I²S-LWR Activation Analysis of Heat Exchangers Using Hybrid Shielding Methodology With SCALE6.1

Mario Matijević, Dubravko Pevec, Radomir Ječmenica
University of Zagreb, Faculty of Electrical Engineering and Computing, Department of Applied Physics
Unska 3, 10000 Zagreb, Croatia
mario.matijevic@fer.hr, dubravko.pevec@fer.hr, radomir.jecmenica@fer.hr

ABSTRACT

The Integral Inherently Safe Light Water Reactor (I²S-LWR) concept developed by a team lead by Georgia Tech is a novel PWR reactor delivering electric power of 1000 MWe while implementing inherent safety features typically reserved for Generation III+ small modular reactors. The main safety feature is based on an integral primary circuit configuration, bringing together a compact core design with 121 fuel assemblies (FA), control rod drive mechanism (CRDM), 8 primary heat exchangers (PHE), 4 passive decay heat removal systems (DHRS), 8 pumps, and other integral components. A high power density core based on uranium silicide fuel (U₃Si₂) is selected to achieve high thermal power which is extracted with PHEs placed in the annular region between the barrel and the vessel. The compact and integrated design of I²S-LWR leads to activation of integral components, mainly made from stainless steel, so accurate and precise Monte Carlo (MC) simulations are needed to quantify potential dose rates to personnel during routine maintenance operation. This shielding problem is therefore very challenging, posing a non-trivial neutron flux solution in a phase space. This paper presents the performance of the hybrid shielding methodologies CADIS/FW-CADIS implemented in the MAVRIC sequence of the SCALE6.1 code package. The main objective was to develop a detailed MC shielding model of the I²S-LWR reactor along with effective variance reduction (VR) parameters and to calculate neutron fluence rates inside PHEs. Such results are then utilized to find the neutron activation rate distribution via ⁶⁰Co generation inside of a stack of microchannel heat exchangers (MCHX), which will be periodically withdrawn for the maintenance. ⁵⁹Co impurities are the main cause of (n,γ) radiative gamma dose to personnel via neutron activation since ⁶⁰Co has half-life of 5.27 years and is emitting high energy gamma rays (1.17 MeV and 1.33 MeV). The developed MC model was successfully used to find converged fluxes inside all 8 stacks of PHEs with respect to MC statistics using the FW-CADIS methodology. For that purpose the S₉ module Denovo, based on forward-adjoint transport theory, was used to find VR parameters (importance map and biased source) to effectively bias MC simulation. Further research is required to account for other activation pathways, i.e. isotopes of iron which may generate ⁵⁹Co through neutron activation and beta decay.

Keywords: I²S-LWR, PWR, shielding, Monte Carlo, activation, SCALE6.1, FW-CADIS.

1 INTRODUCTION

The SCALE6.1 code package [1] with hybrid shielding sequence MAVRIC based on CADIS and FW-CADIS methods developed at Oak Ridge National Laboratory (ORNL) was used for I²S-
LWR [2],[3],[4] modeling. Automatic, adjoint and mesh-based variance reduction preparation has nowadays become a standard when dealing with complex MC models posing deep penetration shielding problem. Such hybrid shielding method utilizes a two-step approach [5],[6]: (1) deterministic transport theory solution for the VR preparation (forward-adjoint multigroup fluxes); (2) accelerated and optimized MC solution using these VR parameters. A well known methodology CADIS [7] (Consistent Adjoint Driven Importance Sampling) from ORNL was developed for shielding problems involving answers in localized regions of phase-space such as point/region detectors. The discrete ordinates $S_N$ solver Denovo [8] is used in CADIS for a quick approximation of space-energy adjoint flux which is subsequently used for VR construction: mesh importance map and biased source. This gives in turn effective biasing of MC simulation towards one specific, localized space region. With the computer hardware advance, it is now possible to handle huge MC models even on workstations, so a slight change of MC paradigm was introduced over the last decade. The MC method has nowadays become routine engineering tool for seeking not only (traditional) point detector results, as illustrated for the PCA benchmark [9] analyses in [10],[11], but radiation field in a sense of phase-space distributions, a characteristics historically typical to deterministic solvers. Following these computing trends, a generalization of the aforementioned ORNL method known as FW-CADIS [12] was developed to address real life MC models with uniformly small errors over large problem domains [13],[14].

