RAVEN/OSCAR-Fusion COUPLING FOR ACTIVATED CORROSION PRODUCTS ASSESSMENTS, SENSITIVITY AND UNCERTAINTY QUANTIFICATION *

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Abstract

Activated Corrosion Products (ACPs) may represent a significant source of radiological hazard in nuclear fusion reactors. Corrosion and erosion phenomena mobilize activated materials which are transported by the working fluid in regions of the cooling system accessed by worker personnel. Predicting contaminant transport in tokamak cooling circuits may benefit radiation exposure assessment, design optimization, waste management, maintenance plan definition, and source terms identification. Several calculation tools have been made available for ACPs determination in nuclear systems. Among these, the OSCAR-Fusion code, developed by the CEA (France), allows to predict ACPs generation and transport in closed water-cooled loops for fusion applications. This work aims to show a straightforward sensitivity analysis methodology and uncertainty quantification. A single ACP assessment involves several neutronics, thermal-hydraulics, geometrical, and water chemistry parameters. Coupling OSCAR-Fusion to RAVEN, a multi-purpose framework developed by INL (USA), allows sensitivity and uncertainty quantification analyses that might provide useful indications to the designers and safety analysts. This work presents a general methodology, showing preliminary results obtained for the EU-DEMO divertor cassette primary heat transfer systems.

Keywords: OSCAR-Fusion, RAVEN, Uncertainty Quantification, Sensitivity, Activated Corrosion Products, EU-DEMO, Divertor, Fusion Power

I. INTRODUCTION

Today, in performing the safety assessment of fusion reactors, the estimation of Activated Corrosion Products (ACPs) plays a fundamental role. In particular, predicting the radioactive contamination of nuclear plants' cooling systems could help decrease workers' exposure to radiation, optimize plant operation and estimate the source term. For this purpose, several computational tools have been developed [1], and some of them are widely used in the fusion reactors framework. These include the French OSCAR (tOol for Simulating ContAmination in Reactors) code, developed by the CEA in collaboration with Framatome and Electricité de France (EDF) to estimate radioactive contamination in the cooling circuits of pressurized water reactors. OSCAR has been recently modified into OSCAR-Fusion to assess the behavior of ACPs inside the Primary Heat Transfer System (PHTS) of fusion facilities, in which high fast neutron flux and corrosion issues could pose a safety concern.

The process governing the ACPs contamination of a PHTS depends on many different physical processes involving neutronics, thermal-hydraulics, geometrical, and water chemistry aspects. In water-cooled nuclear reactors, the corrosion and erosion of activated piping and components of the cooling system cause a release of activated ions and particles into the cooling circuit. In stainless steel pipework, the corrosion induces the generation of two distinctly different oxide films: the inner sub-layer is a chromium-rich protective spinel (chromite), which is adherent to the pipe base metal, reducing the ions exchange with the coolant. The second surface porous layer is instead more loosely attached (ferrite), characterized by large iron-rich tetrahedral crystals. Erosion and dissolution mechanisms produce particles and ions transported by the coolant over the entire loop. The precipitation of particles and ions occurs when the fluid reaches saturation.

There are two types of radioactive corrosion product formation: those produced by neutron activation of ions, particles and deposits mobilized and transported by the cooling fluid from the out-flux regions; and those produced by corrosion and erosion of activated structural materials under direct neutron flux. Materials may transmute under an intense neutron field to give birth to radioactive and unstable material specimens. OSCAR-Fusion allows to consider this activation processes defining a set of homogenized one-group reaction rates in its own database. Preliminary Monte Carlo neutron calculations generally produce these reaction rates with the associated uncertainty bands.

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Because of the intrinsic complexity of the involved phenomena, OSCAR-Fusion relies on several input parameters affected by bias and uncertainties.
A joint activity between Sapienza University of Rome and ENEA allowed the development of a new Python interface to couple OSCAR-Fusion with RAVEN (Reactor Analysis and Virtual control ENviroment) tool. The ACP uncertainty bands will be evaluated through sensitivity analyses, programmed, collected, and statistically manipulated through the RAVEN software tool.
This paper aims to show the coupling capabilities between OSCAR-Fusion and RAVEN, performing statistical analyses to estimate the inventory range of ACP. For this purpose, a thermal-hydraulic model of the EU-DEMO divertor cassette PHTS has been developed, and an 1888-days continuous activation scenario has been simulated with OSCAR. Both neutronic and chemical parameters have been selected to test the developed code-coupling. Transient results have been statistically analyzed through the RAVEN post-processor.

