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ORIGINAL PAPER

Computation of concentration changes of heavy metals in the fuel assemblies with 1.6% enrichment by ORIGEN code for VVER-1000

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Abstract ORIGEN code is a widely used computer code for calculating the buildup, decay, and processing of radioactive materials. During the past few years, a sustained effort was undertaken by ORNL to update the original ORIGEN code [4] and its associated data bases. The results of this effort were updated on the reactor model, cross section, fission product yields, decay data, decay photon data and the ORIGEN computer code itself. In this paper we have obtained concentration changes of uranium and plutonium isotopes by ORIGEN code at different burn-up and then the results have been compared with VVER-1000 results in the first fuel cycle for fuel assemblies with 1.6% enrichment in the BUSHEHR Nuclear Power Plant.

Key words ORIGEN code • burn-up • heavy metals • BUSHEHR Nuclear Power Plant

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Introduction

ORIGEN is a versatile point depletion code which solves the equations of radioactive growth and decay for large numbers of isotopes with arbitrary coupling. The code uses the matrix exponential method to solve a large system of coupled, linear first-order ordinary differential equations with constant coefficients. The general nature of the matrix exponential method permits the treatment of complex decay and trans-mutation schemes. An extensive library of nuclear data has been compiled, including half-lives and decay schemes, neutron absorption cross sections, fission yields, disintegration energies and multigroup photon release data. ORIGEN has been used to compute the compositions and radioactivity of fission products, cladding materials and fuel materials in LWRs, LMFBRs, MSBRs and HTGRs.

One of the problems commonly encountered in the field of nuclear energy is the solution of equations involving nuclear transmutation and decay. To a good approximation, these nuclide chain equations can be represented as a simultaneous system of linear, homogeneous, first-order ordinary differential equations with constant coefficients. In many instances, the matrix of nuclear transmutation coefficients is triangular and the system of equations can be solved using the method of Bateman [4], which has been employed in a number of computer codes. However, each of these codes has generally suffered from an inability to treat more than a few specific types of transmutations and from difficulties encountered in treating feedback despite some progress in these areas.

An alternative approach to solving the same system of equations utilizes the matrix exponential method, which has been employed by Pease and others [4]. Although completely general, this method has been limited in the past by the storage that is required to generate the matrix exponential series and by computational inaccuracies, computational difficulties arise because the nuclide chain equations constitute a classic example of a set of stiff ordinary differential equations, that is, one in which the eigenvalues of the characteristic equation for the system are widely separated. The matrix exponential method has been employed in the ORIGEN code in order to exploit its extreme generality. The limitation on the number of nuclides that can be treated, which results from the necessity to store large arrays, has been overcome by two devices:

1. ORIGEN stores only the non-zero elements of the normally sparse transition matrix and two vectors that are used to locate them.
2. The expansion of the matrix exponential function is performed using a recursion relation which requires storage of only one vector in addition to the solution. Computational difficulties arising from eigenfunctions with very large eigenvalues (corresponding to nuclides with very short half-lives) are avoided by using asymptotic solutions of the nuclide chain equations for the conditions of secular and transient equilibrium.

The ORIGEN code has been designed to be extremely versatile in its applications. It is capable of computing isotopic compositions of fuel, fission products and cladding in both fixed and fluid fuel reactors.

The library of nuclear data that has been compiled for use with the code and is sufficiently extensive to treat U-235 and Pu-239 fuels in both fast and thermal spectra, and fission of U-235 in thermal spectra. The library also contains multigroup photon release rates for the fission products and the heavy metals, which permits the calculation of gamma-ray spectra in spent and refabricated fuels. One other important feature of the code is that the matrix exponential technique has been developed to solve a nonhomogeneous system of equations. This feature makes it possible for ORIGEN to be employed in calculating the accumulation of activity in processing plants, in waste disposal operations, and in the environment.

In this paper we have calculated concentration changes in uranium isotopes (U-235, U-238) and plutonium isotopes (Pu-239, Pu-240, Pu-241, Pu-242) with burn-up (burn-up = 0.0 until burn-up = 10.0 MWD/KgU) by ORIGEN code and have compared with BUSHEHR Nuclear Power Plant (VVER-1000) results for fuel assemblies with 1.6% enrichment. Geometrical specification and material in the reactor core (fuel assemblies with 1.6% enrichment) including: fuel rods, gap gas, coolant, spacer grid, guiding channel and central tube have been considered and material values have been calculated and have been given to input file of ORIGEN code and concentration changes in uranium and plutonium isotopes have been obtained with burn-up and then have been compared with BUSHEHR Nuclear Power Plant (VVER-1000) results.