Due to the integral configuration of I$^2$S-LWR, variation of the neutron flux by many orders of magnitude and complex spatial distribution is expected. To assert confidence in obtained results, shielding analyses were performed independently by two groups, at the Georgia Institute of Technology [15],[16] and at the University of Zagreb. Such parallel work in two independent groups allowed consistent cross-verification of the shielding results.

This paper presents results obtained at the University of Zagreb for the updated shielding model of the I$^2$S-LWR with reactor pressure vessel (RPV), integrated components and biological shield. More specifically, the performance of the SCALE6.1/MAVRIC code was investigated to find well converged neutron fluxes inside stacks of homogenized PHEs. The CADIS and FW-CADIS methodologies were used for the PHX irradiation problem, where the objective was to optimize the fast fluence rate ($E >1$ MeV) simultaneously at 8 PHX locations. The focus was on homogenized microchannel material to asses the MAVRICs effectiveness for deep penetration shielding problem and $^{60}$Co generation which presents activated gamma source. The integral configuration of the I$^2$S-LWR reactor introduces large modular units, such as PHEs, which will most likely be activated by neutrons during reactor operation. Such internal components, made from steel alloys, will introduce potential dose rates to working personnel during routine maintenance operation and periodical core refueling. Thus neutron activation via $(n,\gamma)$ reactions inside heat exchangers needs to be well known because of its radiological importance. Such complex reactor configuration in shielding terms can only be addressed by modern MC codes with advanced VR schemes, utilizing a very detailed level of 3D geometry, which is necessary to capture fine space-energy physics (i.e. phase space) of the reactor model [17],[18].

This paper is organized as follows. Section 2 gives the description of the SCALE6.1 code package with focus on hybrid shielding capabilities in the MAVRIC sequence. Section 3 shows MAVRIC model of the I$^2$S-LWR reactor concept with computational parameters. Section 4 gives shielding analysis of the PHEs irradiation problem with different approaches (CADIS vs. FW-CADIS). Section 5 gives PHE activation analysis results. Section 6 gives discussion and conclusions while the referenced literature is given at the end of the paper.

2 THE SCALE6.1 CODE PACKAGE

The SCALE6.1 code package is still the latest production version of the ORNL’s computing software platform developed in support for the U.S.NRC needs. In the present form the code has versatile ability to perform a whole spectrum of different calculations pertinent for nuclear
engineering activities in wide areas. Some of the possibilities are: criticality, shielding, radiation source term, burnup/depletion and nuclear decay, reactor physics, and sensitivity/uncertainty analyses using well established analytical sequences. The main shielding sequence is MAVRIC, based on the CADIS and FW-CADIS methods utilizing S\textsubscript{N} solver Denovo for VR calculation and subsequent accelerated MC Monaco particle transport. The Denovo code is a fast and robust deterministic program utilizing Koch-Baker-Alcouffe transport sweep algorithm with Krylov multigroup iteration over the orthogonal meshes [8]. A variety of S\textsubscript{N}-like options are available, such as numerical convergence criterion, spatial differencing, within-group acceleration, etc. Inherent flux solution positivity of Step Characteristic (SC) spatial differencing is the best and most important feature of Denovo, which in turn gives the numerical stability for Monaco code. When one looks for a solution in a form of multiple point detectors or over millions of spatial mesh cells, it is necessary to use FW-CADIS which demands for extra forward S\textsubscript{N} run. Such forward solution is used for preparing inversely weighted adjoint source, placed in the region of users interest. For both CADIS and FW-CADIS the particle average weight is inversely related to adjoint flux value throughout phase-space, so locations of high importance (i.e. adjoint flux) will have low-weighted particles and vice versa. This implies that adjoint source location with optimized MC results will present spatial attractor for the source particles, giving "reasonable" MC results in-between regions. This approach was used in I\textsuperscript{2S}-LWR shielding calculations presented in the following chapters.