II. OSCAR-Fusion RAVEN COUPLING

The main objective of this work is to develop functionalities for the sensitivity quantification and Uncertainty Quantification (UQ) of ACP estimates in the water-cooled PHTS of fusion plants to improve the relate safety analysis.
OSCAR-Fusion is one of the most advanced codes for the assessment of the Activated Corrosion Products in fusion applications.
RAVEN (Reactor Analysis and Virtual control ENviroment) is a software tool, developed at the Idaho National Laboratory (INL), that acts as the control logic driver and post-processing tool for different applications [6]. The tool was initially developed to perform parametric and probabilistic analysis based on complex system codes' responses to quantify the safety margins related to safety-related events. Currently, RAVEN is a multi-purpose, probabilistic and uncertainty quantification platform that can be coupled with any system code [7].
A new code interface has been developed to incorporate OSCAR-Fusion within the RAVEN framework. The Python script allows perturbing all the parameters accessible through the RAVEN input deck. In such a way, RAVEN can investigate the system response and the input space using different sampling schemes.
The developed script has three main functions: to interpret the information coming from RAVEN; to translate such information into inputs of the OSCAR-Fusion code; to manipulate output data files to create a database. The "GenericCode interface" module already implemented in RAVEN has been coupled with a module that runs the OSCAR-Fusion executable to deal with the first two steps. A Python output parser has been developed to allow RAVEN to store output data coming from OSCAR-Fusion. This parser aims to create a Comma Separated Values (CSV) file with the Figure Of Merits (FOMs) requested by the user. In Figure 1, the procedural framework used for performing uncertainty quantification studies with OSCAR-Fusion and RAVEN is shown. An OSCAR-Fusion input deck is used as a template. The chosen parameters to be perturbed are specified by the user as strings with special characters. In such a way, RAVEN can identify such parameters and replace the string with values sampled from a specified distribution. After that, a fixed number of OSCAR-Fusion input decks are generated and executed. Once the Hierarchical Data Format version 5 (HDF5) database has been generated, statistical analysis of the output sets can be performed.

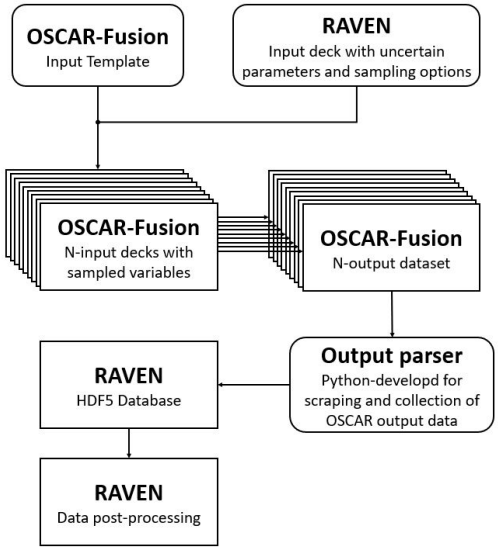

Figure 1. RAVEN/OSCAR-Fusion procedural framework scheme

III. EU-DEMO DIVERTOR REFERENCE DESIGN

The EU-DEMO divertor system is a key tokamak in-vessel component that extracts the power conducted to the tokamak scrape-off layer (the plasma region characterized by open magnetic field lines) whilst maintaining the plasma purity.
The DEMO Divertor comprises 48 toroidal cassettes, three for each toroidal sector of the reactor, to facilitate the remote handling procedure. Each divertor cassette is made of two modular sub-system, the targets Plasma Facing Units (PFUs) and the underlying Cassette Body (CB) that supports the PFUs. The cassette body supports the PFUS while shielding the vacuum vessel from neutrons and performing impurities extraction. The divertor target consists of a plasma-facing armor that must withstand the interaction with the plasma power and particle loads and is subject to erosion.

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As shown in Figure 2, each cassette is formed by a CB, which has a Shielding Liner (SL) and two Reflector Plates (RPs), and two PFUs composed of two components named Inner Vertical Target (IVT) and Outer Vertical Target (OVT).

Since EU-DEMO aims to prove the feasibility as a next-generation fusion power plant, the thermal power deposited on the divertor shall be extracted and converted into electricity. For this purpose, a PHTS has been designed to transfer the thermal power deposited into divertor cassette structures toward a Power Conversion System (PCS) through Heat eXchangers (HXs).

