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STATE-OF-THE-ART FOR PROBABILISTIC PTS ANALYSIS

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ABSTRACT

First attempt of probabilistic pressurised thermal shock (PTS) analysis was done in the US in the 1980s and revised in the next decades. The risk-informed technical bases generated by the USNRC PTS Re-evaluation Project from 1999 through 2008 (using the advanced FAVOR code) resulted in the promulgation of the Revised PTS Rule, 10 CFR 61a in February 2010. In the EU the use of probabilistic PTS analysis in the scope of structural integrity assessment became of interest in the last two decades, but current state-of-the-art for PTS analysis is the use of deterministic assessment.

Within the EU's HORIZON 2020 APAL (**A**dvanced **P**TS **A**nalysis for **L**TO) project the state-of-the-art on probabilistic PTS Analysis as well as on tools and software currently used for probabilistic PTS assessments has been identified. Moreover, recommendations and conclusions were drawn as well as possible improvements identified for use of probabilistic PTS analysis. The performed work and drawn conclusions within the APAL project will be presented in this paper.

An overview of the different types of assessment for probabilistic PTS analysis used by the partners involved in the APAL project is given. In addition to the overview, further information and recommendations are given. This additional information covers several descriptions needed for better understanding of probabilistic assessments (e.g. description, advantages and restrictions of FORM/SORM). Also a simplified benchmark was performed to show the difference in the methods used for calculation of initiation or failure probability. Detailed information about the outcome of the identification of the state-of-the-art on probabilistic PTS Analysis is given in APAL public summary report Deliverable D1.6.

INTRODUCTION

The APAL project was launched in October 2020 with a duration of four years. In total 16 partner (14 European + 2 international partner) work together to develop a guideline for advanced PTS Analysis in the scope of long-term operation (LTO).

The main objectives of this project are development of advanced probabilistic PTS assessment method, quantification of safety margins for LTO improvements and development of best-practice guidance. The project will address multidisciplinary and multi-physics challenges related to reactor pressure vessel (RPV) safety assessment of PTS mitigation. The planned work to achieve these objectives is divided into five parts leading to five technical work packages (WP):

The first part (WP1) consists of an extensive literature review and collection of experience to identify the state-of-the-art of LTO improvements (hardware and software) that may have an either beneficial or adverse impact on the results of PTS analysis. This includes the identification of technology gaps and the definition of possible improvements. Furthermore, the human factor relevant during a PTS event will be identified (and quantified) based on available operator experience and expert judgement.

The second part (WP2) will be extensive thermal hydraulic (TH) assessment, as it is one of the most important steps in the entire PTS analysis. The impact of LTO improvements and human factor on the results of TH analysis will be quantified and later assessed by subsequent structural and fracture mechanics benchmarks (WP3 and WP4). Moreover, the consideration of uncertainties in TH analysis (due to plant data, used computer codes and human factor) and their impact on the entire PTS analysis will be addressed.

The third part (WP3) will be deterministic structural and fracture mechanics analyses to quantify the safety margins (shown in fig. 1) related to LTO improvements and uncertainties in TH analysis. The analyses to be used for deterministic margin assessment will be carried out based on a common deterministic benchmark. This common benchmark will be defined based on the extensive benchmark provided by the NUGENIA+ project DEFI-PROSAFE, for which a solid validation and verification basis is available.

The fourth part (WP4) will be probabilistic margin assessment based on probabilistic fracture mechanics analysis. It allows the quantification of safety margins in terms of risk of failure, which becomes more and more important as conservative deterministic assessments are reaching their limits in demonstrating the safety of RPVs for LTO. An appropriate benchmark for the probabilistic fracture mechanics analysis will be defined based on the extensive benchmark provided by the NUGENIA+ project DEFI-PROSAFE and in accordance with the benchmark performed for deterministic margin assessment. An advanced probabilistic PTS assessment will be performed by considering the TH uncertainties in the subsequent structural mechanics and probabilistic fracture mechanics analyses. In addition, a link between deterministic and probabilistic margin assessment will be established.