3 THE I\textsuperscript{2S}-LWR MC MODEL WITH SCALE6.1/MAVRIC

The Integral Inherently Safe Light Water Reactor (I\textsuperscript{2S}-LWR) is an integral reactor concept developed by Georgia Institute of Technology (Georgia Tech) implementing inherent safety features and delivering an electric power of large PWR (1000 MWe) [2]. Integral primary circuit configuration is limited in size and thus requires a compact design and optimized layout. A novel high power density core based on silicide fuel is composed from 121 fuel assemblies inside reactor pressure vessel. Internal primary heat exchangers are grouped in 4 pairs (8 units in total), based on new micro-channel technology and placed in the annular region between the core barrel and RPV. The control rod drive mechanism and supporting plates are placed above the core. Total of four passive decay heat removal units are also placed outside the core in the annular region, giving passive natural recirculation in case of hypothetical transient scenario. The design details on other reactor vessel internals with CAD images can be found in available I\textsuperscript{2S}-LWR papers [3],[4]. The updated MAVRIC model of the I\textsuperscript{2S}-LWR is depicted in Figures 1 and 2, where one can notice the location of the PHEs.
The SCALE6.1/MAVRIC sequence was used on a workstation with 32 GB of RAM and Core i-5 CPU. CADIS and FW-CADIS methods were explored for PHEs irradiation problem, where we calculated the neutron fast fluence rate \( (E > 1 \text{ MeV}) \) simultaneously at 8 PHE locations. The focus of calculations was on homogenized MCHX material inside PHEs, since that result is useful for later \(^{59}\text{Co} \) activation calculations. The adjoint source was thus set as PHE stacks with energy spectrum of fast neutron spectra. That spectra was later changed to \(^{59}\text{Co}(n,\gamma)^{60}\text{Co} \) cross section (in barns) for the purpose of activation calculation. The silicide fuel in heterogeneous FAs (FA depicted in Figure 2) was uniformly sampled with \(^{235}\text{U} \) fission spectrum and with nu-bar of 2.5. The total thermal power of 2850 MW was halved to mimic neutron spatial gradient on core periphery.
This shielding problem with multiple region tallies (i.e. PHE stacks) requires advanced VR parameters, since internal configuration and water coolant massively attenuate neutrons from the reactor core. The computational SN mesh with $S_{13}/P_1$ parameters completely covers global unit with 135x135x310 voxels. The Monaco was used with 4000 batches/15000 neutrons per batch and with mesh tally of 100x100x260 voxels. The same broad-group shielding library "$v_{7.27n19g}$" in SCALE6.1 was used for both Denovo and Monaco modules, derived from ENDF/B-VII.0 data [19]. One has to note that $S_N$ solver accuracy for a hybrid shielding is not a paramount criterion, since only crude spatial flux profile is good enough for MC acceleration, but that knowledge is not a priori known. In order to benefit from a more accurate $S_N$ solution without raising memory demanding $S_N/P_N$ parameters, Denovo was used with macromaterial option which represents the voxel material as a volume-weighted mixture of elementary (user) materials. With "mmTolerance=0.005" option and about 20 elementary materials, the macromaterial table contained 1013 pseudo materials, which will mitigate rapid changes in $S_N$ flux solution between neighboring cells. The macromaterial option in Denovo solver is a very elegant way to refine $S_N$ solution without calling for extra memory by increasing $S_N/P_N$ parameters.

