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LWR decay heat calculations using a GRS improved ENDF/B-VI based ORIGEN data library

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Abstract. The known ORNL ORIGEN code is widely spread over the world for inventory, activity and decay heat tasks and is used stand-alone or implemented in activation, shielding or burn-up systems. More than 1000 isotopes with more than six coupled neutron capture and radioactive decay channels are handled simultaneously by the code. The characteristics of the calculated inventories, e.g., masses, activities, neutron and photon source terms or the decay heat during short or long decay time steps are achieved by summing over all isotopes, characterized in the ORIGEN libraries. An extended nuclear GRS-ORIGENX data library is now developed for practical appliance. The library was checked for activation tasks of structure material isotopes and for actinide and fission product burn-up calculations compared with experiments and standard methods. The paper is directed to the LWR decay heat calculation features of the new library and shows the differences of dynamical and time integrated results of ENDF/B-VI based and elder ENDF/B-V based libraries for decay heat tasks compared to fission burst experiments, ANS curves and some other published data. A multi-group time exponential evaluation is given for the fission burst power of 4 important fission materials, to be used in quick LWR reactor accident decay heat calculation tools.

1 Development of a GRS improved, ENDF/B-VI based ORIGEN data library

A new nuclear data library GRS-ORIGENX [11] is now developed for practical appliance. In a first step of development, called LIBMAST04, some problems in the former ORIGEN calculation method [2] and/or in the data libraries for structural material activation calculations (LIB1), for the actinide build-up (LIB2) and the fission product generation (LIB3) could be solved, e.g., the tritium, ^{14}C, ^{22}Na, ^{26}Al, ^{60}Fe or ^{93m}Nb production problem. This was achieved by extending the number of neutron reaction channels, the energy groups and the energy range. All cross sections and build-up channels are completely recalculated by point data files JEF-2.2, ENDF/B-VI, JENDL3.2 and EAF97. But the decay data and fission yields of LIBMAST04 were based on ENDF/B-V as in the burn-up program system OREST-96 [10].

In a second step of development LIBMAST06 the decay data – decay energies, probabilities and channels – and 25 fission yield sets are now taken from ENDF/B-VI data bases. The decay energies were analyzed and improved for reactor accident calculation to avoid the slight under-predictions of the reactor decay heat in the first 1000 seconds in ENDF/B-VI. Especially the beta and gamma energies of 70 important fission products were enlarged by 5%. The library was checked for structure material isotope activation, and for actinide and fission product burn-up inventories compared with experiments and standard calculations. The overall data of the new library, compared to elder evaluations, are listed in table 1, last column:

Table 1. Nuclide numbers and data range LIBMAST06 and former ORIGEN versions.

Library	ORIGEN ref. [2]	ref. [10] *)	LIBMAST-04 *)	LIBMAST-06 **)
Number of nuclides				
LIB1	253	700	980	1050
LIB2	101	144	177	177
LIB3	461	847	1116	1195
Range of decay data				
Channels	7	8	8	8
Fission yield sets	5	5	20	25
Delayed n-precursors	0	95	95	225
Number of neutron reactions				
LIB1	6	6	15	15
LIB2	7	7	16	16
LIB3	2	2	15	15
E-Groups	3	3	6	6
Up to MeV	10	10	20	20

*) Decay library based on ENDF/B-V. **) Decay library based on ENDF/B-VI.

1.1 Burst decay heat exponential presentations for ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu

For the most important fission materials ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu we started GRS-ORIGENX decay heat calculations up to 10^{13} seconds. Due to good agreement in fission burst experiments, a time group exponential development was generated by the GRS-WATT10 code for the four isotopes.

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The data represent the exact ORIGENX results inside one, maximum two percent (see last two lines in the tables) starting at discharge up to 10^{13} seconds or 317,000 years. They can be used in quick LWR reactor accident calculations. It should be mentioned, that only the decay heat of the fission products is respected. Decay heat contributions of actinides and of captured delayed neutrons are excluded.

The data fit two simple burst decay power/energy equations, summarizing the time groups m = 1.34 for each fission material l = 1.4

$$\mathrm{Pl}(t) = \sum_{m} \alpha_{lm} * \exp(-\lambda_{lm} * t), \qquad (1)$$

Pl(t) is the power (MeV/s) of material l at time t (s)

$$Q_l(t) = \sum_{m} (\alpha_{lm}/\lambda_{lm}) * \left[1.0 - \exp(-\lambda_{lm} * t)\right], \qquad (2)$$

$Q_l(t)$ is the emitted energy (MeV) of material l at time t (s).

