EVALUATION OF THE OSCAR-4/MCNP CALCULATION METHODOLOGY FOR RADIOISOTOPE PRODUCTION IN THE SAFARI-1 REACTOR

Z. Karriem and O.M. Zamonsky
Necsa, Radiation and Reactor Theory, PO Box 582, Pretoria, 0001, South Africa
zain.karriem@necsa.co.za

Abstract

The South African Nuclear Energy Corporation SOC Ltd (Necsa) is a state owned nuclear facility which owns and operates SAFARI-1, a 20 MW material testing reactor. SAFARI-1 is a multi-purpose reactor and is used for the production of radioisotopes through in-core sample irradiation. The Radiation and Reactor Theory (RRT) Section of Necsa supports SAFARI-1 operations with nuclear engineering analyses which include core-reload design, core-follow and radiation transport analyses. The primary computer codes that are used for the analyses are the OSCAR-4 nodal diffusion core simulator and the Monte Carlo transport code MCNP. RRT has developed a calculation methodology based on OSCAR-4 and MCNP to simulate the diverse in-core irradiation conditions in SAFARI-1, for the purpose of radioisotope production. In this paper we present the OSCAR-4/MCNP calculation methodology and the software tools that were developed for rapid and reliable construction of MCNP analysis models. The paper will present the application and accuracy of the methodology for the production of yttrium-90 (^{90}Y) and will include comparisons between calculation results and experimental measurements. The paper will also present sensitivity analyses that were performed to determine the effects of control rod bank position, representation of core depletion state and sample loading configuration, on the calculated ^{90}Y sample activity.

1. Introduction

The South African Nuclear Energy Corporation SOC Ltd (Necsa) owns and operates the SAFARI-1 research reactor. The SAFARI-1 reactor is a multi-purpose, 20 MW plate-type material testing reactor that is used for radioisotope production. Isotopes are produced in fixed in-core positions and experience irradiation under various geometric configurations and core depletion states.

In order to model the dynamic irradiation conditions of irradiated samples, the OSCAR-4/MCNP calculation methodology was developed. OSCAR-4 is the SAFARI-1 reactor core simulator which is based on the nodal diffusion method [1], while MCNP is the well-known Monte Carlo transport code [2]. This methodology consists of a tool to transfer detailed atom densities from OSCAR-4 to the MCNP model, and an automation code to model the arbitrary sample configurations in MCNP.

This paper is an extension of the work in reference [3], which introduced the OSCAR-4/MCNP calculation methodology and presented the initial performance of a *simplified calculation approach* based on this methodology. Although the OSCAR-4/MCNP methodology is capable of performing high-fidelity calculations in terms of specifying the core depletion state and geometric sample configuration, the calculation approach in reference [3] implemented a simplifying assumption for specifying the core depletion state. The motivation for this was to develop a general system for predicting sample irradiation times. The main results from comparing calculation with experiment for a series yttrium-90 (^{90}Y) samples in reference [3], were that the *simplified calculation approach* showed an under-prediction of the measured activities of 9.1 % with a standard deviation of 5.4 %.

In this work, the irradiation specific (cycle specific) core depletion state was specified for each irradiation. This resulted in a more accurate representation of the experiment, which consisted of an explicit core depletion state, a control rod bank position based on experimental data and detailed sample configuration modelling. The major result from this work was that the use of an irradiation specific core depletion state does not improve the predicted activities. This however allows one to use a generic approach to modelling the core depletion state, which facilitates the development of a generic calculation methodology for planning sample irradiation time.

The sensitivity analyses for the calculated sample activity considered the effect due to sample loading configuration and control rod position. For the loading configuration, a reference sample configuration case was considered and the effect on the activity was determined as a function of neighbouring sample configurations. The sensitivity due to control rod position was performed by varying the rod position around the reference case.

Section 2 gives a description of SAFARI-1, while the analysis codes and methodology are described in Section 3. Section 4 describes the analysis performed in this work, with the results presented in Section 5. The conclusions and future work are presented in Section 6.

2. The SAFARI-1 Reactor

The SAFARI-1 reactor is a 20 MW tank-in-pool type material testing reactor (MTR). The reactor core is contained inside the reactor vessel, which is inside the reactor pool. The reactor vessel is immersed in light water which serves as coolant, moderator and shielding. In the configuration analyzed in this paper, the core contains 26 fuel elements and 6 control rod elements. Apart from the routine molybdenum production, several isotopes are produced through neutron irradiation in the reactor. In this paper we analyze the particular irradiation of yttrium oxide (Y_2O_3) for the production of ^{90}Y. Figure 1 shows a cross section of the MCNP model of SAFARI-1. Sample irradiations typically occur in in-core positions D6 and F6. The results presented in this work were from samples irradiated in the D6 position.

