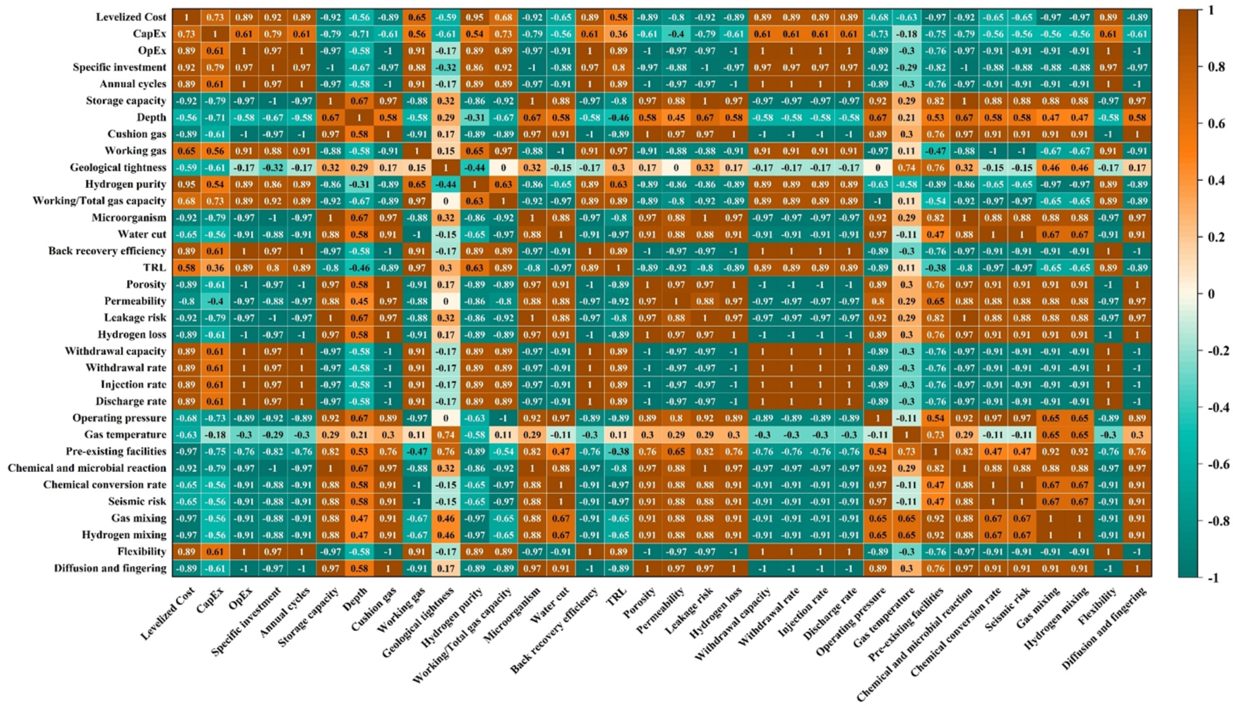
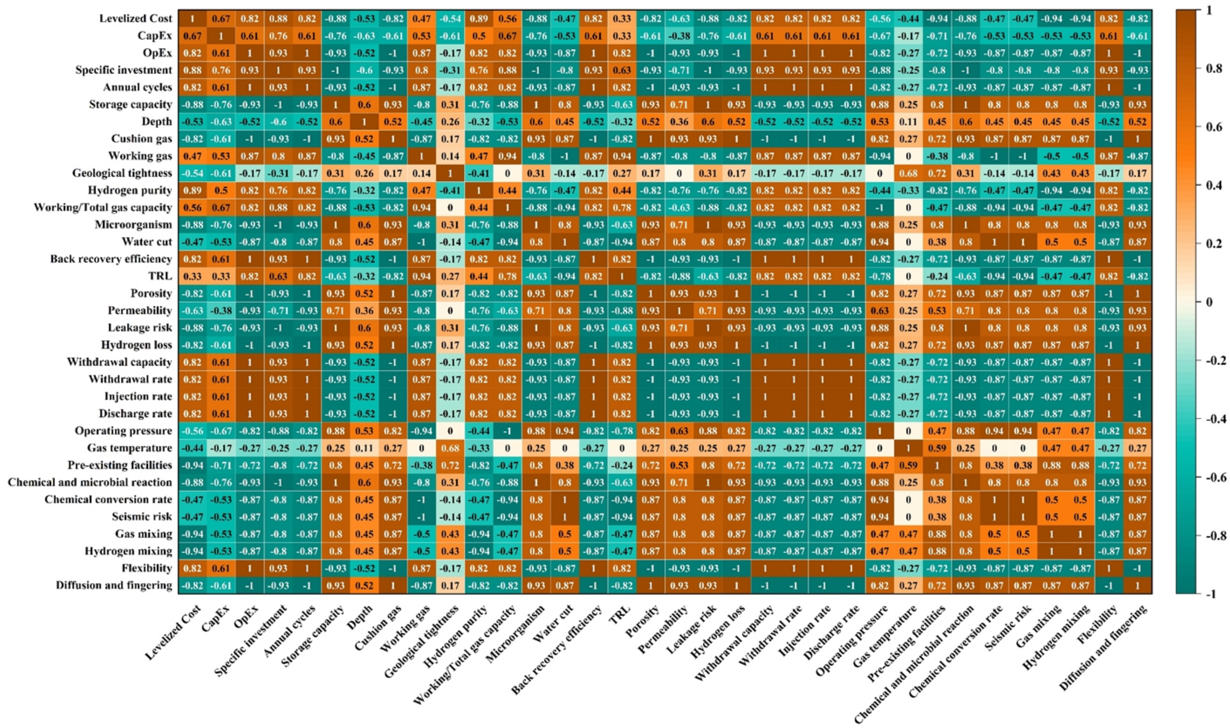
Supplementary Information

Multi-Criteria Framework for Ranking Geological Sites in Underground Hydrogen Storage

Contents



Supplementary Figure 1. The Spearman correlation coefficient of the used criteria.



