Transactions of the SMiRT 27
Yokohama, Japan, March 3-8, 2024
Division VII

PROBABILISTIC MODELING OF PRESSURIZED THERMAL SHOCK

Fabio Pasti[1]

[1] Mechanical Engineer, NRG, Petten, Netherlands (pasti@nrg.eu)

ABSTRACT

A pressurized thermal shock (PTS) is the occurrence of a sudden and catastrophic cleavage fracture in the reactor pressure vessel (RPV) of a pressurized water reactor (PWR). Thick-walled RPVs, particularly those with fractures and weak welds, are vulnerable to dangerous situations due to low temperatures, thermal strains, and radiation embrittlement. A comprehensive understanding of temperature and stress intensity is necessary to determine the probability of a cleavage crack developing and spreading. The critical stress intensity for brittle cleavage fracture is influenced by the ductile to brittle transition temperature. A complex interplay of loads, temperatures, and temperature gradients, combined with radiation damage, is considered to assess the likelihood of cleavage fracture. (IAEA, 2005) The PTS phenomenon can be more complex in multi-loop reactors, as the coolant is distributed through multiple loops with their own pumps, heat exchangers, and pressurizers. Although in multi-loop reactors, the likelihood of high local thermal stresses can be reduced due to the existence of multiple ECC systems distributed over the reactor circumference, the interaction between the cold plumes of ECC systems can influence the temperature field and hence the stress distribution on the RPV wall.

INTRODUCTION

PTS is a Pressurized Water Reactor (PWR) accident scenario, as described by Boyd (2008). When water is under high pressure and a heated reactor pressure vessel (RPV) is suddenly cooled, high mechanical loads might result at relatively low temperatures. This can increase the likelihood of cleavage fracture starting.

A thermal-hydraulic model can be used to obtain the cooling transient with some conservatisms; the coolant must flow as much as feasible while being under the greatest pressure and lowest temperature. Even so, buoyancy-induced forces still predominate the fluid flow in cold legs during a non-symmetric cool-down. This may cause significant temperature gradients in the tangential direction of the RPV. Previous numerical and experimental studies by Versteylen at all (2020 and 2022) have shown that the local thermal gradients and stresses generated during a PTS accident can cause cracking in the reactor vessel and other components. It is, therefore, necessary to comprehend the spatiotemporal behaviour of the RPV temperature in order to identify the high-risk areas for fracture development. A thorough thermo-hydraulic study of such reactors may be used to gain this information.

In the context of PWR accidents, the focus of this year activities is on advancing thermal-hydraulic models. This year, 2 main models are shown: a 3D deterministic model that includes a CFD (computer fluid dynamic) and a FEM (finite element method) analysis and a 1D model named PETO which ultimate goal is to employ a thermal-hydraulic approach to simulate the cooling transient with conservatisms.

The 1D model form the foundation for a probabilistic assessment using a Monte Carlo-based approach. The goal is a better understand of the spatiotemporal behavior of the RPV in a PTS scenario. This analysis is crucial for identifying high-risk areas susceptible to fracture development. The implementation of PETO signifies a step towards a more comprehensive analysis of potential scenarios. This approach ensures the accuracy of our simulations, allowing for a nuanced comprehension of the interplay between thermal gradients, stresses, and reactor vessel integrity. The likelihood of cleavage crack initiation is evaluated with a Master Curve as presented by IAEA (2005).

The remnant ductility at a temperature in the irradiation condition can be assessed using the Reference Temperature for Nil Ductility Transition RT_{NDT}, specified in ASME Section III, which describes the procedures to get the RT_{NDT} from the Nil Ductility Transition (NDT). This information is utilized as input in the Master Curve for brittle cleavage fracture propagation and arrest, along with a few conservative restrictions.

RPV MECHANICAL BEHAVIOR MODELLING USING FEM (DETERMINISTIC)

To evaluate the integrity of the RPV, thermomechanical analyses are conducted, focusing on hypothetical cracks within the structure. A comprehensive CFD simulation is employed to capture all large-scale turbulent fluid features, as shown in Figure 1.