3. Reactor Analysis Codes: OSCAR-4 and MCNP

Reactor operation and irradiation analyses support to SAFARI-1 are provided with two code systems. The first is the OSCAR-4 (OSCAR) code system which is used for reactor reload design and core-follow analysis. OSCAR contains a three-dimensional, multigroup, nodal diffusion code that is developed and maintained in the RRT Section at Necsa [1]. The second, is the Monte Carlo code MCNP [2], which is used to compute detailed 3-D analysis of in-core irradiations and for other transport applications. For radioisotope production, OSCAR and MCNP are used in conjunction, i.e. OSCAR provides MCNP with the appropriate core depletion state for the irradiation analysis [3].

In addition to the analysis codes, dedicated automation tools were developed to support the efficient and reliable use of OSCAR and MCNP. OASYS2MCNP was developed to transfer the core isotopic composition from OSCAR to MCNP. To implement the wide variety of arrangements for sample irradiation in the MCNP model in a relatively user friendly way, the LOAD_IPR (Load Isotope Production Rig) code was developed. Both of these software tools will be described in more detail in Section 3.3.

3.1 SAFARI-1 MCNP Model

Figure 1 shows the MCNP model of SAFARI-1. The model includes the reactor core, as well as the ex-core irradiation facilities. It contains detailed modelling of all the assemblies available in the reactor and has been designed in order to make it easy to implement MCNP variance reduction techniques outside the reactor core.

The reactor core is composed of a 8×9 grid containing various reflector elements on three sides of the core, with fuel elements and irradiation rigs modelled with explicit detail on the inside of the core. A fuel assembly is of the plate-type and consists of 19 plates, with each plate consisting of a Uranium-Silicide-Aluminum (U3Si2-Al) powder dispersed core, enclosed in an aluminum-alloy cladding. The control rods are of the fuel follower type with absorber in the upper section and fuel follower in the lower section of the rod. The reactivity control system contains six identical control rods that are located in positions C5, E5, G5, C7, E7 and G7. The Isotope Production Rigs (IPRs), in which the samples are irradiated, are inserted in positions D6 and F6.

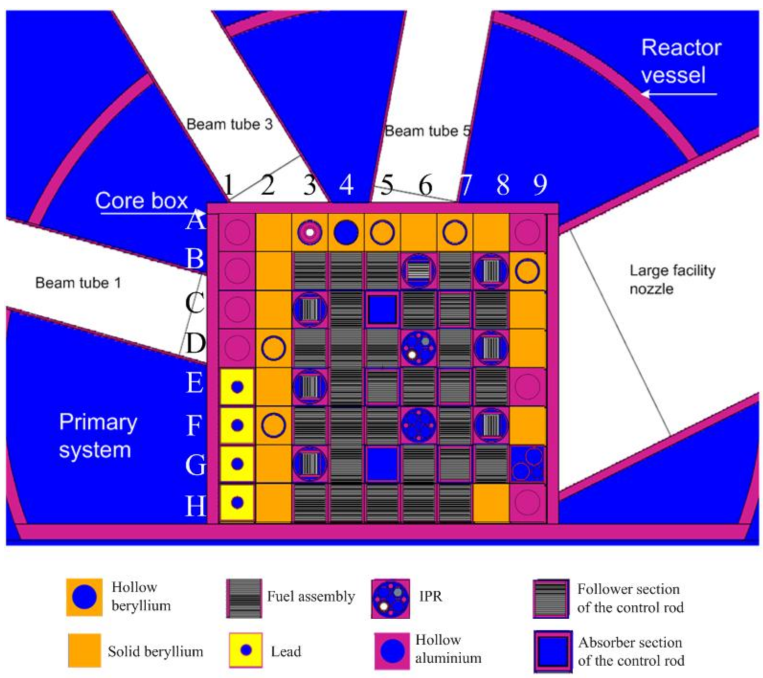

Figure 1 XY view of the core and beam tubes

3.2 Isotope Production Rig

The MCNP model of the IPR is shown in Figure 2. The model of the experimental column configuration for the sample irradiations considered in this work is shown in Figure 2(a). Figure 2(b) shows a top view of the IPR and a horizontal section through the IPR model showing the columns and their location; i.e. 1, 2, 3 and 4. Figure 2(c) shows the modelling of the sample geometry contained in Figure 2(a).

