Photoproduction data for heating calculations

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Abstract

For irradiations in a materials test reactor, the prediction of the amount of gamma heating in the reactor is important. Only a good predictive calculation will lead to an irradiation in which the specified temperatures are reached. The photons produced by fission product decay are often missing in spectrum calculations for a reactor, but the contribution of the photons can be computed effectively using engineering correlations for the amount of fission product decay and the ensuing photon spectrum. The prompt photons are usually calculated by a spectrum code based on the underlying nuclear data libraries.

For most of the important nuclides, the nuclear data libraries contain data for the photon productions rates. However, there are still many nuclides for which the photon production data are missing, and some of these nuclides contribute to gamma heating.

In this paper it is estimated what the contributions to heating are from photon production on nuclides such as ²³⁶U, ²³⁸Pu, ¹³⁵I, ¹³⁵Xe, ¹⁴⁷Pm, ¹⁴⁸Pm, ¹⁴⁸Pm, and ¹⁴⁹Sm. Also, simple arguments are given to judge the effect from photon production on all other (lumped) fission products, and from ²⁸Al decay. For all these calculations the High Flux Reactor is used as an example.

1. Problem statement

In experiments in a research reactor a sizable amount of heat is deposited. Unlike the situation in a fuel assembly in a power reactor, this process is not dominated by fission, but by photons. Therefore it is usually referred to as gamma heating, even though neutrons do contribute to it as well. It is difficult to calculate the amount of gamma heating in an experiment, even if the required accuracy is 'only' 10%. This is because photon production has never received the same sort of attention as neutron reactions typically have. For a start, fission product decay photons are not part of neutron transport data, whereas delayed neutron data are. This problem can for the moment only be solved by making use of approximate correlations (Vander Marck, 2006), or maybe in the near future by using the new photon data in ENDF/B-VII.0 for ²³⁵U and ²³⁹Pu (Chadwick et al., 2006). However, the situation is even more difficult because there are photon production data for almost none of the fission products. Even for the most notorious neutron capturing isotopes, ¹³⁵Xe, ¹⁴⁹Sm, or ¹⁵¹Sm, there are no photon production data. Also, for none of the Cd isotopes photon production data are available from either JEFF or ENDF/B. Since the High flux Reactor (HFR, see Figure 1) in Petten, the Netherlands, has cadmium control rods and cadmium burnable poison, this poses a problem.

This situation, combined with the reports from our experimentalists that our heating predictions

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Figure 1 General lay-out of the High Flux reactor in Petten, the Netherlands

have sometimes been low by more than 10%, led us to re-examine the availability of photon production data for fission products, and some actinides as well. The aim was to find out whether we could explain why heating predictions for the HFR were low.

2. Extent of the problem and short term solution

In the MCNP model of the HFR, only a relatively short list of fission products is taken into account explicitly. These are ¹³⁵I, ¹³⁵Xe, ¹⁴⁷Pm, ¹⁴⁸Pm, ¹⁴⁸Pm, ¹⁴⁸mPm, and ¹⁴⁹Sm. In the data libraries we have used so far, photon production is not present in any of these. Only recently for one of these isotopes, ¹⁴⁹Sm, photon production data were included in ENDF/B-VII.0. For the actinides we model explicitly, the situation is less severe. At present we do not use photon production data for ²³⁶U and ²³⁸Pu. However, for these isotopes there are nuclear data evaluations available today that include photon production data. For the purpose of the present investigation we have chosen JEFF-3.1 for ²³⁶U, and

a beta version of ²³⁸Pu, which is currently under development in Subgroup 26 of WPEC.

To judge the effect of photon production by fission products, we need to have new nuclear data files for the isotopes we model explicitly. We have produced these data using TALYS-1.0 (Koning et al., 2007). All the nuclear structure and reaction models have been implemented into one software package, TALYS, which is used frequently by both the nuclear physics and applied nuclear science communities. It simulates reactions that involve neutrons, gamma-rays, protons, deuterons, tritons, helions and alpha-particles, in the $10^{-5} \text{ eV} - 200 \text{ MeV}$ energy range. With a single run, cross sections, energy spectra, angular distributions, etc. for all open channels over a whole incident energy range are predicted.

The nuclear reaction models are accompanied by a restricted set of parameters, such as optical model, level density, photon strength and fission parameters, and the success of describing experimental data depends on the adequate determination, microscopic or phenomenological, of these parameters. With this model code, we are able to provide full nuclear data evaluations of all isotopes of interest, including all secondary distributions such as photon production data. In fact, all the following quantities can be calculated for any nuclide:

- Total, elastic, and reaction cross sections,
- Non-elastic cross sections per discrete state,
- Elastic and non-elastic angular distributions,
- Exclusive reaction channels ((n,2n), (n,p), etc.)
- Exclusive double-differential spectra,
- Exclusive isomeric production cross sections,
- Discrete and continuum gamma-ray production cross sections,
- Extrapolation of non-threshold cross section down to the thermal energy range,
- Total particle production cross sections, e.g. (n,xn)
- Single- and double-differential particle spectra,
- Residual production cross sections (+isomers),
- Level density tables
- Astrophysical reaction rates,
- Recoils,
- Fission cross section and fission yields.

