VALIDATION OF DECAY HEAT DATA FROM ENDF/B-VI, JEF-2.2, AND JNDC FP (second version) Nuclear Data Libraries

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ABSTRACT

The ENDF/B-VI, JEF-2.2, and JENDL-3.2 evaluated nuclear data files are widely used and accepted for reactor physics calculations. Nuclide cross sections in these files are validated with mathematical benchmarks and critical experiments. This is mostly not the case with fission yields and decay heat data, except for the Japanese data. In this paper, a comparison has been made between two decay heat experiments and calculations using analytical solutions (decaying exponentials) and evaluated data from ENDF/B-VI, JEF-2.2, and JNDC FP files for the fissile nuclides ^{233}U, ^{235}U, and ^{239}Pu. For all these nuclides the decay heat is overestimated for both analytical and evaluated results for short irradiation times (about 20%) and less underestimated for both analytical and evaluated results for long irradiation times (about -10%).

I. INTRODUCTION

In a fission event of a heavy nucleus a recoverable energy (excluding the neutrino energy) of about 190 to 200 MeV is released, depending on the nuclide fissioned. From this recoverable energy about 7.5% is released by decay of the fission products. This decay heat production will continue for a long time after a reactor is shut down. The decay heat production and its time dependence is therefore extremely important in loss of coolant accidents, but also plays an important role in the transportation and storage of spent fuel. The decay heat production can be calculated from the decay rate of fission products if the decay energy for each unstable fission product is known. The nuclide densities of the fission products depend on the decay constants of all the nuclides in a decay chain and to a lesser extend on the cross section for transition to another fission product. For a large number of fission products these data are included into the ENDF/B-VI[1], JEF-2.2[2], and JNDC FP[3] evaluated nuclear data files and need validation by comparison of decay heat measurements. For the calculations, we used the functional module ORIGEN-S from the SCALE-4.2 code system[4] for the decay heat production, using updated ORIGEN-S libraries from ENDF/B-VI, JEF-2.2, and JNDC FP data respectively. Analytical solutions are also retrieved by using a weighted sum of 23 decaying exponentials from the American National Standard for Decay Heat Power in Light Water Reactors[5] and the JAERI standard using 33 exponentials.[3]

II. EXPERIMENTAL DATA OF DECAY HEAT

For validation of decay heat data results are available from two carefully designed and executed experiments of decay heat measurements. Dickens et al.[6] irradiated thin foils of fissile material of about 10 µg for 1, 10, and 100 s, and measured decay heat between 2 and 2000 s after the irradiations, respectively. Yarnell and Bendt[7] irradiated thin foils of 66 mg of fissile material for 20,000 s and measured the total decay heat between 10 and 10^5 s after the irradiations, respectively. The major fissile isotopes in the foils were ^{235}U and ^{239}Pu for the Dickens experiments. In the case of Yarnell and Bendt the fissile isotopes ^{233}U, ^{235}U, and ^{239}Pu were used respectively. The foils used by Dickens et al. were irradiated in a thermal neutron flux of 3.10^{17} n/m^2/s. For the Yarnell and Bendt experiments the neutron flux during the experiments was not specified, a value of 10^{16} n/m^2/s (average thermal flux in a reactor) was used in the calculations. All measurement results are given in MeV/s and are normalised to a fission rate (s^{-1}) in the foil. Hence, calculated results are expressed in MeV per fission. Therefore, the neutron flux value is of little importance.