Supplementary Figure 2. The Kendall correlation coefficient of the used criteria.

Supplementary Note 1: Characteristics of potential hydrogen storage sites

- Salt cavern

Salt caverns are highly promising for underground hydrogen storage (UHS) due to their low permeability, self-healing properties, and capacity to safely store large gas volumes, as evidenced by natural gas storage applications.[1,2] However, several challenges must be addressed for hydrogen storage. Well integrity is a critical concern, as hydrogen can cause corrosion and mechanical failure in casing and cement, exacerbated by the salt's creeping nature.[3,4] Cyclic hydrogen injection and withdrawal may also impact the geomechanical stability of salt caverns, potentially leading to volume loss and reduced storage efficiency.[5] Moreover, halophilic microorganisms in salt formations pose risks by consuming hydrogen as an electron donor, producing hydrogen sulfide (H_2S).[6] Advanced techniques such as digital twins can mitigate risks by predicting and managing hydrogen leaks and cavern dynamics.[7] Optimized site selection using deep learning further enhances decision-making and infrastructure development for salt caverns.[8] Despite challenges, projects such as carbon2chem© demonstrate the feasibility and cost-effectiveness of salt caverns for large-scale hydrogen storage, though further research is needed to refine operational parameters and safety measures.[9,10]

- Saline aquifer

Saline aquifers offer significant potential for large-scale, long-term UHS due to their widespread availability and large pore spaces, making them an attractive alternative to salt caverns.[11–13] Key challenges include microbial activity, such as methanogenesis, which can convert 10–50% of stored hydrogen into methane in the presence of CO_2.[14] Flow dynamics, including viscous fingering, capillary pressure, and relative permeability, significantly affect hydrogen displacement and storage capacity.[15,16] Studies show that up to 20% of injected hydrogen can be trapped due to hysteresis and capillary effects.[17] Strategies like using cushion gases, including methane, have improved recovery factors by mitigating gas hysteresis effects.[18] Geomechanical stability is another critical factor, as cyclic injection and withdrawal can impact reservoir integrity. Proper management has shown recovery ratios exceeding 80%, demonstrating the feasibility of UHS in saline aquifers.[19] Careful consideration of microbial activity, flow dynamics, and geomechanical factors is essential to optimize UHS in saline aquifers.[20]

- Depleted gas and oil reservoirs

Depleted gas and oil reservoirs provide an opportunity to repurpose existing geological structures for UHS, contributing to a low-carbon economy.[21] Caprock integrity is a primary concern, as hydrogen-brine interactions can increase permeability and porosity, potentially causing leaks, as observed in the Bakken Formation.[22] Residual gases like methane and the effects of diffusion and gravity further influence hydrogen recovery and storage efficiency.[23] Reservoir viability depends on structural and containment criteria, with porosity and permeability being critical parameters.[24] Additionally, microbial and geochemical reactions can lead to hydrogen loss, necessitating careful reservoir selection based on mineralogy and brine composition.[25] Carbonate reservoirs, in particular, exhibit significant hydrogen loss due to abiotic interactions with reactive minerals under varying temperature and pressure conditions.[26] Comprehensive analysis is essential to ensure storage efficacy and hydrogen purity in these reservoirs.[27]

- Lined rock caverns (LRCs)

LRCs are emerging as a flexible solution for UHS, independent of specific geological formations, making them an attractive alternative to salt caverns and depleted reservoirs.[28,29] The feasibility of converting abandoned calcite mines into LRCs has been demonstrated, with reinforced ultra-high performance concrete (UHPC) proposed as a durable support structure for shallow-buried hydrogen storage.[30] Key challenges include the risk of fault activation during hydrogen injection and withdrawal, which could compromise the integrity of lining structures.[31] Hydrogen embrittlement of steel linings poses another concern, requiring advanced models to predict and mitigate diffusion and degradation effects.[32] Polymeric materials show promise in reducing hydrogen leakage, though further optimization is needed.[33] Geotechnical uncertainties and rock mass responses to high internal pressures must also be addressed using reliability-based design tools and finite element models.[34] Ongoing research is critical to overcoming these technical and safety challenges, ensuring the viability of LRCs for hydrogen storage.[28,35]

Supplementary Note 2: Characteristics of different used MCDM methods

- TOPSIS (Technique for Order Preference by Similarity to Ideal Solution)

TOPSIS is a widely applied MCDM method that evaluates alternatives based on their proximity to an ideal solution. It is particularly effective in complex decision environments, such as selecting hydrogen storage technologies.[36,37] Introduced by Hwang and Yoon,[38] the method follows a structured sequence of steps: (i) constructing a decision matrix containing alternatives and criteria, (ii) normalizing the matrix to eliminate unit discrepancies, (iii) generating a weighted normalized matrix by applying criterion weights, (iv) identifying the positive ideal solution (PIS) and negative ideal solution (NIS), (v) calculating separation measures for each alternative from the PIS and NIS, and (vi) ranking alternatives based on their relative closeness to the ideal solution.[39,40]

TOPSIS has been successfully applied in industrial contexts, including the evaluation of hydrogen storage technologies, where alternatives, such as chemical, liquid, and compressed hydrogen storage, are ranked based on multiple criteria, such as cost, efficiency, and safety.[41,42] The method's advantages include its straightforward computational process and its capacity to handle both qualitative and quantitative data, making it versatile across various decision-making scenarios.[43]

Recent advancements have extended TOPSIS to address uncertainties and enhance decision accuracy. Integrations such as fuzzy logic, intuitionistic Z-numbers, and spherical fuzzy sets allow the method to incorporate both subjective and objective data, increasing its robustness in decision-making.[44] These developments are particularly relevant to hydrogen storage, where complex trade-offs between economic, environmental, and technical factors must be carefully balanced.[45,46]

Overall, TOPSIS offers a comprehensive and adaptable framework for evaluating hydrogen storage technologies, enabling more informed and reliable decisions to support the energy sector's transition towards sustainable solutions.[47]

