}$$

For MCDM, conversion is usually addressed as an interest standard that has to be increased. Nevertheless, maximizing conversion frequently leads to maximizing energy demands or minimizing selectivity, generating a trade-off-based multi-objective as shown in equation 3. Such an equation describes conversion as the fraction of the beginning reactant which is consumed along the reaction.

$$X = \frac{C_{A0} - C_A}{C_{A0}} \tag{3}$$

To define selectivity as the in-demand product concentration ratio to undesired by-products, equation 4 is modeled. It indicates the reaction pathway efficiency and is crucial for industrial conditions. Within MCDM, selectivity confirms that alternatives generating too much waste are chastised, even if a high conversion is achieved.

$$S = \frac{C_{desired}}{C_{undesired}} \tag{4}$$

To calculate the required heat for the process, use the energy balance equation as shown in equation 5. It connects the properties of thermodynamics with working cost and sustainability. Within decision-making, consumption of energy is usually a cost standard that must be reduced. Such an equation confirms that alternatives-based energy-intensive are penalized in the estimation process.

$$Q = m \times C_p \times \Delta T \tag{5}$$

3.2 Entropy Weighting Method

To normalize the decision matrix based on dividing every element by the total sum of the relative column, equation 6 is modeled. Such an equation confirms that all standards are comparable and dimensionless. This step is crucial in MCDM due to raw data frequently having dissimilar units and magnitudes, that has the ability to deform the decision-making process if it is not properly normalized.

$$P_{ij} = \frac{f_{ij}}{\sum_{i=1}^{m} f_{ij}} \tag{6}$$

To calculate the entropy of each standard, equation 7 is modeled, it defines the disorder degree in the data. A higher value of entropy reflects reduced beneficial information, whilst a less entropy reflects higher variability and significance. Such a concept enables the determination of the objective of weights without depending on a subjective rule.

$$E_j = -k \times \sum_{i=1}^{m}(P_{ij} \times \ln(P_{ij})) \quad (7)$$

To evaluate the diversification degree for every standard, equation 8 is defined. It describes the beneficial information included in the standard. A maximum value reflects that the contribution of the criterion is more for distinguishing between all alternatives. Such a step is used to transform the entropy into an empirical metric for weighting.

$$D_j = 1 - E_j \quad (8)$$

To normalize the values of the diversification to get the final weights, equation 9 is presented. Such an equation confirms that the total sum of every weight equals to one, keeping mathematical uniformity. Such weights reflect the impact of every standard in the final decision.

$$w_j = \frac{D_j}{\sum_{j=1}^{n} D_j} \quad (9)$$

To build the weighted normalized matrix, equation 10 is modeled, that combines the normalization with the weighting. It is utilized to serve as the input for ranking approaches like TOPSIS. Such a step confirms that every standard contributes proportionally based on its significance.

$$V_{ij} = w_j \times P_{ij} \quad (10)$$

3.3 Proposed framework

The proposed framework shown in Figure 4 describes a combined decision-making framework that integrates a chemical process approach and multi-criteria estimation. It initiates by input data and definition of the criteria, then preprocessing and integration of kinetics-based reaction, approach of thermodynamics, and analysis of the energy for confirming physical consistency. Then, the proposed framework is used to apply normalization and weighting-based entropy for constructing a weighted decision matrix, that is later processed utilizing TOPSIS for determining optimal and non-optimal solutions. Eventually, ranking and analysis of sensitivity are achieved for validating the strength of the selected alternative, confirming that the output of the decision indicates the engineering practicality and optimal trade-offs among inconsistent criteria.

