3.8. The Netherlands

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3.8.1. Introduction

In the framework of the IAEA Co-ordinated Research Programme (CRP) on "Potential of the Thorium based Fuel Cycles to Constrain Plutonium to Reduce Long-Term Waste Toxicities", a benchmark calculation on a simple pin cell geometry has been performed.

The purpose of the CRP is to assess advantages and disadvantages of thorium-based fuel cycles with the aim to elaborate a selection of options and guidance for the IAEA's member states on the perspective fuel cycle for the next century. The first stage of the CRP is a benchmark calculation on a PWR pin cell geometry in order to intercompare the differences in cross section libraries and calculation methods of the participants. Of interest are the isotopic composition, cross sections, fluxes and infinite multiplication factors. The specifications of the benchmark have been given in Section 2.1.1.

This document describes the NRG results obtained by the burnup code system OCTOPUS. This code system consists of different modules which take care of the spectrum and burnup calculations. The spectrum calculation was done by the SCALE-4.1 code system. For the burnup calculation ORIGEN-S was used.

Section 3.8.2 describes in detail the calculation with the code system OCTOPUS. In Section 3.8.3 the results of the calculations are presented in the form of pictures, tables and comments. Section 3.8.4. contains the requested numerical output.

3.8.2. Calculation method

The calculations have been done with the burnup and criticality code system OCTOPUS developed at NRG [1]. The code system interconnects all reactor codes available at NRG. OCTOPUS works with modules that are scripts that call interfacing codes and the underlying reactor codes. In the particular case of this benchmark OCTOPUS links the SCALE-4.1 code system with the burnup code ORIGEN-S [2]. SCALE-4.1 is a neutron transport code for pin-cells and assemblies. ORIGEN-S is a point-depletion code.

OCTOPUS uses cross sections form the ECNAF data library, which contains activation and transmutation cross sections for over 750 nuclides mainly based on the JEF2.2 data file [3-4]. SCALE-4.1 uses the EIJ2-XMAS library. This is a 172 group data library for reactor calculations with the XMAS group structure based on JEF2.2. In order to transfer cross sections from one code to the other a generic format is used which can be converted to and from the formats used by the other codes. The format that is chosen is the AMPX weighted format (AMPX-W). All information needed for the coupled spectrum-burnup calculation is passed from one module to the other via a Binary Interface File (BIF).

One other important feature of the OCTOPUS code system is the (optional) use of the PSEUDO-module. This module can be used with the SCALE-spectrum module. It calculates for each burnable zone a fine-group cross-section set, which accounts for the neutron absorption and production of all actinides and fission products not explicitly included in the SPECTRUM-module. These cross sections sets are added to the cross section library of the spectrum code used. For this benchmark a pseudo nuclide was included in the fuel region of the pin-cell. The connection between the modules and the BIF's is presented in Fig. 3.8.1.

3.8.3. Results of the benchmark calculation

The numerical output data as requested in the benchmark specifications are included in this document in Section 3.8.4. In this section a graphical presentation of the results is given. The figures will be commented qualitatively.

3.8.3.1. The infinite multiplication factor: K∞

The infinite multiplication factor is shown in Fig. 3.8.2. Each point in the curve of Fig. 3.8.2 corresponds with one spectrum calculation and subsequent burnup calculation. The time steps at the beginning are small because the xenon buildup, which influences the neutron flux spectrum, takes place on a relatively short time scale. The entire burnup sequence consists of 24 time steps.

3.8.3.2. Isotopic composition of actinides

In Fig. 3.8.3 the depletion of the plutonium isotopes is shown. After the exit burnup of 60 MWd/kgHM nearly all the Pu-239 has been burnt. The mass of Pu-241 first increases and after a while decreases. At the one hand the production of Pu-241 is due to capture in Pu-240 and at the other hand Pu-241 is depleted due to fissioning.

