Development of Clustering Method for Accident Scenarios Using UMAP and Dynamic Time Warping Technique

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ABSTRACT

The enhancement of reactor safety is crucial for the widespread adoption of nuclear energy. In particular, Small Modular Reactors (SMRs), due to their multi-reactor nature and relatively fewer personnel per module, may present more complex accident response procedures compared to large-scale reactors. Therefore, the Korea Atomic Energy Research Institute (KAERI) is developing a system to detect accidents and provide optimal response strategies to operators, with plans for its application to virtual reactors. In this study, we propose a methodology for extracting representative accident scenarios by analyzing various accident progressions and identifying scenarios with similar peak cladding temperature profiles. Although Uniform Manifold Approximation and Projection (UMAP) has been reported to perform excellently in data classification tasks such as image recognition, its effectiveness in time-series data classification remains unverified. Given that UMAP's performance depends on the similarity measure (i.e., metric) used between data points, we applied the dynamic time warping (DTW) method, which is capable of detecting trends and patterns in time-series data, as a metric for UMAP. We then compared the result of accident scenario classification using UMAP with its default metric to evaluate the performance of the DTW-based approach.

Keywords: Severe accident, UMAP, dimensionality reduction, dynamic time warping, machine learning

I. Introduction

To develop new reactor types such as Small Modular Reactor (SMRs), it is essential to conduct probabilistic safety assessment (PSA) to verify the safety of the reactor. In Level 1 PSA, representative accident scenarios are classified for each initial event (IE), and comprehensive risk assessment is performed up to the pre-core damage phase. PSA results are also utilized as reference data to improve the safety system design. Traditional PSA approaches have evaluated safety systems by applying several conservative assumptions that negatively affect reactor states. However, such conservative assessment methods may lead to the design of excessively redundant safety systems, which can increase the levelized cost of electricity for SMRs.

To address this issue, dynamic PSA (DPSA), which assesses risk more progressively and realistically, has been proposed in recent years [1]. DPSA diversifies event timing and branches resulting from events (i.e., branch points) and comprehensively evaluates the risks of scenarios corresponding to all branches [2]. Therefore, DPSA theoretically allows for an infinite number of scenarios to unfold beyond an IE. However, performing safety analysis for all possible scenario is highly inefficient. Thus, it is necessary to identify representative scenarios with similar accident progression and establish safety measures based on theses representative scenarios. This study aims to propose a methodology for deriving representative accident scenarios by applying clustering algorithms to identify the structural relationships among accident scenario data and assigning similar scenarios to the same cluster.

Since risk assessment of nuclear reactors cannot be directly experimented with using real-scaled reactors, severe accident (SA) codes (e.g., MARS, MAAP, MELCORE) are employed to simulate such events. The SA code used in this study is MAAP. MAAP terminates calculations beyond the core damage (CD), a critical event that occurs when the temperature of the nuclear fuel exceeds its melting point. Thus, peak cladding temperature (PCT) is a key thermohydraulic variable that determines whether CD has occurred and provides insight into accident scenarios based on the shape of its curve. Therefore, this study assumes that PCT is the primary thermohydraulic variable that defines accident scenarios and utilizes PCT for accident clustering and deriving representative scenarios. This study developed a methodology for generating random accident scenarios based on the Monte Carlo method. Using this approach, 6,400 random scenarios were produced, followed by the application of dimensionality reduction and clustering algorithms to derive representative scenarios.

In general, previous studies have used uniform manifold approximation and projection (UMAP), a dimensionality reduction algorithm, to compute differences between data points in image datasets [3]. Data points with smaller calculated differences are densely distributed within the latent space. Subsequently, clustering algorithms (e.g., DBSCAN) are applied to the latent space to group nearby data points into the same cluster, completing the clustering process. For image data, two-dimensional data are typically flattened into one-dimensional vectors, and their similarities are calculated using Euclidean distance (ED) for dimensionality reduction. However, due to the characteristics of time-series data, when the graphical representation of data on the x-y plane shifts horizontally along the x-axis (time direction), ED evaluates such data as having low similarity (i.e., large data distance). This indicates a limitation of traditional image-based similarity evaluation methods in assessing the similarity of time-series data, even when the overall shape of the graphs is similar.

In this study, UMAP was employed for dimensionality reduction of time-series data, while soft dynamic time warping (soft-DTW) was used as a substitute for ED [4]. Soft-DTW, an improved algorithm derived from dynamic time warping (DTW) for gradient computation, is a specialized metric for evaluating structural similarities in time-series data. The mathematical details of this approach are discussed in Section 2. Additionally, clustering performance was validated by comparing results obtained using the traditional ED metric. It was observed that the embedding results using the soft-DTW metric made it easier to derive representative accident scenarios specifically for time-series data.