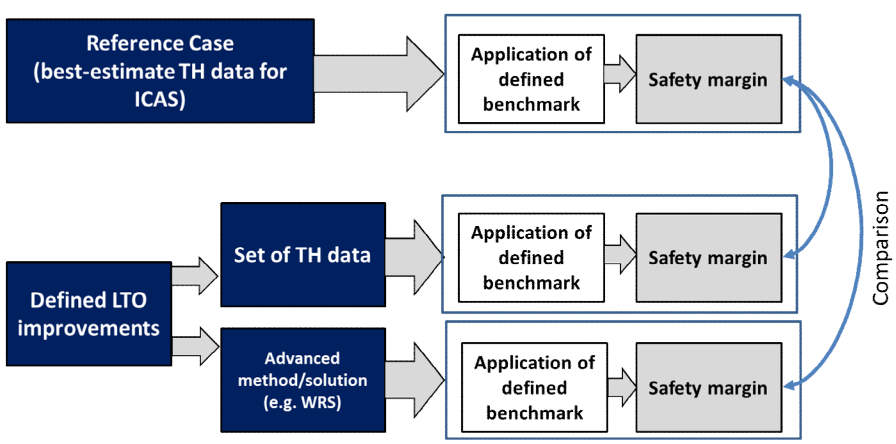

Figure 1: Determination of inherent margins related to LTO improvements

The fifth part (WP5) will gather recommendations and conclusions from performed work to define the best-practices for an advanced PTS analysis for LTO. Close cooperation with Advisory Board, regulatory bodies and end-users during the project will help to increase the acceptance of the best-practice guidance.

STATE-OF-THE-ART FOR PROBABILISTIC PTS ANALYSIS

As part of APAL's WP1, state-of-the-art for probabilistic PTS analysis has been identified. Therefore, a collection of experience on probabilistic PTS analysis and on tools and software currently used for probabilistic assessments has been performed. An overview of the different types of assessment for probabilistic PTS analysis used by the partners involved in the APAL project was gathered, including the following aspects of a probabilistic PTS analysis:

- Methods and software used for calculation of fast fracture initiation or reactor pressure vessel (RPV) failure probability including convergence criterion
- Methods for sampling of distributed parameters
- Summary of distributed input data and basis for distribution parameters
- Consideration of the whole spectrum of PTS scenarios
- Scope of the assessment and treatment of RPV loading
- Events considered (Initiation, Failure, Arrest)
- Fracture mechanics models used
- Overview of performed applications

In addition to the overview, further information and recommendations are given. This additional information covers several descriptions needed for better understanding of probabilistic assessments (e.g. description, advantages and restrictions of FORM/SORM). Also a simplified benchmark was performed to show the difference in the methods used for calculation of initiation or failure probability.

Methods and software used for probabilistic fracture mechanics

An overview of the different tools/software used by the different partners for probabilistic fracture mechanics in the scope of PTS assessment is given in table 1.

Table 1: Software/Tool used by APAL partner for probabilistic PTS analysis

Partner	**Tool/Software**	**Remark**
UJV	PROVER (in-house)	Based on FAVOR and adjusted for VVER
FRA-G	In-House	modular based
OCI/PSI/Tecnatom/JSI	FAVOR	v16.1
IPP	SIF-Master (in-house)	new version under development
KIWA	ISAAC	Probabilistic part = in-house
BZN	In-House	under development
IRSN	In-House	under development
JAEA	PASCAL	v4
GRS	PROST	

For probabilistic fracture mechanics it is common practice to use Monte-Carlo (MC) method for calculation of probability with the general approach, that each Monte-Carlo run gives either “failure” or “non-failure” and finally the probability of failure is simply the sum of failure runs divided by the total number of Monte-Carlo runs. For some tools (like FAVOR and PROVER) each Monte-Carlo run gives a probability of failure (or initiation), because fracture toughness and arrest toughness are not sampled, they remain as distribution resulting in a probability of failure (or initiation) per Monte-Carlo run. With this approach, mean value and standard deviation of failure and initiation probability related to aleatory uncertainties in fracture toughness and crack arrest are calculated. It should be mentioned, that the standard deviation related to these aleatory uncertainties is not an indicator for the convergence of the Monte-Carlo method.