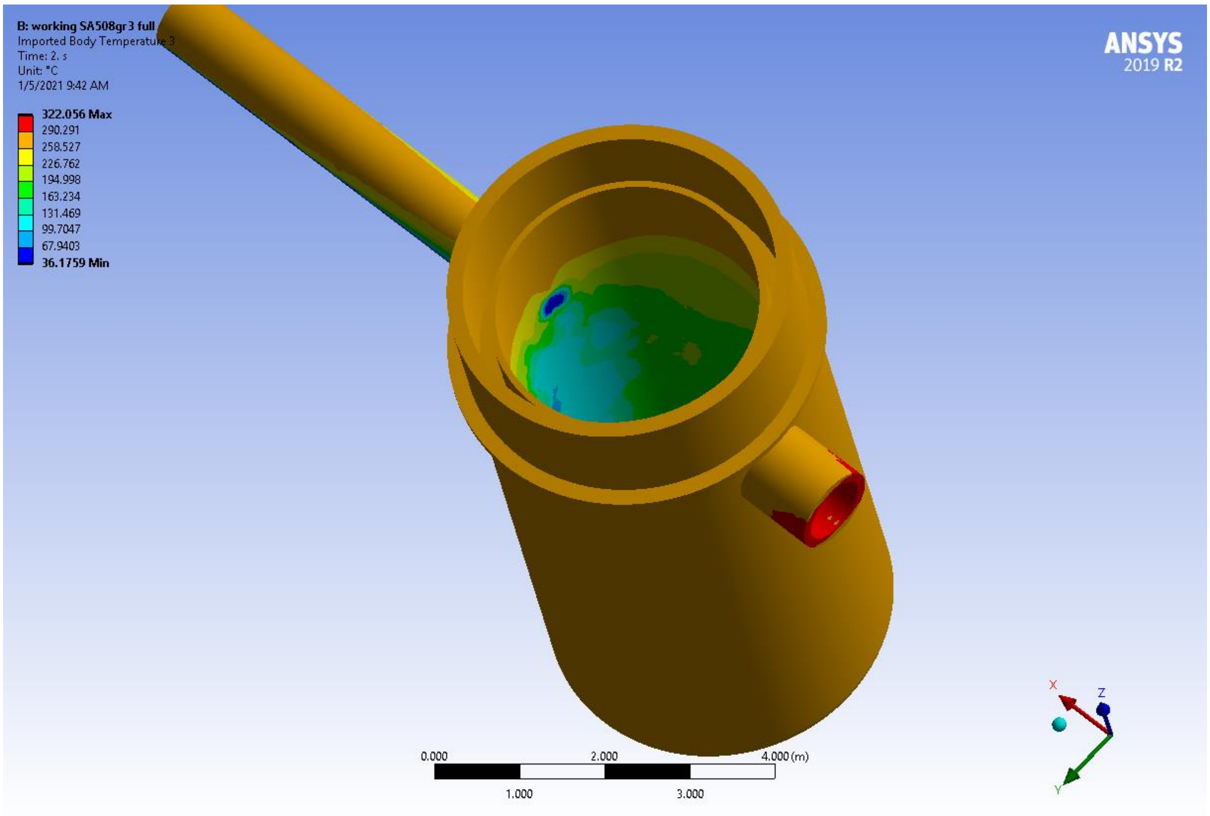

Figure 1. The temperature imported in the full 360 model, the model includes the RPV and inner barrel, temperature profile visualized for time 150 seconds in the transient.

Temperature data is transferred to a designated model containing the crack, provided the model is expansive enough to avoid crack-boundary contact. At each time step, a specific temperature distribution is imported, resulting in a unique thermal stress distribution.

Earlier research by Uitlag-Doolard et all (2020) validates J-integral trends, prompting a consideration of a limited number of time steps. In adherence to ASME code recommendations, a semi-elliptical postulated crack is introduced at the center to represent cracks of unknown actual size.

The assumed crack is positioned directly under the nozzle, based on findings that indicate this location corresponds to maximum J-integral values in a one-loop PWR. The postulated crack adheres to ASME-suggested values, with a depth one-quarter of the wall thickness and a length of 3/2 of the wall thickness.

Stress intensity is calculated using a J-integral path approach and the plain stress assumption, as expressed in Equation (1):

$$K_J = \sqrt{\frac{J_i \cdot E}{1 - \upsilon^2}} \quad (1)$$

The combination of stress intensity at the crack tip and temperature at the crack tip enables the determination of the probability of cleavage initiation using the Master Curve. Equation (2) expresses the critical stress intensity for a certain probability of cleavage initiation:

$$K_{Jc} = 20 + \left[11 + 77exp(0.019(T - T_0)) \cdot \left(\frac{25.4}{B}\right)^{\frac{1}{4}} \left(ln\left(\frac{1}{1-P_f}\right)\right)^{\frac{1}{4}} \right] \quad (2)$$

The critical stress intensity (K_{jc}), temperature (T), reference temperature related to the ductile-to-brittle transition temperature (T_0), wall thickness (B), and probability (P_f) are used to calculate the critical stress intensity at a specific location. The finite element method (FEM) calculations are performed using Ansys software, and the geometry is designed with SpaceClaim. The temperature steps from the larger CFD model are applied to the model, and appropriate constraints are placed on the edges. Tetragonal quadratic elements are used to mesh the sub-model and the larger model for comparison. For these simulations, SA-508gr.3's material attributes were utilized as done by Versteylen (2020).