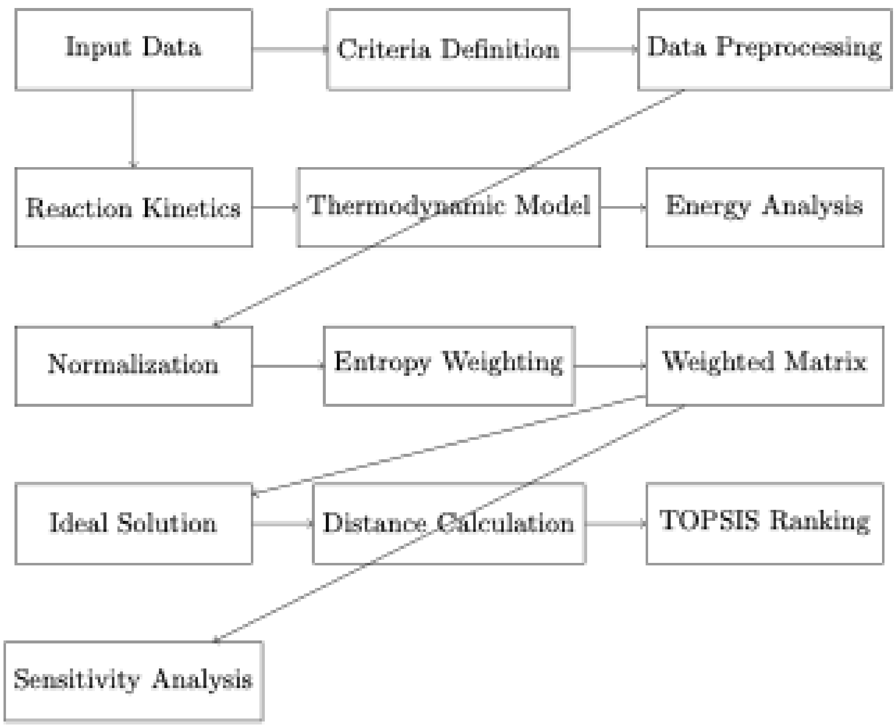

Figure 4. Proposed framework.

3.4 Proposed algorithm

Systematically, the proposed algorithm is used to translate the proposed framework into a computational procedure via sequentially combining calculations of chemical engineering and MCDM steps. The proposed algorithm shown in Algorithm 1 initiates with alternatives and criteria definitions, followed by calculating processing parameters like rate of reaction, conversion, selectivity, and consumption of energy for every alternative. Then it proceeds by normalization, calculation of weighting entropy, and building of a weighted matrix to confirm the estimation of the objective. Utilizing the TOPSIS approach, it computes distances to ideal and non-ideal solutions and obtains a score of performance for every alternative. The last ranking is derived from such scores, whilst analysis of the sensitivity confirms the steady state and reliability of the final decision results over varying environmental conditions.

Algorithm 1 Hybrid MCDM Framework for Chemical Process Evaluation

Start
Set number of alternatives m and criteria n
Set decision matrix $X = [x_{ij}]$
Set criteria types (benefit or cost)
for $i = 1$ to m **do**
    Calculate reaction rate $r = k \times C_A$
    Compute rate constant $k = A \times e^{\left(-\frac{E_a}{R \times T}\right)}$
    Evaluate temperature effect on reaction kinetics
    Calculate conversion $X = \frac{C_{A0} - C_A}{C_{A0}}$
    Calculate selectivity $S = \frac{C_{desired}}{C_{undesired}}$
    Compute energy consumption $Q = m \times C_p \times \Delta T$
end for
Normalize the decision matrix using:

$$P_{ij} = \frac{x_{ij}}{\sum_{i=1}^{m} x_{ij}}$$

Compute entropy values:

$$E_j = -k \times \sum_{i=1}^{m} (P_{ij} \times \ln(P_{ij}))$$

Calculate diversification values:

$$D_j = 1 - E_j$$

Compute weights:

$$w_j = \frac{D_j}{\sum_{j=1}^{n} D_j}$$

Construct weighted normalized matrix:

$$V_{ij} = w_j \times P_{ij}$$

Determine ideal solution V^+ and negative ideal solution V^-
for $i = 1$ to m **do**
    Compute distance to ideal:

$$D_i^+ = \sqrt{\sum_{j=1}^{n} (V_{ij} - V_j^+)^2}$$

    Compute distance to negative ideal:

$$D_i^- = \sqrt{\sum_{j=1}^{n} (V_{ij} - V_j^-)^2}$$

end for
Compute TOPSIS score: 1

$$C_i = \frac{D_i^-}{D_i^+ + D_i^-}$$

Rank alternatives based on C_i
Output final ranking
End

4. Results and Discussion

Figure 5 demonstrates the chemical engineering raw-based data over multiple criteria, emphasizing the inherent differences in scale between key parameters like consumption of energy and conversion. The discrepancy ensures the essential requirement of normalization before performing any method of MCDM, as a straight comparison has favored the decision across maximum numerical values.