The decay power of fission products for longer burn-up times than a fission burst can be constructed by using equation (2) for the reached burn-up time, summing over the fission rates of the four fission materials and combing this expression with equation (1) for the decay time. This method is used, e.g., in [3].

1.2 Burst decay heat calculations compared to measurements and other evaluations in the short time range

In figure 1, a comparison of different library evaluations and the averaged value is made for the burst decay heat of ^{235}U, presented as a curve F*T (power*decay time). Five measurements for the total (gamma plus beta) power were used from 0.4 up to 7×10^4 seconds. It is good to see that LIBMAST06 (full square dots) fits the experimental results (empty circles). The ANS curve ([1], triangular dots) slightly over-predicts, but the ENDF/B-V based LIBMAST04 library (empty square dots) and also the ENDF/B-VI based SCALE5-ORIGENS library (cruciform dots) under-predict the measured data by some percent.

The deviations of codes and single experiments are shown in figure 2, where the zero deviation line is represented by the averaged five measurements. The spreading of the measurements [5–9] against the averaged data is found as ±5%. The most recent gamma and beta measurements taken from [9] (empty square dots, /NZLU35-8/), dated from 1997, are found up to 5% higher than the zero line, whereas the known ORNL-Dickens data ([6], /NZLU35-2/) are up to 5% lower than the averaged value.

In [9] we found the beta values to be reliable over the whole time range of measurements, but the gamma values after 2000 seconds are found to be significantly too low, so for [9] our experimental total results ended at 1000 seconds.

Similar results and good agreement in the short time range we found for ^{239}Pu in seven measurements from 0.7 to 7×10^4 s, ^{238}U in two measurements from 0.4 to 2×10^4 s and ^{241}Pu, where only one measurement from 5 to 10^4 s is available.

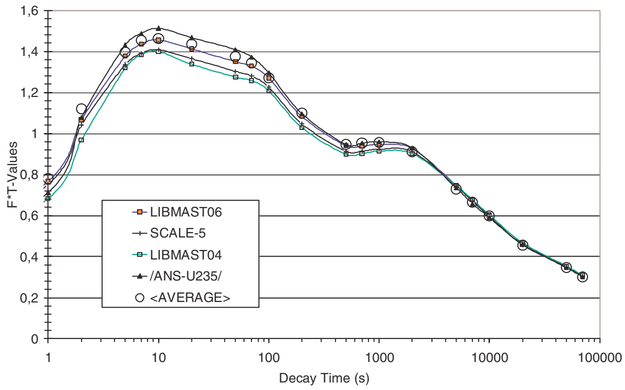

Fig. 1. Experimental average decay heat ^{235}U in comparison to three libraries and ANS [1].

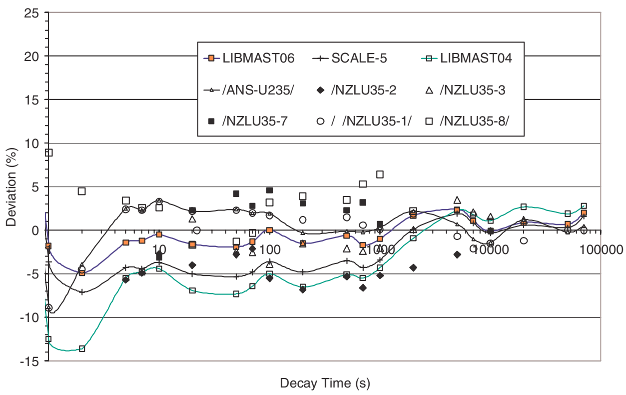

Fig. 2. Deviations of the three libraries and ANS of figure 1 against experimental ^{235}U decay heat.

We noticed that the pandaemonium effect, the great discrepancy between the gamma and beta decay heat in the range between one and 1000 seconds in the ENDF/B-V based data libraries ([10] and LIBMAST04) is now avoided in the ENDF/B-VI based library of this paper.

1.3 Burst decay heat calculations in the long time range

The library was tested against the future German Industry Decay Heat Standard DIN 24563-2 [3] for PWR MOX fuel. An exponential presentation in 24 time groups is here given for four fission materials ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu. The long time range of [3] is limited to 10^9s or ca. 30 years. In the whole decay time range a comparison was made with our LIBMAST06.

In the short time range of ref. [3] at burst decay heat calculations up to 10^4 s we found a slight under-prediction of the averaged ^{235}U experimental data in figure 1 similar to SCALE5/ORIGENS or [6], but for the other fission materials ^{238}U, ^{239}Pu and ^{241}Pu the agreement with our calculation or the experimental data was very good. For the long time decay heat range greater 10^4 s the DIN-LIBMAST06-comparison was made up to 10^{11}s, see figure 3 for ^{235}U and figure 4 for ^{239}Pu.

