Benchmarks for the Scattering Kernel of Graphite

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Abstract

The probability of the transfer of energy between the media and the thermal neutron field is sensitive to the phonon spectra of the graphite lattice, $\rho(\omega)$. Despite more recent, and discrepant, calculations of $\rho(\omega)$, the standard evaluation of the scattering matrix, $S(\alpha,\beta,T)$, is still based on $\rho(\omega)$ (and numerical accuracies) from the early 60's. We have calculated new sets of $S(\alpha,\beta,T)$ based on more recent analysis (experimental and theoretical) of the phonon dispersion law. The sensitivities of reactor physics parameters with respects to the scattering matrices were calculated for 2 benchmarks: 1) measured configurations of ~ 16.6 % enriched pebbles (PROTEUS), and 2) measured configurations of the ~ 4 % enriched prismatic fuels (VHTR). Sensitivities for commercial Pebble Bed Modular Reactors and weapons-grade plutonium fueled reactors were also calculated. Very detailed Monte Carlo models were developed for the MCNP code with coated fuel particle (~ 0.5 mm radius) resolution.

I. Introduction

Two developments during the 90's resulted in the questioning of the scattering matrices for graphite. In the early 90's one of us (JPR) discovered[1] that the temperature coefficients of reactivity of some prototypical New Production Reactors (NPR) were sensitive to the numerical accuracy used with the GASKET[2] code. Later, the analysis of the PROTEUS experiments on High Temperature Gas Cooled Reactors (HTGR) made necessary the critical evaluation of the ability of the present evaluation of the scattering matrices to describe the thermalization process in graphite. One of us (FCD) concluded[3] that despite all the improvements in the simulation of the transport of neutrons the ultimate bias is defined by the evaluated scattering matrices, and that the bias is the same as in the early 60's. Under the auspices of a recent NERI[4] (Nuclear Energy Research Initiative) we made a reevaluation of the scattering matrices of graphite based on more recent calculations of the phonon spectra. Reactor physics parameters were then computed with the two sets of scattering matrices, the standard ENDF-B/VI and the new, for measured benchmarks (pebble bed and prismatic fuels) as well as for a model of the Pebble Bed Modular Reactor (PBMR). Pulsed neutron experiments in bulk graphite were also analyzed.

II. Available Models and Data for the Calculations of the Scattering Matrices.

The GASKET and LEAPR[5] codes are the present standards for the calculations of $S(\alpha,\beta,T)$. Both codes calculate the inelastic scattering in the incoherent approximation that cannot describe the considerable structure detected in the direct measurement[6] of the scattering matrices, the basic input for both codes is the phonon spectra. To this moment all ENDF/B evaluations (since version 3) include sets computed with the Young-Koppel[7] (YK) phonon spectra that used the bond-bending and bond-stretching model (BBS) to compute the tensor forces between neighboring atoms in the graphite lattice. This model was later criticized by Nicklow, Wakabayashi and Smith[8] (NWS) as unable to reproduce the direct measurements of acoustic and optical branches of the phonon dispersion law they made at ORNL. The authors used instead an axially symmetric model (AS) to describe the forces that produces results consistent with their measurements. Then they computed the phonon spectra (NWS) shown in Figure 1 together with the YK spectra.