The target reactor type for the methodology developed in this study is the OPR-1000, which is internationally widespread and has undergone numerous safety validation studies. According to the Level 1 PSA report on the OPR-1000 conducted by Korean Atomic Energy Research Institute (KAERI), there are 14 IEs, each with dozens of sub-scenarios [5]. While this study focused on a case study for the loss of offsite power (LOOP), the methodology could technically be applied to derive representative accident scenarios for other ISs as well. In summary, the academic contribution of this study are as follows:

1. Enhanced clustering performance for time-series data using an improved metric
2. Diversification of reactor accident scenarios based on the Monte Carlo method
3. Derivation of representative accident scenarios based on thermohydraulic data calculation

II. Methodology

This study is organized by two research materials: the generation of accident simulation results from MAAP based on random sampling in Monte Carlo simulations, and the clustering of the derived accident scenarios using UMAP with soft-DTW for dimensionality reduction and DBSCAN for scenario clustering. All research materials were implemented in Python. The UMAP algorithm was applied using the umap-learn library, DBSCAN was utilized via the sklearn libaray, and soft-DTW, as it is an unsupported custom metric, was implemented manually.

II.A. Random scenario sampling

Random Scenario Sampling (RSS) refers to the process of stochastically determining the states of key systems and components of a reactor over time to define accident scenarios. Using the Monte Carlo method, RSS stochastically decides whether each component operates successfully, fails, or the timing of failure if it occurs. However, given that MAAP involves hundreds of components, RSS is applied only to key Structures, Systems, and Components (SSCs) to reduce the computational calculation cost.

When performing random sampling for SSCs, the success or failure of each SSC is sampled based on failure data from conventional PSA. For instance, if an SSC is in standby mode and is activated or fails to be activated, the probability of failure on demand is used to make probabilistic determinations. Secondly, for components already in operation, the time to failure is determined using operational failure rate data. If operator intervention is required, it becomes part of RSS, where the action time required for task execution and the success probability of the task are stochastically calculated. Lastly, as reactors involve interconnected systems, the operation of specific components may depend on the proper functioning of other components, which are designed as combinations of AND/OR gates.

This study conducted a case study by assuming LOOP as a representative IE. Instead of performing RSS for all reactor components, only SSCs related to LOOP were considered. SSCs associated with LOOP can be categorized into power-related components and safety systems. The power-related components include key equipment and human actions that are activated when external power is lost, or additional power supply is required. Major components associated with failures such as fail-to-start or fail-to-run include the emergency diesel generator (EDG) and the alternative alternating current diesel generator (AAC-DG). The power supply from these components is used for HVAC (heating, ventilation, air conditioning) systems and to support the high-pressure safety injection system (HPSIS), which is critical for system recovery during a loss of coolant accident

(LOCA). The HPSIS is a critical safety system in nuclear reactors designed to inject coolant into the reactor pressure vessel during LOCA. The system operates at high pressure, typically capable of injecting borated water even when the reactor is at or near operating pressure (15 – 16MPa). HPSIS consists of high-pressure pumps, borated water storage tanks, injection piping, and associated valves that automatically activate upon detection of accident signals such as low reactor pressure or high containment pressure. The OPR-1000 reactor is equipped with two EDGs connected in parallel, ensuring successful operation as long as at least one of them functions (Figure 1).

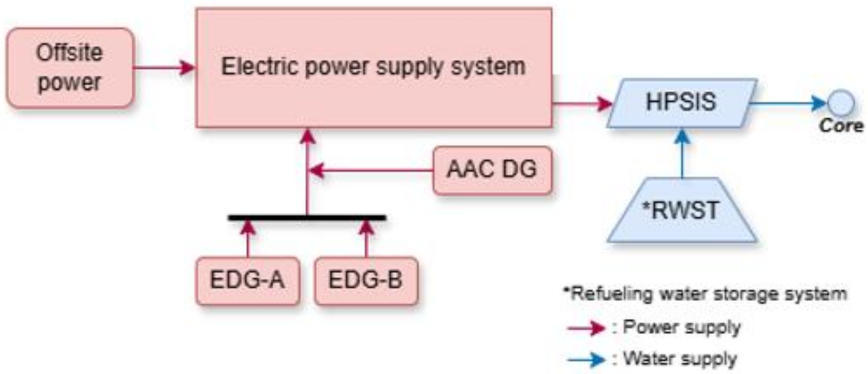

FIGURE 1. Simplified diagram of power-related SSCs in OPR-1000 [5]

