Self-Shielding Effects in Decay Heat Calculations for Tungsten

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ABSTRACT

Precise representation of geometry and energy is essential to properly account for self-shielding effects in tungsten. Up to a factor of 7 overestimation of tungsten decay heat results from homogenization of tungsten and the water cooled heat sink behind it and use of non-self-shielded cross sections in the activation calculations. To correctly estimate tungsten decay heat, 3-D continuous energy Monte Carlo calculations with proper layered heterogeneous modeling should be used to calculate the spectra and reaction rates or effective self-shielded cross sections to be adopted in the activation calculations.

I. INTRODUCTION

Tungsten (W) is an attractive candidate for the plasma facing components in fusion systems. These components have full view of the plasma and are exposed to high energy neutron flux that results in significant activation. The amount of decay heat generated in the tungsten plasma facing material at short times after shutdown has important safety consequences and should be determined accurately. ^{187}W ($T_{1/2}$ = 23.85 h) is the dominant contributor to tungsten decay heat for several days after reactor shutdown. It is produced from the $^{186}W(n,\gamma)$ reaction that is characterized by a giant resonance at 20 eV as shown in Figure 1. Precise representation of the geometry and energy variable is essential to properly account for self-shielding effects. In this paper, the self-shielding effects are assessed for the tungsten plasma facing components of the ITER divertor cassette[1]. Several 3-D calculations have been performed to determine the effect of homogenizing the W with the heat sink material. The importance of using continuous energy treatment with pointwise cross section data for correct W decay heat calculation will be illustrated.

II. CALCULATIONAL MODEL

The continuous energy, coupled neutron-gamma ray Monte Carlo code MCNP-4A[2] has been used in the 3-D neutron transport calculations. The nuclear data used is based on the FENDL-1 evaluation[3]. The detailed geometrical configuration of the divertor cassette has been modeled for 3-D neutronics calculations. The model includes in detail the high heat flux plasma facing components (PFC), the vertical targets, the wings with associated plates, and the gas boxes, as well as the central dome and cassette bodies. Each divertor cassette was divided into 103 regions to provide detailed spatial distribution of the neutron flux. The layered configurations of the dome PFC and vertical targets were modeled accurately with the front tungsten layer modeled separately. Figure 2 shows a vertical cross section of the cassette model at a toroidal location at the center of the cassette.

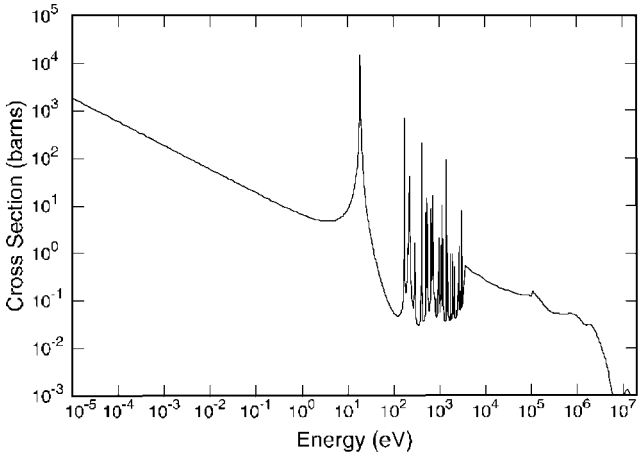

Fig. 1. $^{186}W(n,\gamma)$ cross section.

The regions of interest in this study are the W PFC in the central dome and the inner and outer vertical targets. In the dome, the W layer is 1 cm thick followed by a 2 cm thick heat sink consisting of 75% Cu and 25% H_2O. The top section in each of the inner and outer vertical target has a 1 cm thick W layer followed by 2.5 cm thick heat sink consisting of 82% Cu and 18% H_2O. As shown in Figure 2, each of the vertical targets is divided into upper and lower regions in the calculational model. The divertor cassette model has been integrated with the general ITER model that includes detailed modeling of the first wall and blanket. While Be is used as the plasma facing material at the first walls of the blanket modules, tungsten is used for the inboard and outboard baffle modules above the divertor cassette.