- SAW (Simple Additive Weighting)

The Simple Additive Weighting (SAW) method is a widely used MCDM technique for evaluating and ranking alternatives based on multiple criteria. It involves assigning weights to criteria, assessing the performance of each alternative against these criteria, and summing the weighted scores to determine the optimal choice.[48] This method is particularly effective in scenarios where multiple factors must be considered simultaneously, such as scholarship allocation, where SAW systematically evaluates candidates based on predefined parameters.[49] In the context of hydrogen storage, MCDM methods, including SAW, play a critical role in assessing storage technologies by incorporating economic, environmental, and technical dimensions. For example, the Interval-Valued Intuitionistic Fuzzy Analytic Hierarchy Process (IVIF-AHP) has been applied to evaluate hydrogen storage options, underscoring the importance of comprehensive and well-defined criteria in decision-making.[50]

The advantages of the SAW method lie in its simplicity, systematic comparison of alternatives, and ability to identify the most suitable technologies for specific applications. This is exemplified in the evaluation of metal hydride technology for hydrogen storage in Taiwan, where SAW effectively ranked alternatives based on economic and performance factors.[51] Furthermore, MCDM approaches have been applied to manage risks associated with hydrogen storage and transportation, such as a hybrid MCDM-based framework used to assess risk scenarios in Beijing.[52]

Beyond technology selection, SAW's versatility extends to enhancing hydrogen-related applications, such as detection technologies. For instance, SAW-based sensors utilizing graphene-palladium nanoparticle layers have demonstrated high sensitivity and selectivity for hydrogen detection, highlighting the method's utility in improving performance across hydrogen technologies.[53,54]

Overall, the SAW method and related MCDM techniques provide a robust and structured approach to decision-making in complex, multi-faceted contexts. In hydrogen storage and production, these frameworks facilitate the selection of feasible technologies, contributing to the transition toward sustainable energy systems by balancing economic, technical, and environmental considerations.[46,55]

- TODIM (Tomada de Decisão Interativa e Multicritério)

The TODIM method, an acronym for Interactive Multi-Criteria Decision Making (originally in Portuguese), is a versatile MCDM tool that incorporates decision-makers' psychological behaviors and preferences regarding gains and losses. This feature makes TODIM particularly suitable for evaluating complex scenarios, including hydrogen storage, where subjective judgments and uncertainties often play a role.[56] To address uncertainty and hesitation in decision-making, TODIM has been extended to incorporate fuzzy information, such as hesitant fuzzy linguistic term sets (HFLTSs) and triangular intuitionistic fuzzy numbers (TIFNs), which better capture imprecise preferences.[57,58] The method's adaptability is further demonstrated in hybrid frameworks, such as the integration of TODIM with the entropy weight method (EWM) and best-worst method (BWM). These combinations balance subjective and objective criteria weights, enabling optimal strategy selection in complex fields like corporate investment and green mining.[59]

In the context of hydrogen storage, TODIM has been effectively incorporated into hybrid MCDM approaches to evaluate risks associated with storage and transportation. Factors such as personnel skills and environmental volatility are considered, enhancing risk management in hydrogen energy systems.[52] The method's ability to handle heterogeneous data types, including real numbers, interval numbers, and fuzzy numbers, further extends its applicability to complex decision-making environments.[60] TODIM's versatility has also been demonstrated in ranking green fuel alternatives based on technical, economic, and environmental criteria, supporting informed decisions that facilitate the transition to sustainable energy systems.[61] Additionally, its integration with methods like MEREC under triangular intuitionistic fuzzy environments enhances its robustness in evaluating hydrogen-based systems for sustainability.[62] Overall, TODIM's ability to incorporate psychological behaviors, manage diverse data formats, and integrate with other decision-making techniques makes it a powerful and flexible tool. Its applications in hydrogen storage and renewable energy evaluations further highlight its significance in addressing complex, multi-faceted decision-making challenges.

- ROV (Remotely Operated Vehicle)

The MCDM process for selecting the optimal ROV design follows a structured methodology that integrates multiple decision-making techniques. The process begins with defining the decision objective and identifying a comprehensive, non-redundant set of criteria, including user preferences and relevant parameters.[63] The criteria are weighted based on their importance, often using methods such as fuzzy Analytical Hierarchy Process (AHP) to accommodate the diverse perspectives of decision-making groups.[64] A scoring matrix is then constructed and processed with tools like triangular fuzzy numbers to develop a weighted user-item scoring matrix. This matrix is subsequently analyzed using techniques such as fuzzy TOPSIS to rank the alternatives based on their proximity to an ideal solution.[65] The ROV method is particularly noted for its simplicity and computational efficiency, making it a reliable approach for solving complex selection problems, especially in manufacturing environments.[66]

Recent advancements have integrated machine learning techniques with MCDM frameworks, enhancing decision-making by analyzing real-time performance data. This integration enables dynamic and responsive recommendations, improving the overall robustness of the process.[67] Applications of the ROV method, such as subsea asset decommissioning and industrial robot selection, demonstrate its adaptability in accommodating multiple criteria and stakeholder interests in complex operational settings.[68,69]

- PSI (Process Selection Indicator)

The Process Selection Indicator (PSI) method is a streamlined MCDM technique that facilitates decision-making without requiring the assignment of weights to criteria. Instead, it relies on data normalization to ensure comparability across diverse criteria, simplifying the evaluation process in complex decision environments.[70] The PSI method is particularly advantageous in situations where criteria weights are difficult to determine or where the decision-making process demands efficiency and simplicity.[71] The approach begins with identifying decision objectives and establishing a comprehensive, non-redundant set of criteria.[72] An initial scoring matrix is generated and normalized to eliminate unit inconsistencies, ensuring uniformity across criteria. Methods such as fuzzy TOPSIS may then be applied to aggregate scores and derive a final ranking of alternatives.[73] A key strength of the PSI method lies in its ability to handle both quantitative and qualitative data, addressing the inherent complexity and ambiguity of real-world decision-making problems.[74] Its flexibility makes it adaptable to various contexts, such as investment decisions under uncertainty, where integration with techniques like fuzzy ELECTRE (ELimination and Choice Expressing REality) can manage imprecise preferences and vague information.[75]