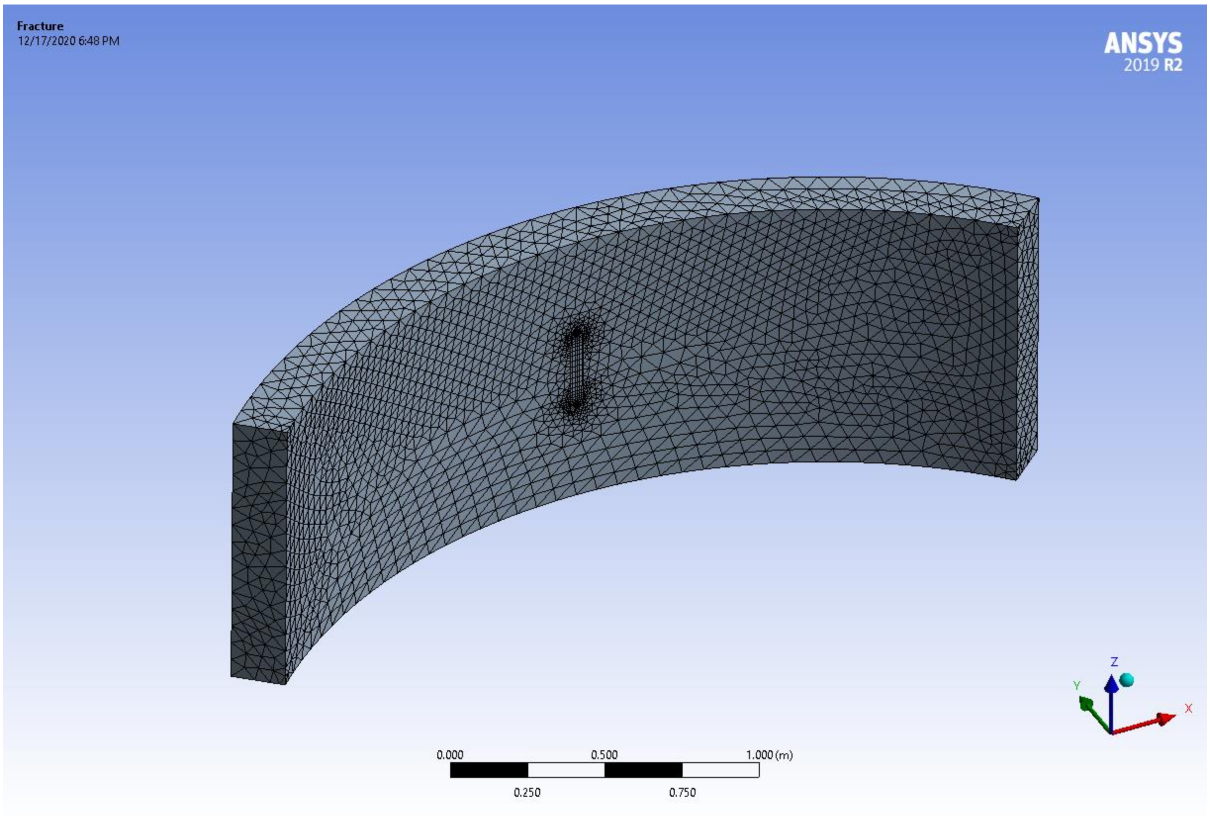

Figure 2. The mesh of the sub-model containing a postulated crack.

The cracks are positioned at points of maximum stress concentration, where, for each time-step, the crack tip exhibits the highest J-integral values. The location and size of these J-integral maxima vary over time. Due to the greatest thermal gradient occurring at the inner surface of the RPV, there is a notable level of thermal stress. However, the absolute maximum is closer to the center of the crack front, corresponding to higher temperatures.

The FEM calculations are executed on the model, incorporating a temperature gradient determined through CFD. Consequently, each time step involves a static structural computation. An illustration of one such computation is depicted in Figure 6.