The convergence of the Monte-Carlo method is an important issue that needs to be addressed as it provides information on how accurate the result is. In this context, the convergence of Monte-Carlo method is attained, if a sufficiently large number of runs are performed to get a stable result. Until now it is more or less common practice to arbitrarily select the number of Monte-Carlo runs based on the expected probability or on an allowable value for the probability. Convergence criteria are not typically used in many cases. To track run-time estimates of the convergence of the Monte-Carlo method, FAVOR and PROVER use visualization of the running-average and running coefficient of variation of the conditional probability of initiation (CPI) and failure (CPF) over the current number of Monte-Carlo trials as the solution evolves. It is recommended to address the convergence of a Monte-Carlo method by a quantification of the coefficient of variation, and/or standard error, of the MC result.

As probabilistic PTS analyses are mostly dealing with very low probabilities ($< 10^{-6}$), an appropriate random number generator is needed to ensure an adequate result not impacted by the limitation of the sequence of random numbers. The choice of appropriate random number generator is always a question of sufficient length of random number sequence and of computation time. Commonly used is the Mersenne Twister Algorithm and other self-made algorithms

The first-order and second-order reliability methods (FORM and SORM) are commonly used probability estimation methods. A brief description of both methods is given in deliverable D1.6. Besides the aim to calculate initiation or failure probability, FORM/SORM is also used for sensitivity study to quantify the impact of different input data and for Importance Sampling. If FORM or SORM is used to calculate the probability of initiation or failure for PTS analysis, some inherent uncertainties due to the method remain, see details in deliverable D1.6:

- Error in finding most probable point
- Goodness of first-order or second-order approximation
- Transformation into standard normal space by inverse sampling
- Approximation for limit state function with no closed solution

In addition to standard Monte-Carlo method, Monte-Carlo with importance sampling is a powerful method to reduce the number of MC runs needed for a given level of precision. The basic idea is, to sample the input data around the most probable point determined by FORM/SORM, i.e. neglecting most of the distributed input data, that might not contribute to failure probability. To compensate the adjusted sampling of input data, a correction of the weight of each contribution is necessary. A brief description of Monte-Carlo with importance sampling is given in deliverable D1.6.

Methods for sampling

For sampling of data from a defined distribution the following methods are commonly used:

- Sampling from (standard) normal distribution: Box-Muller transformation
- Sampling from log-normal distribution: Sampling the logarithm as normal distributed value
- Sampling from arbitrary distribution: Inverse transform method, i.e. $x = F^{-1}(p)$ with $F(x)$ distribution function and $p = U(0;1)$ uniformly distributed between 0 and 1

In order to ensure a representative covering of all possible sets of distributed input data, sampling methods like Latin hypercube sampling or orthogonal sampling can be used. This becomes important, when the number of distributed input data is large and both aleatory and epistemic uncertainties are considered in combination with a relatively low number of Monte-Carlo runs. For typical probabilistic PTS analysis with more than 10^6 Monte-Carlo runs and less than 10 sampled input data, a random sampling is sufficient.

If uncertainties in the input data are separated into epistemic and aleatory the combination of both uncertainties is needed for sampling the input data. For example, in PASCAL v4 a numerical integration method is used to combine epistemic and aleatory uncertainties for sampling of fracture toughness and crack arrest.

Events considered

An overview of the different events considered for a probabilistic PTS analysis is given in table 2.