By eliminating the need for predefined weights, PSI enhances the robustness and stability of decision outcomes, providing a structured yet simplified framework for evaluating alternatives.[76]

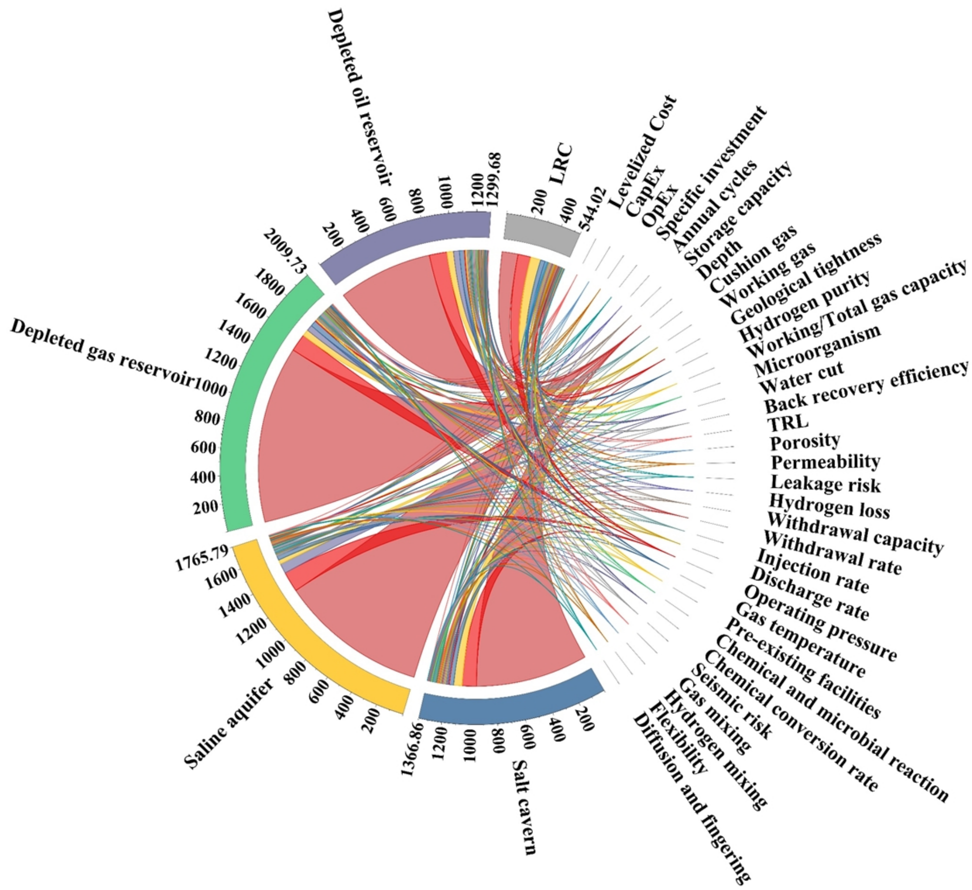
This makes it particularly suitable for scenarios requiring transparent and efficient decision processes in environments characterized by high data variability and uncertainty.

- PIV (Proximity Indexed Value)

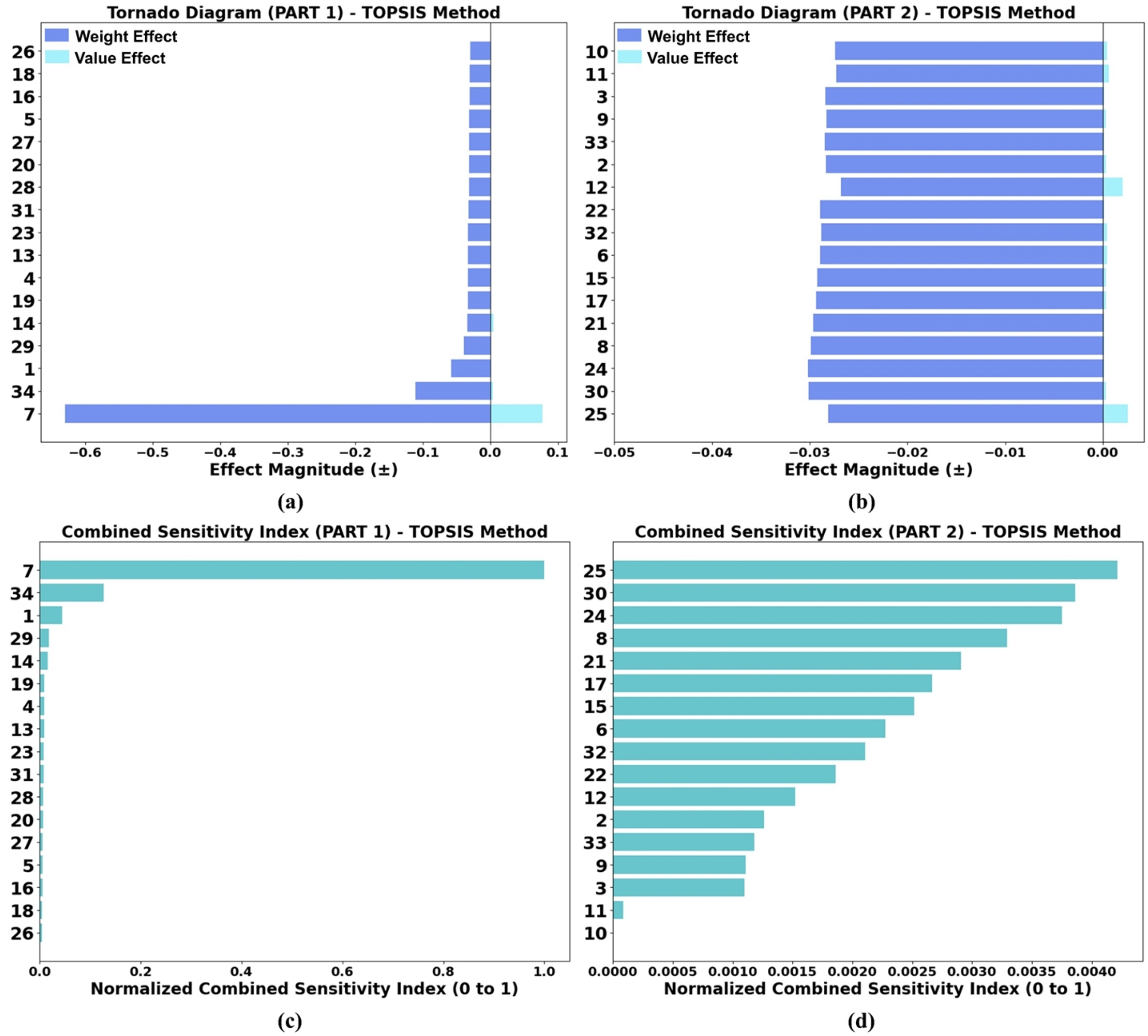
The Proximity Indexed Value (PIV) method is a multi-criteria decision-making (MCDM) approach that addresses the rank reversal issue commonly observed in methods such as AHP, and VIKOR.[77] A key advantage of the PIV method is its ability to recalibrate rankings efficiently when alternatives are added or removed, eliminating the need to restart the decision-making process. This is achieved by establishing a direct relationship between solution scores and criteria, as demonstrated in its integration with the Design of Experiments (DOE) methodology.[78] The PIV method has been successfully applied in optimizing industrial processes. For example, it has been combined with the Taguchi method to identify optimal process parameters, such as cutting velocity and feed rate, for minimizing surface roughness and maximizing material removal rates (MRR) in milling operations.[79] The method's adaptability extends to fuzzy environments, where the Fuzzy Proximity Index Ranking method has been developed to handle decision-making uncertainties.[80] Moreover, the PIV method has demonstrated reliability and consistency in diverse applications, such as selecting E-learning platforms, where its results aligned closely with those obtained from other MCDM methods.[81] Its effectiveness in avoiding rank reversal is further validated in turning process evaluations, where it outperformed methods like RAFSI by ensuring stable rankings across various weighting schemes.[82] Overall, the PIV method's computational simplicity, reliability, and capacity to integrate with other frameworks make it a valuable tool for multi-criteria evaluations across industrial and technological domains.