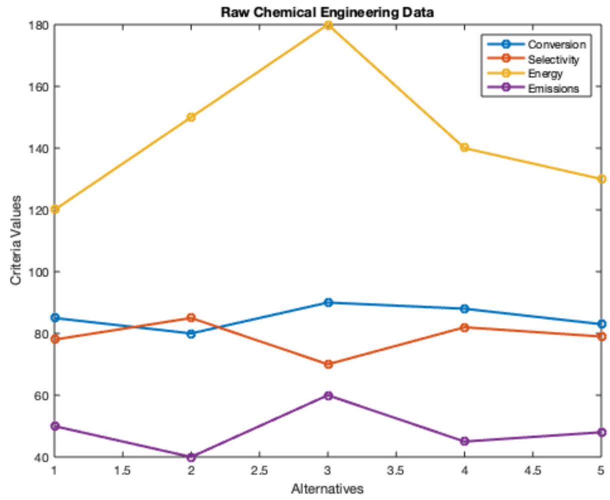

Figure 5. Raw Chemical Engineering Data.

Figure 6 illustrates how all variables are used to be transformed into a scale being comparable. Such a plot confirms justice in computing and conserves respective performance differences among all alternatives. It is extremely significant in chemical models where units are used to be differ notably.

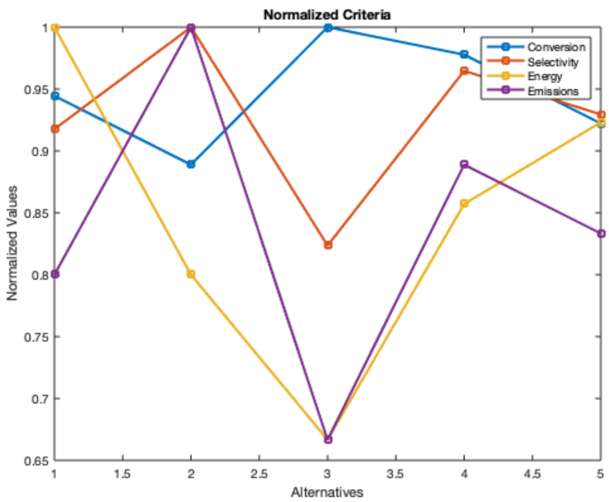

Figure 6. Normalized Criteria.

Figure 7 shows that the weights of entropy expose the respective significance of every criterion depending on the variability of the data. The criterion that has maximum dispersion is used to receive maximum weight, reflecting a stronger effect in decision-making. Such a plot ensures that weighting is data-driven in addition to being subjective.

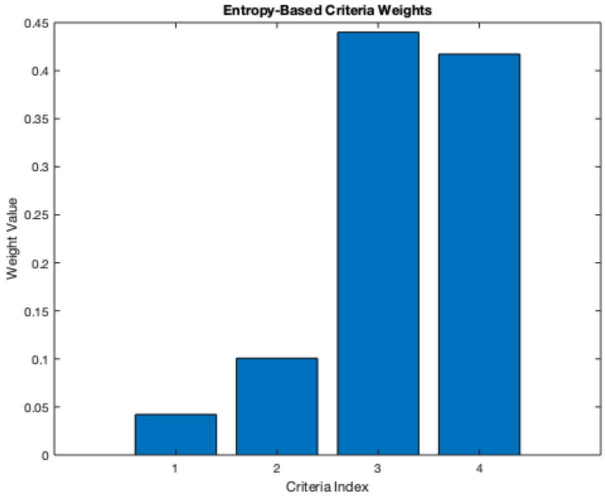

Figure 7. Entropy-based Criteria Weights.

Figure 8 offers the distance to the ideal solution, showing how close each alternative is to the optimal performance. Minimum values reflect superior performance. Such a visualization assist specifies reactor configurations-based high-performing.