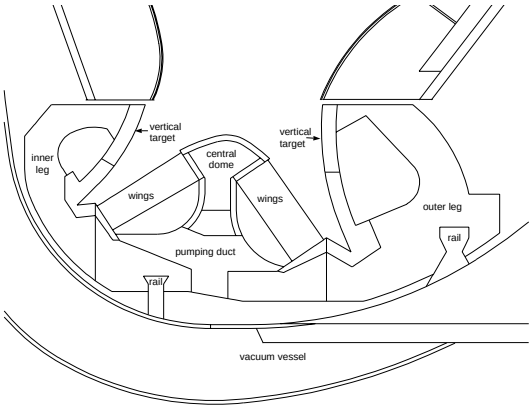

Fig. 2. Vertical cross section at middle of cassette model.

III. NEUTRON ENERGY SPECTRUM

The neutron flux has been calculated in the different components of the divertor cassette. The energy spectra were determined for the VITAMIN-J fine group structure of 175 energy groups used to represent the FENDL data and a coarse group structure of 46 energy groups. The values of the energy integrated neutron flux in the W PFC regions are given along with the one-sigma standard deviation in Table 1. The largest flux occurs in the dome PFC that has a full view of the plasma. Figure 3 gives the neutron spectrum in the W PFC of the dome. The large depression in the spectrum in the W PFC around 20 eV is a result of the giant resonance in the (n,γ) cross section for ^{186}W at 20 eV. The dip in the spectrum in the energy range 3-6 eV represents the effect of the resonance in cross sections for ^{182}W. The shallow dip at ~8 eV results from the resonance in the ^{183}W cross sections.

Table 1. Energy Integrated Neutron Flux in the W PFC of the Divertor Cassette

Zone	Neutron Flux (n/cm^{2}s)	Standard Deviation (%)
Dome PFC	2.16×10^{14}	2.2
Outer Vertical Target		
Upper Region	1.81×10^{14}	3.7
Lower Region	1.46×10^{14}	3.7
Inner Vertical Target		
Upper Region	1.16×10^{14}	4.5
Lower Region	9.70×10^{13}	5.5

IV. GEOMETRICAL MODELING EFFECTS

In the previous 3-D models for the divertor cassette[4,5] the 1 cm thick tungsten PFC was homogenized with the heat sink material. A 6 cm thick zone was used with a homogeneous mixture of W, Cu, SS and H_2O.

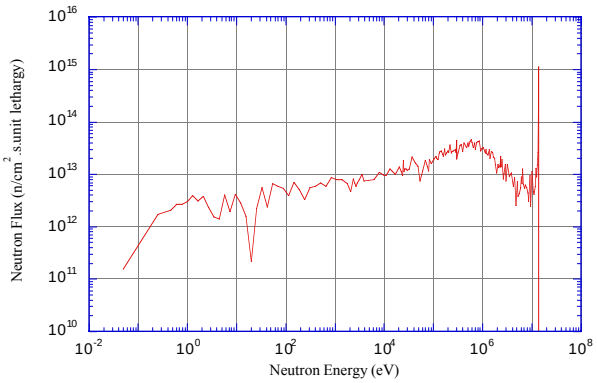

Fig. 3. Neutron spectrum in the W PFC of the dome.

It was pointed out by H. Iida et al.[6] that the improper homogenization of the tungsten with other components can lead to results that are incorrect. The effects of the homogenization of the tungsten armor and substrates on the calculated production rate of ^{187}W were determined using the Monte Carlo code MCNP with a simple cylindrical geometry model. When the W armor and the underlying substrate are homogenized, the ^{187}W production rate is significantly overestimated since the hydrogen in the homogenized zone helps slow down neutrons to the energy of the ^{186}W(n,γ) giant resonance. The overestimate increases as the water content increases. The ^{187}W production rate can be overestimated by up to a factor of two depending on the thickness of the homogenized zone and the water content. This clearly demonstrates that the layered configuration must be modeled correctly to properly account for self-shielding.