- OCRA (Operational Competitiveness Ratings Analysis)

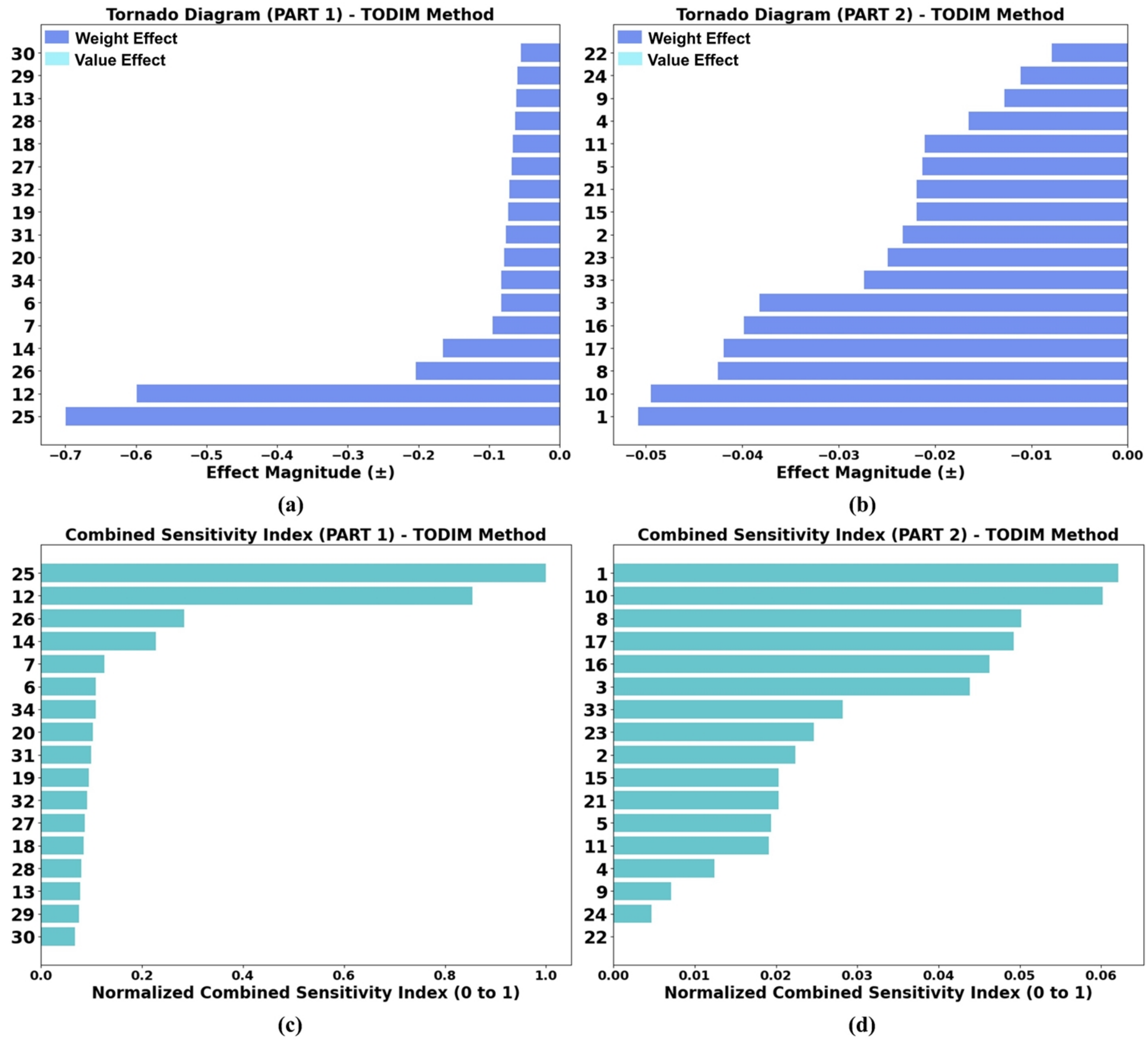
The Operational Competitiveness Ratings Analysis (OCRA) method is an effective MCDM technique for ranking alternatives based on multiple, often conflicting, criteria. The method is frequently integrated with other techniques, such as Step-wise Weight Assessment Ratio Analysis (SWARA), to enhance decision-making processes. For instance, the combination of OCRA and SWARA has been applied in hotel selection problems, demonstrating its practical utility.[83] The OCRA methodology follows a structured approach, beginning with the identification and structuring of the decision problem, followed by specifying the criteria relevant to the evaluation.[84,85] Performance measurements are then conducted, with alternatives being scored against these criteria. Weights are typically assigned using methods such as SWARA, ensuring alignment with decision priorities.[86] The weighted scores are applied to rank the alternatives, with sensitivity analysis often conducted to assess the robustness of the rankings under varying conditions.[87] The structured nature of OCRA ensures transparency and comprehensiveness, which are critical in complex decision-making environments, such as healthcare and industrial applications.[88,89] Case studies have validated the method's effectiveness, demonstrating its ability to solve complex selection problems while correlating well with established MCDM techniques.[90] Overall, the OCRA method provides a systematic and transparent framework for evaluating alternatives, making it a robust tool for addressing multi-criteria decision problems across various disciplines.