In Fig. 3.8.4 the densities of the protactinium and the uranium isotopes are shown. The buildup of the fissile nuclide U-233 is due to neutron capture in Th-232 and subsequent decay of Th-233 via Pa-233. Since the growth of U-233 becomes less during burnup, while the total flux is increasing as will be seen in the next section, one can conclude that fissioning of U-233 contributes more and more to the power.

The concentration of Pa-232 has reached its equilibrium value almost after 100 days. The level of the Pa-233 is increasing slightly during burnup due to increasing total neutron flux. U-234 is produced both by capture in U-233 and capture in Pa-233 and subsequent decay of Pa-234. A little U-235 is produced due to capture in U-234. The nuclide U-232 plays an important role in reprocessing since one of its decay products emits hard gammas. Uranium-232 is formed by (n,2n) reactions on U-233.

In Fig. 3.8.5 the concentrations of the minor actinides are plotted. Am-243 and Cm-244 are the most abundant minor actinides present in the fuel. Cm-244 is mainly produced by neutron capture in Am-243 and subsequent decay of Am-244. Americij-243 is produced by neutron capture of Pu-242 and subsequent decay of Pu-243. Cm-244 decays to Pu-240 with half-life of 18 years, while Am-243 decays to Pu-239 with the much longer half-life of 7370 years.

3.8.3.3. Total neutron flux

The total neutron flux is increasing during the burnup, because the macroscopic fission cross section decreases mainly due to depletion of the fissile nuclides. This is a direct consequence of the constant linear power assumed. In Fig. 3.8.2 is shown that the total neutron flux increases from 2.9×10^{14} to about 3.9×10^{14} $cm^{-2}s^{-1}$ during burnup.

3.8.3.4. Microscopic cross sections

The absorption, fission and (n,2n) cross sections at burnups of and 60 MWd/kgHM are presented in Section 3.8.4. The absorption cross section is the summation of the fission cross section and the neutron disappearance cross-section. The latter is defined as the sum of all cross sections in which a neutron is not in the exit channel. In terms of ENDF/B MT-numbers this means MT = 18 plus MT = 102 through 114. Due to their high cross sections and low lying resonance peaks the nuclides Pu-239 and Pu-240 strongly determine the shape of the flux especially in the thermal region. This is shown in Fig. 3.8.6. If the concentrations of these nuclides change, the averaged microscopic cross sections of all other nuclides change due to the different flux shape. One example of the influence of the changing flux spectrum is the change of the averaged microscopic cross section of Th-232. Since the concentration of Th-232 is virtually constant during burnup, which means that the self-shielding is constant too, a change of the microscopic cross section must be caused by the changing neutron flux spectrum. The averaged microscopic absorption cross section of thorium increases from 0.85 barn at zero burnup to 1.13 barn at a burnup of 60 Mwd/kgHM. The effect of the decrease in self-shielding can be illustrated by the absorption cross sections of Pu-239. At zero burnup σ_a = 68 barn and at a burnup of 60 Mwd/kgHM σ_a = 178 barn.

3.8.3.5. Average energy per fission

In Section 3.8.5 the values of the average energy per fission are shown. This includes energy generated due to the neutron captures of the nuclides in the fuel. Because of the change in composition of the fissile nuclides the average energy per fission changes. In the case of the plutonium/thorium fuel the average energy per fission decreases during burnup. The smooth transition from plutonium fissioning to U-233 fissioning causes the decrease in the average energy per fission during burnup. This is due to the fact that the fissile plutonium isotopes release about 200 MeV thermal energy per fission and U-233 only releases about 190 MeV thermal energy per fission.