Table 2: Events considered for a probabilistic PTS analysis

Partner	Software/Tool	Initiation (brittle/ductile)	Arrest/Re-Initiation	Failure
UJV	PROVER (in-house)	yes/yes	no	no
FRA-G	In-House	yes/yes	yes/yes	yes
IPP	SIF-Master (in-house)	yes/no	no	no
KIWA	ISAAC (in-house)	yes/yes	no	yes(1)
JAEA	PASCAL v4	yes/yes	yes/yes	yes
GRS	PROST	yes/no	no	no
OCI, PSI, Tecnatom, JSI	FAVOR	yes/yes	yes/yes	yes

(1): If initiation and failure are independent events

It is obvious that brittle crack initiation for PTS analysis is always considered as an event. Some tools are assessing only brittle fracture initiation, resulting in probability of initiation, which can be treated as conservative for RPV failure probability. If so, no benefit of possible crack arrest is considered, which leads to inherent safety margin in the RPV failure probability. As the intention of a probabilistic assessment is always to reduce inherent safety margin, it is not advisable to use brittle fracture initiation probability equal to RPV failure probability.

For the determination of RPV failure probability it is common practice to assess crack arrest and possible re-Initiation after arrest. This sequence of events should finally lead to stable arrest with no re-initiation (i.e. no failure) or failure of the RPV. Failure of the RPV is gained, if the crack reaches a pre-defined fraction of the RPV wall (e.g. 80%). The use of an appropriate pre-defined fraction should be verified (e.g. instability of remaining ligament). Nevertheless, it is common understanding that a value in the range of 75% to 90% is appropriate for PTS assessment. Moreover, some tools assess net-section collapse of the remaining ligament directly in addition to the use of a pre-defined fraction of the RPV wall.

Although a potential ductile fracture initiation might be of minor importance for a PTS analysis, it should also be taken into account. It becomes more important when crack arrest is considered, because crack re-initiation may occur in warmer regions of the RPV wall, where ductile initiation becomes more relevant. The consideration should be done either by explicitly considering ductile fracture initiation as an event in the probabilistic tool or by a case-specific evaluation of relevance of ductile fracture initiation by a deterministic approach.

Fracture mechanics models

The use of appropriate fracture mechanics models is an important aspect for PTS analysis, both deterministic and probabilistic ones. For probabilistic PTS analysis it is common practice to use the well-established fracture mechanics models from deterministic analysis, concerning especially the stress intensity factor solutions for the cracks of interest, limit load analysis for cracked structures and ductile crack growth. Fracture mechanics models like brittle or ductile fracture initiation or crack arrest are more or less related to the distributions used for the material properties. The use of different fracture mechanics models (e.g. stress intensity factor solutions or limit load solutions) has an impact on both deterministic and probabilistic results. It is common understanding that several solutions are adequate for the case of interest, but with different amount of inherent margin.

Treatment of loading

Temperature and stress calculations (3D or 1D) are usually pre-processing assessments for probabilistic PTS and it is common practice to transfer transient temperature and stresses over wall thickness at relevant location to probabilistic fracture mechanics.

Most tools are assessing a single location of the RPV (e.g. core weld) with a representative stress and temperature distribution at that location. Only FAVOR, PROVER and FRA-G In-house tool assess the whole beltline region, but with different approach on loading:

- FAVOR and PROVER splits the beltline region into sub-regions with individual properties like chemistry, flaw population. But, the loading condition is the same for all sub-regions.
- With the FRA-G In-house tool it is possible to combine results representative for various sub-regions of the RPV to an overall RPV result. With this approach it is also possible to address different loading conditions for the different sub-regions.

The consideration of cold plume effect for probabilistic PTS analysis is done in many different ways. For the most commonly used tools with 1D Finite Elements (FE) calculations, the use of coolant temperature and heat transfer coefficient in cold plume from mixing calculations leads to appropriate temperature for inside cold plume. But with 1D FE calculation it is not possible to determine thermal stresses in the region of the plume accurately. Using this simplified approach is realistic from the temperature point of view and non-conservative from stress point of view for plume region. It is conservative from both temperature and stress point of view for outside of plume region. The overall conservativeness of this approach is questionable. There are some methods and adjustments that can be used to ensure bounding stresses for cold plume region, but these methods and adjustments need to be verified and inherent margins remain. The common practice to calculate appropriate stresses inside the plume region is to use a 3D FE method with input from mixing codes or fluid dynamics analysis.

Distributed Parameters and flaw distribution

In general, there exists a common understanding which kind of distribution to be used for which kind of data. An overview for the most important input data is given in table 3.