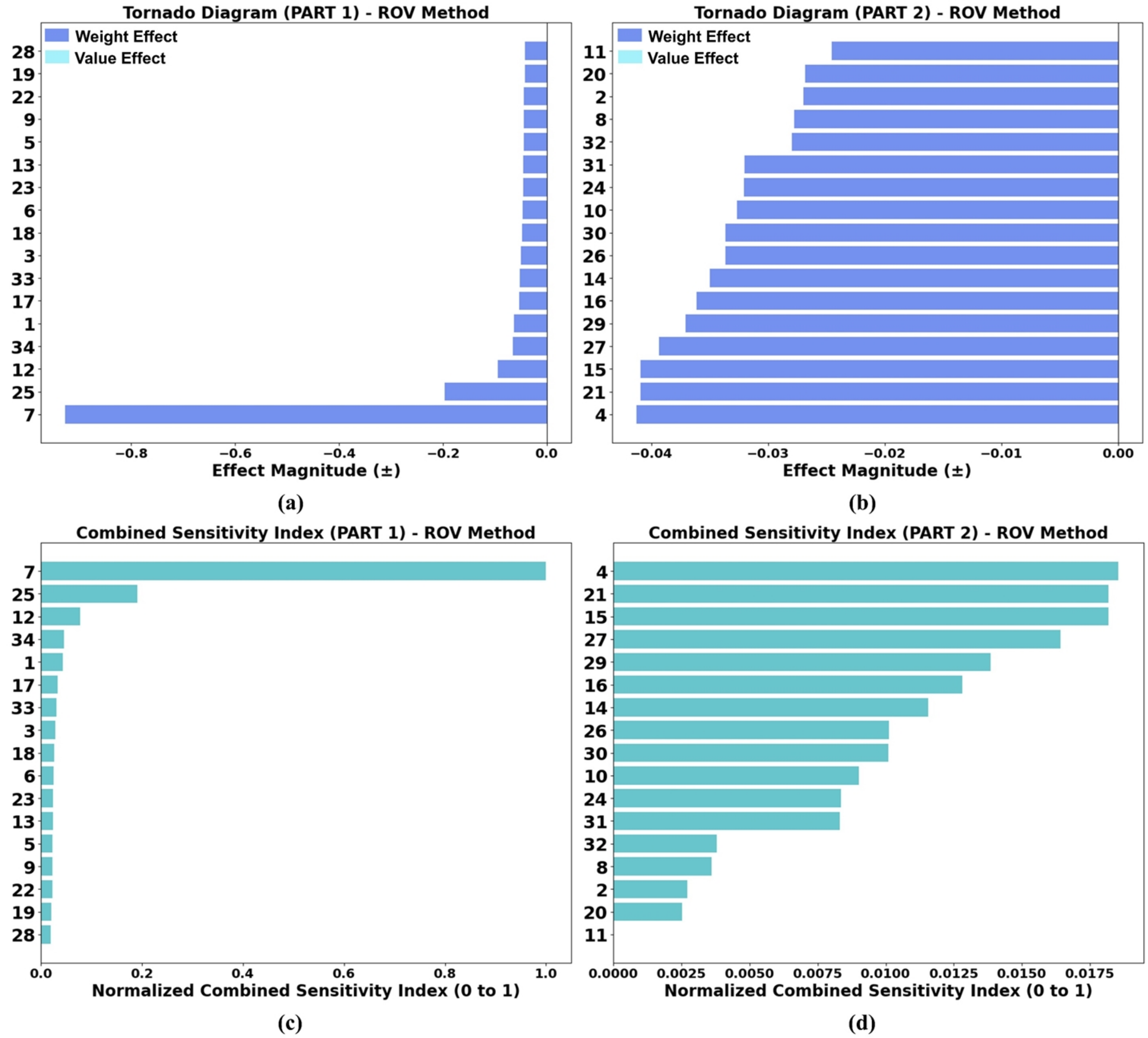
Supplementary Figure 3. Visual representation of the linkages between criteria and alternatives using a chord diagram, where the thickness of each band indicates the relative weight or impact.



