Scattering Law Data for Graphite in a Gas Cooled Reactor

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1. Introduction

A GCR (Gas Cooled Reactor) employs graphite as a neutron moderator and a reflector. At thermal energies, the scattering of the neutrons is affected by the binding characteristics of the scattering nucleus in the moderator. Thus, these effects should be carefully described by well defined scattering laws. The calculations for the scattering laws require an exact shape of the phonon frequency distribution of a material as an input parameter, as well as its lattice structure. Currently several variations of the phonon frequency spectra are available. We have generated different sets of temperature dependent scattering laws for graphite with the module LEAPR of the NJOY using the available phonon frequency spectra. To find out the effect of these different scattering laws on the criticality of a GCR core, MCNP calculations were carried out and their results were compared with each other. As the basis of a comparison, the keff and the temperature coefficients for the moderator and reflector were used.

2. Generation of Cross Section Data

There are three available variations of the phonon frequency spectra for graphite. The first one was computed by Young and Koppel (YK) using the bondbending and bond-stretching model (BBS) in 1965 [1]. The scattering law data for graphite of the current ENDF/B evaluations are based on this YK spectrum. In 1972, Nicklow et al. published a new phonon frequency distribution [2]. They used the axially symmetric model (AS) for the calculation of the spectrum. The last one



Figure 1. Phonon frequency spectra for graphite.

was computed by Hawari et al. based on the central force dynamical theory [3]. Figure 1 shows the comparison of the phonon frequency spectra.

For the calculations of the scattering law data, the module LEAPR of the NJOY [4] was used. It calculates both the elastic and inelastic scattering effects at the thermal energy region. The scattering law data and cross sections for graphite were prepared at temperatures from 300 to 2000 K at 100 K intervals. Figures 2 and 3 show the calculated scattering cross sections for the three different phonon spectra compared at three temperatures. The cross sections for



Figure 2. Elastic cross sections for graphite.



Figure 3. Inelastic cross sections for graphite.

the YK spectrum are largest in the case of an elastic scattering, while they are smallest in the case of an inelastic scattering. For the MCNP [5] calculations of k_{eff} , the thermal MCNP library was prepared using the module ACER of NJOY99.90.

3. Calculations and Results

To investigate the effect of the different phonon frequency spectra, we calculated k_{eff} at temperatures from 300 to 2000 K at 100 K intervals and the temperature coefficients for the moderator and reflector of a gas-cooled reactor and compared those results.

Table 1, 2, and 3 show the calculated k_{eff} when using the different phonon frequency spectra for moderator, central and outer reflector, respectively. The numbers in the 3rd and 4th columns represent the differences in pcm and errors in parenthesis correspond to last digits of standard deviations. The calculated values agree well with each other within 3 σ except for some values written in red. The Figure 5, 6 and 7 shows the calculated temperature coefficients of GCR for the three scattering law data. The results show the tendency that

T(K)	Young&Koppel	Nicklow et al.	Hawari et al.
	@GA	@ORNL	@NCSU
300	1.42599(33)	-67(33)	-15(32)
400	1.42278(33)	-45(32)	-50(32)
500	1.41856(33)	+55(33)	+86(33)
600	1.41488(32)	+45(33)	+41(33)
700	1.41084(33)	+44(33)	-59(33)
800	1.40652(33)	+42(32)	+5(32)
900	1.40257(32)	+73(33)	+139(33)
1000	1.40016(34)	-103(33)	-71(33)
1100	1.39573(33)	+30(34)	-8(32)
1200	1.39159(32)	+82(31)	+71(32)
1300	1.38851(33)	+87(33)	+66(33)
1400	1.38598(33)	+8(33)	+5(33)
1500	1.38294(33)	+9(33)	+25(34)
1600	1.37951(33)	+46(34)	+76(32)
1700	1.37690(33)	+68(33)	-17(33)
1800	1.37462(33)	+35(33)	-3(33)
1900	1.37204(32)	-31(33)	+33(33)
2000	1.36989(33)	-38(33)	-64(33)

Table 1. Effect of moderator with different phonon spectra on the calculations of GCR core, $k_{\rm eff}$.

T(K)	Young&Koppel @GA	Nicklow et al. @ORNL	Hawari et al. @NCSU
300	1.42579(32)	-37(33)	+22(33)
400	1.42980(32)	-30(33)	-40(33)
500	1.43298(33)	-25(32)	-168(32)
600	1.43575(32)	- <mark>98</mark> (32)	-96(32)
700	1.43742(32)	-23(33)	-38(33)
800	1.43871(33)	+13(32)	-17(32)
900	1.44063(32)	-53(32)	+3(32)
1000	1.44260(32)	+23(32)	-75(33)
1100	1.44327(32)	-23(32)	-14(32)
1200	1.44391(31)	+56(32)	+83(32)
1300	1.44591(32)	- <mark>97</mark> (33)	-21(33)
1400	1.44682(33)	-17(31)	-20(31)
1500	1.44751(32)	-17(32)	-53(31)
1600	1.44728(32)	+23(33)	+123(32)
1700	1.44877(33)	+6(33)	-54(32)
1800	1.44990(34)	-32(32)	-32(32)
1900	1.45026(32)	- <mark>97</mark> (33)	-80(31)
2000	1.45078(32)	-96(32)	-65(31)

Table 2. Effect of central reflector with different phonon spectra on the calculations of GCR core, k_{eff} .

T(K)	Young&Koppel	Nicklow et al.	Hawari et al
	@GA	@ORNL	.@NCSU
300	1.42608(33)	-23 (32)	-30 (33)
400	1.42958(33)	-52 (31)	-42 (32)
500	1.43190(33)	-58 (33)	-57 (32)
600	1.43420(33)	-52 (33)	-134 (32)
700	1.43477(32)	+25 (33)	+44 (32)
800	1.43605(32)	+72 (32)	+23 (32)
900	1.43744(32)	-42 (33)	+34 (33)
1000	1.43822(33)	+96 (33)	+66 (32)
1100	1.43915(32)	-22 (32)	-47 (32)
1200	1.43941(34)	+51 (33)	+51 (33)
1300	1.44010(33)	+84 (32)	+48 (32)
1400	1.44061(32)	-41 (33)	+79 (32)
1500	1.44184(32)	-50 (33)	-37 (32)
1600	1.44231(33)	-54 (32)	-40 (32)
1700	1.44290(32)	-57 (31)	-44 (33)
1800	1.44272(33)	-32 (32)	+23 (32)
1900	1.44289(32)	+11 (32)	-55 (33)
2000	1.44363(33)	-77 (32)	-62 (32)

Table 3. Effect of outer reflector with different phonon spectra on the calculations of GCR core, k_{eff} .

moderator temperature coefficient increases and the reflector temperature coefficient decreases, when the temperature increases.

4. Conclusion

To investigate the effect of the different phonon frequency spectra, the k_{eff} and temperature coefficients

for the moderator and reflector of a gas-cooled reactor were calculated and the results were compared with each other. The results show that different phonon



Figure 4. Moderator temperature coefficient in the GCR.



Figure 5. Central temperature coefficient in the GCR.



Figure 6. Outer temperature coefficient in the GCR.

spectra do not make any significant differences to the calculations of the k_{eff} of GCR core, even though there were large differences between the cross sections for the different phonon spectra

The calculated temperature coefficients showed the tendency that the moderator temperature coefficient increases and the reflector temperature coefficient decreases, when the temperature increases.

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