Table 3: Distribution used for most important input data

Input data	**Symbol**	**Distributed**	**Distribution**
Neutron fluence	f	Mostly yes except SIF-Master, ISAAC	Normal
Chemical composition	Cu, P, Ni, Mn	Mostly yes except ISAAC	Normal
Reference temperature	RT_{NDT} or T_0	yes	Normal
Fracture Toughness	K_{IC}	yes	Mostly Weibull IPP, FRA-G: normal based on ASME K_{IC}
Upper shelf (ductile) crack initiation	J_{IC}	Mostly yes except SIF-Master	Normal
Crack arrest	K_{Ia}	FAVOR, FRA-G, PASCAL v4 (1)	Lognormal

(1): Only FAVOR, FRA-G In-House and PASCAL v4 are assessing crack arrest

Concerning postulated flaws it is common practice to assess inner surface (trough clad), embedded and/or underclad cracks. An overview of the different flaw types assessed by the different tools is given in table 4.

Table 4: Type of flaws to be assessed

	Surface cracks	**Underclad cracks**	**Embedded cracks**
PROVER	no	yes	yes
FAVOR	yes	no	yes
ISAAC	yes	no	yes
SIF-Master	yes	yes	yes
FRA-G in-house	yes	yes	yes
PASCAL4	yes	yes	yes
PROST	yes	no	no

The general approach for flaw size distribution is as follows:

- Flaw depth: log-normal or exponential distribution
- Flaw length: log-normal or exponential distribution

When multiple flaws are assessed (FAVOR, PROVER and FRA-G In-house) flaw density and flaw orientation distribution is also required:

- Orientation: Uniform
- Density of surface and underclad cracks: Exponential distribution
- Density of embedded cracks: Poisson distribution

If multiple flaws are simulated in a probabilistic PTS analysis the interaction of the adjacent flaws is currently not considered.

SIMPLE BENCHMARK

To compare the functionality and the results of the different methods (Monte-Carlo, FORM and SORM), a simple benchmark problem has been defined. The randomly sampled input parameters are the crack depth a and the fracture toughness K_{IC}. The parameters are assumed to be normally distributed, since FORM/SORM algorithms can only be applied to normally distributed parameters. The stress intensity factor is calculated with the simple formula $K_I = \sigma\sqrt{\pi \times a}$. The stress σ is assumed to be constant over wall thickness (pure membrane). Crack initiation occurs if $K_I > K_{IC}$. Two example problems have been assumed, as shown in table 5. A stress variation over time was considered with a maximum of σ_{max} = 205.9 MPa. Two different types of Monte-Carlo assessment have been applied:

- Standard MC = randomly sampled values of a and of K_{IC} and each MC runs gives initiation “yes” or “no”
- FAVOR MC = randomly sampled values of a and determination of probability for each MC run by determination of percentile of K_{IC} for applied K_I

Table 5: Examples for simple benchmark

	Crack depth a (m)		Fracture toughness K_{IC} (MPa√m)	
	Mean	Standard dev.	Mean	Standard dev.
Example 1	0.01	0.003	80	20
Example 2	0.03	0.0003	65	0,2

The results for the two example cases are shown in table 6, with initiation probability in the order of 10^{-2} for example 1 and 10^{-4} for example 2. For example 2, the result from standard MC seems not to be fully converged due to insufficient number of MC runs.

Table 6: Results for simple benchmark

	MC runs	Standard MC	FAVOR MC	FORM	SORM
Example 1	100000	1.73E-02	1.70E-02	1.77E-02	1.76E-02
Example 2	200000	2.75E-04	2.87E-04	2.83E-04	2.82E-04

The influence of convergence/error and random number generator on the results of the Monte Carlo method has been investigated in additional examples.