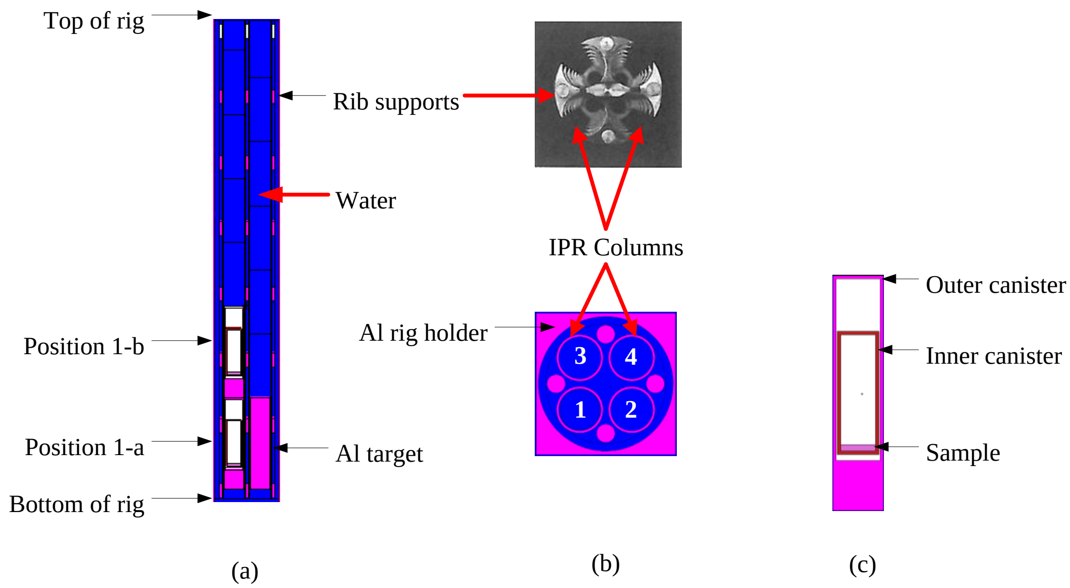

Figure 2 MCNP model of IPR and samples

3.3 OSCAR-4/MCNP Calculation Methodology

The OSCAR-4/MCNP calculation methodology consists of OSCAR-4, MCNP and the two main automation codes OASYS2MCNP and LOAD_IPR as shown in Figure 3. In Step 1, OASYS2MCNP is used to transfer a detailed core depletion state to MCNP. The inputs to OASYS2MCNP are a base MCNP model and a selected core depletion state, which is used to generate a depletion specific MCNP model.

OASYS2MCNP transfers the atom densities of the 37 actinides and fission products [3] and Equivalent Boron Content (EBC) that represents 66 lumped isotopes that are not explicitly tracked in OSCAR-4, to MCNP. The number densities are transferred per assembly in the same axial nodalization that is used in the OSCAR-4 nodal diffusion solver.

Step 2 of the methodology specifies the remaining calculation parameters in the MCNP model, i.e. the control rod position during irradiation and the IPR loading configuration. LOAD_IPR takes the MCNP model generated with OASYS2MCNP and sets the control position, constructs the sample loading geometry and builds the necessary neutron flux and reaction rate tallies for inserted samples. Figure 4 shows the typical rig configurations generated with LOAD_IPR and that was analyzed in this work.