The results presented in this paper stem from "blind" TALYS calculations, i.e. the model calculated results were not adjusted to existing experimental data (this could be done in a next revision if the quality of the photon production data turns out to be essential) but come directly from calculations. These calculations are based on nuclear models, categorized in optical, direct, preequilibrium, compound and fission models. The nuclear models are all driven by a comprehensive database of nuclear structure and model parameters, including the known discrete level scheme of the isotopes under consideration. The results of TALYS were then automatically processed, by a proprietary code TEFAL, into ENDF-6 formatted files. This is the usual format for cross section and particle production evaluations for any isotope. The program TEFAL can put all of the above quantities into this ENDF-6 format automatically. These ENDF-6 formatted files were then processed by NJOY-99.161 to produce ACE formatted files which are subsequently used in our MCNP calculations.

For the remaining isotopes, which are taken into account in the HFR model through lumped fission product pseudo cross sections, we do nothing for the moment. For cadmium one can use the data from JENDL-3.3, which have photon production included.

A final issue is the decay of 28 Al that is produced by capture on 27 Al. The half-life of 28 Al is only 2.2 min., so that after less than an hour the decay of 28 Al is in equilibrium with neutron capture on 27 Al. This implies that for each capture on 27 Al, for which the associated photon production is included in the nuclear data files, this an extra photon production due to the decay of 28 Al, which is *not* included in the nuclear data file.

3. Results and conclusions

The impact of the extra photon production we described in the previous section can be quantified by calculations for the HFR. This reactor has a checkerboard pattern of 33 fuel positions, 6 control rod positions, and 17 in-core experiment positions, see Figure 1. Each position is 7.71×8.1 cm² wide, and the reactor core is 60 cm high. The core is surrounded on three sides by beryllium reflector elements. On the fourth side, on the left in Figure 1, there is a pool side facility with several irradiation rigs. The reactor is operated at 45 MWth for around 300 days per year. The typical radiation heating, averaged over a full experimental position, ranges from more than 10 W/g in row C, to around 3 W/g in rows G and H.



Figure 2 The MCNP model for the full HFR

We have done calculations for the full reactor model using MCNP-4C3, specifying a heating tally for all experimental positions. For each position we calculated (using f6:n,p in kcode mode) average radiation heating in the central 40 cm and the average for the full 60 cm core height. The numbers from MCNP are in MeV/g/'source neutron'. Using a normalization factor based on reactor power (45 MWth), these numbers can be translated to units of W/g. Note that the normalization is based on reactor power vs a similar f6 tally, summed over the whole reactor core. Since the total power is generated mainly in the fuel elements, the calculation of radiation heating in the experimental positions is nevertheless a test whether the photons are produced and transported throughout the reactor core in the correct way.

For the purpose of this calculation, all experimental positions were filled in MCNP with an idealized experiment definition, containing concentric annuli of water, aluminium and stainless steel. This definition represents a typical experimental rig used in the HFR. We performed one reference run with the nuclear data as we have used them until now, which is JEF-2.2 for ²³⁵U and ²⁷Al, and ENDF/B-VI.5 for all other isotopes. For the second run we substituted the new nuclear data as described in the previous section.

The results are shown in the Table below. The values in the table are the extra relative contribution to heating calculated with the new data. In all cases the heating was averaged over HFR experimental positions of $7.71 \times 8.1 \times 60$ cm³.

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The relative contribution to gamma heating from photon production on ¹³⁵Xe, ¹⁴⁹Sm, ¹⁴⁷,¹⁴⁸,^{148m}Pm, for all in-core experimental positions in the HFR.

	Α	В	С	D	Ε	F	G	Н
2				3%		3%		3%
3			3%		3%		3%	
4								3%
5			3%		3%		2%	
6								2%
7			2%		3%		2%	
8				2%		2%		1%

Table 2

The relative contribution to gamma heating from photon production on Cd, for all in-core experimental positions in the HFR

	Α	B	С	D	Ε	F	G	Н
2				3%		4%		2%
3			3%		5%		6%	
4								4%
5			4%		5%		6%	
6								5%
7			4%		5%		6%	
8				3%		4%		5%

The effect of photon production on all the fission products that we have lumped together can be estimated as follows. From MCNP one can get a table detailing the amount of capture per isotope. For all the lumped fission products in the whole reactor model this amount is roughly 60% of the amount of capture on ¹³⁵Xe, ¹⁴⁹Sm, and ^{147,148,148m}Pm combined. Assuming the Q-value for capture on all these fission products is similar to the ones for ¹³⁵Xe and ¹⁴⁹Sm, and that the photons are equally energetic, we can tentatively conclude that photon production on lumped fission products will yield roughly 60% of the effect of ¹³⁵Xe, ¹⁴⁹Sm, and ^{147,148,148m}Pm on photon production, i.e. another contribution of 2%. The spatial distribution of the lumped fission products is different from ¹³⁵Xe, though, because ¹³⁵Xe reaches equilibrium soon, whereas most of the others build up over a longer

time, and therefore accumulate more in older fuel elements.

The contribution of ²⁸Al decay to photon production, and therefore to gamma heating, can be estimated by considering the emitted photon of 1.78 MeV. The amount of capture on ²⁷Al is roughly twice the amount of capture on ¹³⁵Xe and ¹⁴⁹Sm, but the photon energy of 1.78 MeV is only a quarter of the Q-value of ¹³⁵Xe. This would lead to a crude estimate that ²⁸Al decay has half the effect of capture on ¹³⁵Xe and ¹⁴⁹Sm, i.e. an extra 1.5% contribution to gamma heating. However, the spatial distribution of capture on ²⁷Al is different from the ¹³⁵Xe distribution, so this estimate is very crude indeed.

All in all we find an effect on gamma heating of up to 7% from fission products and ²⁸Al, and 5% for cadmium. We conclude that a more rigorous treatment of all these affects may lead to much improved nuclear heating predictions for the HFR.

References

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