Convergence analysis for standard Monte Carlo method

The biggest drawback of standard Monte Carlo method is the large number of simulations needed for a sufficiently accurate result. Depending on the complexity of the problem, this can result in long runtime. To investigate the error and convergence of the Monte Carlo method additional example cases were investigated with an a-priori defined sufficiently large number of MC runs, see table 7. Error bands of the standard MC are calculated by (CPI_i is the failure probability in the i-th simulation):

$$e_i = \sqrt{\frac{(i \times CPI_i + 2) \times [i \times (1 - CPI_i) + 2]}{(i+4)^3}} \tag{3}$$

Table 7: Additional examples for simple benchmark

	MC runs	Crack depth *a* (m)		Fracture tough. K_{IC} (MPa√m)	
		Mean	Standard dev.	Mean	Standard dev.
Example 3 – high CPI	$50 \cdot 10^6$	0.03	0.001	85	15
Example 4 – small CPI	$200 \cdot 10^6$	0.03	0.001	80	4

The results for example 3 are shown in Figure 2. It can be seen, that FAVOR MC converges much faster than standard MC. After approximately 6 million simulations the expected result of 5.82×10^{-2} lies within the calculated error band of standard MC method. At the end, after 50 million simulations the standard MC method converges to the result of FAVOR MC. The FORM and SORM results lie a little bit higher than the MC results. This is because FORM and SORM are less exact for high failure probabilities.

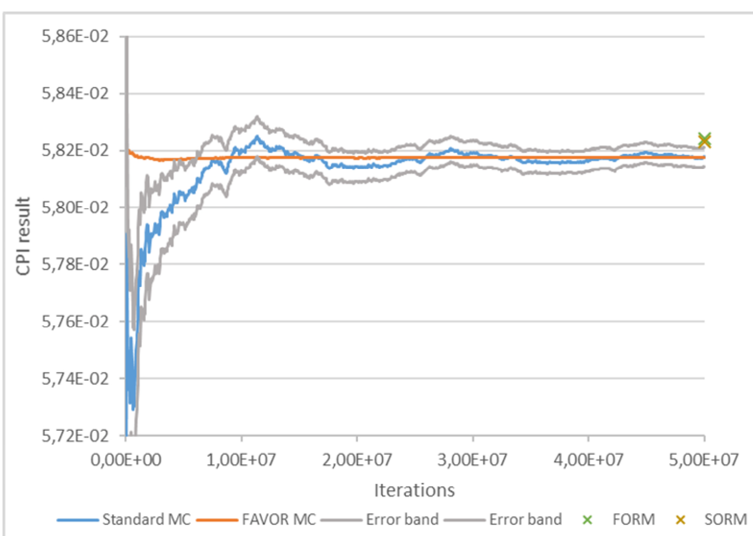

Figure 2: Convergence of MC – example 3

The results for example 4 are shown in Figure 3. The FORM and SORM results agree better with the FAVOR MC result than in the example 3 with higher CPI. Moreover, the Standard MC shows some periodic behaviour which is due to the limitation of the random number generator (EXCEL's Rnd() has been used). Even for further increased number of simulations the Standard MC will not coincide with expected CPI of 3.3×10^{-6} due to the repetitiveness of the random number sequence.