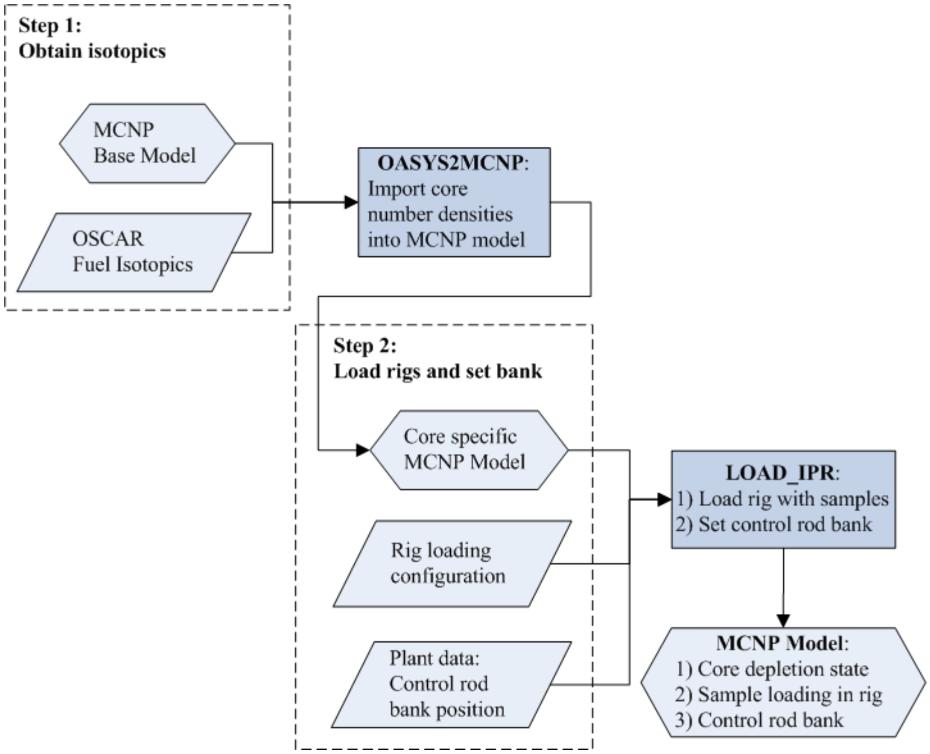

Figure 3 OSCAR-4/MCNP Methodology

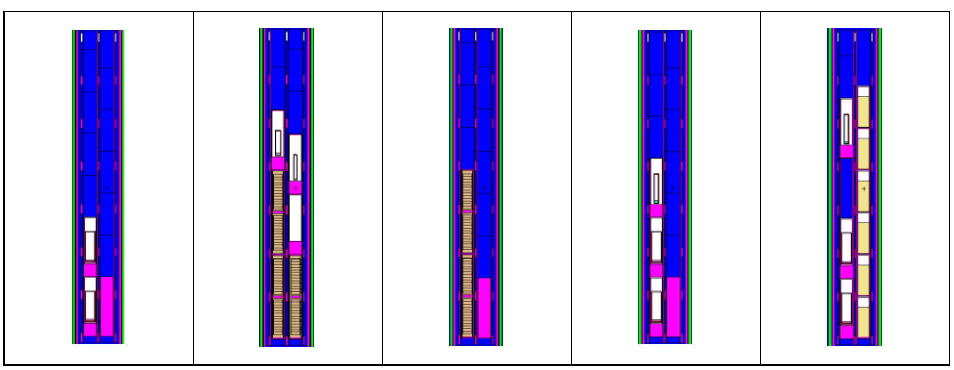

Figure 4 Sample IPR column loading configurations generated with LOAD_IPR

4. Calculations

This section describes the calculations that were performed in this work. A description of the reactor operation during isotope production is given, which is followed by a description of the experimental data set and the application of the OSCAR/MCNP methodology. Finally the sensitivity analyses that were performed in this work are introduced.

4.1 Reactor Operation

Research reactors are typically designed as multi-purpose machines for accommodating various reactor experiments and irradiation applications. As such the arrangement of samples in the IPRs can vary depending on customer demand and requirements. In addition, individual columns can also be removed during the cycle to either remove- or re-insert samples into the desired positions.

4.2 Experimental Data Set

In order to validate the OSCAR/MCNP methodology, calculations were compared to a series of measured activities obtained for the production of ^{90}Y. The data set used in this work is identical to that used in reference [3] and consists of 33 irradiations of Y_2O_3 samples that were irradiated during 2013. Each irradiation case contained two samples per irradiation, giving a total of 66 experimental data points. Reference [3] also presented the initial comparison of the methodology with experiment.

The locations of the sample irradiations considered in this paper are as shown in Figure 2(a). Note that while the Y_2O_3 samples were always loaded in the 1-a and 1-b positions, other sample loading configurations above the Y_2O_3 and in neighbouring columns included the loading variations similar to that shown in Figure 4.

4.3 Application of OSCAR-4/MCNP Methodology

This section describes the application of the OSCAR/MCNP methodology that was applied in reference [3] and the main difference to the approach taken in this work. The major variables that are considered of importance for the accurate modelling of the experiment are:

i) Experimental information – sample composition, sample mass, irradiation- and decay time; and measurement uncertainty;
ii) Irradiation rig sample configurations;
iii) The control rod bank position during irradiation; and
iv) The core depletion state.

The maximum activity measurement uncertainty was 1 %. The control bank positions were obtained from the SAFARI-1 reactor plant data at intervals of 4.2 seconds. The core depletion state can be generated with OSCAR-4 at any given time. In all, the OSCAR/MCNP methodology therefore allows for the modelling of a specific irradiation. However, the detailed application of this methodology is impractical since it would involve many MCNP calculations. For reasons of practicality, additional assumptions are required, which are discussed below.

For the IPR loadings during the irradiation, the sample configurations in neighbouring columns varied in practice. This detail was not taken into account; instead the sample configuration that dominated the irradiation period was used as the geometric configuration. Also, the addition and removal of molybdenum rigs during the operation were not taken into account in this work.

During reactor operation the control rod bank location is not static. In practice, the control rods are constantly adjusting over the irradiation period, which is impractical to model. An irradiation specific average control rod bank position was therefore used in the calculations. The assumption of an average bank was motivated by the fact that the average bank extraction over the irradiation period is only about 3 cm.

The above assumptions relating to sample loading and control rods were identical to that used in reference [3]. In reference [3] however, a *typical* time dependent core depletion state consisting of 4 core states was used in all 33 calculations. The core cycle selected as a depletion basis in reference [3] was Cycle 8 of 2013 (C2013-8). In this work however, the irradiation specific core depletion state was used in the irradiation calculation.

