

Integrated Safety Margin Quantification–Leveraging Probabilistic Considerations in Safety Demonstration

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Abstract: Nuclear safety demonstration has traditionally relied on deterministic approaches, in which predefined accident scenarios are analyzed to verify compliance with safety criteria and to evaluate safety margins. While probabilistic methods have been developed in parallel to assess risk and identify significant accident sequences, their integration into safety margin quantification remains limited. This work proposes an Integrated Safety Margin Quantification (ISMQ) framework that leverages probabilistic considerations to enhance deterministic safety analyses.

The proposed methodology incorporates probabilistic insights to systematically explore a wide range of accident scenarios, accounting for different configurations of available safety systems as well as uncertainties in physical and modeling parameters. By embedding uncertainty quantification within a two-loop framework, the approach captures both variability in system conditions and uncertainties affecting accident progression, while maintaining computational efficiency through the use of optimized deterministic sampling techniques.

In addition, a machine-learning-based exploration is employed to identify the most penalizing scenario, thereby complementing the realistic safety margin assessment.

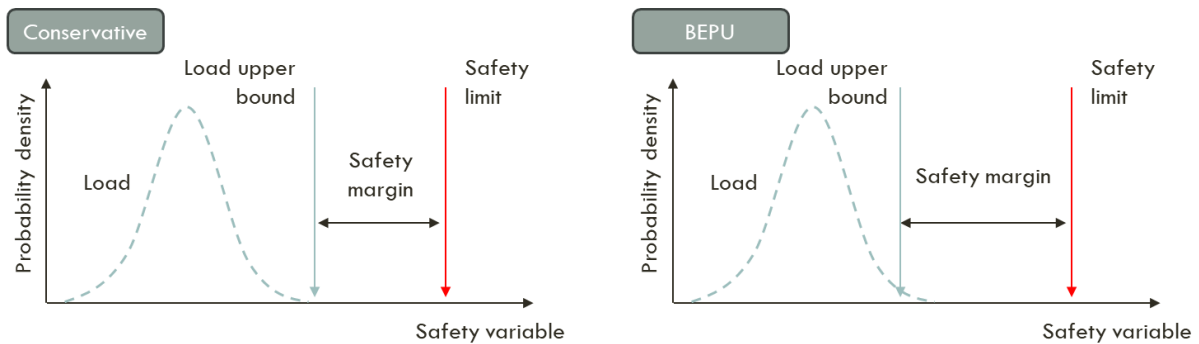
By integrating probabilistic considerations into the safety demonstration, the proposed approach extends beyond existing deterministic evaluations to provide a more comprehensive characterization of safety margins. This includes the identification of relevant and risk-informed scenarios, the assessment of the distance between best-estimate system responses and safety limits, and the quantification of the likelihood of exceeding these limits. The framework thus supports a more informed and realistic evaluation of safety margins.

1. INTRODUCTION

Nuclear safety demonstration has traditionally relied on Deterministic Safety Analyses (DSAs), in which predefined accident scenarios are analyzed to verify compliance with safety criteria and to evaluate safety margins. DSAs have been initially conducted using a conservative approach, combining conservative computer codes, penalizing assumptions regarding system availability, and conservative initial and boundary conditions [1]. This approach intends to justify a conservative load upper bound, bounding all sorts of uncertainties, while being still below the safety limit imposed by the authorities (see left part of Figure 1).

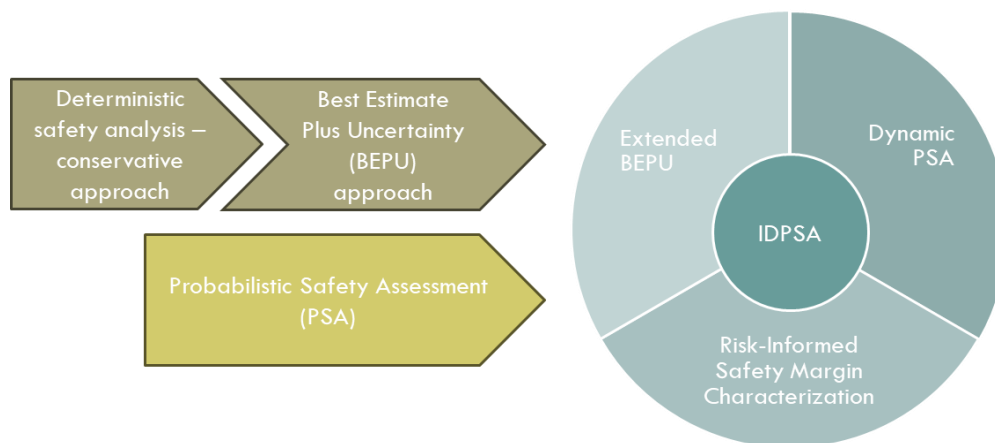
In 1989, the US Nuclear Regulatory Commission (NRC) updated its licensing framework to permit the Best Estimate Plus Uncertainty (BEPU) approach as an alternative to traditional conservative methods [2]. Since then, BEPU has been widely adopted across the nuclear industry [3], particularly for Loss-of-Coolant Accidents (LOCAs), because it explicitly incorporates uncertainties in physical phenomena and modeling while maintaining conservative assumptions on system availability [3], [4]. This approach evaluates safety margins by determining an upper bound of the load distribution (commonly 95% probability at 95% confidence), providing a more realistic yet still robust basis for safety demonstration.

