Decay Heat Calculations for Reactors: Development of a Computer Code ADWITA

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Abstract

Estimation of release of energy (decay heat) over an extended period of time after termination of neutron induced fission is necessary for determining the heat removal requirements when the reactor is shutdown, and for fuel storage and transport facilities as well as for accident studies.

A Fuel Cycle Analysis Code, ADWITA (Activation, Decay, Waste Incineration and Transmutation Analysis) which can generate inventory based on irradiation history and calculate radioactivity and decay heat for extended period of cooling, has been written. The method and data involved in Fuel Cycle Analysis Code ADWITA and some results obtained shall also be presented.

Decay Heat Generation in a Reactor

The heat generated in an operating reactor is effectively removed such that thermal equilibrium and energy balance is maintained within prescribed limit. When the reactor is shutdown the radioactive materials that remain in the reactor at the time of shut down continue to decay and release energy. This requires effective cooling must be maintained to keep reactor core form damage due to overheating. Decay heat generated in a reactor just after cessation of neutron fission chain reaction (scram) is about 6% of the operating thermal power which comes down to about 0.1% after 40 days. [Fig-4]This means even after cessation of neutron chain reaction the cooling system must perform with efficiency not less than 6% of that at full power.

Calculation of decay heat in reactors

The method of decay heat estimation relies on the measurements over practical time intervals as well as on calculation for predictions over very long time intervals. Neutron cross sections, fission yields and decay data together with operational history are the basic inputs to such calculations. A code used to calculate decay heat is required to generate isotopic inventory that would be present at the shutdown, based on operational history of the reactor and follow up the decay heat generation over an extended period of time.

The decay heat calculation is done based on standard prescription and algorithm for such calculations. The American National Standard for Decay Heat Power in Light Water Reactors (the ANS standard) ANS-5.1 is one of such standard. Other standards for the decay heat calculation are the JAERI standard (for both LWRs and FBRs) , JAERI-M-91-034 and the German standard, DIN 25463.

The decay standard prescribes fission product decay heat power and its uncertainty for a fission pulse and for infinite reactor operation (usually an irradiation of 10^{13}s represents infinite irradiation). Decay heat power from activation products in reactor materials is not specified in the standard and thus the decay heat power is related to the operating power of the reactor only via the fission rate and the recoverable energy per fission during operation. The decay data standard is based on summation calculation and experimental data. Due to scarce experimental data for decay times longer than 10^5 seconds the standard largely depends on calculated data for decay times beyond 10^5 to 10^9 seconds respectively. [1]

The reference [3] describes in detail the methodology of decay heat calculation based on interpolation of decay heat tables according to interpolation parameters such as (a) heat generation rate of the assembly, (b) cycle and cycle times of the assembly, (c) fuel burnup of the assembly, (d) specific power of the fuel, (e) assembly cooling time. The decay standards state explicitly the domain of parameter values to which it can be applied and prescribe correction if the interpolation parameters do not fall in to the applicability domain because of any of the following, like cooling time shorter than that used for making table, operating power larger than used in table, enrichment different from that in the table.

Codes for decay heat generation calculation

The codes for decay heat calculation are used extensively for the safety assessments of all types of nuclear plant, handling of fuel discharges, the design and transport of fuel-storage flasks, long time management of the radioactive waste and thus have far reaching consequence on safety and sustainability of nuclear energy. [2] The codes used for the decay heat calculation for the licensing purposes use the decay data tables according to the regulatory requirement. Such codes are based on realistic decay heat measurements and details of the operational history. The ORNL-LWRARC is such a code. [1,3]

The other kind of decay heat calculation codes are required to generate the inventory at the shutdown based on irradiation history before embarking on decay heat calculation based on radioactive transitions. The example of such codes is ORIGEN and its versions [4, 5], CINDER [6], and DCHAIN [7]. The inventory generation and subsequent decay heat calculation in such codes depends on the reactor specific neutron flux dependent cross section library and a decay data library. ADWITA (Activation Decay Waste Incineration and Transmutation Analysis) is an inventory generation and decay calculation code based on matrix exponential method [4, 5] and series solution of generalised Bateman equation for the transmutation chains through Transmutation Trajectory Analysis (TTA). [8, 9]