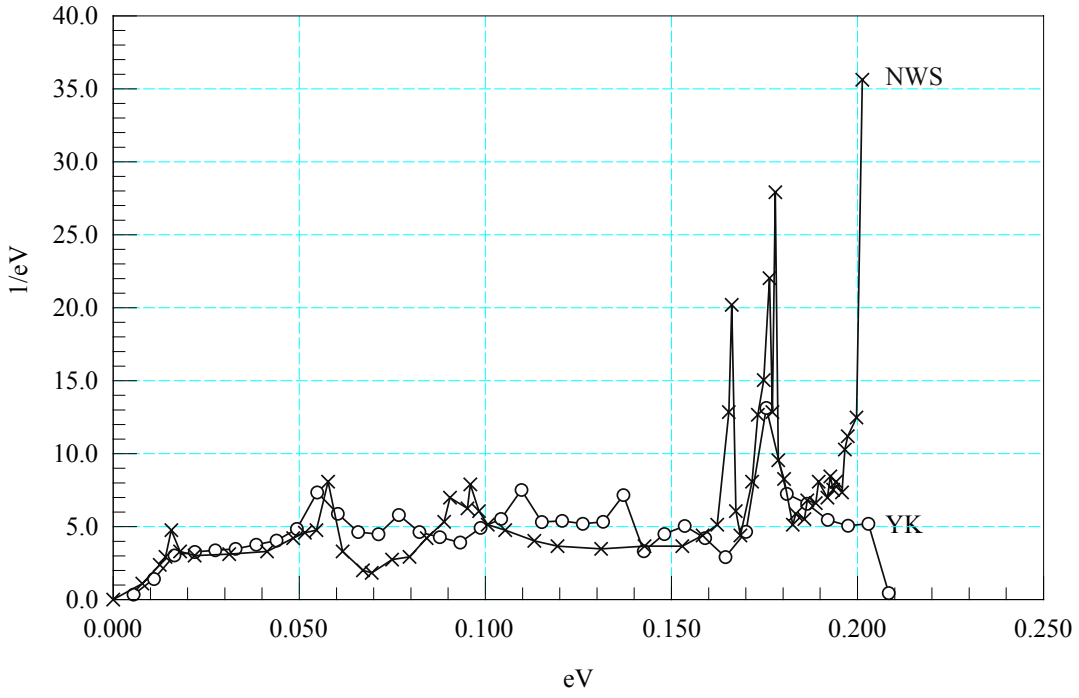

Figure 1: Distributions of oscillators in graphite (or Phonon Spectra) according to Young-Koppel (YK) and Nicklow, Wakabayashi and Smith (NWS). The variable frequency (f) is measured in energy units (E) (E=hf, h Planck constant)

III. Test with Prismatic Fuel Benchmarks

The Japanese facility VHTRC is the source of one of the experimental benchmarks[9] available to test the new calculation of the scattering matrices. In particular we made detailed calculations of the VH1-HP experiment, which consisted in the measurement of k_{eff} as function of the isothermal temperature in simple (or "clean") geometries. The critical assemblies consisted of 12 prismatic fuel elements containing 12 fuel rods each with 4 %

enriched uranium oxide. We used the continuous energy code MCNP4C code for detailed simulation of the configurations. The random distributions of the coated fuel particles were simulated with an explicit cubic lattice of kernels with the appropriate coatings. Table 1 is a summary of the available experimental data.

Table 1
VH1-HP Experiment in the VHTRC[a]

T(K)	k_{eff}	T Coefficient (pcm/K)
298.65	1.008	-15.6
344.35	1.001	-17.9
374.05	0.996	-18.1
423.65	0.987	-17.7
472.75	0.979	-17.3

a: no error available

Calculations were performed at 296, 400 and 500 K and compared with the results of Table 1 with the proper interpolations. The comparison is shown in Tables 2 and 3 for respectively k_{eff} and the temperature coefficient of reactivity. The differences for the k_{eff} are less than a dollar but with k_{eff} systematically larger than the measured values. The differences are smaller for the scattering matrix calculated with the NWS phonon spectrum. No significant differences between YK and NWS models were found for the temperature coefficient of reactivity.

Table 2
Effect of the Scattering Matrix $S(\alpha,\beta,T)$ on the Calculations[a] of the VH1-HP Experiment, k_{eff}

T(K)	YK Sab	Diff (pcm)	NWS Sab	Diff (pcm)
296	1.01368(35)	568(35)	1.01119(35)	319(35)
400	0.99774(35)	645(35)	0.99531(35)	402(35)
500	0.98142(35)	686(35)	0.97952(35)	496(35)

a: Monte Carlo calculations, errors in parenthesis correspond to last digits

Table 3
Effect of the Scattering Matrix $S(\alpha,\beta,T)$ on the Calculations[a] of the VH1-HP Experiment
Isothermal Temperature Coefficients of Reactivity (pcm/K)

T(K) Range	YK Sab	NWS Sab	Experiments
296-400	-15.1(5)	-15.2(5)	-17.5
400-500	-16.7(5)	-16.2(5)	-17.5

a: Monte Carlo calculations, errors in parenthesis correspond to last digits

Calculations were also made at 296 K for MOX fuel with weapons grade Pu mixed with depleted U oxide. The results for the case of the same enrichment (4 % fissile Pu) were k=1.07404(40) for the YK case and k=1.07267(40) for the NWS case.