Figure 1: Safety margin in DSA – conservative approach vs. BEPU approach



The first Probabilistic Safety Assessment (PSA) was carried out in the WASH-1400 study in 1975 [5], emerging as a complement to DSA. While DSA examines a limited set of predefined scenarios, PSA systematically evaluates combinations of initiating events, system failures, and human errors to identify risk-significant accident sequences. It adopts a best-estimate approach and provides an overall measure of plant risk, supported by uncertainty analyses to strengthen result reliability.

Figure 2: Evolution of deterministic and probabilistic safety analyses



Since the early 2000s, risk-informed approaches promoted by the US NRC, Nuclear Energy Agency (NEA), and International Atomic Energy Agency (IAEA) have driven the development of Integrated Deterministic–Probabilistic Safety Assessment (IDPSA) methods (see Figure 2). IDPSA generally includes three main approaches: Extended BEPU (EBEPU), which integrates PSA insights on safety system availability into BEPU analyses [3]; dynamic PSA, which combines system physics with stochastic behavior to capture time-dependent accident evolution [6] and event dependencies [7], though its industrial use remains limited by complexity and computational cost; and Risk-Informed Safety Margin Characterization (RISMC), which probabilistically evaluates safety margins (i.e. probability of respecting safety limit) by focusing on the most relevant and likely accident sequences [8].

This work proposes an Integrated Safety Margin Quantification (ISMQ) methodology that incorporates probabilistic approaches to account for all relevant uncertainties in safety analysis. It provides a realistic evaluation of safety margins by analyzing key scenarios, quantifying the gap between best-estimate loads and safety limits, and estimating the probability of exceedance. The approach is complemented by advanced machine-learning-based sensitivity analysis to identify the most penalizing conditions.

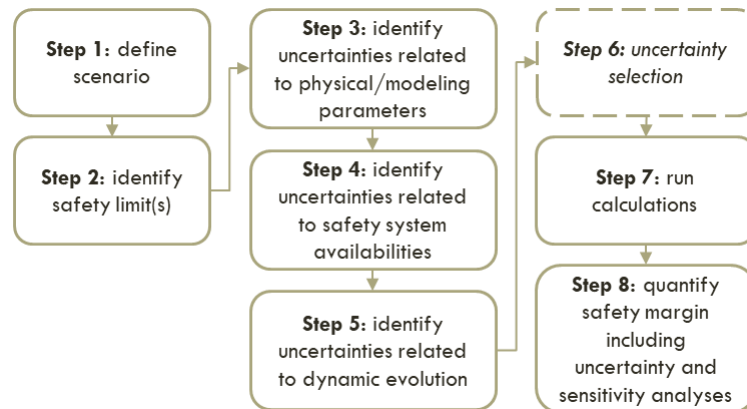
The ISMQ methodology is explained with a reactor application in §2. The approach is then compared with BEPU in §3 to illustrate its capability of offering additional insight into safety margin. Finally, conclusion and perspectives are provided in §4.

2. METHODOLOGY OF INTEGRATED SAFETY MARGIN QUANTIFICATION

2.1. Overview of the Methodology

The proposed ISMQ methodology is designed to be general and adaptable to a wide range of safety studies, without being limited to a specific reactor design. As a scenario-based approach, it is applied to defined accident scenarios, including initiating events, safety system configurations, and operator actions. Its overall process is illustrated in Figure 3 and detailed in §2.2 with a reactor application.

Figure 3: Integrated safety margin quantification methodology



The ISMQ methodology uses uncertainty as its starting point and provides a comprehensive framework for its treatment in safety analysis. It considers:

- probable safety system configurations (similar to EBEPU), linked to aleatory uncertainties such as failures on demand, failure times, and recovery times in PSA models [9];
- physical and modeling uncertainties (similar to BEPU), including both aleatory (e.g. initial and boundary conditions) and epistemic (e.g. model parameters) components [9];
- dynamic accident evolution uncertainties, related to system actuations and operator actions (based on Dynamic Event Tree (DET) approach), generally treated as aleatory [9], [10];
- sample probabilities, used to ensure the representativeness of each simulation;
- a two-loop treatment of uncertainties, with an inner loop for dynamic evolution uncertainties and an outer loop for all others, optimizing computational cost.

Rather than classifying uncertainties by nature (aleatory vs. epistemic), the approach prioritizes their impact on accident evolution. This enables efficient computation while capturing possible scenario bifurcations and diverse end states.