The EU-DEMO Divertor Cassette PHTS selected as a reference for this study consists of two separate cooling circuits equally distributed over the two sides of the tokamak building. Each cooling loop is operated at 3.5 MPa with a mass flow rate of 860 kg/s serving the cassette bodies pertaining to 8 tokamak sectors. The coolant inlet and outlet temperatures are respectively of 180 °C and 210 °C. Each cooling loop consists of one heat exchanger (Hex in Figure 4), one Main Coolant Pump (MCP), one PRessuriZer (PRZ) and the connecting piping between these components (see Figure 3). Into the circuit there are also the distributors (DIS in Figure 4), the Hot Feeding Pipe (HFP in Figure 4), the Cold Feeding Pipe (CFP in Figure 4), the Cold Leg (CL in Figure 4) and the Cross OVer pipe (COV). The black arrows in Figure 4 are representative of the flow direction.

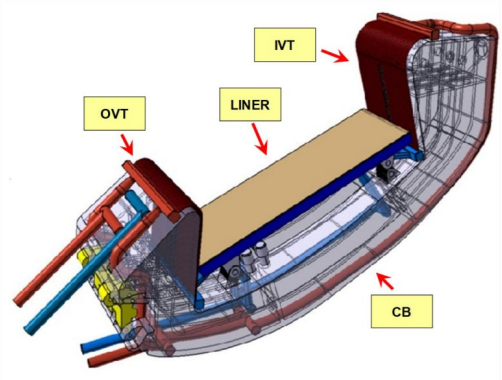

Figure 2. EU-DEMO divertor assembly

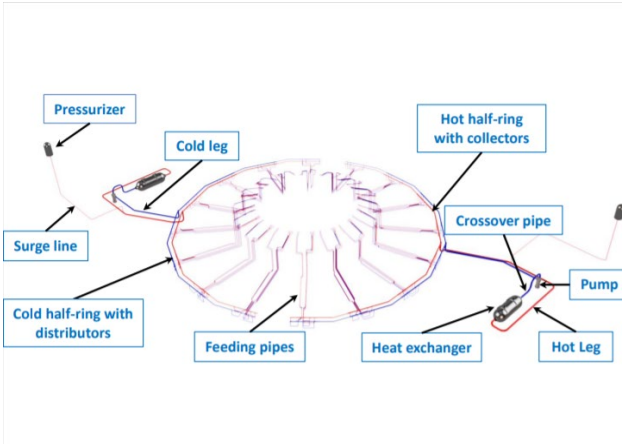

Figure 3. Overview of EU-DEMO divertor cassette PHTS

The PHTS shall interface with a Chemical Volume Control System (CVCS), which plays a crucial role in maintaining coolant purity and chemical composition. Since a specific design was not made available, a scaled CVCS model was derived from [10].

IV. OSCAR-Fusion MODEL DESCRIPTION

OSCAR-Fusion modeling requires the nodalization of the whole PHTS in a simplified closed loop made of one-dimensional regions with assigned conditions of bulk coolant temperature, wall temperature, pressure, neutron flux, wet surface, hydraulic diameter, coolant velocity, and turbulence regime parameter. The Divertor Cassette PHTS has been subdivided into 57 regions: its schematic representation is shown in Figure 4. The Divertor Cassette PHTS main parameters are reported in Table 1.

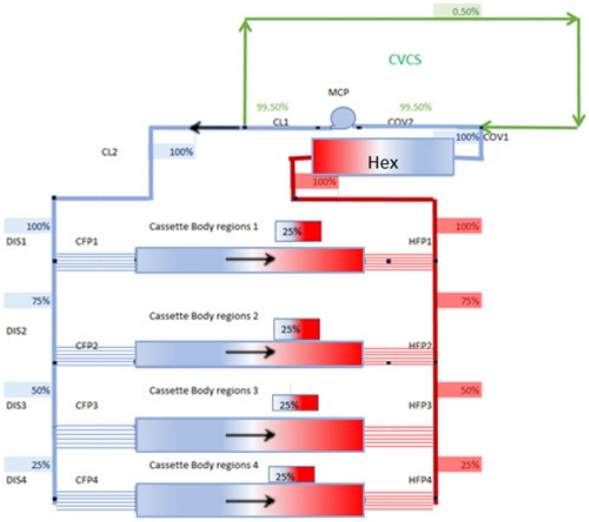

Figure 4. DEMO Divertor Cassette PHTS nodalization scheme

Table 1. Divertor Cassette PHTS main parameters

Parameter	Value
Mass flow rate	860 kg/s
Total wet surface	10448 m^2
EUROFER wet Surface	3256 m^2
SS316L wet surface	1087 m^2
INCONEL 660 wet surface	6105 m^2
Volume	192 m^3
Water mass	1.66 x 10^5 kg
Roughness	2.5 μm
Efficiency of filter and resin	99%
Li	0.275 ppm
H_2	25 cm^3/kg_{water}