III. DECAY HEAT CALCULATIONS

The functional module ORIGEN-S of the SCALE code package solves the nuclide density equations for over 100 actinides and over 1000 primary and secondary fission products during irradiation and a subsequent decay time interval. It uses a library with cross section and decay data for all these nuclides. The ORIGEN-S library as supplied with the SCALE code package was updated[8] in the Netherlands in a joint effort of the Interfaculty Reactor Institute (IRI) and the Netherlands Energy Research Foundation (ECN), using all available data from the JEF-2.2 evaluated data file. The data of ENDF/B-VI can also be used to update the ORIGEN-S library, as this file has the same ENDF-6 format. The JENDL-3.2 file does not include fission yield and decay heat data. These data are available in the JNDC FP file. Those nuclides in the ORIGEN-S library not present in the ENDF/B-VI, JEF-2.2, or JNDC FP file, were effectively removed from the ORIGEN-S library. For a proper calculation with ORIGEN-S the irradiation and decay time intervals had to be taken sufficiently small to avoid error messages. To compare the calculational results with the measurements data all the time instances at which measurements were reported were included in the ORIGEN-S input specification.

As the measurement results are reported in MeV per fission, proper normalisation of the calculational results was needed. The normalisation is obtained from the total burnup obtained in the foil and calculating the fission rate using the prompt energy release per fission as calculated by ORIGEN-S.

The decay heat measurements are also compared with analytical solutions (using a weighted sum of 23 decaying exponentials) from the American National Standard for Decay Heat Power in Light Water Reactors and the JAERI standard using 33 exponentials.

Results of the Dickens benchmark are given in Fig. 1 and 2 for ^{235}U and in Fig. 3 and 4 for ^{239}Pu. The results for the Yarnell and Bendt benchmark are given in Fig. 5 and 6 for ^{233}U, in Fig. 7 and 8 for ^{235}U, and in Fig. 9 and 10 for ^{239}Pu. For all the benchmarks firstly the analytical results including measurements are displayed and secondly the results from evaluated data files including measurements are displayed.

IV. COMPARISON OF CALCULATIONS WITH EXPERIMENTS AND DISCUSSION

The results of the Dickens case and the Yarnell and Bendt case differ because of the different irradiation times. In the Dickens case the irradiation time is much shorter, leading to less build-up of fission products and hence to lower values of the decay heat. By including the material from the seals of the foils in the calculation it was found that their activation plays no role in the decay heat. The neutron spectral parameters were also varied during the irradiation, but this led only to minor changes in the total decay heat In the experiments only the decay heat due to fission products was measured, by measuring separately the β- and γ- energies. Hence, the contribution of the actinides can be excluded from the calculations.

Dickens: In Fig. 1 and 2 the experimental, analytical, and evaluated results are displayed for decay heat from ^{235}U. The analytical ANS 5.1 and JAERI results are both about 10 to 25% higher than the experimental results for 1, 10, and 100 s irradiation time. The JAERI analytical solution is slightly better than the ANS 5.1 result. The same discrepancies between experimental and evaluated results are found for the ENDF/B-VI, JEF-2.2, and JNDC evaluated data used. The best results are from the ENDF/B-VI evaluated data. A remarkable discrepancy is found for the long irradiation time (100 s) and long waiting time (5000 s) for both analytical and evaluated results. There is good agreement between analytical and evaluated results. In Fig. 3 and 4 the experimental, analytical, and evaluated results are displayed for decay heat from ^{239}Pu. The analytical and certainly the evaluated results are better than the results for the ^{235}U benchmark. Notice the different scales for the (c-e)/c plots. The results of the different evaluated data are closer than in the ^{235}U benchmark.

Yarnell and Bendt: In Fig. 5 and 6 the experimental, analytical, and evaluated results are displayed for decay heat from ^{233}U. No analytical data are available for ^{233}U from ANS 5.1. The analytical result from JAERI shows a difference from about –5% for short waiting times to about 0% for long waiting times. The evaluated results have discrepancies from about –10 to –5% for JEF-2.2 and ENDF/B-VI data, while the discrepancies for JNDC data ranges from about -5 to 0%. In Fig. 7 and 8 the experimental, analytical, and evaluated results are displayed for decay heat from ^{235}U. Both ANS 5.1 and JAERI analytical results have good agreement with the experimental results, certainly the ANS 5.1 result. The evaluated results show discrepancies from about –5 to 0% for JNDC and JEF-2.2 data, with larger discrepancy for the ENDF/B-VI data. In Fig. 9 and 10 the experimental, analytical, and evaluated results are displayed for decay heat from ^{239}Pu. The analytical results show a discrepancy of about –5% for ANS 5.1 over the whole decay time, while the JAERI result shows a discrepancy from about –10 to –5% for short to long waiting times. The evaluated results show discrepancies from about -15 to 0% for short to long waiting times. The discrepancies at waiting time of 10^5 s are about +5 to