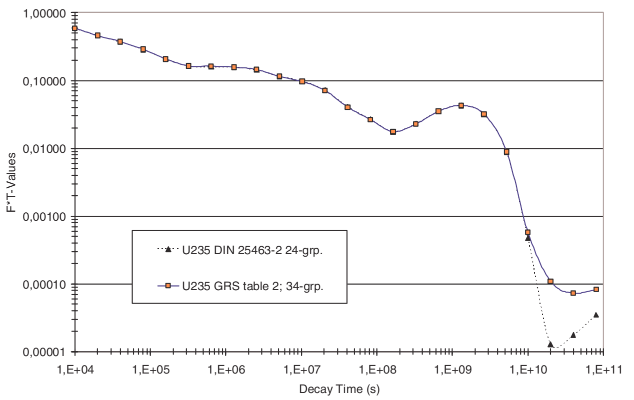

Fig. 3. ^{235}U decay heat GRS-LIBMAST06 and DIN 25463-2 in the long time range.

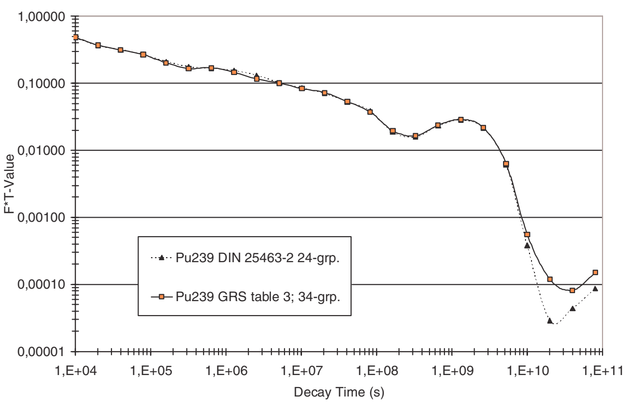

Fig. 4. ^{239}Pu decay heat GRS-LIBMAST06 and DIN 25463-2 in the long time range.

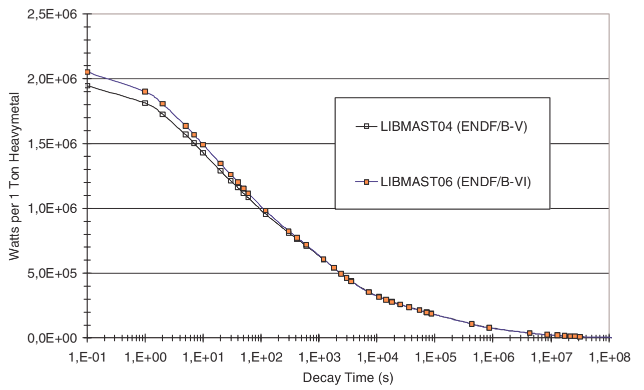

Fig. 5. Decay heat of PWR UO2 at a burn-up 40 GWd/tHM, calculated with OREST-V04 (ENDF/B-V decay data) compared to OREST-V06 (ENDF/B-VI decay data).

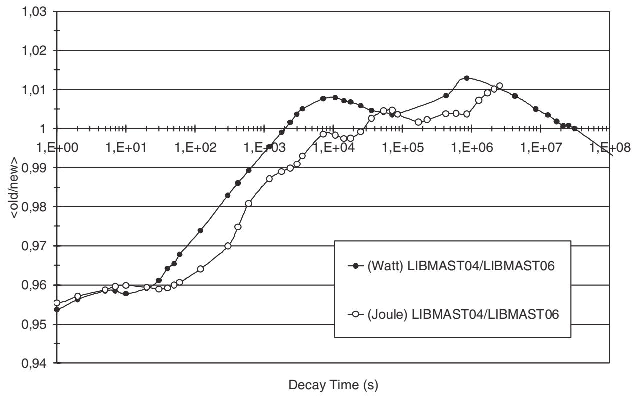

Fig. 6. Library comparison of the decay power and emitted decay energy calculated from figure 5.

The figure 3 for uranium-235, the most important fission material in UO_2 fuel, shows clearly that both exponential presentations, DIN or LIBMAST06, are in very good agreement in a time range up to 10^{10} s or ca. 317 years. Same is true for plutonium-239, figure 4, which is in MOX fuel the most important fission material, and for ^{238}U and ^{241}Pu (not shown). Beyond such long decay times of 10^{10} s a more detailed evaluation with more groups than 24 should be used; for example our evaluation, which had been developed up to 10^{13} seconds.

2 Burn-up calculations and decay heat

Fission burst analysis is only one (important) aspect of the methods to prove a library. But in the short pulse all other neutron activation processes which lead to other long living decay heat emitting isotopes are neglected, which normally occur in the neutron flux during the reactor burn-up time periods. The build-up of ^{134}Cs by neutron capturing in the fission product ^{133}Cs is the most known and most important example.