Human actions related to the power systems come into play when EDGs fail following a LOOP, and offsite power is not restored, leading to the declaration of a Station Blackout (SBO). After the SBO is triggered, the operator activates the AAC-DG. Similarly, if the AAC-DG fails before offsite power is restored, the Technical Support Center (TSC) attempts to recover power using a mobile diesel generator (MDG). The safety systems are activated following SBO to circulate feedwater and cool down the reactor core, necessitating the operation of the auxiliary feedwater system (AFWS) pumps. The turbine-driven pump (TDP) of the AFWS must be activated proactively, and if the AFWS fails, the motor-driven pump (MDP) is engaged. The operation of the TDP and AAC-DG determines the feasibility of sealing coolant leakage caused by the reactor coolant pump (RCP). If sealing the coolant leakage fails, a LOCA will occur.
If both the TDP and MDP fail, the operator initiates feed and bleed (F&B) operations, which involve a deliberate LOCA by the operator. Additionally, during the initial stage of an SBO, the pressure safety valve (PSV) may become stuck open, which can also trigger a LOCA. Following a LOCA, cooling is attempted through the insertion of control and safety rods (CSR) and by employing the safety injection system (SIS), such as the HPSIS and low-pressure safety injection system (LPSIS). The operational status, failure timing, and other parameters of all the mentioned equipment are randomly sampled using the Monte Carlo method based on the given failure data. Similarly, human actions, including action time and mission success probability, are also stochastically sampled.

II.B. Scenario labeling method

This study aims to cluster scenarios and extract representative scenarios solely based on PCT data. Although the proposed methodology follows an unsupervised approach, assigning labels to each scenario enables an effective evaluation of the clustering results by comparison with the labeled data. Therefore, this section explains the labeling methodology for accident scenarios that occur in OPR-1000 reactor following a LOOP event. The possible accident scenarios after an IE, under the system conditions described in Section 2.1, are summarized in Figure 2. In Figure 2, each branch point represents a decision point, with the lower branch indicating the failure of the corresponding component or action. For example, after a LOOP occurs, if the emergency diesel generator (EDG, referred to as DG in Figure 2) operates successfully and the pressure safety valve (PSV) re-closes, core damage (CD) does not occur, regardless of whether the AFWS operates or fails but is mitigated by a successful F&B operation. These scenarios are labeled as LOOP-1 and LOOP-2, respectively.
Similarly, if the AFW fails and F&B also fails, CD occurs, and this scenario is labeled as LOOP-3. The labeling process systematically assigns labels to all possible scenarios based on the sequence of events and outcomes shown in Figure 2. If the EDG operates but the PSV becomes stuck open, a small-loss-of-coolant accident (SLOCA) scenario unfolds (Figure 3). When a LOOP occurs, the EDG may either fail to start or fail during operation, and these two cases are categorized as separate events due to their significantly different occurrence frequencies. However, once the EDG fails, the subsequent safety measures do not vary significantly. Therefore, scenarios following an EDG failure are collectively categorized as SBO scenarios (Figure 4).

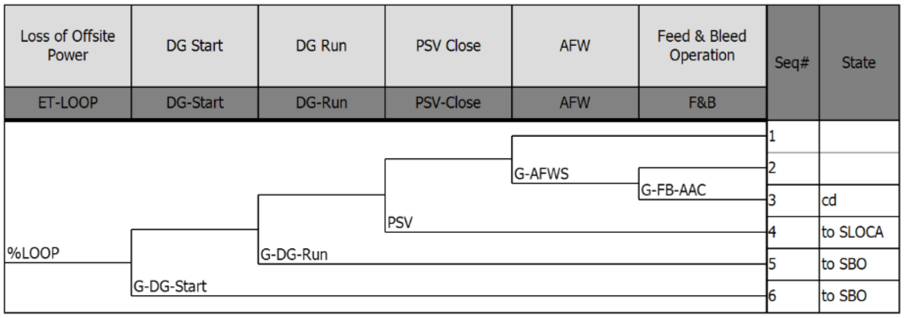

FIGURE 2. Event tree summary beyond LOOP [5]

In Figure 2, when the fourth sequence occurs, it is assumed that detailed scenarios, as depicted in Figure 3, exist. Even if the PSV becomes stuck open, no CD occurs if the SIS and AFW (i.e., AFWS in Figure 8) operate successfully. Furthermore, even if the AFW fails, successful execution of F&B ensures that CD does not occur. In all other cases, CD is inevitable. If both the SIS and AFW succeed (Seq#1 in Figure 3), the scenario is labeled as LOOP-SLOCA-1. Similarly, scenarios for Seq#2 to Seq#4 are named LOOP-SLOCA-2, LOOP-SLOCA-3, and LOOP-SLOCA-4, respectively.