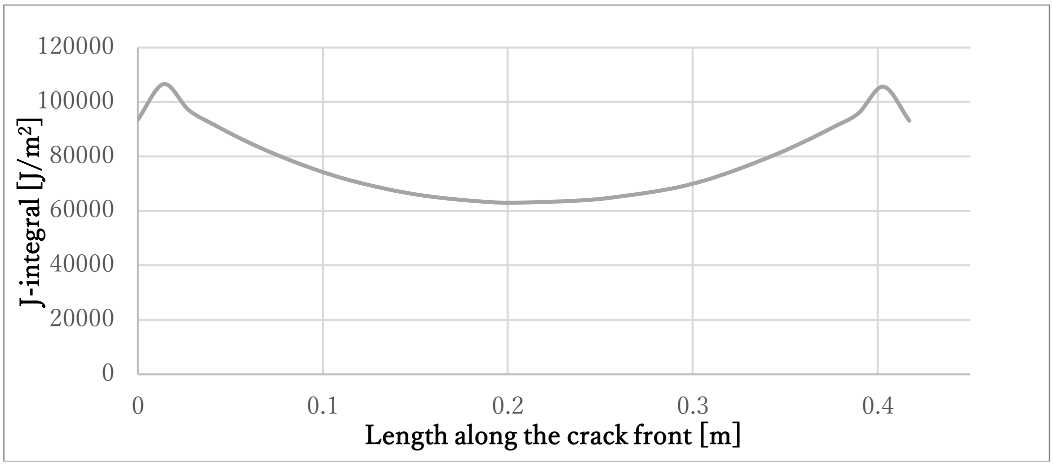

Figure 3. Example of a J-integral path integral curve (time of 300 seconds of the transient)

The J-integral fit, see chapter 2.1, can be used to predict the maximum K_{Jc} as function of the temperature. The fit of the J-integral has been multiplied by 1.5 % in order to capture the eventual fluctuations of the J-integral.

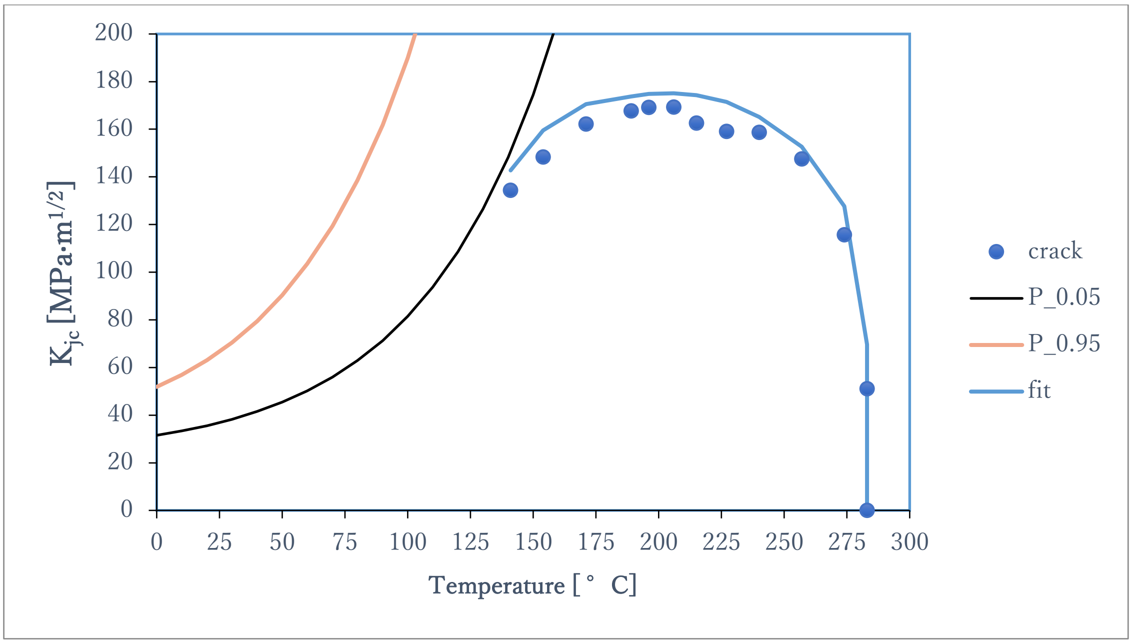

Figure 4. The Master Curve applied to the probability for cleavage fracture initiation for the deeper and more shallow crack.

The probability for fracture increases as the temperature decreases, which means that the highest estimated probability occurs at the end of the transient. In this case that temperature is 120 °C.

1D MODEL - RADIATION EMBRITTLMENT

The main parameter that describes the material irradiation is called ductile-to-brittle transition temperature, which in this document is denoted by RT_{NDT}. This is the temperature at which a material behaviour changes from ductile to brittle when the temperature drops. This phenomenon is especially important for metallic materials. The ductile-to-brittle transition temperature varies based on the chemical and structural qualities of the material. High carbon content materials, such as carbon steel, generally have a greater transition temperature, whereas low carbon content materials, such as stainless steel, have a lower transition temperature.

The ductile-to-brittle transition temperature of materials can be considerably influenced by neutron irradiation. When materials are exposed to neutron irradiation, the neutrons can interact with the atomic structure, causing atoms to be displaced and various forms of defects to occur, such as vacancies, interstitials, and dislocations. The presence of these imperfections can modify the material's mechanical properties, particularly its transition temperature. Irradiation with neutrons tends to raise the transition temperature, moving it to higher values. This is generally known as the "neutron embrittlement" effect. An increase in ductile-fragile transition temperature is particularly dangerous because it makes brittle behaviour possible at temperatures close to atmospheric temperatures, which is the temperature range at which the various maintenance or reactor safety operations take place. In other words, the higher the value of the RT_{NDT} the higher the value of Conditional Probability of Initiation (CPI).