In order to illustrate the effect of homogenization, we performed two calculations using the detailed 3-D model developed here. In the first one, the 1 cm thick W in the dome PFC is modeled separately followed by a 2 cm thick heat sink layer consisting of 75% Cu and 25% H_2O. In the second calculation, a homogeneous composition of 34% W, 49.5% Cu and 16.5% H_2O is used in the front 3 cm of the dome. The ^{187}W production rate is given in Table 2 for both cases. The results for the homogenized case are given per unit volume of W in the mixture. The homogenization effect is clear from these results. The value in the front 1 cm is overestimated by a factor of 1.63 when W is homogenized with the heat sink. Figure 4 compares the neutron spectra in the front 1 cm of the dome PFC when W is modeled separately or homogenized with the heat sink back zone. The results are given for 46 neutron energy bins. The softening of the spectrum in the homogenized case is clearly demonstrated.

The effect of homogenization was investigated also by E. Cheng using one-dimensional (1-D) discrete ordinates calculations[7]. These results indicated that homogenization results in a factor of 1.33 overestimate in the calculated W decay heat. This is in good agreement with the effect found from the 3-D results taking into account the lower water content (18%) used for the heat sink in the 1-D calculation. In addition, J-Ch. Sublet modified his previous 3-D model to include a layered configuration for the dome PFC[8]. The TRIPOLI results are in good agreement with the MCNP results presented here. The total energy integrated flux and ^{187}W production rate are 2.26×10^{14} n/cm^{2}s and 3.28×10^{12} nuclides/cm^{3}s compared to 2.16×10^{14} n/cm^{2}s and 3.82×10^{12} nuclides/cm^{3}s from the MCNP calculation presented here. This is an excellent agreement taking into account the differences in codes and modeling. The ^{187}W production rate from the recent TRIPOLI calculation is about a factor of 4 lower than that obtained previously using the model in which the W PFC is included in a single 6 cm thick homogenized zone[5].

Table 2. Effect of W Homogenization on ^{187}W Production Rate (nuclides/cm^{3}s)

Separate 1 cm W Layer	3.8×10^{12}
Homogeneous 3 cm Zone	
Average Over Front 1 cm	6.2×10^{12}
Average Over Back 2 cm	4.4×10^{12}
Average Over Whole 3 cm Zone	5.0×10^{12}

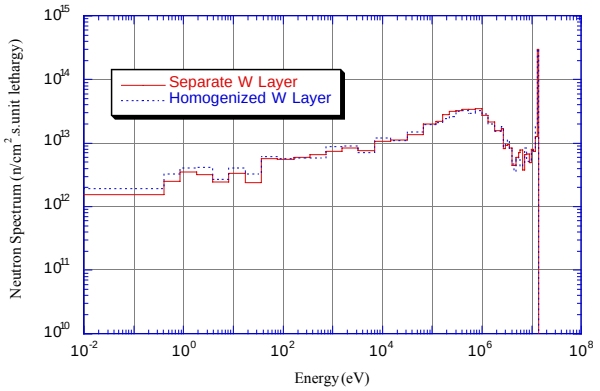

Fig. 4. Effect of homogenization on the neutron spectrum at the W PFC of the dome.

V. EFFECTS OF ENERGY REPRESENTATION

Since the Monte Carlo calculations use pointwise cross section data (continuous energy), the resonance self-shielding effects are treated correctly. Therefore, the neutron energy spectra and reaction rates calculated directly from MCNP take into account the self-shielding effects. This is contrary to the multi-group calculations where the cross sections in each energy group are calculated from the pointwise data using standard weighting spectra. Although some self-shielded multi-group data can be used in the neutron transport calculations to partially account for self-shielding, the multi-group activation libraries do not include self-shielded cross sections. For example, the FENDL activation libraries[9,10] include multi-group cross sections generated from the pointwise data using the VITAMIN-E weighting spectrum. In the energy region from 1 to 100 eV, a smooth 1/E spectrum is used. Since the actual spectrum has a big dip at 20 eV, the multi-group activation data overestimate the ^{186}W(n,γ) cross section at the giant 20 eV resonance. Hence, using the correct neutron energy spectrum that accounts for self-shielding as obtained from the MCNP calculations with the multi-group activation data that does not include self-shielding effects in the activation code will result in overestimating the reaction rates and decay heat.