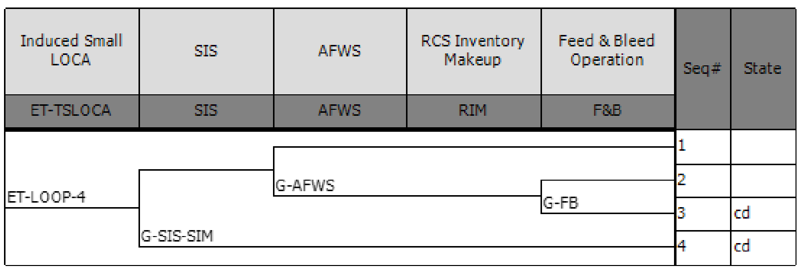

FIGURE 3. Event tree summary of SLOCA [5]

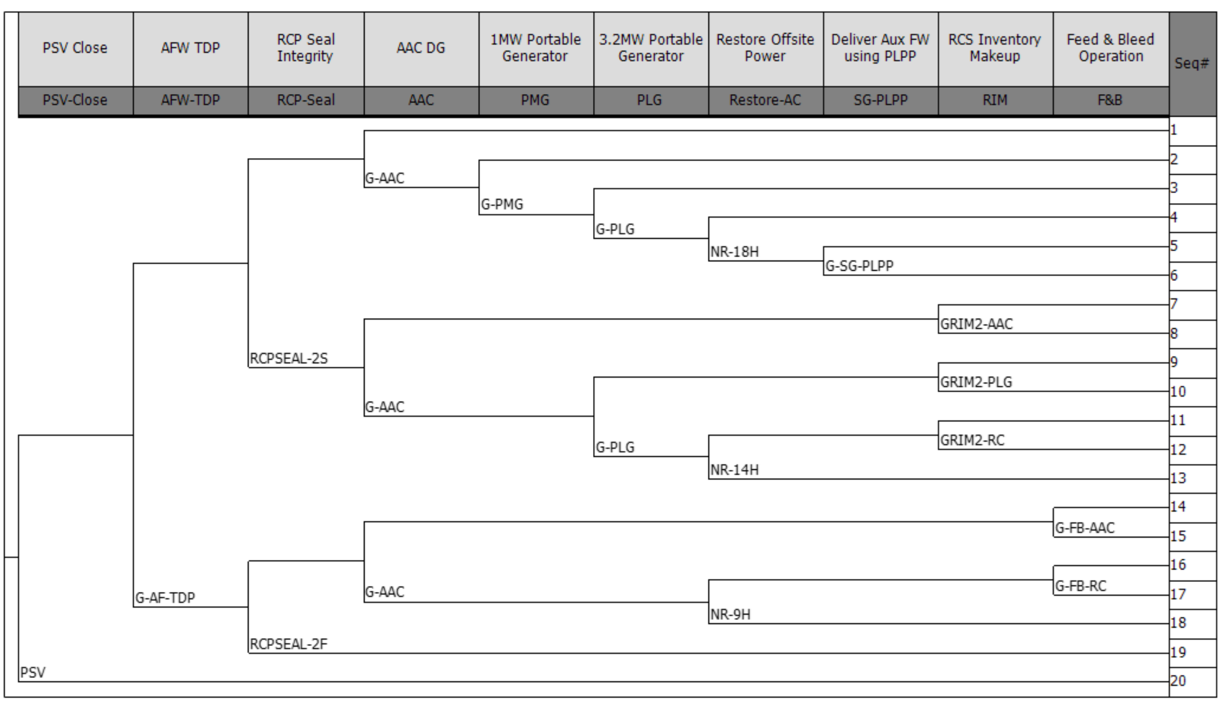

FIGURE 4. Event tree summary of SBO [5]

In Figure 2, Seq#5 and Seq#6 represent scenarios leading to SBO (Station Blackout). The potential accident scenarios stemming from these sequences are depicted in the event tree format shown in Figure 4.
If power recovery using EDG fails, the scenario evaluates the presence or absence of a PSV stuck condition, AFW (i.e., AFW TDP in Figure 4), and RCP seal integrity, proceeding through four stages of power recovery attempts. Subsequently, strategies such as utilizing PLPP for secondary-side cooling of the SG or performing F&B are employed to remove the heat generated in the reactor core. After EDG failure, 20 possible SBO accident scenarios are considered. Each scenario is assigned a sequence number (i.e., Seq# in Figure 4) and is labeled as LOOP-SBO-1 through LOOP-SBO-20.