Using LIBMAST06 of the GRS-ORIGENX code, six improved standard ORIGEN card image libraries were generated for our burn-up systems 1D OREST and 3D KENOREST [4]. In the next figures the heat production of UO2 and MOX PWR fuel after realistic burn-ups of 40 GWd/tHM in a standard fuel assembly is shown for the ENDF/B-VI improved library LIBMAST06 compared to LIBMAST04, which is the elder ENDF/B-V decay data based library with same updated neutron cross sections.

It should be mentioned, that in the following figures only the decay heat of the actinides and fission products is respected. Decay heat contributions of activated structure materials and of captured delayed neutrons are excluded.

In figure 5 the UO_2 decay power after the reactor shut down up to one month is shown for the elder and the improved library.

In figure 6 a quotient old/new is generated for the production of the decay power and the time integrated emitted decay energy. The differences of these realistic calculations with all fission and neutron capturing processes show, that the older library under-predicts the decay power (full circles) up to 1000 s, and under-predicts the emitted energy (empty circles) up to 10^4 s. But it is interesting to see that – starting from these time points up to 10^7s – the elder ENDF/B-V based library gave a slightly higher decay heat (ca. 1%).

Analogous data as shown in figures 5–6 had been generated with the same burn-up and reactor power for a typical MOX fuel assembly as shown in figures 7–8. The

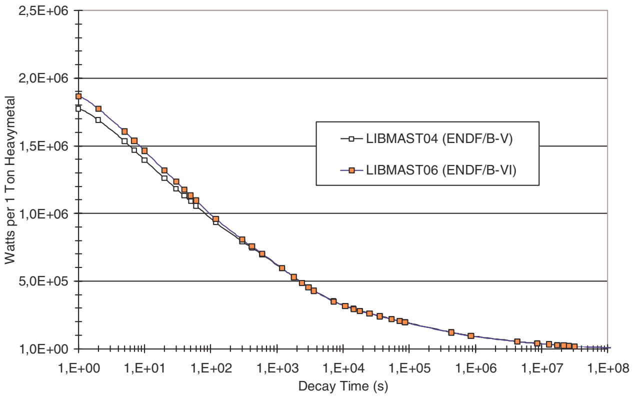

Fig. 7. Decay heat of PWR MOX at a burn-up 40 GWd/tHM, calculated with OREST-V04 (ENDF/B-V decay data) compared to OREST-V06 (ENDF/B-VI decay data).

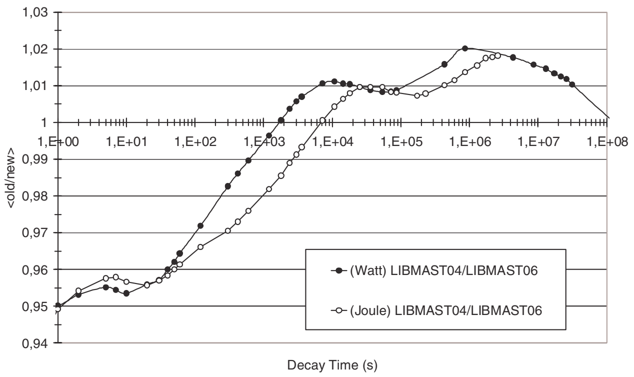

Fig. 8. Library comparison of the decay power and emitted decay energy calculated from figure 7.

maximum MOX decay heat under-predictions arrive 5%, the over-prediction in the time range 10^4–10^8 s arrive a maximum of 2%.

3 Conclusions

A new GRS-ORIGENX library was developed with 16 neutron reactions and 8 decay channels based on ENDFB/F-VI decay data and fission yields and cross section point data for 500 capturing isotopes. The library is used in activation, shielding and burn-up tasks. In the short time range the decay energies of the 70 most important ENDF/B-VI fission product isotopes were enlarged by 5%. For a comparison good agreement with experimental fission burst decay heat experiments for ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu could be shown. A multi-group time exponential evaluation was generated, which can be used in quick reactor accident calculations, representing the exact results of GRS-ORIGENX inside 1% or maximal 2% from discharge up to 10^{13}seconds. A long time calculation compared to the future German Industry Decay Heat Standard for PWR MOX fuel is in good agreement between 1up to 10^{10} seconds for ^{238}U, ^{239}Pu and ^{241}Pu and between 10^4 up to 10^{10} seconds for ^{235}U. The library is available in the GRS-ORIGENX format or in the standard ORIGEN format for the HTGR, LWR and FBR reactor type.

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