In summary, the MCNP model in this work therefore contains a high level of detail pertaining to the three main calculation parameters. That is, each calculation uses a representative IPR loading configuration, control rod bank position and a core depletion state that is specific to the particular irradiation.

The series of MCNP models that were constructed for each of the 33 cases were executed and the total neutron scalar flux, ϕ, and the ^{89}Y capture cross-section, σ_{cap}, were computed for each sample. The activity of each sample was then calculated using Eq. (1)

$$A^{90}(t) = N^{89}\phi\sigma_{cap}\left(1-e^{-\lambda t_{Irrad}}\right)e^{-\lambda t_{Decay}} \quad \text{[Bq]} \tag{1}$$

where $A^{90}(t)$ is the ^{90}Y activity at time $t = t_{Irrad} + t_{Decay}$, t_{Irrad} is the irradiation time, t_{Decay} is the decay time, N^{89} the number of yttrium-89 (^{89}Y) atoms present and λ is the decay constant of ^{90}Y ($\lambda = 1.0814\times10^{-2}$ hr^{-1}). The removal of ^{90}Y by neutron capture was verified to be negligible and therefore neglected in Eq. (1).

4.4 Sensitivity Analyses

Reference [3] showed that the OSCAR/MCNP calculation approach results in an under-prediction of the measured activities. In order to analyze the possible origin of this difference and the effects of different calculation parameters on the activity, various sensitivity calculations were performed.

The first sensitivity analysis was performed to determine the dependence of the predicted activity on the core depletion state. The use of irradiation specific core depletion states in this work provides results that can be compared to the generic depletion model that was employed in reference [3]. The second sensitivity was the variation of the IPRs sample loading configuration around the irradiated samples; while the third was the effect of the control rod position. The details for these calculations are described and presented in Sections 5.2 and 5.3.

5. Results and Analysis

For the purpose of gaining some insight into the axial flux in the IPR, Figure 5 shows a typical axial flux profile for the unperturbed (empty IPR column configuration) and perturbed thermal flux in Column 1 of the irradiation rig. The control rod insertion depth relative to the rig and axial flux distribution are also illustrated.

One notices that the unperturbed flux shows several axial flux depressions, which result from the structural ribs in the rig design. Comparing the unperturbed flux profile to the perturbed flux profile, one sees that the perturbation in the column due to the sample is fairly local. The thermal flux depression in the perturbed case is most likely due to the replacement of the moderator by the void inside the sample canisters. The calculated average unperturbed thermal flux in positions 1-a and 1-b are in the region of about $3\times10^{+14}$ to $3.5\times10^{+14}$ n.cm^{-2}.s^{-1} respectively.

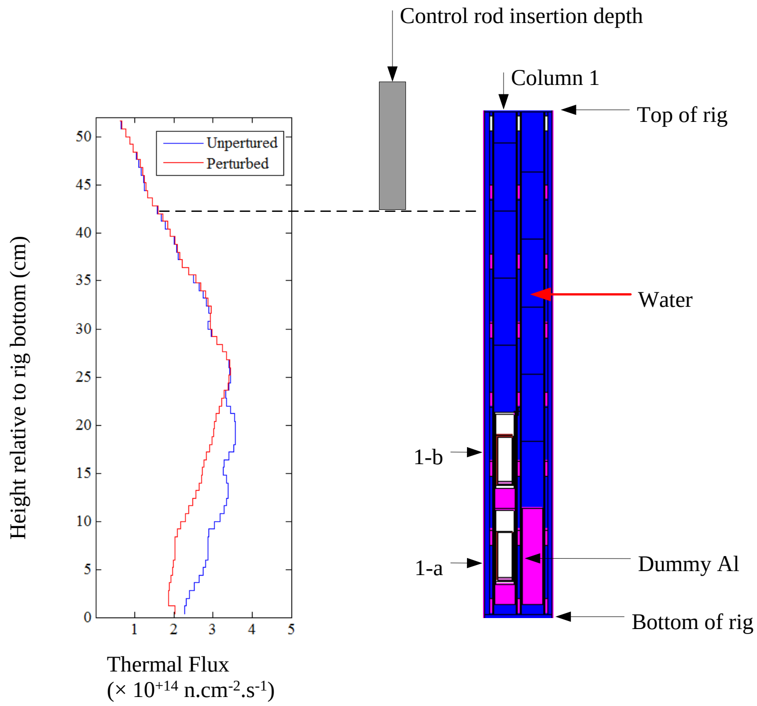

Figure 5 Example of thermal flux suppression in Column 1

5.1 Comparison of calculation with measurement

Figure 6 shows the results of the comparison of the calculated and measured activity with the ratio of calculation to experiment, (C/E – 1) %, for the two approaches to model the depletion state of the core. That is, it shows the results from reference [1] as the "Generic Core Depletion State" and the results from the present work as "Irradiation Specific Depletion State". The relative errors for the MCNP results in both cases were in the order of 2 %. Note that the data points 55 to 62 are where the two core depletion modelling approaches coincide and should be identical for the two cases. These results however, are not identical because the core depletion states for these irradiations were also reselected.