2.2. ISMQ Methodology Description and Its Application

This section details the ISMQ methodology through its application to a generic 3-loop Gen-II 1000 MWe PWR. The case study considers a Design Basis Accident (DBA) involving a 3 to 8" Small-Break Loss of Coolant Accident (SBLOCA) on a cold leg. Simulations are performed using a validated, industry-standard thermal-hydraulic code modeling the core and Reactor Coolant System (RCS). This application aims both to illustrate the methodology and to demonstrate its feasibility with standard analysis tools.

2.2.1. Step 1: Define Scenario

The scenario is defined by specifying the initiating event, initial and boundary conditions, available safety systems, and operator actions, either through a deterministic (DSA) or risk-informed (PSA-based) approach.

In this application, the scenario considers a 3 to 8" SBLOCA on the cold leg of loop B, with the break size range derived from both the safety report and the PSA model. Following reactor, reactor coolant pump, and main feedwater trips, key safety systems include the Auxiliary Feedwater (AFW), accumulators, and Safety Injection (SI).

2.2.2. Step 2: Identify safety limit

The safety limits for the scenario must then be defined. In LOCA analyses, a Peak Cladding Temperature (PCT) limit of 1200 °C is typically used [11], [12]. However, due to the thermal-hydraulic code's coarse core discretization, which cannot capture local temperature peaks, a more conservative limit of 600 °C is adopted to account for this limitation and associated uncertainties [13].

2.2.3. Step 3: Identify uncertainties related to physical/modeling parameters

This step addresses uncertainties related to initial and boundary conditions, physical modeling, and system performance. A Phenomena Identification and Ranking Table (PIRT) analysis is used to identify relevant parameters—either from existing studies or developed specifically—focusing on those most influential on the figure of merit (i.e. the safety limit). These parameters are then treated as sources of physical/modeling uncertainty and sampled according to their distributions, in line with the BEPU approach.

Parameter identification and characterization rely on three sources: model development insights, sensitivities from safety reports (e.g. break size), and literature on SBLOCA PIRT analyses. A comprehensive set of 46 applicable uncertainty parameters is defined and, when needed, their ranges and distributions are adapted to the specific model and inputs (see Table 1 for 12 of them which are discussed in the current paper). Since thermal-hydraulic codes rely on imperfect models, properly identifying and quantifying these uncertainties is essential; in this work, literature-based distributions are considered sufficiently representative.

Table 1: Uncertainty parameters with intervals and distributions (partial list)

#	Parameter	Description	Variation range	Distribution
1	breakSize	Break size	(3, 8) inch	Uniform
5	criticFlow	Critical flow model - break discharge coefficient	(0.7544, 1.2456)	Normal
7	UPinitT	Upper header – initial temperature	(586.95, 596.95) K	Uniform
12	coreHyDiam	Core – hydraulic diameter	(0.98, 1.02)	Normal
18	intactHLtemp	Intact loop – hot leg temperature	(600.5, 604.5) K	Normal
19	intactCLRough	Intact loop – cold leg wall roughness	(0.5, 2.0), a=2.0952, b=2.6190	Beta
38	accuInitInv	Accumulator – initial inventory	(30.5607, 32.1429) m ³	Normal
42	PSI	Safety injection – trigger pressure	HPSI: (10.84, 12.33) / LPSI: (1.99, 2.26) MPa, a=2.2503, b=1.2839	Beta
43	accuInitP	Accumulator – initial pressure	(4.3, 4.86) MPa	Normal
44	AFWdelay	Delay of the auxiliary feed water system	(24, 56) s, a=1.8791, b=2.5750	Beta
45	RCPtripDelay	Reactor coolant pump – trip delay (after reactor trip)	(0, 600) s, a=1.0465, b=2.0455	Beta
46	SIdelay	Delay of safety injection	(15, 27) s, a=1.1362, b=2.1282	Beta

2.2.4. Step 4: Identify uncertainties related to safety system availabilities

This step addresses uncertainties related to safety system configurations. Discrete uncertainties (e.g. number of available system trains) are identified, while continuous parameters (e.g. flow rates) are

treated as physical uncertainties in Step 3. The probability of each configuration is derived from PSA data, following an approach similar to EBEPU. To reduce computational cost, configurations are grouped based on their likelihood and impact, prioritizing the most probable or most penalizing cases.

For the 3–8" SBLOCA scenario, the key systems are AFW, accumulators, and SI. The AFW is simplified to a representative configuration (2 Steam Generators (SG) at nominal flow and 1 at half flow), as differences with the most probable case (i.e. all 3 SG at nominal flow) are negligible. For accumulators, two are assumed available while the one on the broken loop is lost. The SI system configurations are derived from the “Success” sequences in the PSA event tree (see Figure 4), leading to a limited set of representative cases based on HPSI or LPSI availability (i.e. #1-3 in Table 2), which are retained as the main uncertainties for system availability. Note that in the PSA model, 3-8” break corresponds to Medium-Break LOCA (MBLOCA).