To illustrate this effect, we initially used the neutron flux calculated by MCNP in the activation code DKR-PULSAR2.0[11] to calculate the decay heat for W. As predicted the value obtained is different from what we get using the exact ^{187}W production rate calculated by MCNP. Although the flux calculated by MCNP and used by DKR-PULSAR2.0 is correct with the proper self-shielding due to the continuous energy treatment, DKR-PULSAR2.0 couples this with the multi-group activation cross section that does not include self-shielding. Hence, the cross section used in DKR-PULSAR2.0 at the group including the 20 eV resonance is higher than it should be if we use the correct flux distribution inside the group for cross section weighting. As a result, we are multiplying the exact energy integrated group flux by an overestimated group cross section leading to an overestimate of the production rate and decay heat.

Based on the MCNP calculation, the ^{187}W production rate is 3.8×10^{12} nuclides/cm^{3}s. Assuming that the ^{187}W concentration reaches equilibrium and using a conversion factor of 1.16×10^{-13} W/Bq for ^{187}W and for the pulse scenario of 1 hour on-1 hour off over a month (360 pulses) we get decay heat of 0.22 W/cm^3 at shutdown that drops by 4% in 1 hour to 0.214 W/cm^3. The DKR-PULSAR2.0 calculation gave 1.53 W/cm^3, which is higher by a factor of ~7. The ^{187}W production rate calculated by DKR-PULSAR2.0 is 2.7×10^{13} nuclides/cm^{3}s, which is higher than that calculated by MCNP by about the same factor. In this initial DKR-PULSAR2.0 calculation, FENDL/A-1.0[9] data in 46 energy groups were used. The effect is expected to be lower when a finer group structure is used. E. Cheng used the neutron energy spectrum in the W PFC of the dome as

calculated by MCNP to perform activation calculations using the REAC code with the FENDL/A-2.0[10] activation data in 175 energy groups without self-shielding[7]. The resulting ^{187}W production rate is 6.98×10^{12} nuclides/cm^{3}s, which is a factor of 1.83 higher than that calculated directly by MCNP with self-shielding taken into account[12]. These results clearly demonstrate the overestimation of activation resulting from using an accurately calculated spectrum from MCNP in activation codes with non-self-shielded activation data. It is interesting to note that some cancellation of error might result if non-self-shielded multi-group data are used in the transport calculation instead of the accurate continuous energy MCNP calculation. The error cancellation is not quite full because the flux is not determined only by the cross section of interest with the giant resonance. This effect was demonstrated by comparing the ^{187}W production rate for a simple 1-D geometry from MCNP to that from ANISN that showed a factor of 1.2 increase.

VI. ACCOUNTING FOR SELF-SHIELDING IN MULTI-GROUP ACTIVATION

In order to fix the problem of proper representation of self-shielding in multi-group activation calculations, one can bypass the reaction rate calculation in the activation code and use the correct reaction rate calculated from MCNP for reactions with big resonances and which produce dominant radionuclides. Alternatively, one can calculate from MCNP the effective multi-group cross sections for the reactions of interest and modify the activation library to include these self-shielded cross sections. This approach was used in the final activation calculations that were performed using the FENDL/A-2 activation data in the 175 group structure. Unfortunately, this modification is problem dependent and will be different for each cell depending on the material composition.