To obtain the value of RT_{NDT} and consequently the master curve, the first step is to calculate the reference temperature T_0. Usually, T_0 is a reactor-specific parameter that must be determined by Charpy testing of the materials used in the RPV. For the purpose of developing and testing the PETO code, a model derived from Charpy tests conducted on WF-70 welds was used to get the T_0 value, as proposed by Yoon (2000). WF- 70 welds are relatively copper-rich welds that have been made available for testing in order to obtain fracture toughness data. The reference temperature can be obtained by fitting the results contained in table 1. The resulting expression of the reference temperature as a function of the neutron fluence is

$$T_0 = [1 - exp(C_1 \cdot f)] \cdot (C_2 \cdot f + C_3) + C_4 \tag{3}$$

where C_1 through C_4 are constants and f is the neutron fluence. From the T_0 value obtained, it is necessary to derive an alternative reference temperature for unirradiated materials, RT_{NDT0} . This new reference temperature is defined, according to ASME Code Case N-629 as T_0 + 19.4◦C, as shown by William et all (2016).

Due to neutron irradiation, as mentioned above, RT_{NDT0} shifts to higher temperatures. This temperature shift is a function of several parameters such as the neutron fluence and the RPV chemical composition. The study of the transition temperature shift is a particularly complex subject both from the point of view of the physical phenomena involved and in terms of practical study. Various ways exist to estimate this shift, and the one used was derived from a database of Charpy shift values, based on the nickel, copper and phosphorous sampled content in wt% respectively, is the neutron fluence $f_0(r)$ at the r position from the inner surface and on the exposure time.

The RT_{NDT} calculation is uncertain both due to aleatory and epistemic causes. The former are simply due to the material variability. While the latter is mainly due to the conservative definition of RT_{NDT}. Because of epistemic uncertainty, the actual fracture-toughness transition temperature is virtually always overestimated. Therefore, the epistemic uncertainty can be sampled from a Weibull distribution and eventually the reference transition temperature can be expressed as

$$RT_{NDT} = RT_{NDT0} - \Delta RT_{epi} + \Delta RT_{NDT} \tag{4}$$

1D MODEL - PROBABILISTIC APPROACH

The deterministic model that results in the instantaneous conditional probability of initiation CPI(t) time evolution, has many inputs that can actually vary. In fact, in addition to ΔT_{epi}, with its Weibull distribution, there are other parameters such as the chemical properties of the materials that are not necessarily constant throughout the vessel. In order to obtain a more accurate result from the deterministic model, these inputs can be replaced by probability distributions. In doing so, each time the deterministic model is run, several parameters are randomly extracted each time. This consequently leads to a distribution of the final results.

A probabilistic tool functions as a shell on an existing deterministic tool. This is because the probabilistic tool can be used for any deterministic tool. The probabilistic method implemented is a Monte Carlo method due to the possibility of randomly extracting parameters for each iteration. The relation which calculates the transition temperature shift can be written as

$$\Delta T30\left(\widetilde{Ni},\widetilde{Cu},\tilde{P},f_0,t_{ex},T_c\right) = A\ exp\left(\frac{19310}{Tc+460}\right)\ (1\ +\ 110\ \cdot \tilde{P})f_0(r)^{0.4601}\ +\ B(1\ +\ 2.4\tilde{N}i^{1.25}\ )\ f(\widetilde{Cu})\ g(f_0(r))\ +\ Bias \quad (5)$$

where the tilde above a variable indicates that it is a randomly sampled value.
The output resulting from each iteration is the CPI(t) time evolution. Out of each time evolution, it is possible to extract the highest value during the transient as

$$CPI_i = \{cpi_i(t^m)\} \qquad for\ 1\ \leq\ m\ \leq\ n \quad (6)$$

where $CPI_i(t)$ is the instantaneous conditional probability of initiation time evolution obtained in the i-th iteration and n is the number of time steps in the transient. After the iterative process, the final result of the Monte Carlo simulation carried out in the PETO code is the value of the conditional probability of initiation for the postulated crack type. This value is obtained by averaging the values obtained after each iteration as shown below

$$CPI = \frac{\sum_{n=0}^{\infty}(CPI_i)}{n} \quad (7)$$

where n is the number of iterations and CPI_i is the conditional probability of initiation computed in a single iteration. If this calculation and extraction procedure is repeated a large number of times, it is possible to see that the results will converge towards a final result. The number of iterations is strictly related to the accuracy desired. In fact, the higher the accuracy the higher the number of iterations necessary. The problem related to a high number of iterations is the computation time needed to carry out the whole calculation.