V. VARIABLES SAMPLING AND MAIN RESULTS

Preliminary calculations have been performed to verify the effectiveness of the RAVEN-OSCAR coupling.
A dummy operational scenario of 1888 days continuous irradiation has been chosen as a trade-off between test needs and calculation overhead.
The first step to perform an uncertainty analysis is the identification of the variable affected by the uncertainty that can influence system response. The probabilistic random Monte Carlo sampling method has been used to propagate the input uncertainty in this work. The total number of runs has been selected using the Wilks formula [11].

$$\beta = 1 - \alpha^N - (N-1)(1-\alpha)\alpha^{N-1} \quad (1)$$

Where N is the number of code runs, α is the desired probability content, and β is the confidence level. The previous formula is valid for a two-sided tolerance interval and if only one FOM is investigated. For the chosen probability and confidence level of 95%, a minimum of 93 code runs is required. In consideration of the potential failures of code runs, a total of 100 code runs have been performed.
In this work, two different uncertainty analyses have been carried out, running a total number of 200 OSCAR-Fusion simulations.
There are several models for corrosion and release rates in OSCAR-Fusion. An empirical model, named Moorea's law in OSCAR-Fusion [13], was adopted in the present work. Specific correlations adjust the corrosion and release rates according to the pH, temperature and ion concentration conditions. For the use of this Moorea's law, two parameters must be defined: the Short Term Corrosion Rate (STCR) and Long Term Corrosion Rate (LTCR). Assuming the default parameters proposed in OSCAR-Fusion for the Moorea's law yielded a corrosion rate of 2.5E-12 g/cm^2/s at the beginning of the scenario.

In the first study, the Moorea's law for corrosion rates have been selected as uncertain input parameters. A uniform distribution has been selected for both short and long-term Moorea corrosion rates. The upper and lower bounds of associated distributions are reported in Table 2.
The upper bound and lower bound have been chosen considering an uncertainty of ± 50% of the default parameter values proposed in OSCAR-Fusion. The uncertainties associated with STCR and LTCR were arbitrarily chosen considering the lack of experimental corrosion data for specific materials (e.g. EUROFER) under DEMO operating conditions.
The second study has been conducted perturbing nuclear reaction rates. In this case, a normal distribution has been associated with each nuclear reaction. The perturbed variables and the associated distribution parameters are reported in Table 4.

Table 2. Sampling of Moorea law corrosion rates

Corrosion-release rates (Uniform distribution) [g/s/m^2]		
Parameter	Lower Bound	Upper Bound
Moorea law STCR	8.0E-7	2.4E-6
Moorea law LTCR	2.3E-7	6.9E-7

Short term and long term corrosion rates are OSCAR-Fusion input parameters and are constant values used depending on the time of the simulation, as shown in Table 3 are functions of time:

Table 3. STCR and LTCR meaning

Time (month)	Correlation for any material
$t \leq 2$	STCR
$2 < t \leq 12$	Function of both STCR and LTCR
$t > 12$	LTCR

Table 4. Sampling of nuclear reaction rates [14]

Nuclear reaction rates (Normal distribution) [1/s]				
Parameter	Mean	Sigma	Lower Bound	Upper Bound
Co-59(n,g) Co-60m	6.26E-10	1.15E-11	5.34E-10	7.18E-10
Cr-50(n,g) Cr-51	2.75E-10	4.86E-12	2.36E-10	3.14E-10
Cr-52(n,2n) Cr-51	3.47E-12	1.73E-13	2.08E-12	4.86E-12
Cr-52(n,p) V-52	1.45E-12	8.19E-14	7.95E-13	2.11E-12
Fe-54(n,a) Cr-51	1.33E-12	1.14E-13	4.15E-13	2.25E-12
Fe-54(n,g) Fe-55	4.14E-11	1.12E-12	3.24E-11	5.04E-11
Fe-54(n,np) Mn-53	8.03E-12	4.69E-13	4.27E-12	1.18E-11
Fe-54(n,p) Mn-54	7.74E-12	3.28E-13	5.11E-12	1.03E-11
Fe-56(n,2n)	5.90E-12	4.48E-13	2.31E-12	9.48E-12