In general, the results show an under-prediction of the measured activities in both cases. One also notices that the use of the explicit core depletion state in the calculations improves the predictions, but only in the order of a few percent. A normal fit to 63 of the 66 data points, neglecting points 2, 6 and 14, yields a mean under-prediction of μ = 7.5 % with a standard deviation of σ = 6.0 %. The corresponding results in reference [3] were μ = 9.1 % (σ = 5.4 %). The exclusion of the three cases were made on the basis that it did not follow the general trend in the data and due to their relatively large over-prediction. The inclusion of these data points result has a negligible effect on the sample mean and variance.

Although there is an average improvement of the predicted activity with the specification of irradiation specific core depletion states, this improvement does not compensate for the initial average under-prediction of 9.1 % that was obtained in reference [3]. In addition, the results of the present work show that the initial approximation of using a generic approach to model the core depletion state is not a poor approximation. This knowledge in turn could be used for the development of a generic calculation model that may be used for future irradiation design calculations.

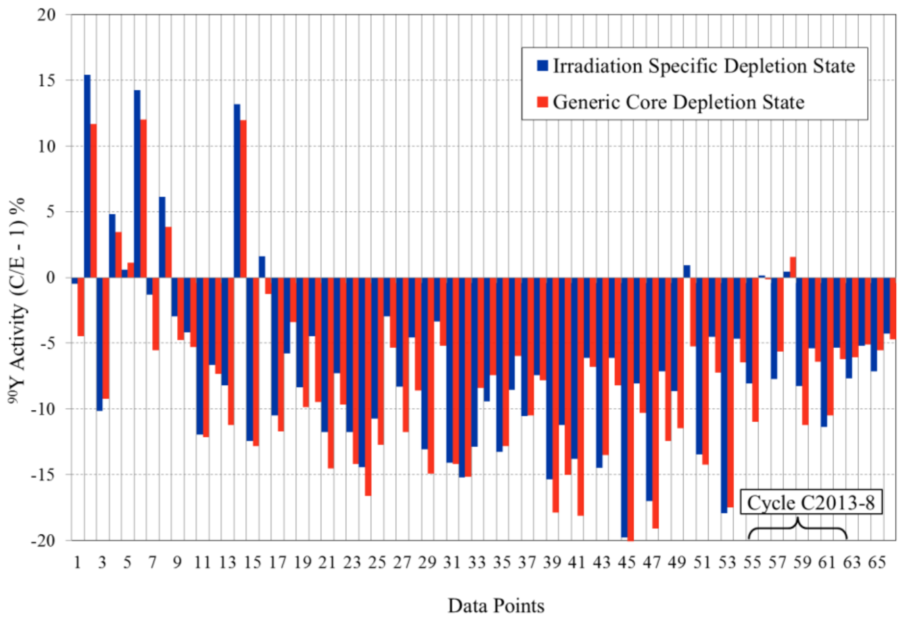

Figure 6 ^{90}Y activity comparison between calculation and experiment [(C/E - 1) %] for two core depletion approximations

5.2 Sensitivity of Loading Configuration

The IPR loading configuration has many degrees of freedom and as such, may influence the resulting activities in the samples in a variety of ways. This degree of freedom also poses a challenge in isolating the impact of the loading configuration on the neutronic parameters, like total neutron flux and flux spectrum, which ultimately determines the sample activity. Numerous IPR loading sensitivity calculations were performed in this work, but only a limited number of cases are presented in this paper.

Three sets of sensitivity calculations are presented in Figure 7 to Figure 9. Each figure shows four sample loading configurations and the relative change in ^{90}Y activity with respect to reference Case 1; which is identical in all three data sets. The reference case consists of two samples in positions 1-a and 1-b of Column 1 as shown in Figure 5. Columns 2 to 4 of the IPR, contained dummy aluminum targets. The numbering scheme for the IPR columns is given in Case 1 of Figure 7. In all the cases, core position F6 does not contain an IPR.

In each of the three sensitivity analysis, the loading configuration was changed by successively replacing the dummy aluminum targets in Columns 2 to 4 (Cases 2 to 4). In

Figure 7 the sample neighbouring columns were replaced by columns of empty containers to determine the effect of water replacement on the activity. In **Figure 8** and Figure 9, the neighbouring columns were replaced by columns of tellurium oxide (TeO) and iridium (Ir) targets respectively.