1D MODEL - DEMOSTRATION CASE

The PETO 1D code consists of two parts: deterministic (to be implemented) and probabilistic. The output data from the deterministic part serve as input for the deterministic part whose ultimate purpose of this first PETO code version is to calculate the CPI. It should be pointed out that several simplified assumptions have been made, especially in the simulation of the deterministic part of the code in order to optimise calculation times. In fact, the main objective of this project is the creation of a functioning logical structure for future developments involving the implementation of more accurate models. The main function of the deterministic part of the code is to generate physically plausible inputs for the fracture mechanics analysis module.

In this demonstration case the crack type selected has been the axial crack on the internal wall. In the following figure, the letters "A" and "B" are referred to the crack points as shown in figure 5. The simplified analysis results in the K_i shown in figure 5.

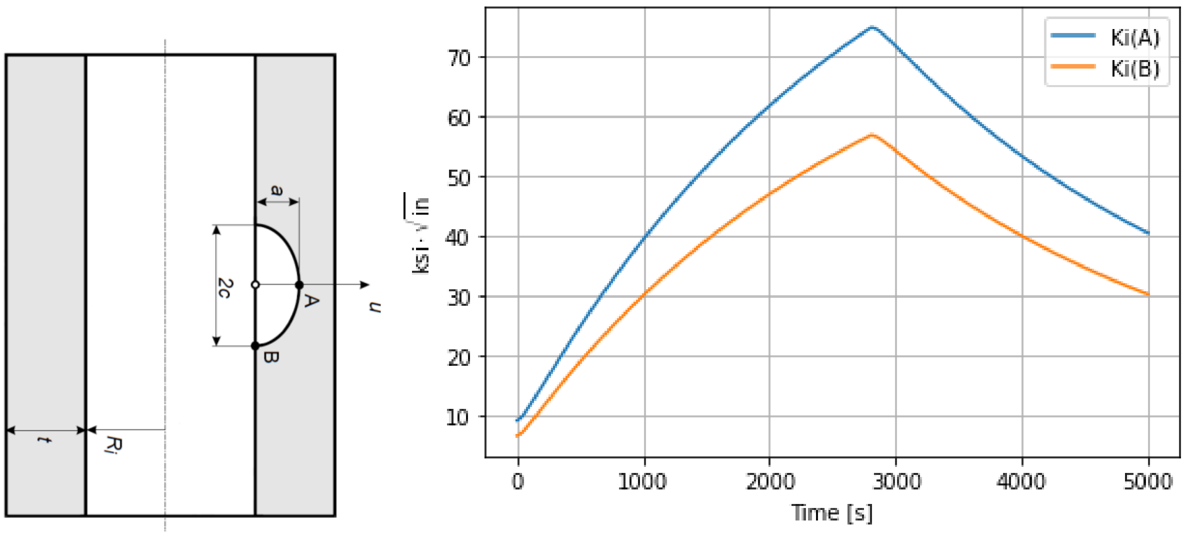

Figure 5. K_i time evolution

As expected from the theory the stress intensity factor is higher at the point "A". It is important to highlight the trend this parameter has. The following figure shows the resulting reference transition temperature distribution resulting after the iteration process.

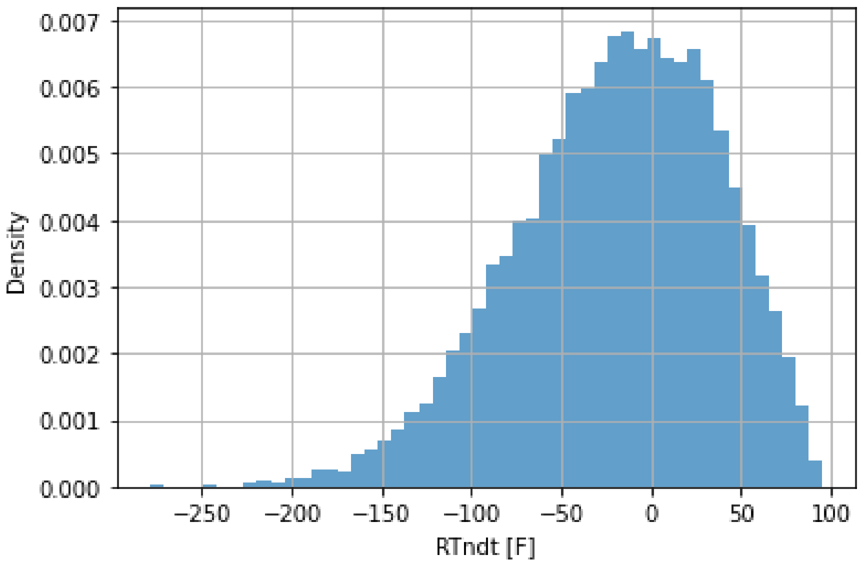

Figure 6. RT_{NDT} values from Montecarlo

The RT_{NDT} distribution shown in Figure 6 is derived by applying the procedure described in the previous section.