Fe-55				
Fe-56(n,p) Mn-56	1.74E-12	7.09E-14	1.17E-12	2.30E-12
Fe-57(n,g) Fe-58	4.76E-11	2.29E-12	2.92E-11	6.59E-11
Fe-58(n,g) Fe-59	2.72E-11	4.20E-13	2.38E-11	3.05E11
Mn-53(n,g) Mn-54	1.68E-09	1.91E-10	1.47E-10	3.21E-09
Mn-55(n,2n) Mn-54	9.74E-12	5.40E-13	5.41E-12	1.40E-11
Mn-55(n,g) Mn-56	2.72E-10	6.14E-12	2.22E-10	3.21E-10

OSCAR-Fusion results of all completed runs have been statistically analysed through the RAVEN BasicStatistic post-processor. A dynamic statistic analysis has been performed chosing time as pivot parameter.

The selected FOM-1 for the Moorea parameters UQ analysis (Case Study 1) is the activity of Co-60 trapped in resins [Bq], while for the neutronic reaction rates (Case Study 2), the selected FOM-2 is the total activity trapped in resins.

In relation to the time-dependent analysis, Figure 4 shows the main statistical parameters evaluated along with the simulation time for Case study 1. While in Figure 5, the standard deviation of the FOM-1 is shown. As expected, the standard deviation is a monotonically increasing function of time.

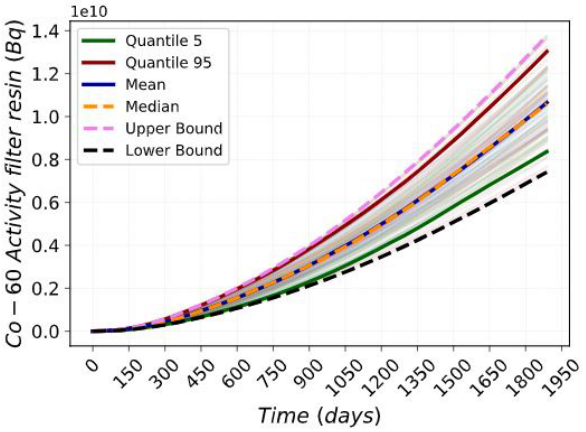

Figure 4. Main statistical parameters evaluated during the simulation for Co-60 activity in resins (Case Study 1)

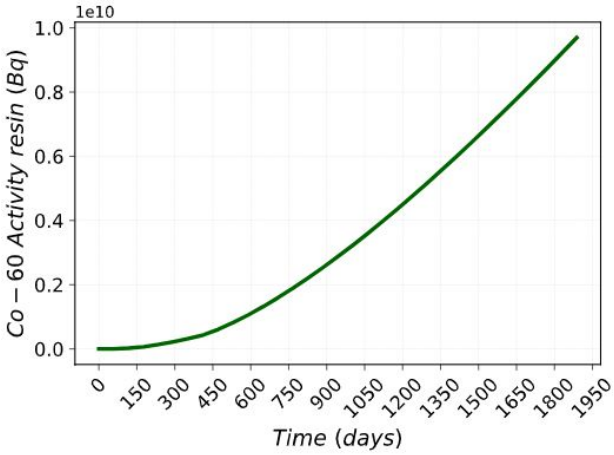

Figure 5. Standard deviation of Co-60 activity in resins evaluated during the simulation (Case Study 1)

In Table 5, the main statistical parameters evaluated at the end of the simulation are reported. The range variability of the FOM-1 output parameters is 19% lower with respect to the input parameters. In particular, for case study 1, the ratio between the upper and lower bounds is 2.43, while the ratio between the upper and lower bounds of input parameters distribution is around 3.