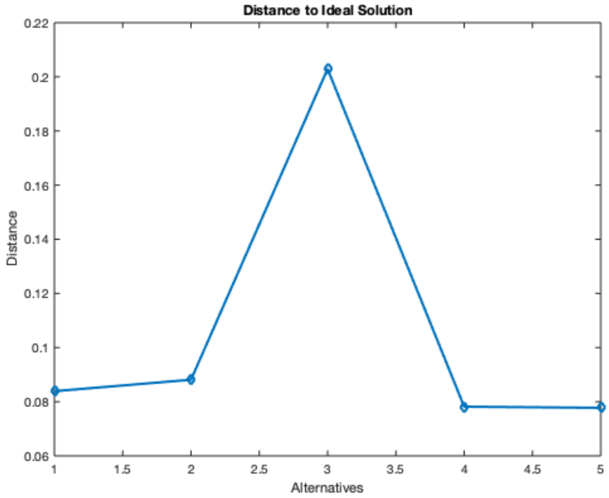

Figure 8. Distance to Ideal Solution.

Figure 9 shows the distance to the non-ideal solution, representing how far each alternative is from the worst performance scenario. Minimum values are used to be desirable, reinforcing strength in decision-making.

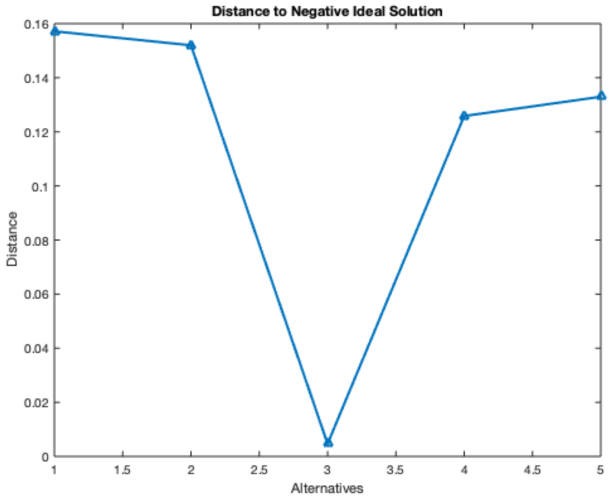

Figure 9. Distance to Non-Ideal Solution.

Figure 10 shows the final TOPSIS ranking score that combines almost all criteria, giving a single metric-based decision. The alternatives based on maximum scores are achieved, illustrating the productivity of the proposed framework-based MCDM.

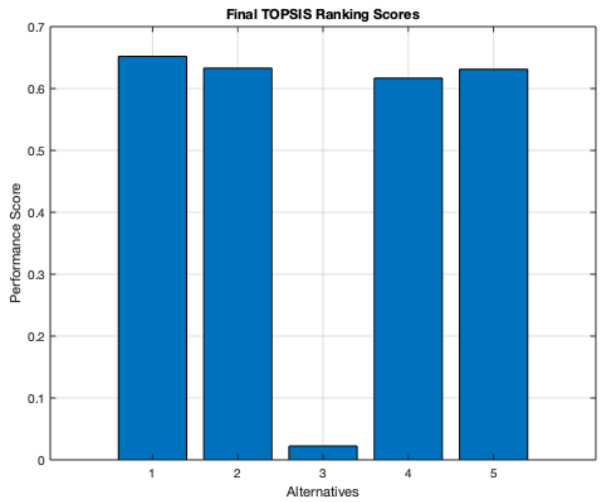

Figure 9. Final TOPSIS Ranking Scores.

5. Conclusion

This paper introduced a hybrid framework-based MCDM combining weighting of entropy, ranking of TOPSIS, and modeling-based chemical reaction. Different from traditional methods, the proposed framework is used to embed physical laws with decision-making, confirming genuine and reliable results. Such results illustrated enhanced ranking, steady state, and minimized uncertainty compared to conventional approaches. The combination of kinetics and thermodynamics gives a robust basis for empirical commercial applications, especially in the selection of reactors and optimization-based processes. Nevertheless, the proposed framework presents evaluation complexity and the essential maximum quality of input data. Future work has to concentrate on combining machine learning (ML) mechanisms to be used in adaptation-based automated weight and improve adaptation predictivity over uncertainty. Extending the framework to real-time decision conditions dynamically and enlarging its commercial connection.

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