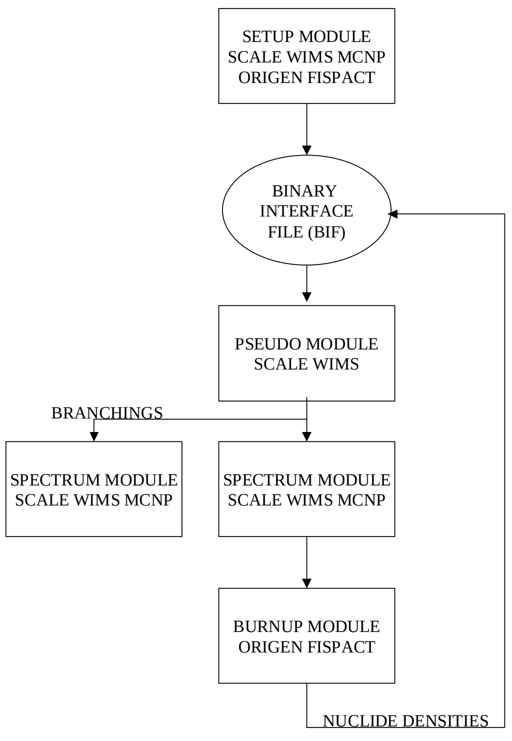

FIG. 3.8.1. The scheme of OCTOPUS burnup and criticality code system.

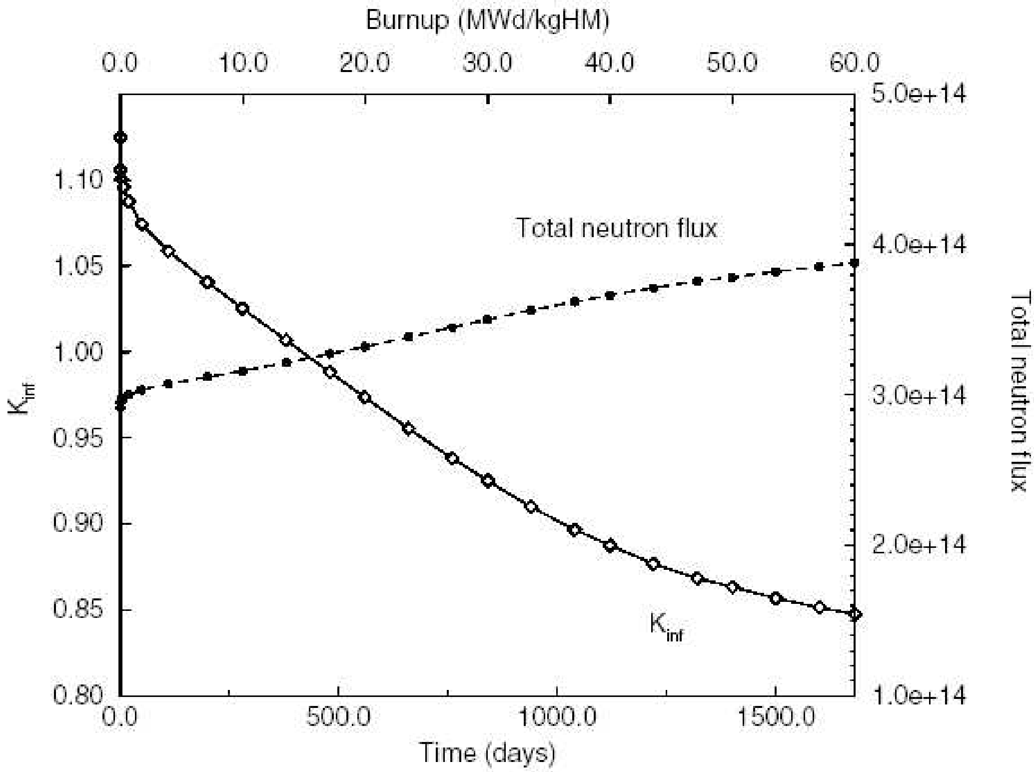

FIG. 3.8.2. k_{inf} and total neutron flux as function of burnup.