Cross section data libraries

Reactor physics design codes usually needs to consider limited number of nuclides which are required for the spectrum and reactivity calculations but decay data codes require reactor specific flux dependent transition rates for exhaustively large number of nuclides which are vital not only for the reactor design calculation but also for the backend process of the fuel cycle. The reactor physics codes usually use about few hundred nuclides explicitly while discharge fuel inventory include few thousands nuclide. The cross section data for the point reactor fuel cycle code used for the generation of inventory and decay data can be obtained from the spectrum calculation code used for the reactor design. The space time averaged cross section data for the nuclides which are explicitly used in spectrum calculation can be obtained for the use in fuel cycle analysis code by flux-volume weighting of self-shielded time dependent microscopic cross section.[10] Table 1 and 2 present capture and fission cross section for some isotopes calculated for PHWR220 library used by code ADWITA. The data for the nuclides, which are not used explicitly in the spectrum codes, can be obtained by weighting the point data with the spectrum specific to the region of the isotope of interest. As example the isotopes belonging to set of fission product can be collapsed with the spectrum specific to the fuel region. Likewise isotopes prevailing in in structural materials or used as soluble poison in coolant or moderator can use spectrum prevailing in those regions. Figure 1 shows a typical BOC (Beginning of Cycle)spectrum prevailing inthe average pin, three rings of fuel and in homogenized lattice cell in PHWR220 19 rod cluster geometry as obtained in 172 energy groups WIMS convention. The data for the nuclides which cannot be obtained from the spectrum collapsing because of lack of complete set of data (in the form of ENDF file) but have piece wise spectrum specific measured or calculated data can be obtained by weighting of such piecewise data keeping in to account the difference between the spectrum for which data is reported and the spectrum of interest for which data is to be obtained. The EXFOR (Experimental Nuclear Reaction Data), CINDA (Computer Index of Nuclear Reaction Data) and NSR (Nuclear Science References) databases (all available online at https://www-nds.iaea.org/) are rich source of such measured piecewise data.

The fission product yield data is required for the inventory generation codes.The individual and cumulative fission product for fission by different incident energy of neutron is given in MT454 and MT459 of file8 in ENDF/B data file.The fission yield of a nuclide I due to fission of nuclide J is required to be multiplied with the fission cross section of nuclide J to obtain corresponding transition matrix element. This requires the fission product yield must correspond to the neutron spectrum for the system of interest for which fission cross section data has been obtained. The library for code ADWITA uses individual fission yields from MT454. The ENDF/B-VII.0 release includes fission product yields for fission of 31 actinides. As of now, explicit fission yields from fission of 6 actinides, namely ^{232}Th, ^{233}U, ^{235}U, ^{238}U238,^{239}Pu and ^{241}Pu is used in

Decay Data Library

The calculation of transitions and heat generation due to radioactive transitions requires a decay data library with details like decay half-life, branching ratios and energy release (Q value) associated with the decay. Library should also provide isotopic abundances of isotopes and toxicities if output in terms of elemental composition and corresponding toxicities are required. As of now code ADWITA do not support elemental compositions as input and output, nor does it give toxicity. The nuclear wallet card from BNL and MT457 in file8 of ENDF/B-VII.0 release, which is basically ENDF translation of BNL nuclear wallet card database, is the source of decay data file.

Figure1 Typical PHWR-220 Spectrum

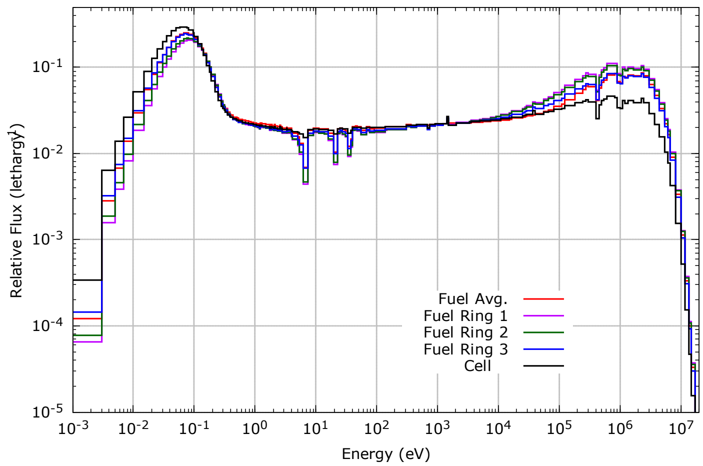


Table 1 Some actinide cross section data for PHWR220 library (barn)