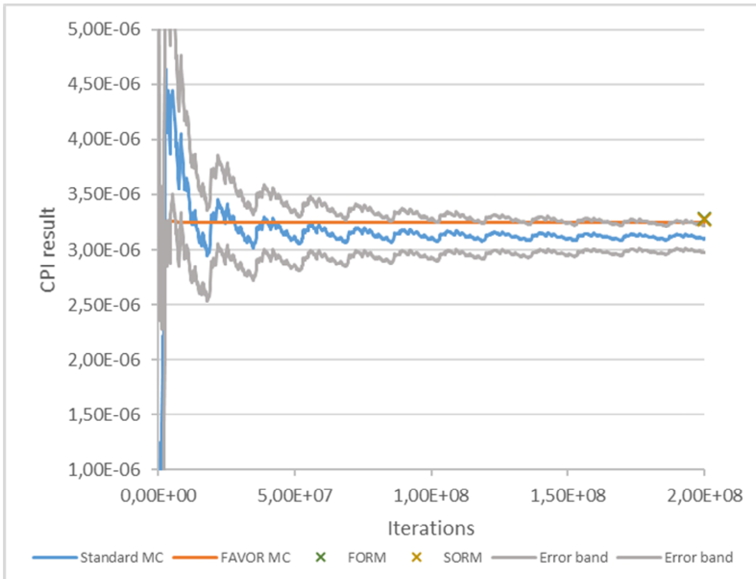

Figure 3: Convergence of MC – example 4

Influence of random number generator

The importance of an appropriate random number generator has been demonstrated for example 4 (see Figure 3). Therefore, example 4 has been repeated with a better random number generator. The Mersenne Twister algorithm has been selected. The results of the standard MC method with the Mersenne Twister random number generator are shown in Figure 4. With the appropriate random number generator, it can be seen that standard MC is in good agreement with the other solutions from 80 million MC runs on.

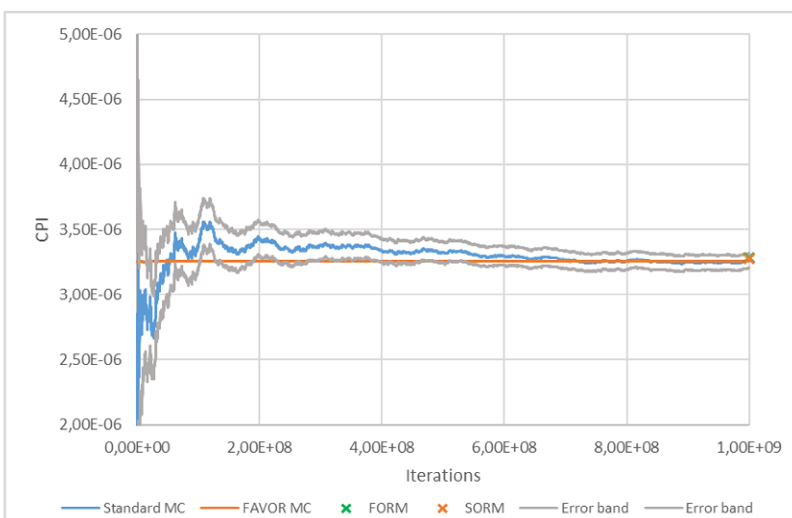

Figure 4: Convergence of MC with Mersenne Twister – example 4

CONCLUSIONS

Based on the performed work within WP1 of APAL project conclusions on state-of-the-art for probabilistic PTS analysis were drawn:

- It is common practice to use Monte-Carlo method for probabilistic PTS analysis, but other methods like FORM/SORM are also used, although some restrictions or uncertainties remain when using such probability estimation methods for PTS analysis.
- Important aspects for the use of Monte-Carlo method are convergence criteria and random number generators to ensure a stable solution.
- There exists a common understanding on the type of distributed parameters used for probabilistic PTS analysis and on sampling methods.
- For the events considered in a probabilistic PTS analysis it is obvious to take brittle crack initiation into account. The determination of RPV failure including crack arrest, re-initiation and ductile initiation or ductile crack propagation within a probabilistic PTS analysis is still challenging, but becomes more important in future assessments.
- The different treatment of loading by the different tools used is an important aspect to consider, when comparing and interpreting results. The common practice to calculate appropriate stresses inside the plume region is to use a 3D FE method with input from mixing codes or CFD analysis.
- Considering flaws in the RPV there are mainly two approaches used: Either based on a single flaw postulated at region of highest loading and highest embrittlement or the assessment of multiple flaws distributed in the RPV wall.

Some of the aspects identified will be further investigated within the APAL project in the upcoming work packages.

ACKNOWLEDGEMENT

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NOMENCLATURE

CPF	Conditional Probability of Failure
CPI	Conditional Probability of Initiation
FE	Finite Elements
FORM	First Order Reliability Method
LTO	Long-Term Operation
MC	Monte-Carlo
PTS	Pressurized Thermal Shock
RPV	Reactor Pressure Vessel
SORM	Second Order Reliability Method
TH	Thermal Hydraulic
WP	Work Package

REFERENCE

APAL Deliverable No. D1.6, Cueto-Felgueroso C. et al., (2021). *Public Summary report of WP1*