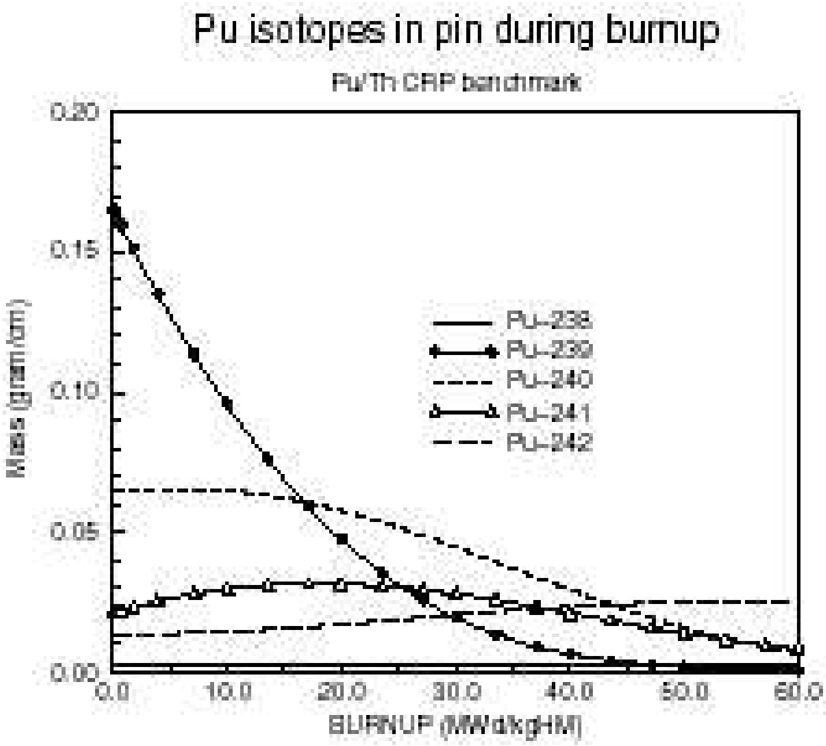

FIG. 3.8.3. Plutonium composition as function of burnup.