Nuclide	(n,f)	(n,g)
Th-232	0.015	3.534
U-232	26.390	20.870
U-233	154.150	15.650
Pa-233	0.048	27.480
U-234	0.306	35.100
U-235	150.580	27.280
U-236	0.136	5.340
U-237	0.433	126.640
U-238	0.062	1.100
Np-237	0.337	59.150
Np-239	0.374	28.600
Pu-238	4.930	132.290
Pu-239	260.300	122.160
Pu-240	0.360	141.830
Pu-241	321.260	111.465
Pu-242	0.262	29.800
Pu-242	0.262	27.570
Am-241	2.331	214.440
Am-242	2105.220	407.730
Am-243	0.295	57.090
Cm-242	0.995	6.570
Cm-243	193.590	36.710
Cm-244	0.744	15.144

Isotope	PHWR (Calc.)
43-Tc-99	11.54
46-Pd-107	2.82
48-Cd-113	12393.2
55-Cs-137	0.084
55-Cs-135	3.54
62-Sm-151	3495.27
63-Eu-155	1624.97

Table 2 Some LLFP capture cross section in PHWR220 library

The code ADWITA can generate inventory based on irradiation or burnup history and continue with the decay of inventory for extended period of time. In one of the input files the name of the cross section file, name of the decay data file together with burnup history is required to be given. In other input file isotopic composition in grams of the nuclides in all three categories, namely activation products, actinides and daughters, and fission products, needs to be given. The code generates three output files, one each for the activation products, actinides and daughters, and fission products, which contain isotopic composition in

The figures 2 through 4 present some typical results for a 19 rod cluster 220 MWe Indian PHWR obtained from the code ADWITA for burnup of one ton natural uranium up to 10 GWD/t with power density 19.77 MW/t and subsequent decay. The nuclide ID in Fig 2 is Z*10,000+A*10 of the isotope.

Figure2 Actinide compositions vs. burnup

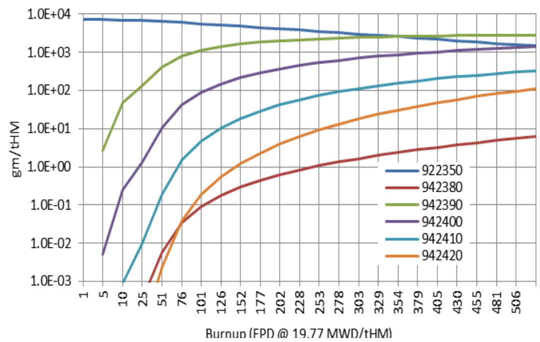


Figure 3 Decay heat generation rateVs. cooling time

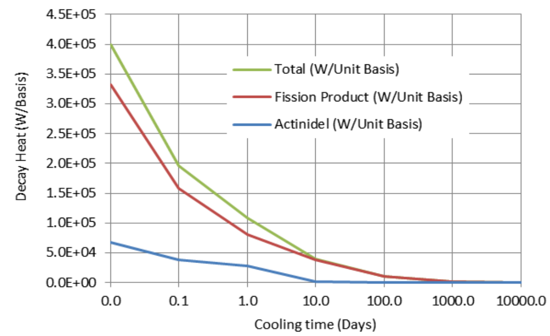
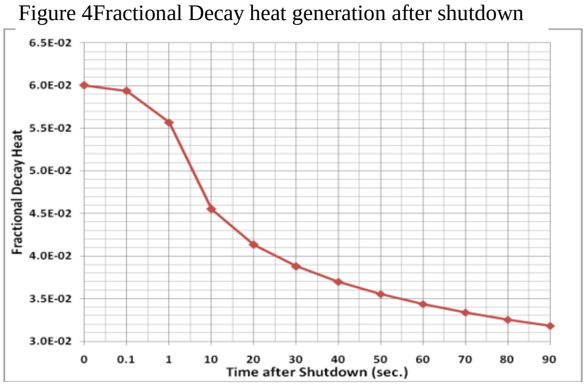