+10%. The best results are retrieved from JNDC and JEF-2.2 evaluated data.

V. CONCLUSIONS

The decay heat is overestimated for all the nuclides used in the Dickens benchmark (short irradiation times) for both analytical and evaluated solutions by about +10 to 25%. There is good agreement between the independent analytical and evaluated decay heat calculation results. For short irradiation times, JAERI shows the best results for the analytical solution for decay heat and ENDF/B-VI shows the best results for the evaluated solution for decay heat.

The decay heat is underestimated for all the nuclides used in the Yarnell and Bendt benchmark (long irradiation times) for both analytical and evaluated solutions by about -5 to -10%, except for decay heat from ^{239}Pu at very long waiting times. For long waiting times (after 1000 s) the agreement between experiments and calculations is rather good. The best solutions for decay heat for long irradiation times are from JNDC data.

Summarising the results, it can be stated that this comparison of decay heat is a useful contribution to the validation of the evaluated data of the ENDF/B, JEF, and JNDC FP nuclear data files for decay heat production.

REFERENCES

1. ENDF-102 Data Formats and Procedures for the evaluated Nuclear Data File ENDF-6, BNL-NCS 44945, Brookhaven (July 1990).
2. JEF-2.2 radioactive decay data, JEF report 13, OECD Nuclear Energy Agency (1994).
3. JNDC Nuclear Data Library of Fission Products (Second Version), Japan Atomic Energy Research Institute, JAERI 1320 (September 1990).
4. SCALE-4.2 – A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, ORNL, CCC-545 (November 1993).
5. American National Standard for Decay Heat Power in Light Water Reactors, ANSI/ANS-5.1-1979, Illinois, USA (1979).
6. J.K. Dickens et al. Fission Product energy release for times following thermal fission of ^{235}U between 2 and 14000 seconds, report ORNL/NUREG-14, Oak Ridge National Laboratory (1977).

   J.K. Dickens et al. Fission product energy release for times following thermal fission of ^{239}Pu between 2 and 14000 seconds, report ORNL/NUREG-34, Oak Ridge National Laboratory (1978).
7. J.L. Yarnell and Ph.J. Bendt, Calorimetric fission product decay heat measurements for ^{239}Pu, ^{233}U, and ^{235}U, Report NUREG/CR-0349, LA-7452-MS, Los Alamos Scientific Laboratory, USA (1978).
8. J.E. Hoogenboom and J.L. Kloosterman, Generation and validation of ORIGEN-S libraries for depletion and transmutation calculations based on JEF-2.2 and EAF-3 basic data, Nucl. Eng. and Design, **170** (1997) 107-118.