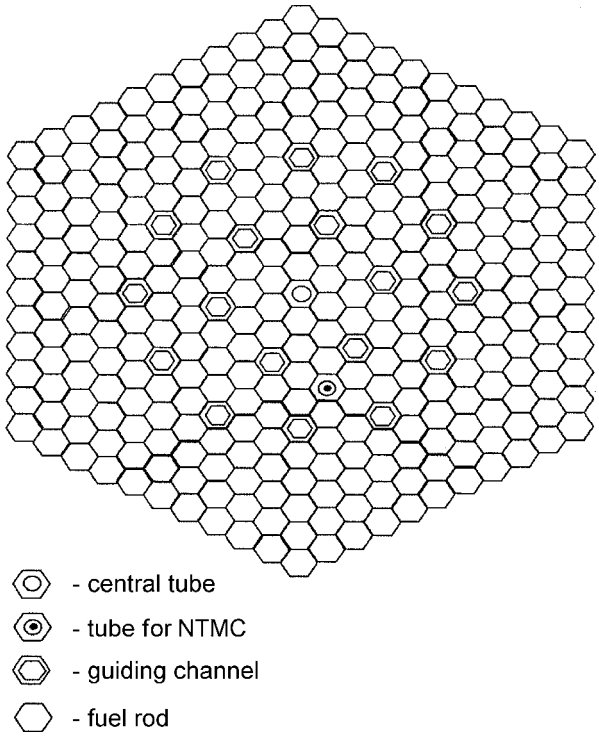

Fig. 1. Arrangment of elements in fuel assemblies with 1.6% enrichment [1].

Arrangement of elements in the fuel assemblies with 1.6% enrichment

Figure 1 shows fuel assemblies with 1.6% enrichment in the reactor core. BUSHEHR Nuclear Power Plants have enrichments of 1.6%, 2.4%, 3.62% at the first fuel cycle [1]. Concentration changes have been considered only for 1.6% enrichment with burn-up in the first fuel cycle.

Figure 2 shows power peaking factor for symmetry section of 60 degrees (in 1/6 core) for the first end of

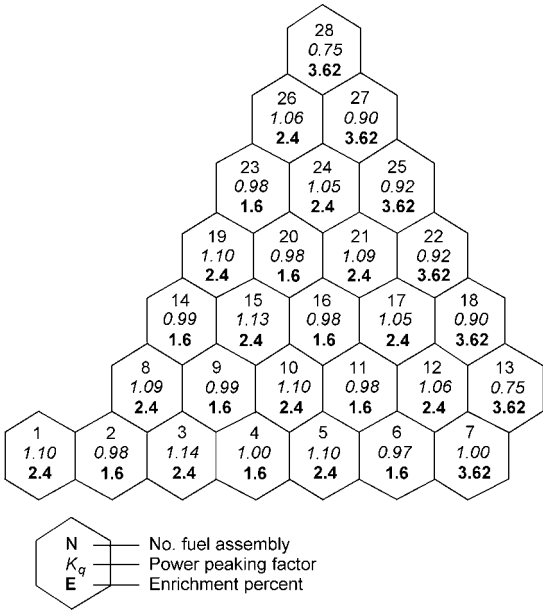

Fig. 2. Power peaking factor for symmetry sector of 60 degree (1/6 core) and value of enrichment of fuel assemblies [1].

Table 1. Specification of fuel rods and gap in the reactor core [1]

Parameters	Values
Fuel	UO_2 pellets
Pellet density, kg/m^3	$(10.4…10.7) \times 10^3$
Hellium pressure under fuel rod cladding, MPa	2.0×0.25
Outside diameter of cladding, nominal, m	9.1×10^{-3}
Inside diameter of cladding, nominal, m	7.73×10^{-3}
Outside diameter of pellet, nominal, m	7.57×10^{-3}
Diameter of pellet central hole, nominal, m	1.5×10^{-3}
Pellet height, m	$(9.0…12.0) \times 10^{-3}$
Fuel rod length, m	3.842
Height of fuel stack in the cold state, m	3.53
Number of fuel rods in the fuel assembly, pcs	311
Pitch between fuel rods, nominal, m	12.75×10^{-3}
Core flow area in the core, m^2	4014

cycle, H10 = 90%, xenon equilibrium poisoning H10 = 90% (that is No. 10 group control rods have been entered 10% in the core) and also values of enrichment for fuel assemblies have been shown [1]. As we know, the core total thermal power is 3000 MWth [1], therefore with using from power peaking factors of Fig. 2, the thermal power of fuel assemblies of 1.6% enrichment is 977.3006 MWth.

Geometry and material of the reactor core

Geometrical specification and material in the reactor core are included (material mass values have been calculated and have been given to input file of ORIGEN code).

Fuel rods

Material of the fuel rods is UO_2 with enrichments of 1.6%, 2.4%, 3.62%. In this paper we have considered fuel assemblies of 1.6% enrichment and the number of fuel assemblies of 1.6% enrichment is 54 and the number of total fuel assemblies is 163 in the reactor core.

Table 1 shows the specification of fuel rods [1], therefore we can obtain the mass of fuel rods with 1.6% enrichment.

Gap gas (gap gas is helium)

Gap is including:
1. Gap between fuel rod and fuel cladding (outer gap).
2. Gap in the center of fuel rod (inner gap).

Specification of the gap has been shown in Table 1 [1].