Table 5. Main statistical parameters evaluated at the end of the simulation

	Case Study 1	Case Study 2
Parameter	Value [Bq]	Value [Bq]
Lower Bound	2.32E+10	1.05E+12
Quantile 5	2.54E+10	1.09E+12
Mean	4.17E+10	1.23E+12
Median	4.35E+10	1.23E+12
Quantile 95	5.48E+10	1.36E+12
Upper Bound	5.66E+10	1.43E+12
Standard deviation	9.69E+09	7.83E+10

The Pearson's and Spearman's coefficients have been used to quantify the linear correlation between the variables [15][16]. For both coefficients, it can be assumed that: if the coefficient is higher than 0.5 (or lower than -0.5) the correlation is significant; if it is between 0.2 and 0.5 (or -0.2 and -0.5) the correlation is moderate; otherwise, it is weak. As expected, the STCR shows a significant correlation only during the first 500 days of operations while the LTCR after 450 days (see Figure 6).

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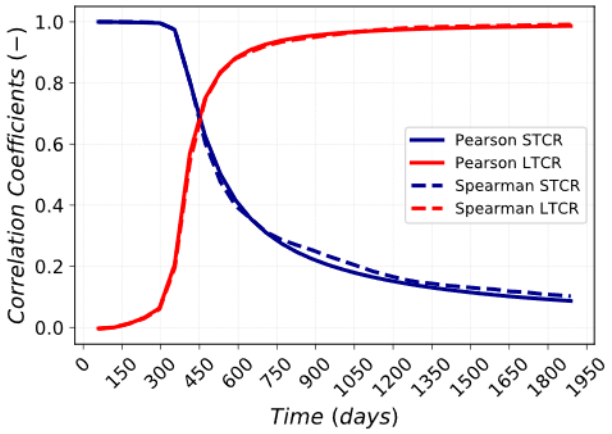

Figure 6. Pearson's and Spearman's correlation coefficients between FOM-1 and perturbed values

Figure 7 shows the FOM-1 as a function of the Long Term Corrosion Rate. From the physical point of view, the activated EUROFER in the underflux regions contributes more to the FOM-1 as its corrosion rate increases. From Figure 7 is also possible to notice the strong linear correlation between the LTCR and the FOM-1 at the end of the simulation.

Concerning Case Study 2, conducted by perturbing the neutronic reaction rates, the main statistical parameters related to the total activity trapped in resins are shown in Figure 8. While in Figure 9, the time-dependent standard deviation of the FOM-2 is shown. Numerical values are summarized in Table 5 in the third column.

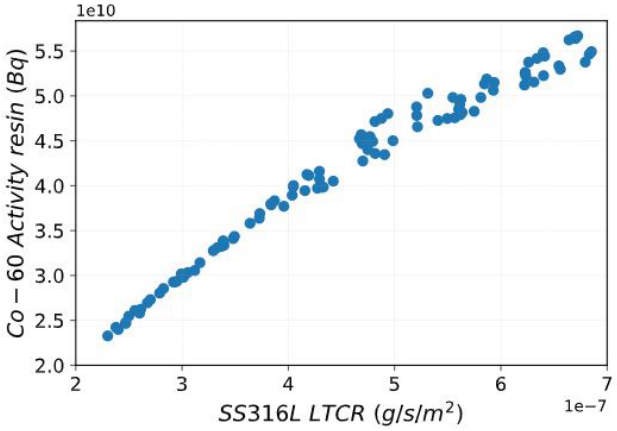

Figure 7. Co-60 activity in resins vs. LTCR at the end of the simulation

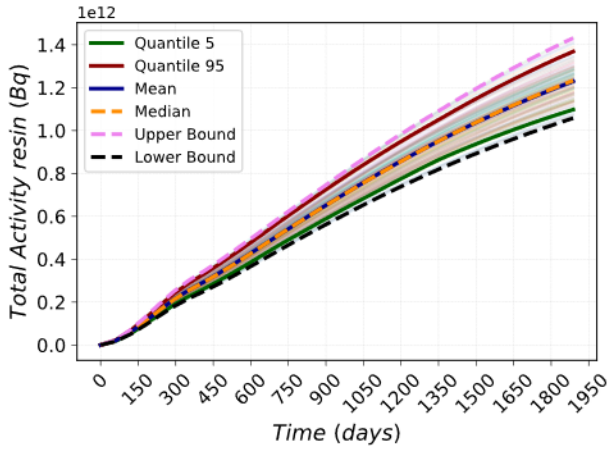

Figure 8. Main statistical parameters evaluated during the simulation for total activity in resins (Case Study 2)