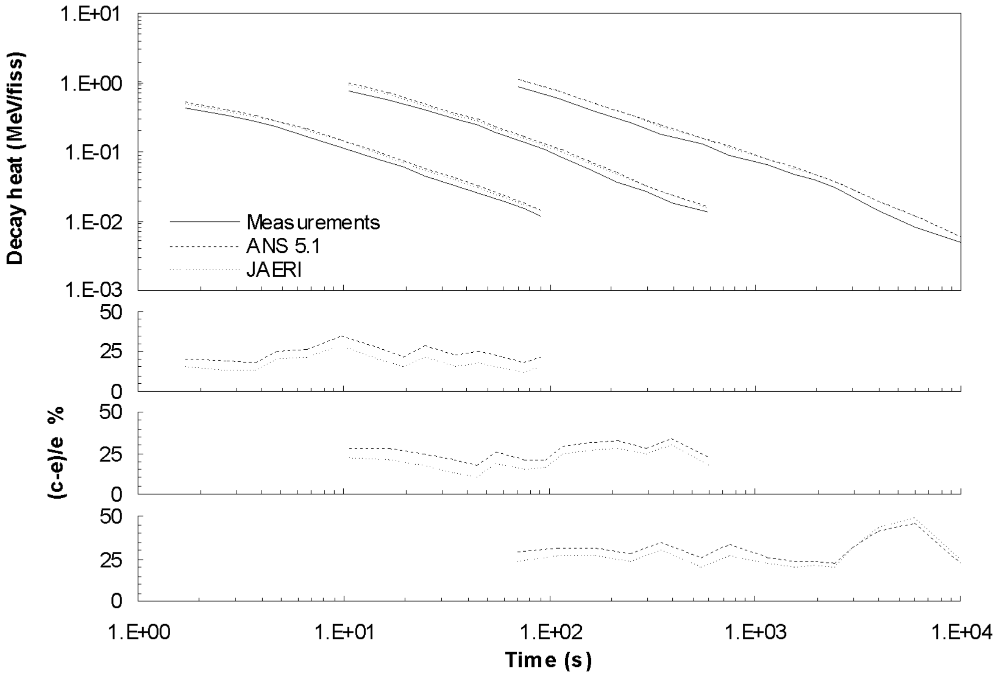

Fig. 1. Dickens, decay heat from ^{235}U for 1, 10, and 100 s irradiation time (analytical results)

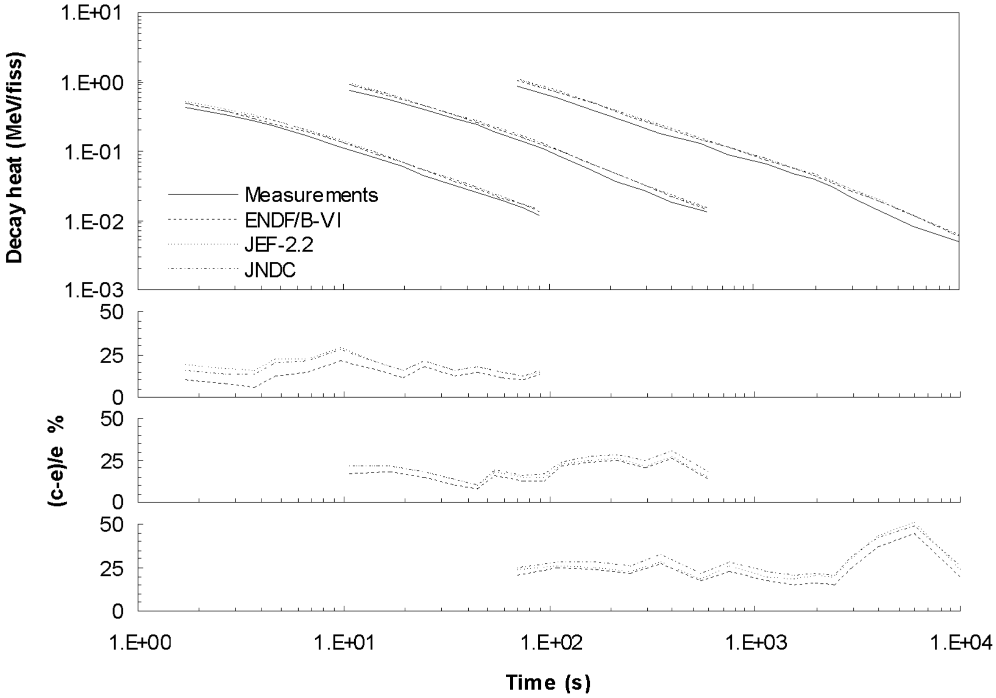

Fig. 2. Dickens, decay heat from ^{235}U for 1, 10, and 100 s irradiation time (evaluated results)