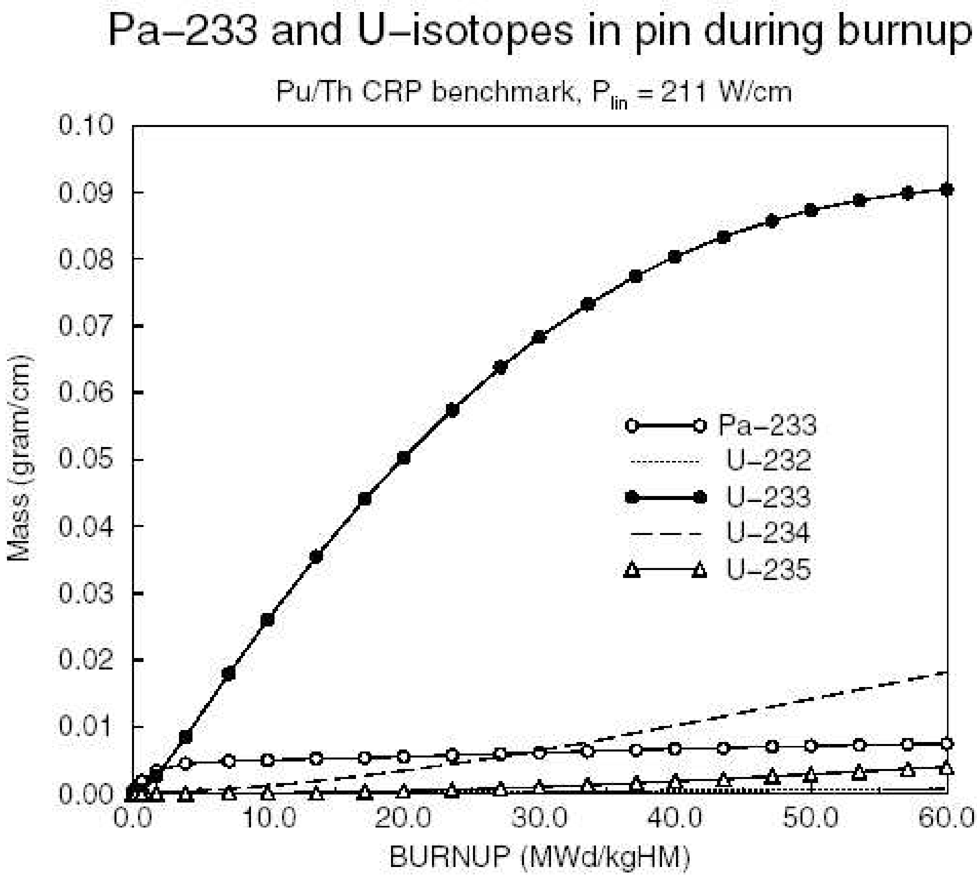

FIG. 3.8.4. Protactinium-233 and uranium as function of burnup.

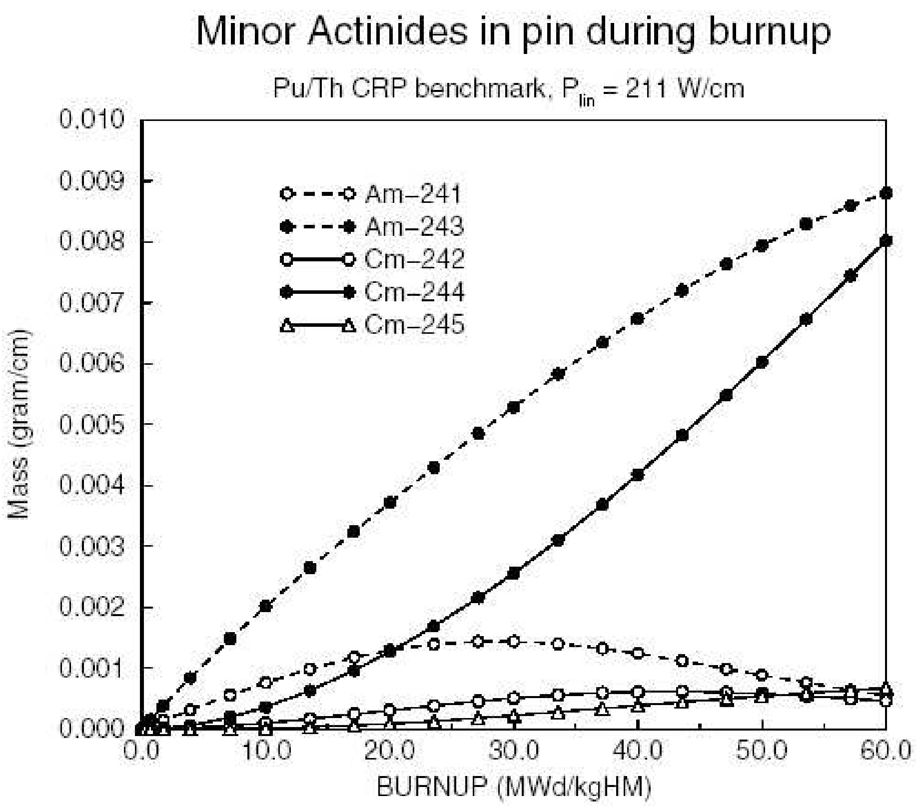

FIG. 3.8.5. The formation of minor actinides as function of burnup.