Figure 4: Simplified MBLOCA event tree

MBLOCA cold leg	HPSI injection	LPSI injection	LPSI recirculation	HPSI recirculation	No.	Conseq.	%
					1	Success	99.38%
					2	Success	0.37%
					3	Core melt	0.04%
					4	Success	0.12%
					5	Core melt	0.00%
					6	Core melt	0.09%

Table 2: Safety injection system configurations with probabilities

# of configuration	No. of sequence	Configuration	Probability
1	1&2	2 HPSI trains	95.84%
2	1&2	1 HPSI train	4.04%
3	4	2 LPSI trains	0.12%
4	4	1 LPSI train	0.00%

2.2.5. Step 5: Identify uncertainties related to dynamic evolution

This step focuses on uncertainties related to system actuation and operator action timing, treated separately in an inner loop to capture their impact on accident evolution. These include parameters such as operator response times and system actuation setpoints, which can alter the course of the scenario and potentially lead to different outcomes (bifurcations).

Only parameters likely to influence accident dynamics are included in this loop; others may be handled with physical/modeling uncertainties. The approach can also account for additional system failures triggered during the transient, allowing key interactions between systems and processes to be represented, similar to dynamic PSA but with reduced complexity. Samples of these dynamic uncertainty parameters are generated from their respective distributions, with selected parameters identified as most relevant.

In this application, parameters #42–46 in Table 1 are identified as potentially significant uncertainties related to dynamic accident evolution.

2.2.6. Step 6: Uncertainty selection

This step aims to identify the most influential uncertainty parameters for further analysis using a quantitative PIRT (sensitivity) approach. While safety system availability uncertainties were preselected in Step 4, this step focuses on physical/modeling and dynamic evolution parameters.

Since PCT remains well below its limit in many cases, the Minimum Collapsed Core Level (MCCL) is used as the Figure of Merit (FoM). To limit computational cost, the Wilks' formula (first order one-sided 95/95) is applied, leading to 59 samples, combined with Latin Hypercube Sampling across parameter distributions. The analysis is repeated for three SI configurations ($59 \times 3 = 177$ simulations in total), though mainly the 2LPSI case is discussed in the current paper due to much larger margins in others. Sensitivity is evaluated using Pearson and Spearman coefficients, representing respectively linearity and monotony between input and output. Results of the 2LPSI case are provided in Figure 5 for the 10 most sensitive parameters.

Figure 5: Sensitivity analysis – 2LPSI case (top 10 parameters)



Applying a selection threshold of 0.2 in the 2LPSI case results in five key parameters—three related to physical/modeling uncertainties (breakSize, criticFlow, intactHLtemp) and two to dynamic evolution (PSI, RCPtripDelay)—balancing representativeness and computational cost.

2.2.7. Step 7: Run calculations

This step defines the final computational scheme to obtain a representative evaluation of safety margins. In addition to comprehensive simulations, it incorporates a machine-learning-based sensitivity analysis to identify the most penalizing conditions. This approach enhances the methodology by providing complementary insight, predicting worst-case consequences along with their typically low probabilities of occurrence.

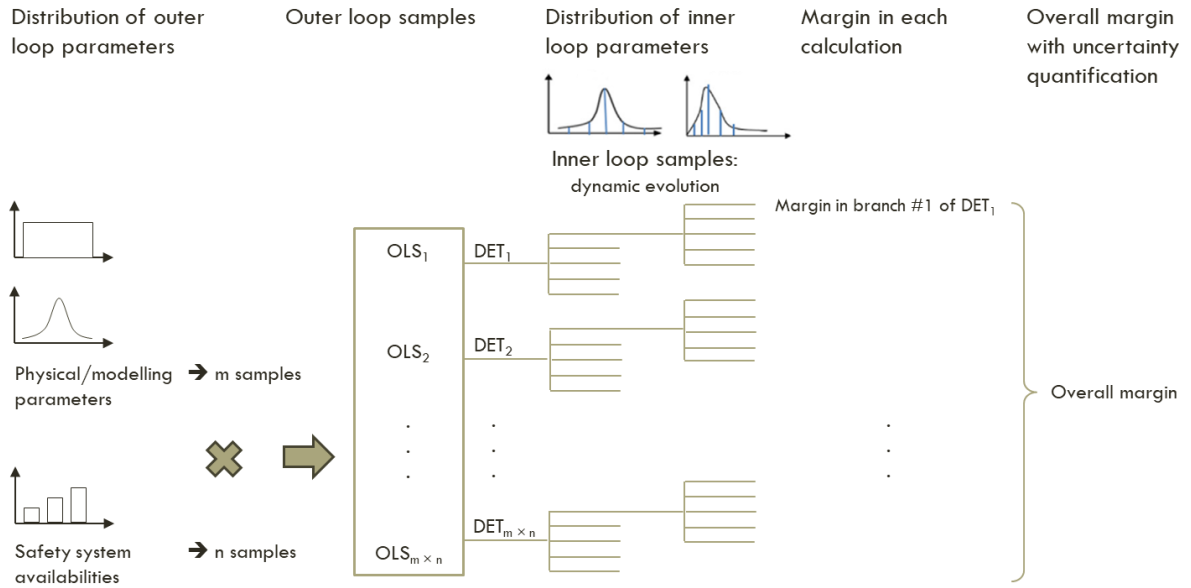
Complete set of calculations for representative safety margin measurements:

The final computational scheme (see Figure 6) is defined, where selected uncertainties are treated through a two-loop structure to ensure a representative and computationally efficient safety margin evaluation:

- Outer loop: covers physical/modeling uncertainties and safety system configurations;
- Inner loop: handles uncertainties related to dynamic accident evolution using a Dynamic Event Tree (DET) approach.