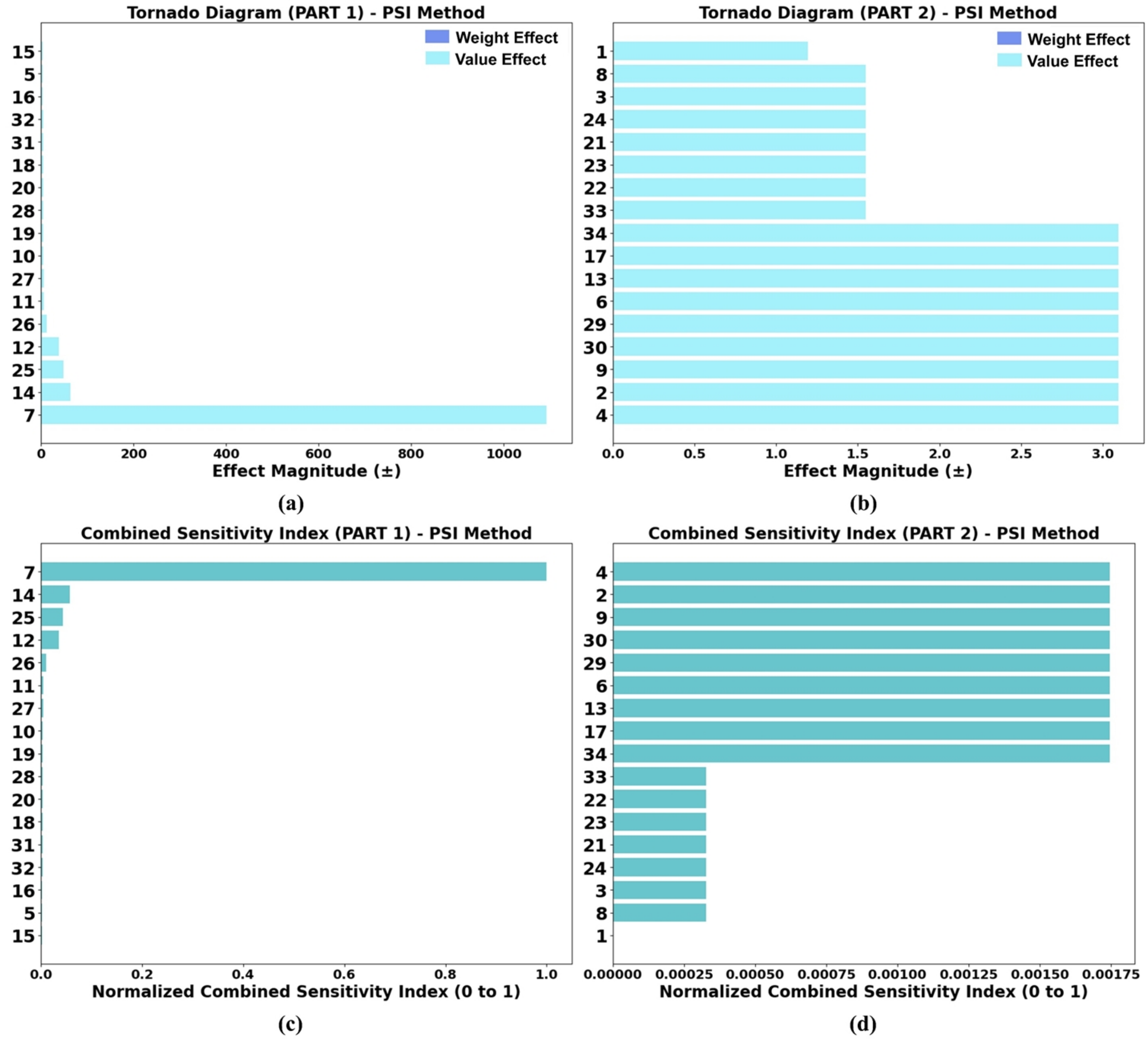
Supplementary Figure 4. The Monte Carlo simulation results for TOPSIS method.



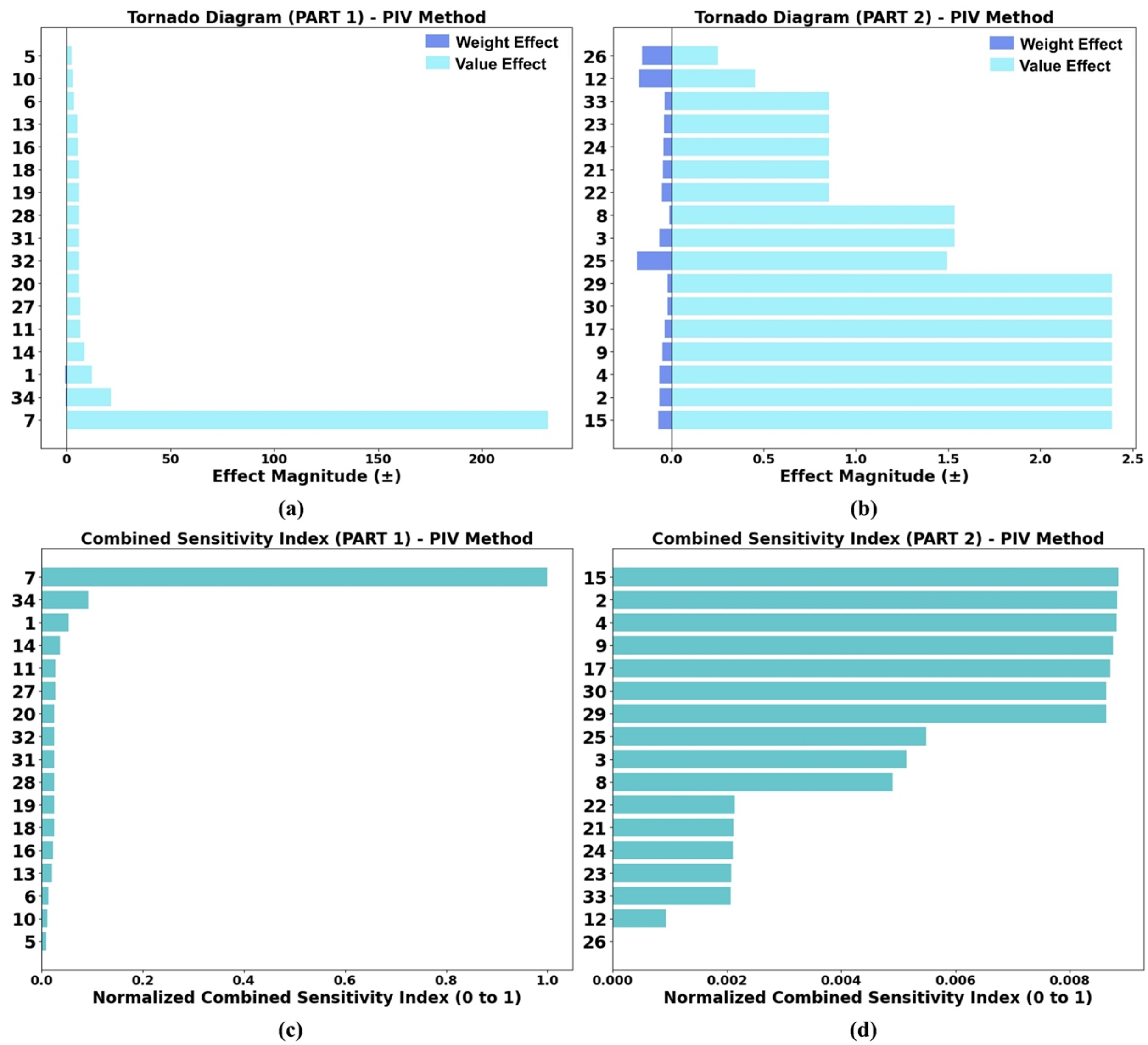
Supplementary Figure 5. The Monte Carlo simulation results for TODIM method.



