Calculation of the energy produced from radiative capture in SAFARI-1

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Abstract. The knowledge of the fission Q-value is important for the safety analysis of a nuclear reactor. This value is around 200 MeV/fission in all nuclear reactors, where the energy released from radiative capture (Qγc) is the main source of differences between reactors. In this work, we present a detailed calculation of (Qγc) produced in SAFARI-1 using the MCNP-5 (Monte Carlo N-Particle) code. MCNP is a probabilistic transport code that has the capability of solving general geometries with continuous energy data. In particular, we calculate the reaction rate of the nuclides that contributes majorly to the heating in the SAFARI-1 core. From the nuclear reaction rate and the energy released per radiative capture reaction (binding energy), the total energy produced from radiative capture was calculated. In previous work, the radiative capture energy was calculated as an energy deposition using MCNP-5. From the energy deposition calculation, (Qγc) was calculated as 5.42 MeV/fission. Using the energy production method, (Qγc) was calculated as 5.31 MeV/fission. Typical values for (Qγc) ranges between 3 - 12 MeV/fission. This work takes a closer look at how to arrive at these values using the two methods in MCNP-5.

1. Introduction

The knowledge of the recoverable fission Q-value is important for the safety analysis of a nuclear reactor. Physicists and engineers require the reactor specific Q-value to normalize calculated quantities to the total power of the reactor. The fission Q-value of a nuclear reactor is the sum of all the radiation energy components such as energy released from fission products, neutrons, prompt and delayed photons, beta decay and neutrinos. Radiative capture photons also forms part of the components that make up the Q-value, however, (Qγc) is not released in the fission process but recovered after fission in the core. It is important to note that the Q-value is calculated per fission event in the reactor core. Another important fact to note is that the mass of the neutrino is extremely small, consequently, there is no interaction with matter, and all the energy released from neutrinos is lost in the reactor. Although the energy released from neutrinos cannot be recovered from the fission process itself, part of the energy can be recovered from radiative capture. Almost all the components that make up the fission Q-value can be approximated from nuclear data libraries, with the exception of the energy deposited from radiative capture (Qγc). This component is reactor specific due to the fact that it is dependent on the materials present in the core. The process of radiative capture involves the capture of a neutron by the medium with the formation of an unstable compound nucleus. The subsequent release of nuclear binding energy in the process of de-excitation of the compound nucleus is done through the emission of gamma radiation. The deposition of the energy of these gamma rays in the system is the so called ($Q\gamma c$). The Q-value contribution from radiative capture may range from 3 - 12MeV/fission [1]. As a result of this energy range, it can be seen that the radiative capture component may add a significant difference to the estimated Q-values which most scientists generally accept as 200 MeV/fission.

The goal of the paper is to present a method of calculating the reactor specific energy deposition from radiative capture released in SAFARI-1 per fission event. We followed the methodology used in [2] for the Advanced Test Reactor. We use MCNP-5 to calculate the total number of radiative capture reactions produced per fission in the core and then multiply it by the energy released per reaction (binding energy). In a previous work [3], MCNP was used to calculate the energy deposition in SAFARI-1 applying a different approach. Previously, MCNP was used to calculate the heat deposited in the reactor from radiative capture by tracking the gammas produced in the de-excitation of the compound nucleus from birth to death. In this work, we also aim to verify the value that was previously calculated. A description of the MCNP model of SAFARI-1, as well as the procedure to calculate the energy deposited from radiative capture is presented in the following sections. In the last section of the paper, the results for the calculations are documented and discussed.

2. Description of SAFARI-1

SAFARI-1 is a 20 MW tank in pool type material testing reactor (MTR), located at Necsa, Pelindaba, South Africa. 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. The reactor core consists of 26 fuel assemblies and 6 control rod assemblies. The control rod assembly consists of two regions namely the absorbing region and the followers that contain fuel. Apart from the molybdenum production assemblies, it contains several positions for neutron irradiation of samples. For this work, the sample positions were filled with water. SAFARI-1 uses 19.7 % enriched uranium as fuel. Surrounding the core is a beryllium reflector and the aluminium core box.

3. SAFARI-1 Analysis Codes

The two main codes used in support of the operation of SAFARI-1, are the OSCAR-4 code system and MCNP. The OSCAR-4 (OSCAR) code system, which is developed and maintained in the Radiation and Reactor Theory (RRT) Section at Necsa, is used for reactor reload design and core-follow analysis. It contains a three-dimensional, multigroup, nodal diffusion code which performs the calculations in a six energy group structure for homogeneous nodes. During core depletion analysis, OSCAR tracks the depletion history of each fuel element in the reactor core [4].