II.C. Soft-DTW method

Soft-DTW builds upon DTW by introducing a mathematical trick to make DTW differentiable. This section first outlines the general features of the DTW algorithm and then provides a detailed explanation of soft-DTW. While UMAP supports various custom metrics, the custom metric must calculate both the distance and the gradient between two time-series datasets. Hence, this study adopted soft-DTW instead of DTW. The soft-DTW can be applied for two vectors which has different length of series. P and Q are defined as time-series data and their lengths are m and n. First, the two time-series are arranged to form a matrix E (with shape $m \times n$). The (i, j)-th element of E represents the squared Euclidean distance between the points p_i and q_j. The warping path (W) represents the set of mappings between P and Q and can be expressed as follows:

$$\begin{gathered} W = [w_1, w_2, \dots, w_K] \\ \max(m, n) \le K < m + n - 1 \end{gathered} \tag{1}$$

At this point, every element of W corresponds one-to-one with the elements of the matrix E. The k-th element of W, denoted as w_k, represents the warping distance. The objective is to find the path among all possible warping paths that minimizes the total sum of the warping distances. This is referred to as the minimum warping path cost (WPC_{min}) and is mathematically expressed as follows:

$$WPC_{min}(P, Q) = \min\left(\frac{1}{\mathrm{K}}\sqrt{\sum_{k=1}^{K} w_k}\right) \tag{2}$$

Starting from i=0, j=0, the cumulative warping distance D for the k-th warping distance is defined as follows:

$$D(i, j) = E(i, j) + \min\begin{pmatrix} D(i-1, j-1) \\ D(i-1, j) \\ D(i, j-1) \end{pmatrix} \tag{3}$$

where the initialization $D(0, 0)$=0.
However, due to the second term in Equation (3), which involves selecting the minimum among three elements, DTW suffers from being non-differentiable. To address this limitation, soft-DTW replaces the non-differentiable operation in Equation (3) with a differentiable alternative. In soft-DTW, the minimum function used in Equation (3) to choose the smallest value among three terms is replaced with a differentiable approximation called the softmin. The softmin function is defined as:

$$\mathrm{softmin}_{\gamma}(a_1, a_2, \dots, a_n) = -\gamma \log \sum_{i} e^{-\frac{a_i}{\gamma}} \tag{4}$$

where γ>0 is a smoothing parameter that controls the trade-off between strict minimum selection and a softer, differentiable approximation. This replacement ensures that the resulting cumulative distance is differentiable, enabling the computation of gradients and facilitating the use of soft-DTW in optimization problems.
In this study, to calculate the distance between two time series data, features are extracted from all elements of the two data sets (P, Q). This is because the number of scenarios is relatively small and the sequence length is not particularly long, so clustering takes only one to two days to compute. However, if additional scenarios are added for the further works, it could take several weeks or more corresponding to the number of scenarios. In such cases, time could be saved by applying a warping window that restrictively searches only the neighboring indices of each time series data element.

III. Results

This section presents the results of clustering 6,400 accident scenarios using soft-DTW as the metric for UMAP-based dimensionality reduction and DBSCAN for clustering. Typically, clustering large-capacity data requires two primary steps. First, it is necessary to reduce the dimensionality of the data and project it into points. Previous studies have utilized convolution methods for feature extraction from deep learning or t-distributed stochastic neighborhood embedding (t-SNE), which has been conventionally used as a dimensionality reduction algorithm. However, UMAP was employed in this study because it is implemented as a library in Python and offers advantages of being faster and more accurate than existing methods, while requiring fewer hyperparameters. Second, an algorithm is needed to form clusters among adjacent points. DBSCAN is commonly utilized due to its advantage of requiring fewer hyperparameters. DBSCAN is an algorithm that explores the neighborhood of embedded points and forms clusters when the number of points exceeds a minimum threshold within the search radius. Therefore, the hyperparameters of DBSCAN are the point search radius and the minimum number of points required within the radius for cluster formation. This study used default sets of hyperparameters of UMAP and DBSCAN.