Figure 4Fractional Decay heat generation after shutdown



The tables 3, 4 and 5 below gives some results obtained from ADWITA and that from reference 15. The table 3 gives the amount of ^{235}U and ^{239}Pu at 0, 4000, and 8000 MWD/t burnup as obtained from ADWITA and that given in reference 15 [p 26-27].

Table 3 ^{235}U and ^{239}Pu content [15 P 26-27]

Burnup	0.0 GWD/t	4.0 GWD/t	8.0 GWD/t
^{235}U (g/kg)			
PPV-Canada	7.1138	3.7859	1.9957
WIMS-Romania	7.1137	3.7465	1.9606
CLU B-India	7.1138	3.7962	2.0195
ADWITA	7.1138	3.8290	2.0520
^{239}Pu (g/kg)			
PPV-Canada	0.0	1.9412	2.4136
WIMS-Romania	0.0	2.0949	2.7282
CLU B-India	0.0	1.9309	2.4895
ADWITA	0.0	2.0811	2.6486

The table 4 and 5 are the radioactivity and decay heat generated by fission products during cooling up to 1.0E10 sec after a burnup of 7500 MWD/t [15, p102-103]. The difference in result can be due to difference in method, data libraries, and specific power used for the burnup. In case of ADWITA an specific power density of 33.155 MWt/tHM has been used to attain a burnup of 7500 MWD/t. Please refer to reference 15 for the details about quoted results.

Table 4 Radioactivity (Curies/Ton) of Fission Products [15, P102]

Time (s)	0.0E00	5.0E00	1.0E01	1.0E02	1.0E03	1.0E04	1.0E05	1.0E06	1.0E07	1.0E08	1.0E10
Argentina	1.50E+08	1.39E+08	1.34E+08	1.08E+08	7.43E+07	4.75E+07	2.86E+07	1.38E+07	3.48E+06	2.38E+05	8.13E+01
Pakistan	1.51E+08	1.39E+08	1.34E+08	1.09E+08	7.54E+07	4.85E+07	2.84E+07	1.37E+07	3.49E+06	2.47E+05	1.20E+02
ADWITA	1.49E+08	1.33E+08	1.27E+08	9.77E+07	6.96E+07	4.54E+07	2.80E+07	1.34E+07	3.32E+06	2.24E+05	5.66E+01

Table 5 Thermal Power (Watt/Ton) of fission products [15, P 103]

Time (s)	0.0E00	5.0E00	1.0E01	1.0E02	1.0E03	1.0E04	1.0E05	1.0E06	1.0E07	1.0E08	1.0E10
Argentina	1.68E+06	1.49E+06	1.40E+06	1.06E+06	6.08E+05	2.82E+05	1.40E+05	6.26E+04	1.44E+04	9.16E+02	1.97E-01
Pakistan	1.69E+06	1.49E+06	1.40E+06	1.06E+06	6.10E+05	2.83E+05	1.37E+05	6.16E+04	1.42E+04	8.46E+02	2.63E-01
ADWITA	1.78E+06	1.46E+06	1.35E+06	8.98E+05	5.36E+05	2.55E+05	1.25E+05	5.66E+04	1.31E+04	7.97E+02	1.41E-01

It is evident from table 4 and 5 the values obtained from ADWITA are in general smaller than the result quoted in the reference 15. The reason for such occurrence can be either difference in methodology or difference in library and cross section or both. The reading of the reference suggests the methodology as well as data is different for all the three cases. The code ADWITA uses custom library made for the PHWR220 from the most recent data releases while the reference result has apparently used modified LWR cross section library.

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