4 ANALYSIS OF PHE IRRADIATION PROBLEM

Two different shielding methodologies (CADIS and FW-CADIS) were investigated with MAVRIC sequence. The adjoint source was defined as PHE stacks with focus on MCHX material. The aim was to calculate a well converged fast fluence rate above 1 MeV, which is radiologically important issue. The mesh-based importance map (i.e. weight windows) derived from such adjoint source represent a "recipe" how to bias transport of source neutrons towards desired locations of PHEs. This transport biasing is in strict (i.e. consistent) accordance with source biasing governed by neutron importance function [1].

4.1 CADIS solution for PHEs irradiation

The $S_N$ representation of the CADIS adjoint source distribution is depicted in Figure 3. One can notice the absence of spatial gradient, which means constant adjoint source intensity in phase-space by definition of method [7]. Since $I^S$-LWR massively attenuates neutrons outside of the core, spatial shadowing is expected along axial direction of PHE stacks. The axial and radial reactor midplanes of fast neutron fluence rates are depicted in Figures 4 and 5. The detailed mesh tally covering one PHE is depicted on Figure 6. The adjoint $S_N$ calculation took 1.88 h while final Monaco took 19.3 h.

![Figure 3: CADIS adjoint source through PHX stacks](image)
Maximum neutron fluence rate at the bottom of the first module is about 2000 n/cm²/s and is falling off rapidly in axial direction. CADIS fluence indicates that $S_N$ forward flux weighting is necessary step in adjoint source preparation, since only MC reasonable results can be found in the
lowest module closest to the core. No neutron transport can be found beyond the first heat exchanger module. Inherent characteristic of CADIS is spatial shadowing if adjoint source is not highly localized. The first layers of the bottom module will get all the neutrons and prevent deep penetration leaving upper white areas without results. This heavy shielding problem is a suitable test-case for the FW-CADIS methodology.

4.2 FW-CADIS solution for PHEs irradiation

From previous MAVRIC calculations it is evident that obtaining fast fluence rate simultaneously at 8 locations of PHE stacks is a significant shielding problem. The motivation for using FW-CADIS is an additional Denovo forward S_N calculation for redistribution of adjoint source in phase-space. Such DOAS (Distribution of Adjoint Source) is constructed by inverse weighting with integrated forward flux approximation, so that heavy-shielded regions with small neutron population in reality will receive MC particle "boost". With such approach the spatial shadowing in PHE stacks should be eliminated, giving well converged fluxes. The FW-CADIS adjoint source is depicted in Figure 7, covering all 8 PHE units [20]. The forward S_N calculation took 11 h, the adjoint S_N calculation took 1.77 h while final Monaco took 3.56 days.

One can easily notice the effect of adjoint source redistribution in phase-space. This new adjoint source distribution is in accordance with the independent FW-CADIS calculation which predicts the region between CRDM plate and top CRDM plate as the most problematic one – the PHE stacks as an adjoint source are reinforced in that region. The satisfactory Monaco MC results with uniform relative errors throughout PHEs are depicted in Figure 8. Maximum fluence rate at the bottom of PHE stacks is similar to previous CADIS results.
Fast fluence rate in some representative reactor axial planes are depicted in Figures 9, 10 and 11. One can notice gradually degradation of MC statistics from the bottom of PHE stacks (below 10% on average) to the top (below 20% on average). Regarding the model complexity and many orders of flux attenuation, one can say that satisfactory, well converged results were obtained in reasonable amounts of time, demonstrating capabilities of SCALE6.1/MAVRIC.
Important thing to notice is a fast neutron streaming and reflection off the biological shield and from the RPV skirt, giving local amplifications of the neutron field inside MCHX material. This is a major mechanism for activation heat exchangers axially. Since the RPV skirt is a necessary component to bear a reactor weight, suitable neutron absorber should be present in reality to prevent fast neutron leakage, such as additional layer of concrete. The fast neutrons reflection off the RPV skirt is depicted in Figure 12.