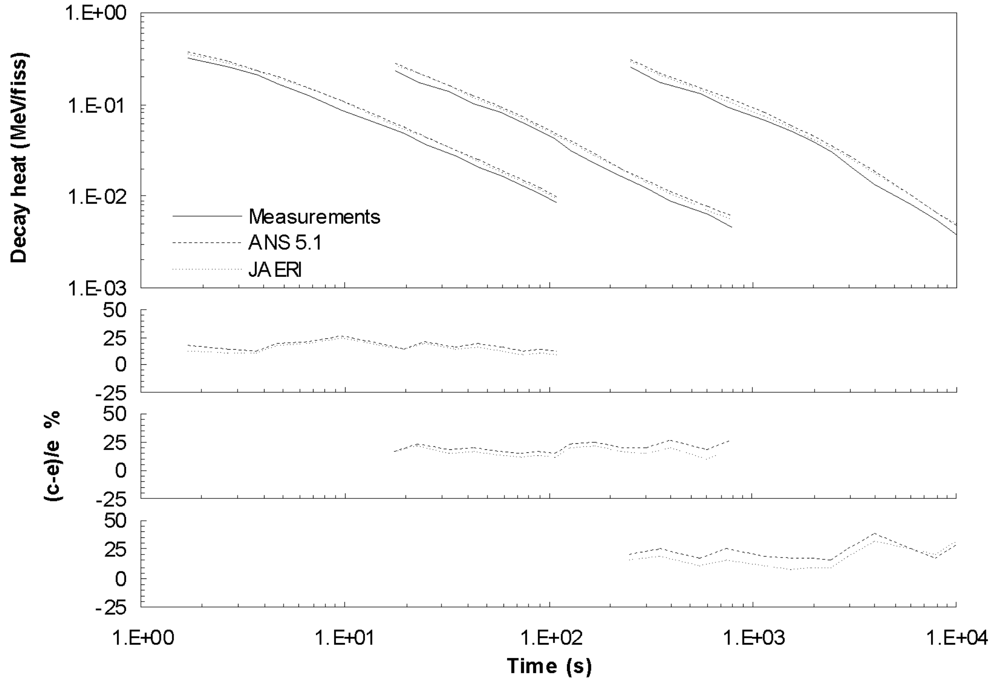

Fig. 3. Dickens, decay heat from ^{239}Pu for 1, 10, and 100 s irradiation time (analytical results)