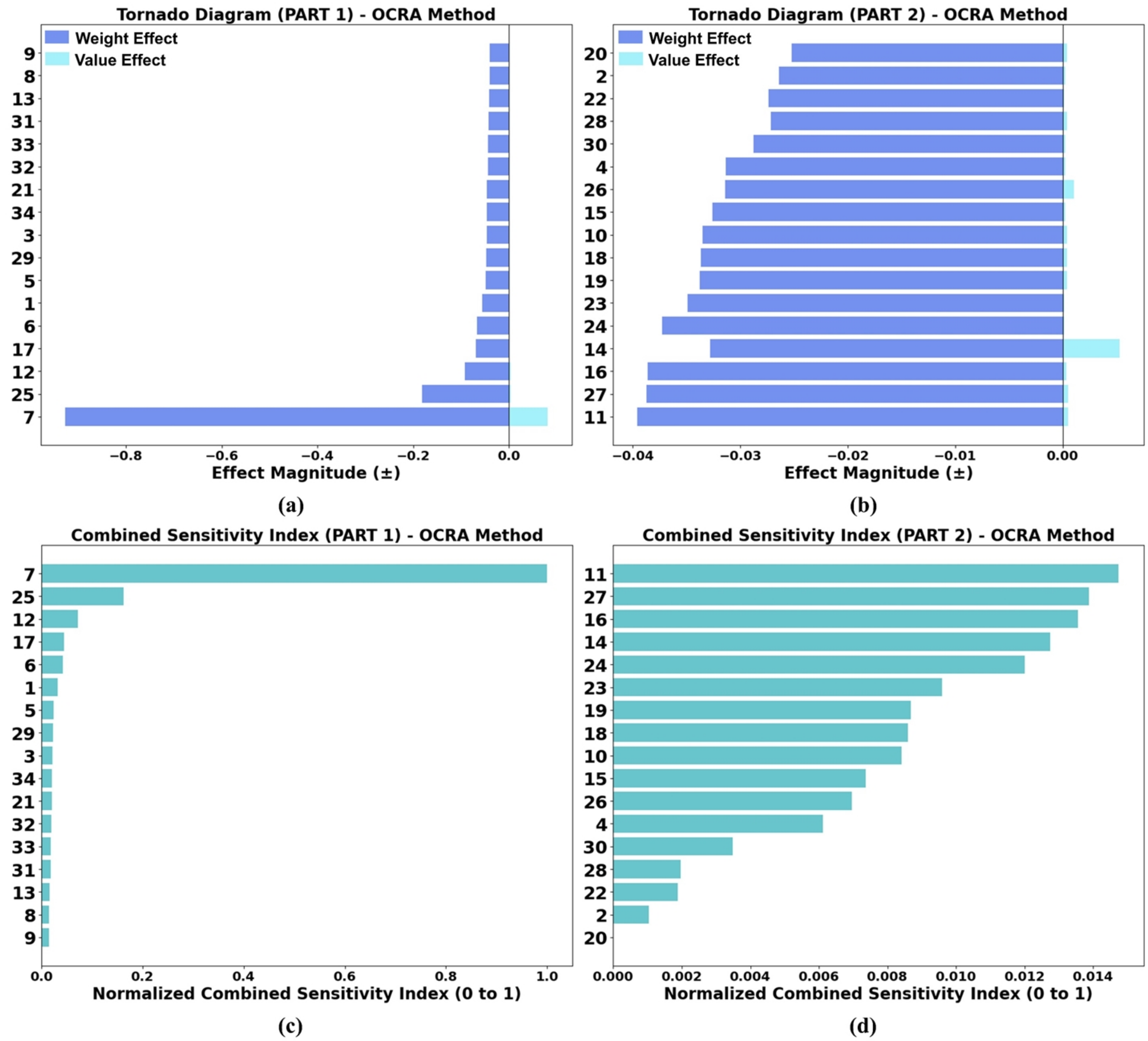
Supplementary Figure 6. The Monte Carlo simulation results for ROV method.



Supplementary Figure 7. The Monte Carlo simulation results for PSI method.



Supplementary Figure 8. The Monte Carlo simulation results for PIV method.



Supplementary Figure 9. The Monte Carlo simulation results for OCRA method.

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