We repeated the MCNP calculation for the divertor to calculate the ^{186}W(n,γ) reaction rate in the W PFC of the dome in 175 energy bins. The reaction rates were used along with the calculated neutron spectra to determine the effective reaction cross sections in each energy group. These group cross sections take into account the effect of self-shielding since MCNP uses pointwise data and the calculated effective cross section is weighted by the actual pointwise flux from MCNP. Figure 5 compares the effective self-shielded cross section to the non-self-shielded cross section in FENDL/A-1.0. This demonstrates the large self-shielding effect particularly at the resonances as expected. About an order of magnitude self-shielding is observed at the 20 eV resonance. Despite the possible difference in evaluated data, the self-shielding effect is clearly demonstrated. The non-self-shielded FENDL/A-1.0 and -2.0 cross sections for ^{186}W(n,γ) are nearly identical. The results indicate that it is essential to modify the production rate of ^{187}W in the activation calculation by replacing it with the value obtained directly from MCNP to properly account for self-shielding. The reaction rates in the front 1 cm W PFC of the dome and vertical targets as calculated by MCNP are given in Table 3. The reaction rates calculated by MCNP account properly for resonance self-shielding and are used in the activation calculations.

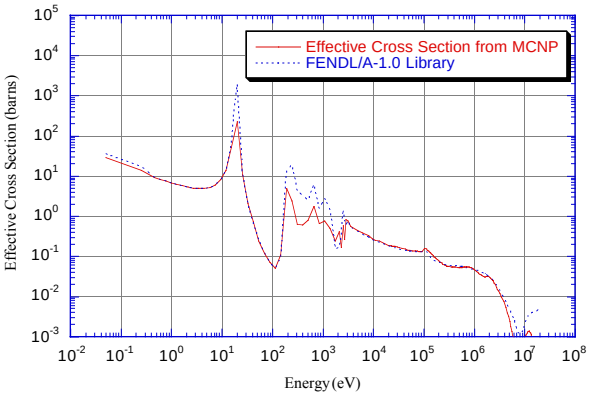

Fig. 5. Comparison between ^{186}W(n,γ) cross section from MCNP with self-shielding and from FENDL/A.

Table 3. ^{187}W Production Rate (nuclides/cm^{3}s) Calculated by MCNP

Dome PFC	3.82×10^{12}
Outer Vertical Target	
Upper	2.43×10^{12}
Lower	1.89×10^{12}
Inner Vertical Target	
Upper	2.03×10^{12}
Lower	1.53×10^{12}

VII. SUMMARY AND CONCLUSIONS

The amount of decay heat generated in the tungsten plasma facing material at short times after shutdown has important safety consequences and should be determined accurately. ^{187}W ($T_{1/2}$ = 23.85 h) is produced from the ^{186}W(n,γ) reaction that is characterized by a giant resonance at 20 eV. Precise representation of the geometry and energy variable is essential to properly account for self-shielding effects. Several 3-D calculations have been performed for the ITER divertor cassette using the continuous energy Monte Carlo code MCNP to determine the effect of homogenizing the W with the heat sink material. The results indicate that homogenization

can lead to decay heat results that are significantly overestimated due to the enhanced spectrum softening. The ^{187}W production rate can be overestimated by up to a factor of two depending on the thickness of the homogenized zone and the water content. This clearly demonstrates that the layered configuration must be modeled correctly to properly account for self-shielding in tungsten.

Since the Monte Carlo calculations use pointwise cross section data, the resonance self-shielding effects are treated correctly and the directly calculated neutron energy spectra and reaction rates take into account the self-shielding effects. Using the correct neutron energy spectrum from the MCNP calculations with the multi-group activation data that does not include self-shielding effects results in overestimating the reaction rates and decay heat. The ^{187}W production rate is overestimated by up to a factor of seven depending on the group structure used in the activation calculation. To fix this problem, the reaction rate calculation in the activation code can be bypassed and the correct reaction rate calculated from MCNP for reactions with large resonances that produce dominant radionuclides can be used. Alternatively, one can calculate from MCNP the effective multi-group cross sections for the reactions of interest and modify the activation library to include these self-shielded cross sections.

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