Unlike traditional methods that separate aleatory and epistemic uncertainties, this framework organizes them based on their impact on accident progression (i.e. transient development), reducing the total number of simulations. The outer loop generates combinations of physical/modeling samples and system configurations, while the inner loop explores dynamic sequences for each case.

Figure 6: Computational scheme – uncertainty handling in two loops



For the 2LPSI case, a limited number of key parameters ($m = 3$) enables the use of standard deterministic sampling in the outer loop, while DET sampling is applied in the inner loop for the 2 dynamic evolution related parameters.

Standard deterministic sampling is a structured method that generates input samples by symmetrically varying each parameter around its mean (μ_i) using its standard deviation (σ_i). For m uncertain inputs, it produces $2m$ samples (positive and negative deviations), ensuring balanced coverage of the input space. This approach is simple, preserves symmetry, and efficiently captures the effect of uncertainties with a limited number of simulations [14], [15]. The sample matrix for 3 inputs, thus 6 samples is provided here-below:

$$\Sigma_{std} = \begin{vmatrix} \mu_1 - \sqrt{3}\sigma_1 & \mu_1 & \mu_1 & \mu_1 + \sqrt{3}\sigma_1 & \mu_1 & \mu_1 \\ \mu_2 & \mu_2 - \sqrt{3}\sigma_2 & \mu_2 & \mu_2 & \mu_2 + \sqrt{3}\sigma_2 & \mu_2 \\ \mu_3 & \mu_3 & \mu_3 - \sqrt{3}\sigma_3 & \mu_3 & \mu_3 & \mu_3 + \sqrt{3}\sigma_3 \end{vmatrix} \quad (1)$$

For the inner loop, four samples are selected for RCPtripDelay at cumulative probabilities of 0.05, 0.35, 0.65, and 0.95 due to its high sensitivity, while three samples are chosen for PSI at cumulative probabilities of 0.05, 0.5, and 0.95. This results in $6 \times (4 \times 3) = 72$ simulations, balancing accuracy and computational cost. Deterministic sampling is chosen for its efficiency and ability to preserve symmetry in the sample space, making it well-suited when the number of uncertain parameters is small.

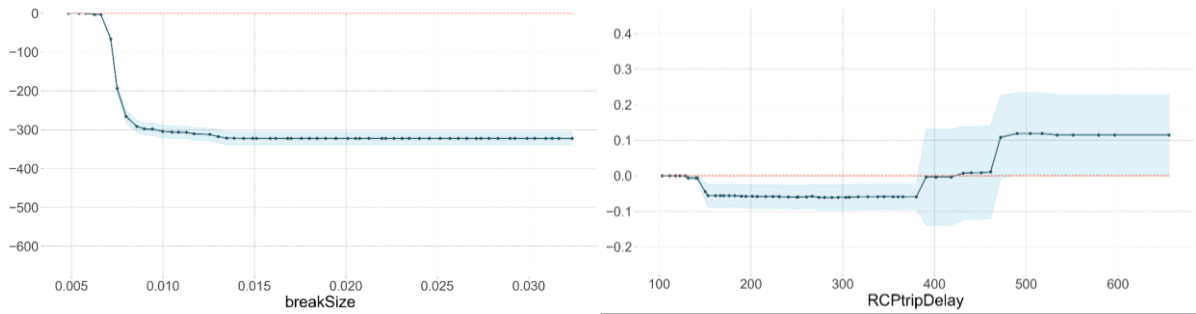
Exploring the most penalizing case – Partial Dependency Plot technique:

This sub-step complements the main simulations by using machine-learning-based sensitivity analysis to better understand input–output relationships and identify the most penalizing conditions. A combination of random forest modeling and Partial Dependence Plots (PDPs) is used to map how each input parameter influences the FoM across its full range.

Unlike traditional sensitivity metrics (e.g. Pearson or Spearman coefficients), PDPs reveal nonlinear effects, trends, and thresholds by isolating the impact of individual variables while averaging out others [16]. The random forest model—trained on simulation data—ensures robust predictions and captures complex interactions [17].

Applied to the 2LPSI case (59 simulations), this approach enables the identification of a most penalizing scenario, defined by specific parameter values that maximize the FoM (PCT), along with their associated (generally low) probabilities. This worst-case scenario provides valuable complementary insight beyond the representative safety margin evaluation, highlighting the most critical system conditions.