The results obtained with the soft-DTW metric were compared and analyzed against those obtained using the Euclidean metric. To generate the dataset, 6,400 accident scenarios were randomly sampled based on the Monte Carlo method. The input data for these scenarios was simulated using MAAP, and the corresponding PCT data was extracted. PCT was calculated for a duration of 72 hours following the IE and recorded at 50-second intervals. In this study, the sampling time (i.e., 50-second intervals) was determined intuitively. If the sampling time were shorter than 50 seconds, the sequence length for each scenario would become excessively long, thereby requiring an impractically long time to perform clustering. Furthermore, since the soft-DTW utilized in this study has a clustering time that increases proportionally to the square of the sequence length, an appropriate sequence length was determined empirically. Figure 5 illustrates the scaled PCT results for all scenarios. The scaling ensures that the average value of the entire PCT curve for each scenario is normalized to 1, providing a consistent basis for comparison. This figure represents the scaled PCTs of all 6,400 accident scenarios.

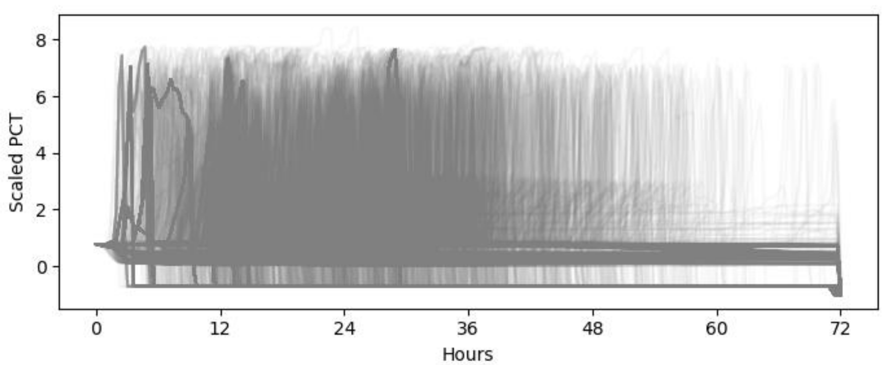

FIGURE 5. Scaled PCTs corresponding to every LOOP scenario

The fact that PCT results repeat across multiple scenarios indicates that, regardless of the random actions, component failures, or timing of events following the reactor IE, the thermohydraulic progression of the reactor eventually converges into a limited set of outcomes. To quantitatively analyze this, UMAP and DBSCAN algorithms were used to cluster scenarios exhibiting similar PCT trends, and the results were compared.

UMAP was employed to embed the PCTs of the 6,400 accident scenarios into a 3-dimensional space (i.e., latent space). Instead of using traditional metrics from UMAP, soft-DTW was applied to measure the similarity between time series data. The embedded data scattered in the 3D space are shown in Figure 6. The left graph in Figure 6 represents the embedding results using the traditional Euclidean metric in UMAP, while right graph shows the embedding results with the soft-DTW metric applied in this study.

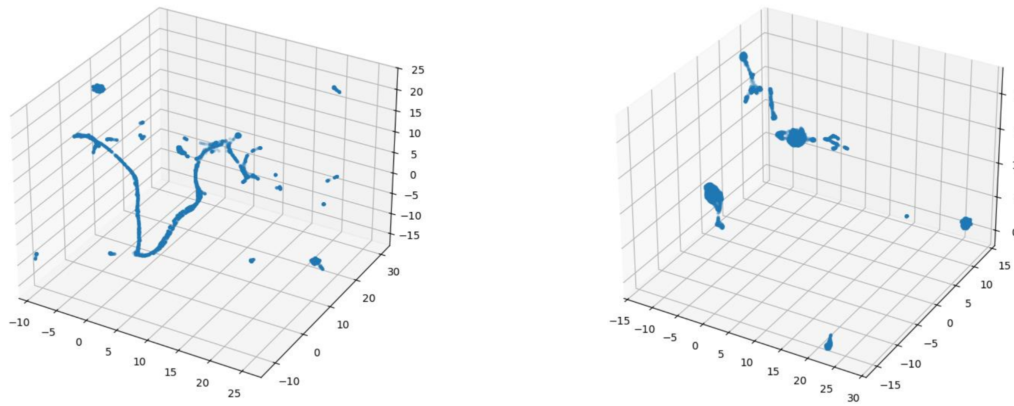

FIGURE 6. Embedded results (ED: left, soft-DTW: right)

Visually, it can be observed that the ED embedding has more scattered points that spread wider, with some forming clusters in the shape of a curved line. In contrast, the soft-DTW embedding generally shows a cloud-like shape where the data points are clustered. However, assessing the performance of the metric solely based on the visual appearance of the scattered data is challenging. To gain further insight, DBSCAN was used to cluster the scattered embedded data, and a more detailed analysis was conducted to identify which data points belong to each cluster. The results from DBSCAN are shown in Figure 7. Data points identified as noise in DBSCAN were labeled as -1, so the minimum value on the color bar in the figure is -1.