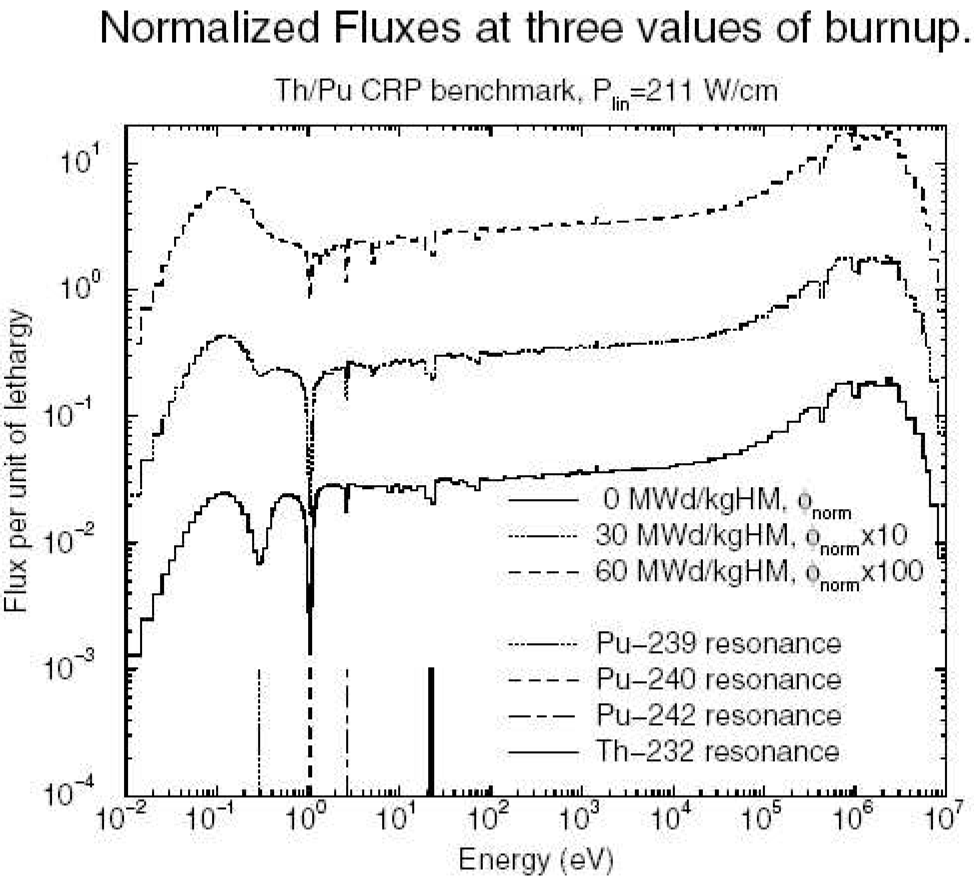

FIG. 3.8.6. Normalized flux at zero, half way and final burnup.

3.8.4. Numerical results of the benchmark

3.8.4.1. The infinite multiplication factor: K_∞.

	0 MWd/kgHM	30 MWd/kgHM	40 MWd/kgHM	60 MWd/kgHM
k_{inf}	1.12479	0.925198	0.887499	0.847561

3.8.4.2. Isotopic composition of the actinides

nuclide concentrations 1/(barn x cm)

nuclide identifier = 10000xZ + 10xA + M,

where:
Z = the atomic number;
A = the atomic mass of the nuclide; and
M = the metastable state of the nuclide.
M = 0 is the groundstate, and M = 1 is the first metastable state of the nuclide.

TABLE 3.8.1. NUCLIDE CONCENTRATIONS [1/(cm^2s)]