Figure 7: Partial dependency plots – input parameters' impact on maximum PCT



The PDPs of the two most sensitive parameters are shown in Figure 7. For example, the PDP for breakSize indicates that, when isolating its effect from other variables, the maximum PCT is highest at the smallest break size and decreases as the break size increases. Based on the PDP analysis, the most penalizing case is defined by the following parameter values and estimated probabilities:

- breakSize = 0.00456 m² (5/59)
- criticFlow = 0.9054 (3/59)
- intactHLtemp = 602.5 K (20/59)
- PSI = 2.08×10⁶ Pa (10/59)
- RCPtripDelay = 695 s (9/59)

2.2.8. Step 8: Quantify safety margin

This final step quantifies multiple dimensions of the safety margin, as illustrated in Figure 8:

- the individual margin for each simulation:

$$m_j = \begin{cases} \text{limit} - \text{load}_j, & \text{if } \text{load}_j < \text{limit} \\ 0, & \text{if } \text{load}_j > \text{limit} \end{cases} \quad (2)$$

- the *probabilistic safety margin*, representing the probability that the safety limit is not exceeded:

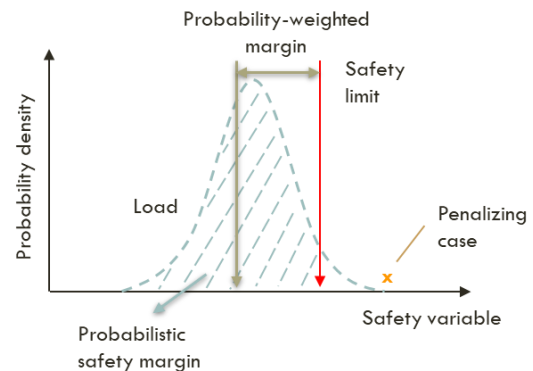
$$p = \sum_{j=1}^N p_j, \quad \text{with } p_j = \begin{cases} w_j, & \text{if } \text{load}_j < \text{limit} \\ 0, & \text{if } \text{load}_j > \text{limit} \end{cases} \quad (3)$$

- and the *probability-weighted margin*, measuring the average margin of compliant cases while accounting for their likelihood:

$$m = \frac{\sum_{j=1}^N m_j \times w_j}{p} \quad (4)$$

Together, these metrics provide a realistic characterization of safety by combining both the likelihood of meeting the limit and the remaining margin to it, avoiding overly conservative or overly optimistic interpretations. Acceptance criteria can then be defined depending on the scenario type. The previously identified most penalizing case further complements this assessment by highlighting extreme but unlikely conditions.

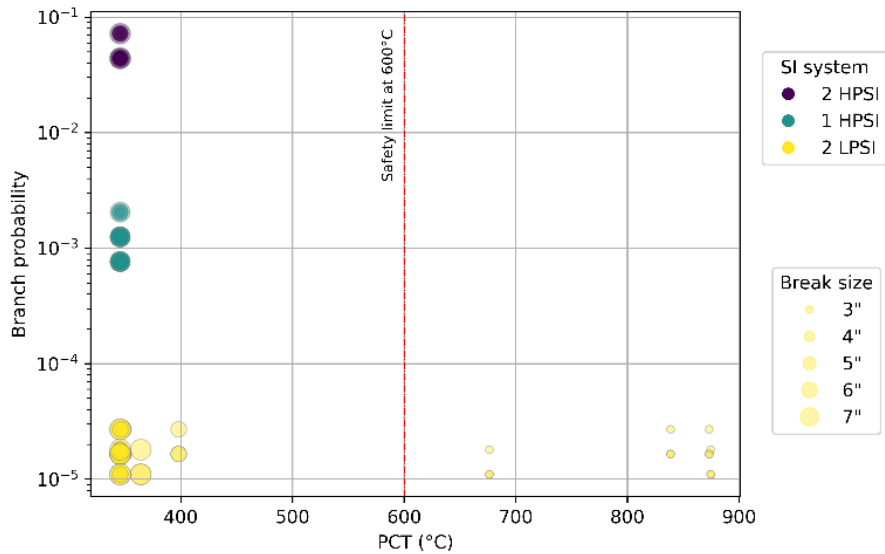
Figure 8: Safety margin quantification complemented by penalizing case



Results in Figure 9 and Table 3 show that configurations with HPSI exhibit large margins, with no exceedance of the safety limit. In contrast, the 2LPSI case includes some exceedances, leading to a probabilistic safety margin of 0.8333, although the remaining cases still maintain a substantial margin.

Overall, the probabilistic safety margin is nearly unity (0.9998), and the probability-weighted margin remains high, indicating significant global safety margins.