From Figure 7, one notices that there is no significant change in the relative activity for IPR position 1-a, i.e. there is little effect when replacing the solid aluminum target with a mostly empty canister. The effect of replacing the water in locations adjacent to position 1-b, results in a relative reduction of the activity by a maximum of 16 %.

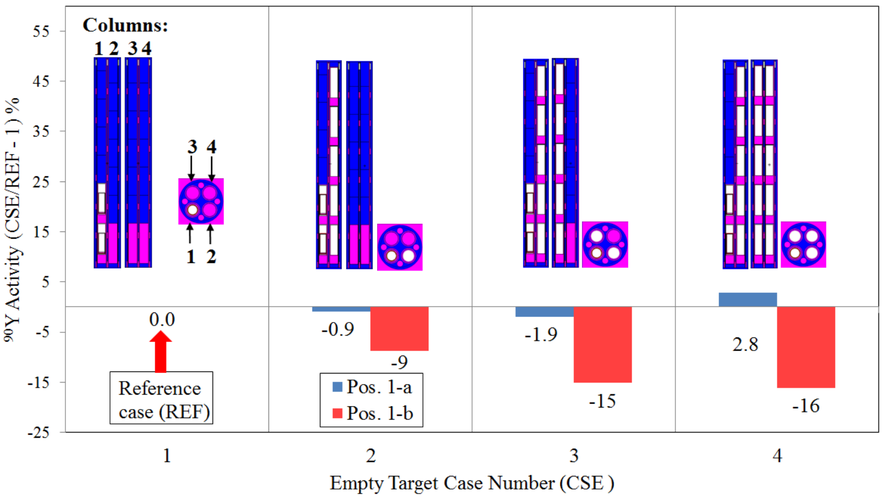

Figure 7 Sensitivity with empty target canister

Similar effects are observed for the TeO and the Ir target cases in **Figure 8** and Figure 9 respectively, except that there is a noticeable reduction in the activities for both positions 1-a and 1-b. The maximum reduction in the activity for the TeO and Ir cases, are 25 % and 33 % respectively.