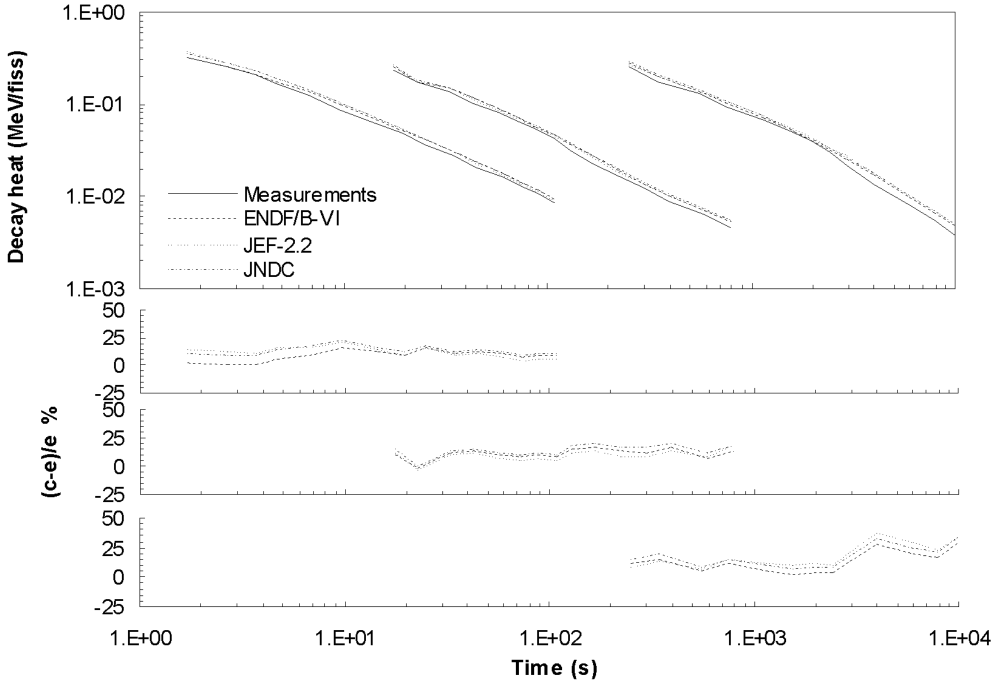

Fig. 4. Dickens Decay heat from ^{239}Pu for 1, 10, and 100 s irradiation time (evaluated results)

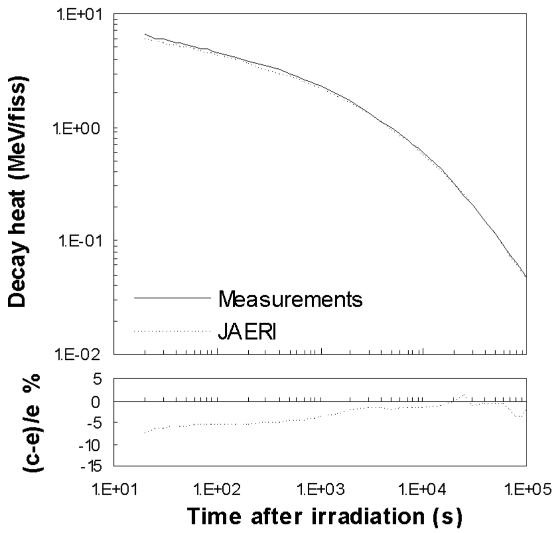

Fig.5. Yarnell&Bendt, decay heat from ^{233}U for 20,000 s irradiation time (analytical results)

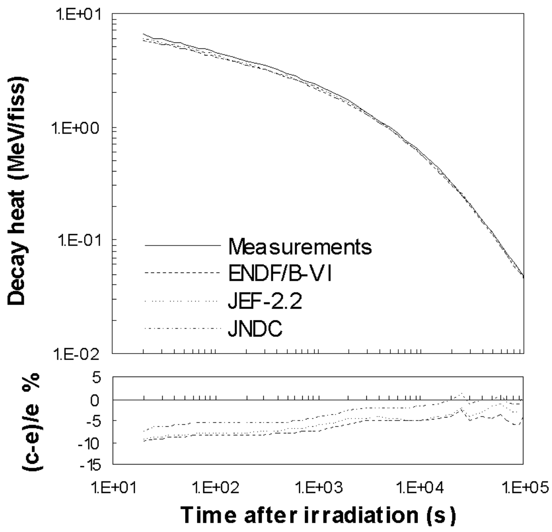

Fig. 6. Yarnell&Bendt, decay heat from ^{233}U for 20,000 s irradiation time (evaluated results)