IV. Test with Pebble Bed Experiments

Seven deterministic and three realizations of random distributions of pebble bed configurations were measured at the PROTEUS facility[9]. The uranium fuel for this case is enriched to16.6 % and the neutron spectrum is harder than in the previous case of Section III. Of the seven deterministic distributions, three contained polyethylene rods to simulate the effects of water ingress. The four measured deterministic configurations with only graphite as moderator and reflector are described in Table 4.

Table 4
Deterministic Pebble Bed Configurations in the PROTEUS Facility
Results from Experiments and Calculations

Case	Core Name[a]	Packing	Comments	Measured[e] k	Calculations[e] YK Sab	Calculations[e] NWS Sab
1	1 State 1	hcp[b]	22 layers m: f=1:2 Sequence AB, AB…	1.0318 (6)	1.0329 (7)	1.0341(6)
2	1a	hcp	21 layers m: f=1:2 Sequence AB, AB	1.0145 (6)	1.0176 (7)	1.0189(7)
3	2	hcp	16 layers m: f=1:2 17 layers m: f=1:0 Sequence AB, AB Reflected with graphite pebbles	1.0106 (6)	1.0162 (6)	1.0174(6)
4	5	CHPOP[d]	22 layers m: f=1:2 Sequence ABC, ABC 23rd layer F=138 pebbles M= 223 pebbles	1.0111 (5)	1.0120 (6)	1.0138(6)

a : Names in PSI documents
b: Hexagonal close packing
c: Bottom reflector channels empty and then filled
d: Column hexagonal point-on-point packing.
e: Error in the last digit between parenthesis

Table 5
Deterministic Pebble Bed Configurations in the PROTEUS Facility
Differences Between Calculated and Measured k's

Case	Core Name[a]	pcm[b] YK Sab	pcm[b] NWS Sab
1	1	115(96)	227(94)
2	1a	311(96)	437(96)
3	2	565(84)	678(88)
4	5	91(84)	266(87)

a : Names in PSI documents
b: Error in the last digit between parenthesis

For this case the calculated[10] k_{eff} are also systematically larger than the measured ones by a fraction of a dollar for both scattering matrices. The small improvement, by using the NWS scattering matrix, observed in the previous case has disappeared in this one.

V. Pulsed Neutron Test

Reference 3 contains a summary of theoretical and experimental results on the neutron decay constant, λ, as a function of the size (or the buckling B) of the graphite media $\lambda = \lambda(B^2)$. The decay constant of a pulse of neutrons injected in bulk graphite is sensitive, for small size media, to the thermalization properties. Table 6 summarizes the results for B^2 of 40 and 60 $1/m^2$ a region with a "chronic" bias of ~ + 4%.

Table 6
Decay constants of Neutrons in 1.74 g/cc Graphite Cubes

$B^2(1/m^2)$	Side (cm)	λ (1/s) YK Sab	λ (1/s) NWS Sab	λ (1/s) Exp
40.	82.	842.	867.	820.
60.	66.	1206.	1254.	1160.

The values under label "Exp" in Table 6 are values averaged from five different experiments. For each experiment the decay constants were interpolated according the experimenter's expansion of λ in power of B^2. The new evaluation of the scattering matrix does not resolve the biases.

VI. Applications to Pebble Bed Modular Reactor Designs

ENDF-B/VI and the new evaluation of $S(\alpha, \beta, T)$ were used in calculations of the proposed South African Pebble Bed Modular Reactor (PBMR)[11]. The 440,000 pebbles (330,000 fuel pebbles for the annular core and 110,000 moderator pebbles for the internal graphite reflector) were modeled explicitly together with the coated fuel particles, and their coating, of the fuel pebbles. For the case of 7 g of U/pebble, 8 % enrichment, fresh fuel, 2 temperatures (half core at 800 K and the other half at 1200K) and 10 cm external graphite reflector (which is a crude simulation of the effects of the total insertion of the external control rods) the results are: k_{eff}=1.04933(64) for the YK $S(\alpha, \beta, T)$ and k_{eff}=1.04979(62) for the NWS $S(\alpha, \beta, T)$.