	0 MWd/kgHM	30 MWd/kgHM	40 MWd/kgHM	60 MWd/kgHM
902300		1.99738E-08	2.66202E-08	3.93323E-08
902320	2.11000E-02	2.06456E-02	2.04631E-02	2.00579E-02
912310		2.06328E-06	2.31721E-06	2.37571E-06
912330		2.26210E-05	2.47680E-05	2.79479E-05
922320		9.23719E-07	1.49241E-06	2.54699E-06
922330		2.54433E-04	2.99339E-04	3.36896E-04
922340		2.39808E-05	3.75794E-05	6.72831E-05
922350		3.60476E-06	6.78927E-06	1.47382E-05
922360		2.35243E-07	5.90704E-07	2.25522E-06
922370		6.22406E-10	1.57728E-09	6.01748E-09
922380		3.31807E-10	6.91969E-10	3.06229E-09
932370		2.23173E-08	4.87085E-08	1.89977E-07
932380		6.13735E-11	1.45367E-10	6.38593E-10
932390		1.67812E-11	2.17215E-11	3.10352E-11
942360		3.96932E-13	4.98487E-13	7.14752E-13
942370		3.27285E-12	3.23564E-12	2.84032E-12
942380	9.72000E-06	8.17818E-06	8.54297E-06	8.18189E-06
942390	5.99000E-04	7.08363E-05	2.34028E-05	2.74119E-06
942400	2.32000E-04	1.61752E-04	1.06364E-04	2.41181E-05
942410	7.69000E-05	1.00379E-04	7.57607E-05	2.91171E-05
942420	4.78000E-05	7.31808E-05	8.38980E-05	8.91505E-05
952410		5.18667E-06	4.45826E-06	1.98443E-06
952420		1.17795E-08	1.18450E-08	6.45866E-09
952421		7.78570E-08	6.60042E-08	2.81144E-08
952430		1.88889E-05	2.40517E-05	3.14022E-05
962410		8.82669E-13	1.07916E-12	7.89001E-13
962420		1.80664E-06	2.18697E-06	1.65886E-06
962430		4.91356E-08	7.91052E-08	9.47679E-08
962440		9.09773E-06	1.48483E-05	2.85139E-05
962450		7.95648E-07	1.36685E-06	2.37964E-06
962460		7.83224E-08	2.26761E-07	8.70984E-07
962470		1.03602E-09	3.95592E-09	2.19781E-08
962480		5.66398E-11	3.23235E-10	3.44533E-09
972490		6.18007E-13	3.98013E-12	4.73533E-11

3.8.4.3. Total neutron flux

TABLE 3.8.2. TOTAL NEUTRON FLUX [1/(cm^2s)]

	0 MWd/kg_{HM}	30 MWd/kg_{HM}	40 MWd/kg_{HM}	60 MWd/kg_{HM}
Fuel	2.9131317E+14	3.5005688E+14	3.6624260E+14	3.8775357E+14
Clad	2.9255918E+14	3.5062147E+14	3.6663592E+14	3.8785461E+14
Moder	2.9300243E+14	3.5120984E+14	3.6725799E+14	3.8851187E+14

3.8.4.4. Microscopic cross sections

microscopic cross sections (barn) at 0 and 60 MWd/kgHM

nuclide identifier = 10000xZ + 10xA + M,

where:
Z = the atomic number;
A = the atomic mass of the nuclide; and
M = the metastable state of the nuclide.
M = 0 is the ground state and M = 1 is the first metastable state of the nuclide).