The next three figures show how the PETO code calculates the CPI value during each iteration. Once the various parameters necessary for the calculation of RT_{NDT} have been randomly extracted using equation 5, as mentioned in the previous section, it is possible to obtain the fracture toughness evolution.

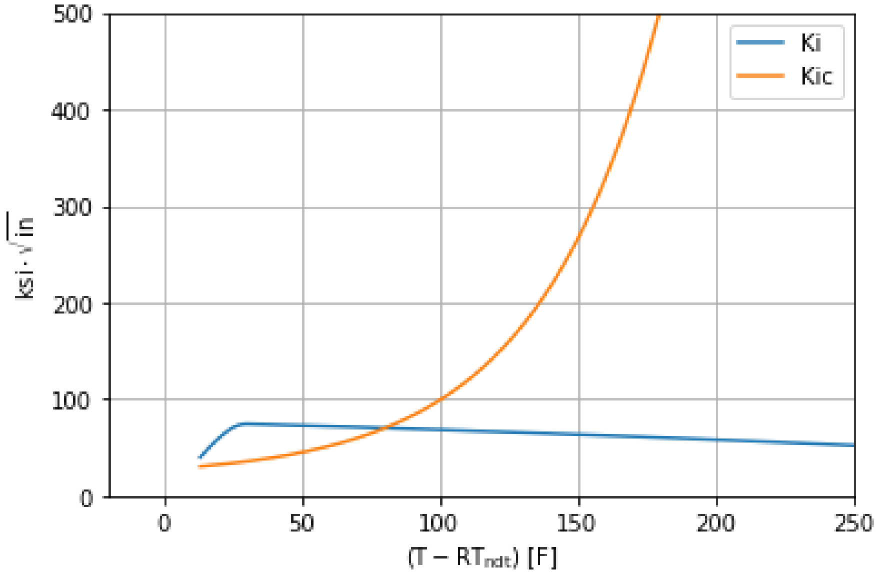

Figure 7. Time evolution of the stress intensification factor and the fracture toughness represented as a function of the temperature difference between the crack and RT_{NDT}.

By simply looking at the step, it is possible to see whether the CPI value becomes greater than 0 during the transient. This is possible simply by referring to the first of the two listed criteria which states that CPI > 0 if $K_i > K_{ic}$.

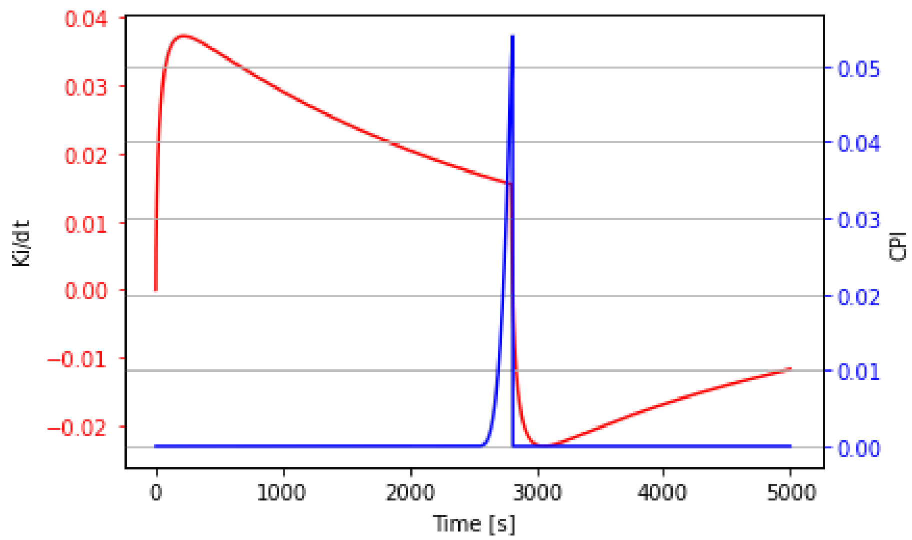

Figure 8. CPI and K_i gradient time evolution

The time evolutions of CPI and K_i's gradient are shown in the graphs above. Both have been represented because according to the second criterion considered in LEFM de the K_i gradient is negative CPI = 0. In fact, as we can see in Figure 25, around 2800 seconds when the gradient becomes negative, the value of CPI goes to zero. As also explained above, the value extracted at the end of each iteration will be the maximum value assumed during the simulated transient. In this case, the value obtained in the single iteration reported is CPI_i = 0.05. The following histogram shows the final output resulting from the demonstration case.