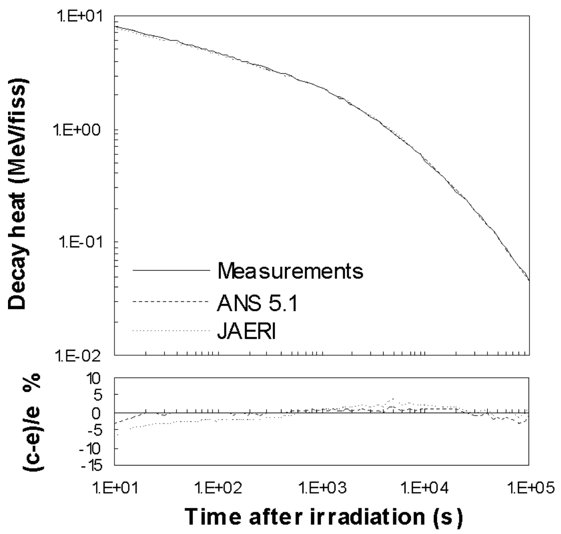

Fig.7. Yarnell&Bendt, decay heat from ^{235}U for 20,000 s irradiation time (analytical results)

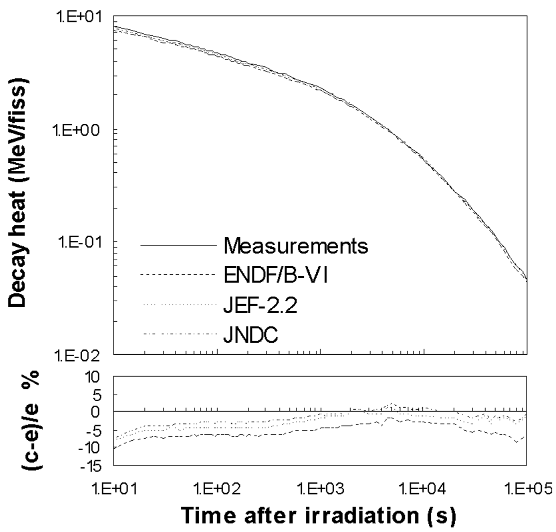

Fig.8. Yarnell&Bendt, decay heat from ^{235}U for 20,000 s irradiation time (evaluated results)

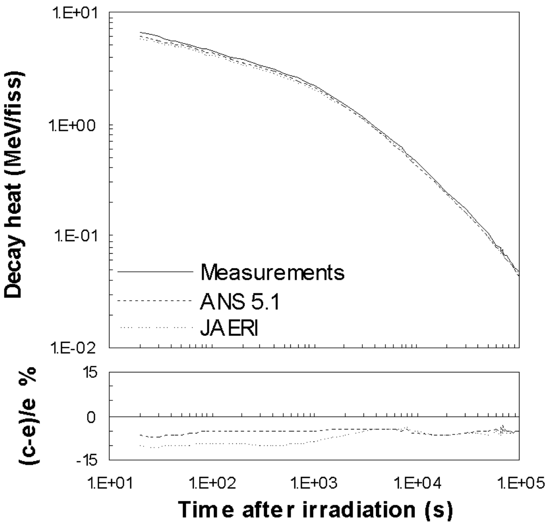

Fig.9. Yarnell&Bendt, decay heat from ^{239}Pu for 20,000 s irradiation time (analytical results)

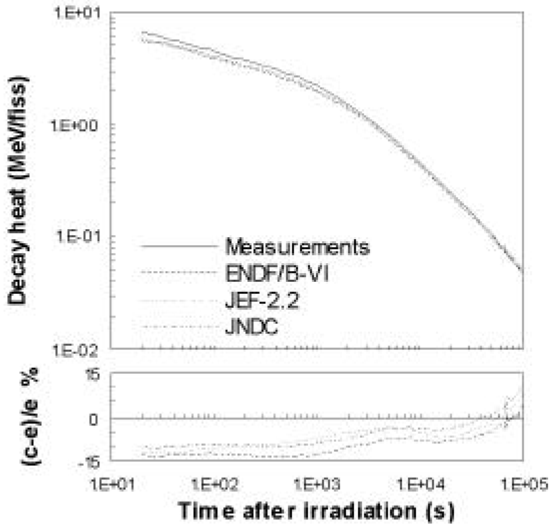

Fig.10. Yarnell&Bendt, decay heat from ^{239}Pu for 20,000 s irradiation time (evaluated results)