Figure 9: Branch probability vs maximum PCT

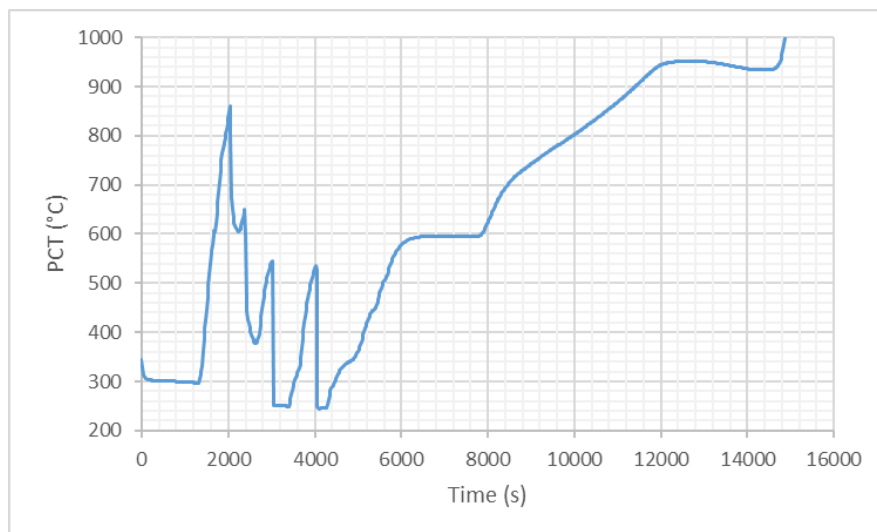


The most penalizing case (Figure 10) confirms that severe conditions can lead to large PCT increases due to insufficient depressurization and coolant injection (simulation capacity of 1000°C exceeded at the end of the calculation), but its probability is extremely low (3.78E-05, and 4.53E-8 if the probability of the 2LPSI case further considered). This highlights the complementarity of the approach: the full set of simulations provides a representative safety assessment, while the penalizing case reveals rare but extreme risk scenarios.

Table 3: Probabilistic safety margin and probability-weighted margin

Case	Probabilistic safety margin	Probability-weighted margin (K)
2 HPSI	1	254.3
1 HPSI	1	254.3
2 LPSI	0.8333	208.4
All	0.9998	254.2

Figure 10: Most penalizing case as defined based on PDPs



3. COMPARISON WITH BEST ESTIMATE PLUS UNCERTAINTY APPROACH

The BEPU approach aims to determine an upper bound of system response (e.g., 95% coverage at 95% confidence). The safety margin is then defined as the distance between this upper bound and the safety limit, as conceptualized in the right part of Figure 1. In contrast, the ISMQ methodology provides a probabilistic perspective. As illustrated in Figure 8, it evaluates:

- the probability of not exceeding the safety limit,
- the average distance (margin) between the safety limit and the probability-weighted load of compliant cases,
- and a penalizing worst-case scenario with a very low estimated probability.

The 2LPSI case is used for comparison because it presents a significant risk of exceeding the 600°C PCT safety limit. For BEPU, 59 simulations were generated using the Wilks 95/95 approach combined with LHS, all with equal probability. Among these, 5 cases exceeded the safety limit. The focus is on the upper bound (95th percentile), which in this case lies above the safety threshold (see Figure 11). For ISMQ, 72 simulations were performed using a multi-loop sampling strategy, resulting in runs with unequal probabilities. Here, 12 cases exceeded the limit, while the majority (60 cases) remained well below it (see Figure 12). Because of unequal probabilities, weighted statistical analysis is required.

The comparison shows that:

- BEPU emphasizes a conservative upper bound, which exceeds the safety limit.
- ISMQ provides richer insight:
 - a high (conditional) probability (0.8333) of meeting the safety limit,
 - a large average safety margin (208.4 K) for compliant cases,
 - and identification of a highly penalizing extreme case (over 1000°C), albeit with negligible probability (3.78E-05).

Overall, ISMQ offers a more comprehensive and informative characterization of safety by combining probability, margin, and extreme-case analysis, whereas BEPU focuses primarily on bounding behavior.