Differential effects in the flux spectra within the kernels are shown in Figure 2 for the temperatures of 800 and 1200K. The figure shows the ratio of the fluxes computed with both scattering matrices within energy bins.

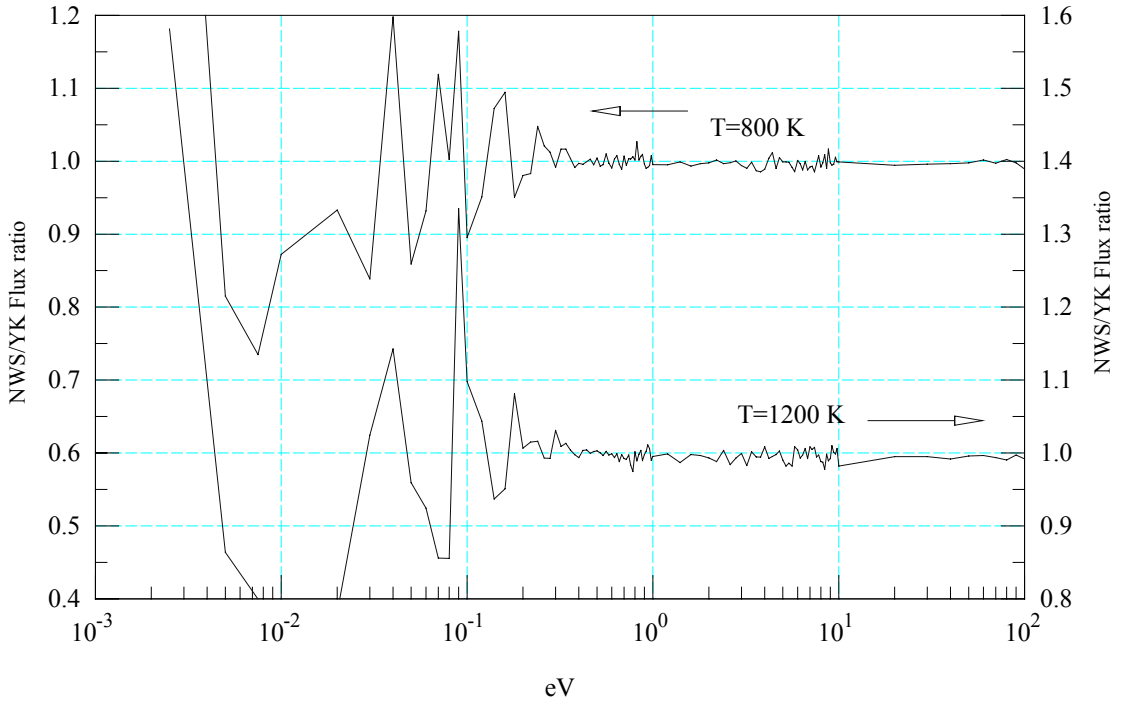

Figure 2: Ratio of the neutron flux spectra inside fuel kernels computed with the NWS $S(\alpha,\beta,T)$ and the YK $S(\alpha,\beta,T)$ at the temperatures of 800 and 1200K.

In general the ratio of the neutron flux spectra (normalized in the same way) fluctuates around unity for good resolution energy bins in a way that the energy average of the cross sections are not very sensitive to the fluctuations.

VII Conclusions

A more recent calculation of the phonon spectra of graphite was used to calculate new scattering matrices for this moderator. The calculation of this newer phonon spectra includes the consideration of new and direct measurements of the phonon dispersion law that preclude the type of interatomic forces used in the calculation of the phonon spectra presently used in the ENDF-B data files (from version III to VI). Calculations were then made with the two scattering matrices for experimental benchmarks in two thermal systems that have some differences in the spectra. Some improvements for k were observed for the case of the more moderated system while slightly worse agreements exist for the system with less moderation.

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