TABLE 3.8.4. MICROSCOPIC CROSS SECTIONS

	0 MWd/kgHM			60 MWd/kgHM		
	SIGMA-ABS	SIGMA-FIS	SIGMA (N,2N)	SIGMA-ABS	NUCLIDE SIGMA-FIS	SIGMA (N,2N)
902300	2.39011E+01	7.02859E-02	6.30347E-0	1.95142E+01	6.27926E-02	5.56113E-03
902320	8.49193E-01	2.64410E-02	6.41957E-03	1.13212E+00	2.34336E-02	5.65989E-03
912310	3.43930E+01	4.26555E-01	4.24246E-03	5.14408E+01	3.85337E-01	3.74945E-03
912330	2.51083E+01	1.74255E-01	1.74513E-03	2.13351E+01	1.54669E-01	1.54123E-03
922320	2.56036E+01	1.49390E+01	3.11247E-03	2.82785E+01	1.65733E+01	2.77855E-03
922330	4.02880E+01	3.51551E+01	3.36468E-03	6.21158E+01	5.54029E+01	2.95478E-03
922340	2.22236E+01	5.65110E-01	6.16813E-04	1.90972E+01	5.27656E-01	5.50979E-04
922350	2.83248E+01	2.21161E+01	4.45086E-03	5.59127E+01	4.57966E+01	3.91303E-03
922360	1.05971E+01	3.56991E-01	3.15559E-03	8.63515E+00	3.08996E-01	2.77735E-03
922370	2.07333E+01	5.87340E-01	8.94844E-03	4.00685E+01	6.25727E-01	7.84089E-03
922380	7.92269E+00	1.13534E-01	4.64700E-03	7.23446E+00	1.00790E-01	4.09127E-03
932370	2.76985E+01	5.63459E-01	9.47485E-04	3.41883E+01	5.08507E-01	8.43972E-04
932380	8.25749E+01	7.48734E+01	5.65892E-03	1.73722E+02	1.57743E+02	4.97627E-03
932390	1.47395E+01	6.63625E-01	1.40592E-03	1.50134E+01	6.00058E-01	1.23564E-03
942360	2.68673E+01	1.39698E+01	1.20173E-03	3.84232E+01	1.96987E+01	1.07031E-03
942370	1.03081E+02	8.42578E+01	8.61504E-04	2.17628E+02	1.75111E+02	7.61526E-04
942380	1.73033E+01	2.04971E+00	3.15369E-04	3.63563E+01	2.52468E+00	2.80248E-04
942390	6.83990E+01	4.40855E+01	1.25423E-03	1.78121E+02	1.13973E+02	1.11049E-03
942400	4.95735E+01	6.59336E-01	1.52586E-03	1.26929E+02	6.16305E-01	1.34854E-03
942410	7.16909E+01	5.42661E+01	8.39213E-03	1.62759E+02	1.21833E+02	7.35902E-03
942420	2.36292E+01	4.97854E-01	2.57304E-03	1.78495E+01	4.46165E-01	2.26686E-03
952410	6.47173E+01	9.61650E-01	7.17547E-04	1.15965E+02	1.25616E+00	6.35437E-04
952420	2.33107E+02	8.95142E+01	1.65527E-03	5.53647E+02	1.83088E+02	1.45273E-03
952421	3.52077E+02	2.87143E+02	4.52328E-03	8.70527E+02	7.06021E+02	3.96576E-03
952430	5.06533E+01	4.74513E-01	1.95508E-03	4.17313E+01	4.23033E-01	1.71900E-03
962410	1.08542E+02	9.91149E+01	1.67822E-04	2.32468E+02	2.12145E+02	1.46885E-04
962420	4.95190E+00	1.01799E+00	4.31725E-04	5.59685E+00	1.18399E+00	3.88580E-04
962430	7.18032E+01	6.13304E+01	1.41869E-03	8.74651E+01	7.36996E+01	1.24944E-03
962440	1.80149E+01	1.04057E+00	1.78854E-03	1.53880E+01	9.63577E-01	1.57743E-03
962450	7.48131E+01	6.46135E+01	1.57724E-03	1.57262E+02	1.36000E+02	1.39709E-03
962460	3.74549E+00	6.77336E-01	1.97097E-03	3.33720E+00	6.04834E-01	1.74164E-03
962470	3.10501E+01	1.90076E+01	1.19287E-02	4.03327E+01	2.45006E+01	1.04651E-02
962480	8.29884E+00	8.32402E-01	2.49872E-03	7.60976E+00	7.52782E-01	2.19761E-03
972490	1.46732E+02	3.46302E-01	7.98240E-03	2.05614E+02	3.09741E-01	6.99766E-03

3.8.4.5. Average energy per fission

AVERAGE ENERGY PER FISSION (MeV per fission)

This value includes energy generated due to neutron captures of the nuclides in the fuel zone of the pin cell.

	0 MWd/kgHM	30 MWd/kgHM	40 MWd/kgHM	60 MWd/kgHM
Energy	207.891	205.775	204.411	202.009

REFERENCES TO SECTION 3.8.

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[2] HERMANN, O.W., WESTFALL, R.M., ORIGEN-S, SCALE Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms, Oak Ridge National Laboratory, Oak Ridge, Tennesee, USA (1989).

[3] KLOOSTERMAN, J.L., New European Cross-Section Data libraries for ORIGEN-S Based on JEF2.2 and EAF3. Technical Report ECN-R-95-008, Netherlands Energy Research Foundation (ECN), Petten, The Netherlands (1995).

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