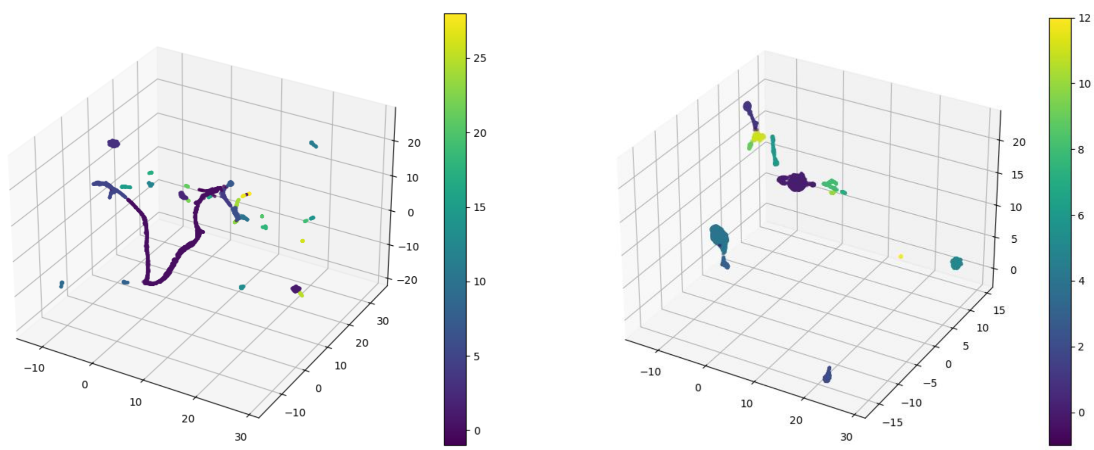

FIGURE 7. Clustered results (ED: left, soft-DTW: right)

To derive representative accident scenarios for each cluster, the most effective method is to identify data points near the centroid of the cluster. However, if the cluster shape is skewed (e.g., a curved line), the centroid may lie outside the cluster structure, leading to the potential for selecting an inappropriate representative scenario. In Figure 7, the cluster with the most data points takes the form of a twisted curve. In fact, the centroid of this cluster lies outside its structure, meaning that the samples close to the centroid cannot be considered representative of the cluster. In contrast, using the soft-DTW metric, it was confirmed that the centroids of all clusters lie within their respective structures. However, in the case of the ED metric, it was found that for 7 out of 29 clusters, the centroid lies outside the cluster structure. Consequently, the ED metric demonstrates limitations when used for deriving representative scenarios in time series data analysis. As a result, the total number of clusters classified by DBSCAN, excluding noise, is 13. The PCT results representing each cluster are shown in Figure 8.