For detailed transport calculations, the Monte Carlo code MCNP, version 5.1.51 [5], is used. MCNP is a general-purpose Monte Carlo N-Particle transport code that is used in RRT for neutron, photon and coupled neutron/photon transport. MCNP's general geometry modelling capability and the use of pointwise cross-sections are amongst its main features that makes it so applicable for the analysis of complex problems. In general OSCAR and MCNP are used in conjunction, i.e. OSCAR provides MCNP with the appropriate core depletion state for the detailed transport analysis.

4. MCNP Model of SAFARI-1

The MCNP model for SAFARI-1 that was developed at RRT is shown in Figure 1. It includes the reactor core, the core box, the reactor tank and the beam tubes. Inside the reactor tank is a grid plate with a rectangular arrangement of 89 positions where different assembly types can be loaded. The core is surrounded by a beryllium reflector and some aluminium and lead assemblies. Positions D6 and F6 contain the Isotope Production Rigs (IPRs) for irradiation of samples but for this work they are filled with water.

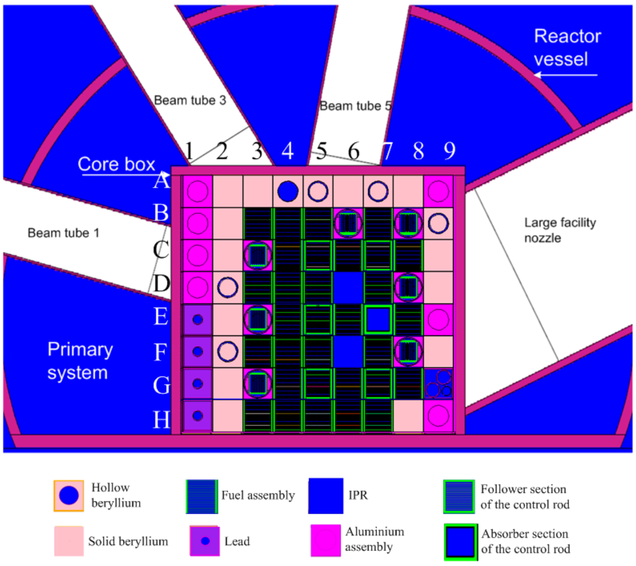

Figure 1: MCNP model of SAFARI-1

Figure 1 shows a planar view of the model with the fuel, control rod elements and control rod fuel follower, at the active regions of these components. The fuel elements are MTR type fuel with 19 plates each. The fuel plates consist of a Uranium-Silicide-Aluminium (U3Si2-Al) powder dispersed core, enclosed in an aluminium-alloy cladding. The control rod assemblies consist of an upper absorber section and a lower fuel section connected through a rigid aluminium coupling mechanism. The absorbing section consists of an aluminium box that contains a cadmium layer as an absorber. The fuel section, also called the control rod follower, is similar to the fuel elements but is constructed inside an aluminium box and contains only 15 plates.

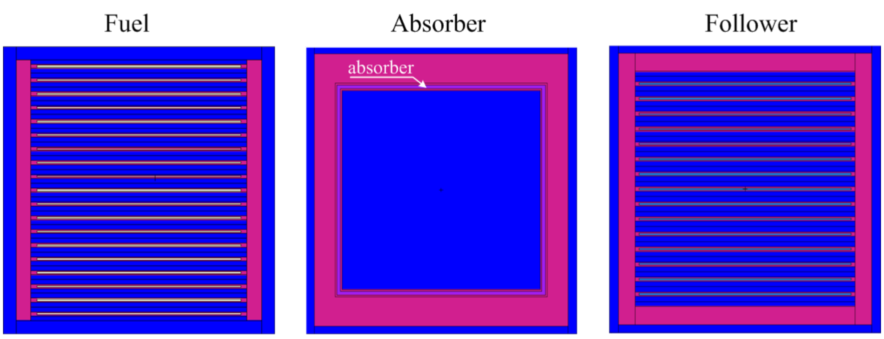

Figure 2: View of the fuel element, absorber and fuel follower

5. Methodology

MCNP is a probabilistic transport code that has the capability of solving generalized geometries using continuous energy data. For this work, MCNP-5 was used to calculate the total number of capture reactions produced from every isotope that contributes majorly to the heating in SAFARI-1. The ENDF-VII library was utilized. The MCNP radiative capture nuclear reaction rate is given by Equation (1). Note that the reaction rate is calculated for isotopes present in every cell of SAFARI-1. The MCNP model of SAFARI-1 consists of more than 3 000 cells.