5 PHE ACTIVATION CALCULATION

Neutron activation of cobalt impurities inside PHE’s steel is a possible source of dose rates to maintenance personnel. The problematic $^{60}$Co is mostly produced via $(n,\gamma)$ reaction on natural $^{59}$Co, coming as steel impurity, but other pathways exist from iron $^{58}$Fe transmuting again to $^{59}$Co. In this model the presumed level of stable isotope $^{59}$Co in MCHX area of PHEs was 0.05 w/o which is upper limit defined by AP1000 Design Control Document [21]. Fast neutron streaming will produce thermalized neutron spectrum interacting with $^{59}$Co inside PHEs, thus generating radioactive $^{60}$Co which is gamma emitter (1.17 MeV and 1.33 MeV) with half-life 5.27 years. The short half-life and high energy gamma ray emission makes the $^{60}$Co very important isotope to track during reactor operation. In this study a fixed neutron source was used at the moment, without time-dependent burnup effects inside reactor core. The continuous $(n,\gamma)$ cross section [22] for $^{60}$Co formation is

![Figure 11: Monaco fast fluence rate with relative errors in PHE planes (bottom)](image1)

![Figure 12: RPV skirt reflection impact on PHEs irradiation](image2)
shown in Figure 13, while multigroup representation in v7_27n19g shielding library is shown in Figure 14.

Figure 13: Cross section $^{59}\text{Co}(n,\gamma)^{60}\text{Co}$ important for thermalized neutrons

Figure 14: Multigroup representation of the $^{59}\text{Co}(n,\gamma)^{60}\text{Co}$ cross section

The MAVRIC sequence was used with PHE stacks as adjoint sources with $^{59}\text{Co}(n,\gamma)^{60}\text{Co}$ reaction as neutron spectrum (response function number MT=102). The forward $S_N$ calculation took 11 h, the adjoint $S_N$ calculation took 4 h while final Monaco took 2.3 days. The mesh tally results covering one of the PHE stack is shown in Figure 15.
A detailed MCHX steel activation study was performed by Georgia Tech taking into account time-dependent decay and isotope activation tracking using ORIGEN-S depletion sequence [1],[23]. This method used a problem-dependent decay library with 1-group cross section derived from multigroup libraries weighted with correct neutron spectrum. Conclusion was that $^{60}$Co was 6 orders less than the initial impurity $^{59}$Co, but still emitting radiologically important high energy photons. Using such detailed gamma source in separate shielding calculations, where PHE was isolated in dry air, the maximum gamma dose rate obtained at the bottom of PHE was $0.127\pm0.3\text{ mrem/h}$ [21].

6 DISCUSSION AND CONCLUSION

The updated shielding model of the I$^2$S-LWR reactor was prepared to reflect the necessary design changes within the RPV and integrated components. The SCALE6.1/MAVRIC shielding sequence was used for simulation of the PHEs irradiation problem. The objective was to find fast neutron fluence and $^{60}$Co activation rates in all 8 PHE units simultaneously. The aforementioned hybrid S$^N$-MC methods (CADIS and FW-CADIS) were used to calculate radiation field distributions. The CADIS method demonstrated serious limitations in form of spatial shadowing inside PHEs, since adjoint source wasn't highly localized. This was a good example of a very difficult shielding problem which could be solved only by means of FW-CADIS and adjoint source redistribution in phase-space. The Monaco converged results over all 8 PHE stacks were found to be acceptable with respect to MC statistics. The specific task was to investigate the neutron activation in the MCHX part of PHE since it is a component likely to be handled during routine maintenance/refueling activities. Fast neutron streaming in the cavity region was identified as an important factor for MCHX activation, since the RPV skirt and biological shield reflect neutrons back inside the vessel. In reality a suitable neutron absorber will fill such void space beneath the RPV skirt. Such shielding calculations are important part of the overall I$^2$S-LWR design process, since they identify potential radiological issues important for achieving ALARA (As Low As Reasonably Achievable) principle in practice.

ACKNOWLEDGMENTS

This work was supported by the Croatian Science Foundation under the grant number 3522.
REFERENCES


[22] IAEA Nuclear Data Services. Website: [https://www-nds.iaea.org/](https://www-nds.iaea.org/)