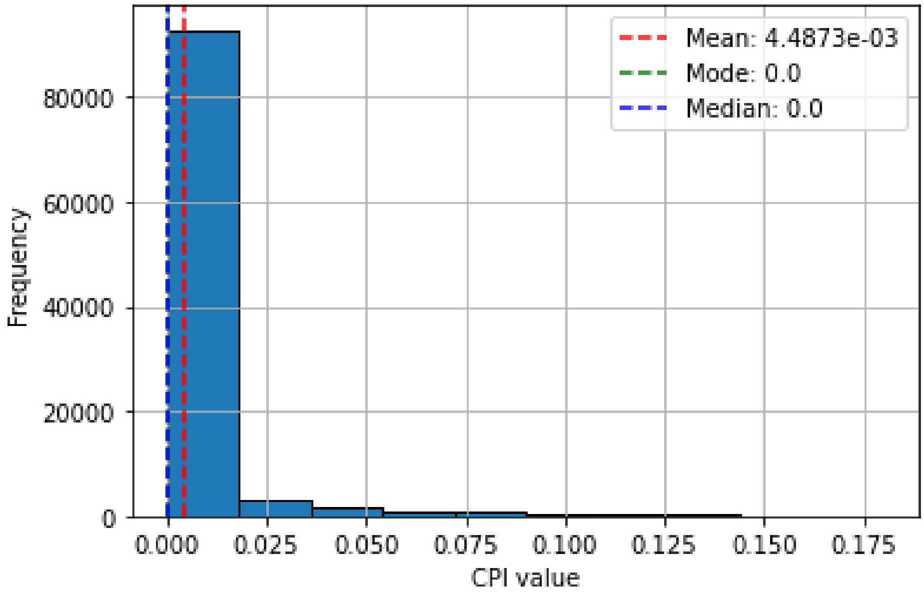

Figure 9. CPI values from Montecarlo

More specifically, in Figure 9 the distribution of probability values is shown. It is clear how the vast majority of the iterations returned CPI_i values very close or equal to zero. In fact, the mode of the distribution is zero as reported in the plot. Finally, in this particular demonstration case with the above-presented input parameters, the probability is CPI = 0.022.

CONCLUSION

In conclusion, this paper introduces a two-part approach: a deterministic 3D model that includes CFD and FEM followed by a simplified 1D probabilistic model based on assumed conditions.

This paper shows the first steps for developing the probabilistic approach in PTS analyses for NRG. The results shown in the demonstration case highlight how this code can be used to analyse many different situations in a short time. This version of PETO is and will be the basic structure for subsequent and more sophisticated versions of the code. For the time being, the current version of the code processes an input describing the evolution of coolant temperatures during a transient. . It should be mentioned that numerous simplifying approximations were used in the development of this version of the PETO code, due to the complexity of the phenomena studied any case, the simplifications made are to be considered conservative.

The future direction involves developing a concise 1D code that mirrors the 3D model and integrating it with the probabilistic component. Additionally, there is a plan to expand the study by incorporating a thermo-hydraulic model for a more comprehensive analysis. This multi-dimensional strategy aims to enhance understanding and application in various domains, paving the way for more sophisticated modeling and simulation in the future.

REFERENCES

Boyd, C., "Pressurized Thermal Shock, PTS," *THICKET,* pp. 463-472, (2008).

IAEA, "Guidelines for Application of the Master Curve Approach to Reactor Pressure Vessel Integrity in Nuclear Power Plants," VIENNA, (2005).

Server W. and others. “Application of Master Curve Fracture Toughness for Reactor Pressure Vessel Integrity Assessment in the USA”. In International Journal of Pressure Vessels and Piping: 79.8 (2002), pages 701–713.

Versteylen, C., Uitslag-Doolaard, H., Stefanini, L. and Blom, F. "A combined CFD and FEM analysis of pressurized thermal shock applied to the probabilistics of cleavage fracture," *Procedia Structural Integrity*, vol. 28, pp. 1918-1929, (2020).

Versteylen, C., Siccama, N.B., Uitslag-Doolaard, H., Brigante, F., Pallaoro, E. and De Haan-De Wilde, F.H.E., "Towards a Probabilistic Analysis of Pressurized Thermal Shock," *Pressure Vessels and Piping Conference,* (2022).

Uitslag-Doolaard, H., Stefanini, L., Shams, A. and Blom, F., "Numerical Prediction of a Single Phase PTS Scenario for the Crack Assessment in an RPV Wall," in *International Congress on Advances in Nuclear Power Plants (ICAPP 2019),* Juan-les-pins, (2019).

Williams, P.T., Dikson, T.L., Bass, B. and Klasky, H., "Fracture Analysis of Vessels – Oak Ridge FAVOR, v16.1, Computer Code: Theory and Implementation of Algorithms, Methods, and Correlations," Oak Ridge, ORNL/LTR-2016/309, (2016).

Yoon, K.K., “A Direct Fracture Toughness Model for Irradiated Reactor Vessel Weld Material Based on Reference Temperature”. In *Nuclear Engineering and Design*: 198.3 (2000), pp.253–259.