$$\text{Radiative capture reaction rate} = N_i \int \varphi(\vec{r},E)\sigma_{ci}(\vec{r},E)dEdV \qquad (1)$$

where:

- N_i = number density of isotope (atoms/barn/cm)
- $\varphi(\vec{r},E)$ = energy dependent neutron flux (n/cm^2/neutron born in the system)
- $\sigma_{ci}(\vec{r},E)$ = radiative capture cross section for isotope (barns).

The i^{th} isotopes in Equation (1) are from the elements that contribute majorly to radiative capture heating in the core. Table 1 shows a list of elements present in the different components of the core. From Figure 1 and Table 1 it can be seen that the majority of the core consists of hydrogen and aluminium. Impurities may be present in the material compositions and were not taken into account for this calculation.

Table 1: List of elements present in the reactor core

Hydrogen	**Aluminium**	**Cadmium**	**Silicon**	**Beryllium**	**Uranium**
Water coolant Primary system	Fuel plates Follower Structural assembies	Control rod Irradiation devices	Fuel meat Follower	Fuel meat Follower	Reflector

In order to calculate the number of capture reactions produced per fission in the core, the MCNP capture reaction rate obtained with Equation (1) is multiplied by $\frac{\nu}{k_{eff}}$ (number of neutrons produced per fission). Binding energy is released during radiative capture. By multiplying the total number of capture reactions produced per fission, by the binding energy released per radiative capture, the total amount of radiative capture energy released in the core per fission event can be calculated. Table 2 lists the various nuclides with their associated binding energies that were used for the final calculations.

Table 2: Binding energies of the nuclides present in SAFARI-1

Target element	Target isotope	Compound nucleus	Binding energy (MeV)
Aluminium	Al-27	Al-28	7.7307
Silicon	Si-28	Si-29	8.4751
	Si-29	Si-30	10.617
	Si-30	Si-31	6.5940
Hydrogen	H-1	H-2	2.2245
Cadmium	Cd-106	Cd-107	7.9243
	Cd-108	Cd-109	7.3197
	Cd-110	Cd-111	6.9741
	Cd-111	Cd-112	9.3979
	Cd-112	Cd-113	6.5401
	Cd-113	Cd-114	9.0421
	Cd-114	Cd-115	6.1386
	Cd-116	Cd-117	5.7669
Uranium	U-235	U-236	6.1386
	U-238	U-239	5.7669
Beryllium	Be-9	Be-10	6.8149

6. Results

Calculations were performed using MCNP-5 for 100 active cycles with a well converged fission source. 200 000 histories were simulated for each cycle. Individual calculations were performed for nuclides contributing to radiative capture in the SAFARI-1 core. Table 3 shows the results that were obtained using the above methodology.

Table 3: Calculated energies from radiative capture in SAFARI-1

Target element	Energy due to radiative capture	% Contribution
Uranium	1.77	33.24 %
Hydrogen	1.62	30.46 %
Aluminium	1.18	22.22 %
Cadmium	6.04×10^{-1}	11.38 %
Beryllium	1.30×10^{-1}	2.46 %
Silicon	1.27×10^{-2}	0.24 %
Total	5.31	100 %

From Table 3, it can be seen that the total energy recovered from radiative capture was calculated as 5.31 MeV/fission. As expected, the highest contributor is uranium due to it having a high capture cross-section. Hydrogen and aluminium are also high contributors which could be because the majority of the core is made up of it.

7. Conclusion

By calculating the radiative capture reaction rate in MCNP-5, we calculated the total energy produced from radiative capture in SAFARI-1. This was calculated to be 5.31 MeV/fission. Previously [3], ($Q\gamma c$) calculated as 5.42 MeV/fission by tracking all the gammas produced in the de-excitation of every compound product. The reason for the difference could be due to the fact that we did not consider impurities in the recent radiative capture calculation. The difference is small, around 2 %; therefore we can have confidence in our results. Future work will focus on the inclusion of the heat deposited from the decay products of radiative capture, since some of the product nuclei undergo radioactive decay.

8. References

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