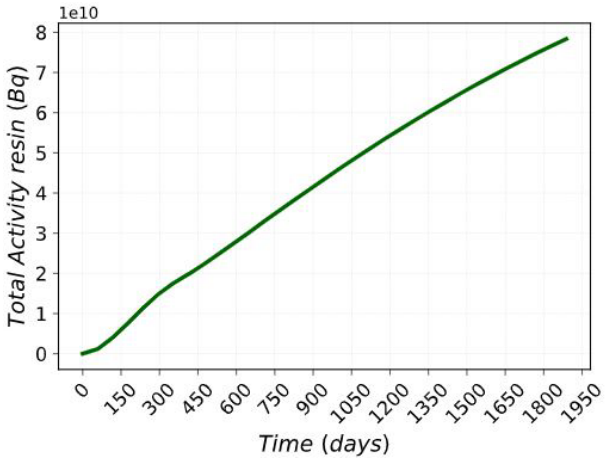

Figure 9. Standard deviation of total activity in resins evaluated during the simulation (Case Study 2)

The Spearman's and Pearson's correlations for Case Study 2 are shown in Figure 10 and Figure 11, respectively. The Fe-56(n, 2n)Fe-55 and Fe-54(n, p)Mn-54 reaction rates are linearly correlated with the total activity trapped in resins.

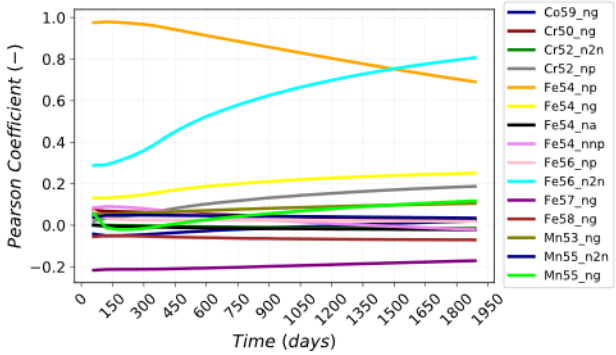

Figure 10. Pearson's correlation coefficient between total activity in resins and neutronic reaction rates

The correlation is linear only for Fe-56(n, 2n)Fe-55 and Fe-54(n, p)Mn-54, because they are the two primary ones responsible for the total activity in resins. The Fe-56(n, 2n)Fe-55 and Fe-54(n, p)Mn-54 correlation coefficients are between 0.2 and 1.0.

In particular, for Fe54(n, p)Mn-54, the correlation is linear and significant because the correlation coefficient is between 0.5 and 1.0 for the entire simulation. Instead, for Fe56(n, 2n)Fe-55 the correlation coefficient is initially between 0.2 and 0.5, where the correlation is moderate, and after about 900 days up to the end of the Case Study, is between 0.5 and 1.0, where the correlation is significant.

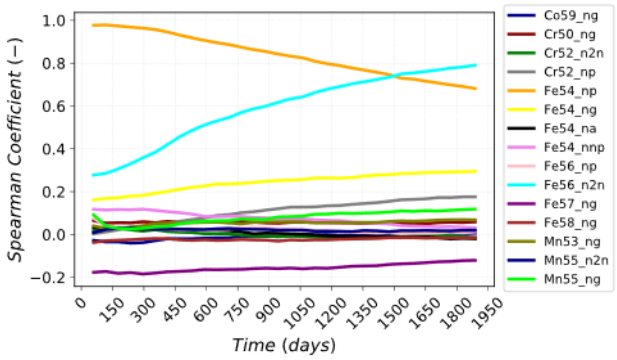

Figure 11. Spearman's correlation coefficient between total activity in resins and neutronic reaction rates

VI. SUMMARY AND CONCLUSIONS

The developed code coupling between RAVEN and OSCAR-Fusion has been successfully tested by performing two separate uncertainty analyses for an operational scenario characterized by continuous irradiation of the EU-DEMO divertor cassette PHTS. For both the analyses, the Monte Carlo probabilistic method has been applied to propagate input uncertainty and the Wilks approach to define the number of simulations performed. The Moorea's law corrosion rates for the EUROFER and the neutronic activation rates for the same materials have been considered as input uncertainty parameters, while the activity of Co-60 and the total activity trapped in resins have been selected as FOM-1.

The correlation analysis, evaluated both in the time-dependent and scalar value approach, underlined a statistical linear correlation between the Moorea coefficients and the activity trapped in resins.

Considering the preliminary nature of this analysis, more detailed studies will be performed to better quantify uncertainties associated with ACP formation and transport for more complex systems.

VII. ACKNOWLEDGMENTS

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