Figure 11: BEPU – histogram and fitted distribution of maximum PCT

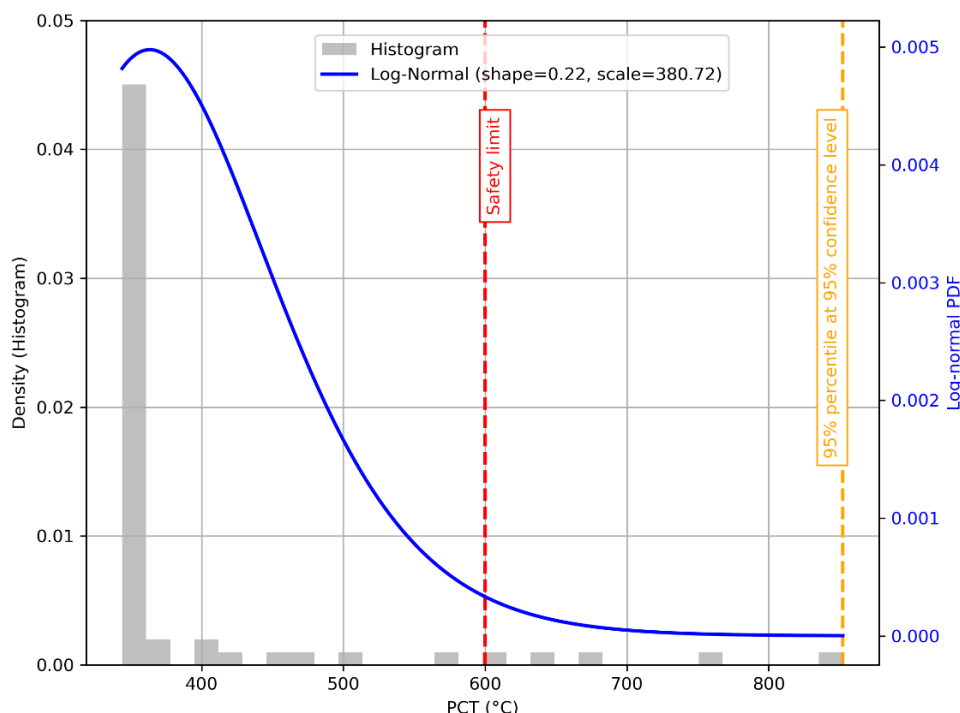
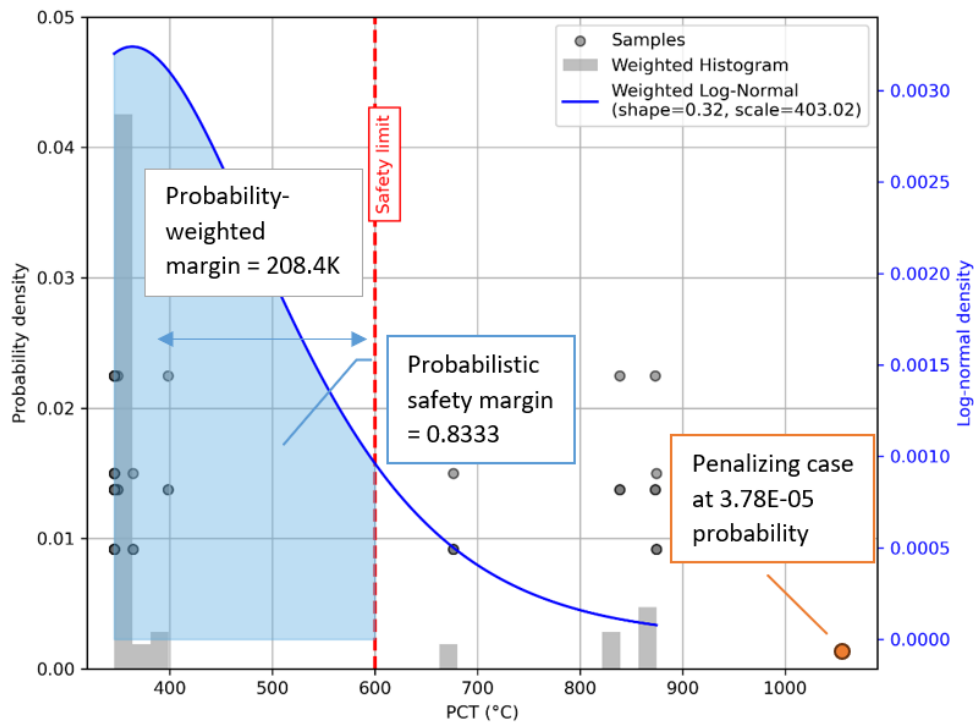


Figure 12: ISMQ – weighted histogram and fitted weighted distribution of maximum PCT



4. CONCLUSION AND PERSPECTIVES

The ISMQ methodology integrates DSA and PSA into a unified framework that captures a wide range of uncertainties. By reducing excessive conservatism in scenario definition and input assumptions based on probabilistic considerations, it enables more realistic safety evaluations, supports larger demonstrated safety margins, and can help reduce regulatory burden—ultimately improving the economic competitiveness of nuclear energy.

Compared with existing IDPSA approaches, ISMQ provides a more comprehensive treatment of uncertainty. EBEPU accounts for system availability and input uncertainties but yields a deterministic safety margin; whereas RISMC incorporates possible scenarios and input uncertainties, producing a probabilistic safety margin. ISMQ combines both perspectives by considering probabilities of system availability and accident scenarios, while introducing dynamic PSA to capture parameters influencing accident evolution. It delivers a probabilistic safety margin, complemented by a deterministic margin for non-exceeding cases. Together, these metrics demonstrate both low failure probability and the absence of cliff-edge effects, making the method particularly relevant when only a small fraction of simulations exceed safety limits while most retain substantial margins.

In addition, ISMQ evaluates the most penalizing scenario together with its (typically very low) probability, thereby characterizing the residual risk associated with rare but extreme system trajectories.

The approach is flexible and applicable to both research and industrial contexts, and is especially valuable for:

- Passive systems, where performance depends on complex interactions between physical phenomena and system behavior during accident evolution.
- Highly uncertain phenomena (e.g., creep failure, severe accident conditions), where outcomes are strongly dependent on evolving physical states.
- Complex operator actions, particularly those with uncertain timing or execution; further integration of human reliability models could enhance realism.

More broadly, ISMQ provides a powerful framework for reactor design optimization, enabling risk-informed trade-offs between safety and economic performance throughout iterative design processes.

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