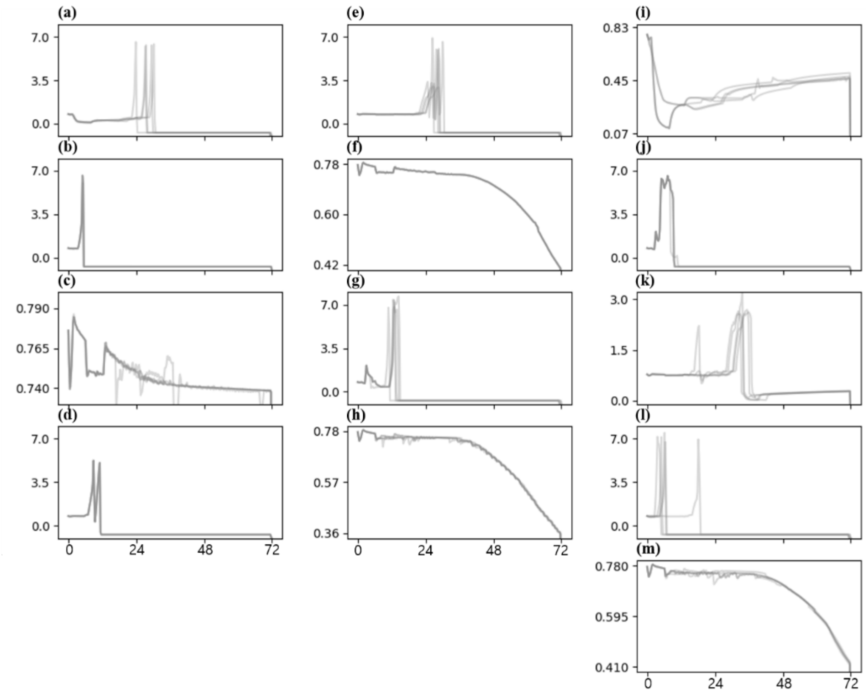

FIGURE 8. Extracted representative scenarios

However, as previously analyzed in the LOOP event tree, it was confirmed that there are total of 27 possible scenarios. Some scenarios, such as LOOP-1 and LOOP-SBO-1, involve the activation of AFW and the restoration of power after an IE, meaning they can be categorized as the same type of scenario. Therefore, the actual number of accident scenarios will be fewer than the 27 possible outcomes. By excluding identical accident scenarios in the event tree, the total number of fundamentally different accident scenarios is identified as 19. However, this number is still greater than the number of clusters derived in this study. There are two possible reasons for this.

First, the scenarios classified as noise in DBSCAN. Since the hyperparameters of DBSCAN (e.g., epsilon, minimum number of samples) and UMAP's parameters have not been fine-tuned, it is possible that the samples classified as noise could be reclassified into a few additional clusters. To achieve this, fine-tuning of DBSCAN and UMAP parameters may be required. The second reason could be due to missing data during the preprocessing step. In this study, clustering was performed after excluding approximately 1,100 data points from the MAAP simulation results with unusually short sequence lengths. Including those data points and performing follow-up research could yield more clusters.

IV. Discussion and Conclusion

This study derived representative accident scenarios from 6,400 randomly sampled LOOP scenarios. The number of scenarios used in this study was determined intuitively. However, since fewer clusters were found compared to the number of scenarios derived using conventional PSA methods, it is considered that the accuracy of clustering performance verification would improve if additional scenarios were supplemented to address the shortfall. Among the various IEs that can occur in nuclear power plants, LOOP is the most complex and has the largest number of possible scenarios, so more than 6,400 samples would be required for accurate verification. However, other IEs (e.g., large break LOCA, steam generator tube rupture) have relatively simple accident sequences, so it is considered that representative accident scenarios can be derived with fewer samples. In other words, the complexity of safety system is determined by the type of IE, and the appropriate number of samples is determined by the complexity of the safety system. The correlation between these two factors can be mathematically analyzed or empirically derived in the future works.

If accident scenarios can be analyzed based on time-series data in this manner, it becomes easier to numerically present the failure limits of safety functions. For example, the results in Figure 8 (m) show that the PCT curve does not exhibit any sharp peak but follows a downward-sloping curve. This indicates that CD did not occur during 72 hours. Therefore, we can analyze the minimum power recovery time to avoid CD in case of IE. Likewise, safety equipment operation start time, and average operation time can be analyzed to avoid CD.

In this study, MAAP simulation results with excessively short sequence lengths were excluded from clustering target. The ratio shows that 1,100 out of 7,500 scenarios were excluded, representing approximately 14.67% of the total. In comparison, the proportion of missing scenarios among the 19 possible scenarios is approximately 31.57%, suggesting that some of the excluded 1,100 scenarios may correspond to the missing scenarios. The reason for excessively short sequence lengths in MAAP simulations could be due to computational instability, as the MAAP code simulates reactor accidents with the nature of high uncertainty. Alternatively, the input scenarios may represent impossible reactor conditions, causing the MAAP calculation to terminate prematurely. Finally, there is a possibility that these are very short scenarios that terminated normally. However, since the underlying cause of short sequence lengths in MAAP simulations has not yet been identified, future research that elucidates this issue could contribute to the validation of representative accident scenario studies.

Furthermore, scenarios generated based on the existing DPSA concept are theoretically infinite in variety, which has limitations in calculating total risk. However, if representative accident scenarios can be derived for each IE, the number of scenarios used in risk calculation becomes finite. Consequently, if this study is supplemented, it will become possible to calculate total risk targeting representative accident scenarios derived using DPSA. This is expected to contribute to realistic risk calculation by making fewer conservative assumptions compared to the conservatively calculated and highly evaluated risks in existing PSA.

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