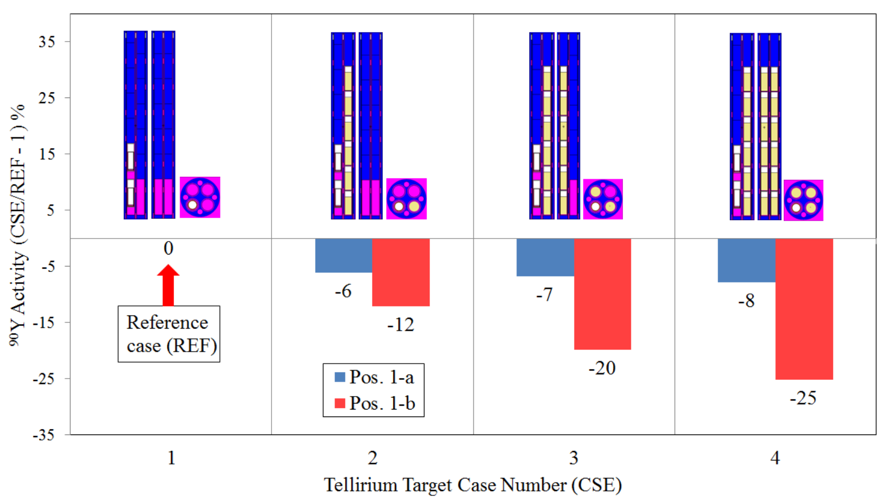

Figure 8 Sensitivity with TeO targets

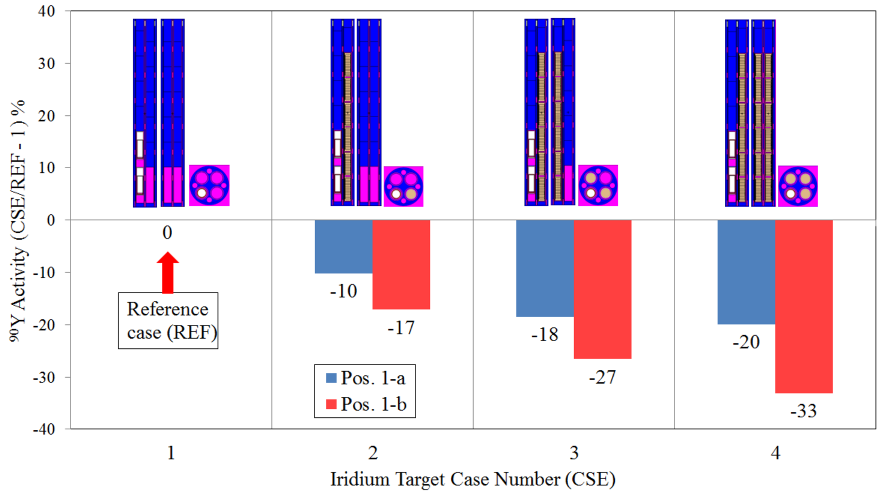

Figure 9 Sensitivity with Ir targets

The results obtained in this section show a general reduction of the relative activity with the replacement of water in neighbouring samples, with a pronounced effect in the TeO and Ir cases. For the TeO and Ir cases, the reduction in activity is not only due to the replacement of water in the columns, but also due to the increased neutron absorption in these targets.

5.3 Sensitivity of Control Rod Bank Position

Figure 10 shows the effect on activity due to control rod movement. The five cases show the control rod bank position and the relative axial flux profile in the column that contained the samples. Case 3 is the reference case. In Cases 1 and 2 the control rod is inserted 10 and 5 cm respectively; while in Cases 4 and 5 the rods are withdrawn 5 and 10 cm respectively.

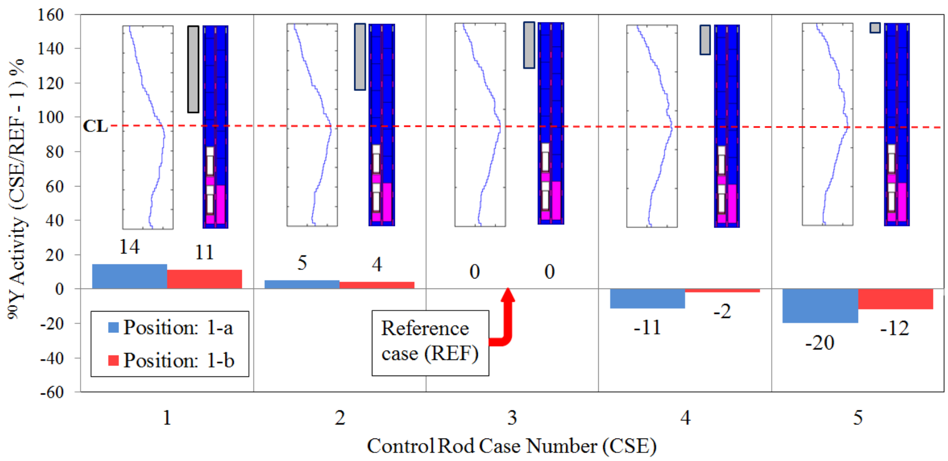

Figure 10 Sensitivity due to control rod movement (CL = Core Centre Line)

The observed effect of the activity is due to the shift of the axial flux profile with the control rod movement. The sensitivity coefficient for position 1-a is 0.6 $\%.cm^{-1}$ and 1.6 $\%.cm^{-1}$ for position 1-b.

6. Conclusions

This paper is an extension of the work in reference [3], which reported the ability of the OSCAR-4/MCNP calculation methodology to predict the activity resulting from in-core irradiations for the production of ^{90}Y. The main contributions in this work consisted of the use of irradiation specific core depletion states and sensitivity analysis on the calculated activity with respect to the rig loading configuration and control rod bank position.

The use of irradiation specific core depletion states, results in an average under-prediction with a mean of μ = 7.5 % (σ = 6.0 %) as compared to the use of a generic core depletion state result of μ = 9.1 % (σ = 5.4 %) [3]. Statistically these results are indistinguishable and as such, verify that the calculated activity is insensitive to the use of irradiation specific core depletion states and that a generic approach can be used for modelling the core depletion state in the OSCAR/MCNP methodology.

The sensitivity analyses performed with different loading configurations show a relative under-prediction of the activity. More specifically, the activity is under-predicted with the replacement of water and the introduction of more absorbing material in the vicinity of the sample. The under-prediction ranges from 0.9 to 33 %, which is the range in which the majority of the (C/E - 1) results are obtained. This result may imply the use of an incorrect or inaccurate representation of the loading configuration around the irradiated samples.

The sensitivity with control rod position shows that the activity may be either over-predicted with rod insertion, or under-predicted with rod extraction. With the modelling approach we adopted for the control rods and with only 3 cm rod extraction during irradiation, we are confident that rod position is not the cause of the observed under-predicted results.

At this time, it is unclear what exactly causes the under-prediction of the measured activities. Since the primary calculated result is the ^{89}Y capture rate, future work will include analyses to determine the effects that influence the neutron flux in the sample. This work will include re-evaluation of the approach to modelling multiple loading configurations during irradiation and considering other input uncertainties.

7. Acknowledgements

The authors thank Rian Prinsloo for providing the core depletion states for the irradiations.

8. References

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