We obtained axial temperatures and power distribution and gap conductance (h_g) (Table 5) in the reactor core and in the fuel assemblies of 1.6% enrichment with CITATION [3] and RELAP [2] codes (using specifications of Tables 1, 3 and 4. Values of the obtained axial temperature distribution have been shown in Table 2 then we interpolated axial temperature distribution and we obtained equations for inner gap (Eq. (1)) and outer gap (Eq. (2)) with height:

$$(1)\quad Tingap = 0.0305529(1.55346 + x)\cdot(28.1263 - 9.71958x + x^2)\cdot(18.3586 - 8.46276x + x^2)\cdot(18.3744 - 0.602171x + x^2)\cdot(0.996295 + 1.19186x + x^2)$$

$$(2)\quad Toutgap = -0.00323791(-7.3744 + x)\cdot(21.9524 - 9.16381x + x^2)\cdot(17.4946 - 4.11285x + x^2)\cdot(1.63358 + 1.86795x + x^2)\cdot(23.029 + 2.77103x + x^2)$$

Base of axial direction is the core bottom. Then we integrated the axial temperature distribution from Eqs. (1) and (2) in the axial direction and we obtained volumetric average temperature whose values are 898.028°C (for inner gap) and 474.894°C (for outer gap). The volumetric average temperature for inner gap and outer gap was used in the calculation of gap mass (perfect gas equation has been considered).

Coolant

The coolant passes through and around each fuel rod. Axial temperature distribution is obtained for coolant by RELAP code [2] in the fuel assemblies of 1.6% enrichment (Table 2). Values of the obtained axial temperature distribution have been shown in Table 2, and we interpolated the axial temperature distribution to obtain the following equation:

$$(3)\quad Tcool = 0.00320553(2.07898 + x)\cdot(28.1925 - 10.3233x + x^2)\cdot(24.4262 - 7.59207x + x^2)\cdot(11.7168 - 2.14237x + x^2)\cdot(5.4307 + 2.14193x + x^2)$$

Table 2. Value of temperature of inner gap, outer gap, coolant, power with height in the fuel assemblies of 1.6% enrichment

$\left[H = \frac{100H}{H_0}\right]^*$	Total power [MWth]	Power in the fuel assemblies 1.6% enrichment [MWth]	Inner gap temperature (°C) in the fuel assemblies 1.6% (average)	Outer gap temperature (°C) in the fuel assemblies 1.6% (average)	Coolant temperature (°C) in the fuel assemblies 1.6% (average)
5	160.3394	52.23326	534.877	292.998	374.525
15	322.2288	104.97146	733.111	295.908	432.153
25	406.7072	132.49173	929.342	299.694	480.570
35	427.7665	139.35215	1085.05	303.972	515.332
45	411.945	134.19803	1172.38	308.431	534.732
55	378.5677	123.32481	1176.73	312.750	538.250
65	334.5641	108.98989	1097.8	316.575	525.757
75	276.09	89.94057	949.371	319.576	497.444
85	194.2519	63.28083	757.565	321.556	454.501
95	87.48582	28.49998	322.635	322.635	400.525
Sum of powers and averages for temperatures	3000	977.3	898.028	474.894	309.406

* where: H_0 = height from core bottom, H_0 = height of active core = 3.53 m.

Table 3. Fuel thermal conductivity with fuel temperature in the reactor core [1]

Temperature [°C]	0	200	300	400	500	600	1300	1800
Thermal (K) conductivity	17.2	19.3	20.1	20.5	20.9	21.8	31.2	33.4

Table 4. Cladding thermal conductivity with clad temperature in the reactor core [1]

Temperature [°C]	0	227	827	1227	1427	1627	2227	2827
Thermal (K) conductivity	8.15	6.7	3.75	2.8	2.5	2.4	2.5	3.5

Table 5. Gap conductance (h_g) with linear power in the fuel assemblies of 1.6% enrichment in the reactor core [1]

Linear power, W/m	Gap conductance for thickness 0.08 mm
0	1790
5000	1814
8800	1886
11600	2072.34
21100	2465.26
26400	3336
34700	3942.72
36100	4468.29
41400	5393.35
42200	6437.19
44800	7470.87

Then, the top equation integrated in the axial direction allows to obtain volumetric average temperature that is equal to 309.406°C. The coolant temperatures in the inlet and outlet are 291°C and 321°C and the coolant densities in inlet and outlet are 743 kg/m^3 and 675 kg/m^3 [4], therefore the average density is 709 kg/m^3. Then, we can obtain the coolant mass in the fuel assemblies with 1.6% enrichment (coolant flow area has been considered in calculation).

Different materials in the fuel assemblies with 1.6% enrichment

Included are the following materials:
1. spacer grid,
2. guiding channel,
3. central tube,
4. tube for ICID (in the core instrumentation detectors).

Specification of the materials have been shown in Table 6 [1], then we have obtained the mass of top materials.

CPS absorber rods (control rod protection system)

In Table 7 specification of CPS absorber rods has been shown [1].

As we know, ten percent of the length of the CPS absorber rods of group No. 10 are in the reactor core in the steady state (thermal power is 3000 MWth), therefore we can calculate the mass of CPS absorber rods of group No. 10 for ten percent of the length.

Figure 3 shows arrangement of CPS absorber rods in the core for first fuel cycle.

Results

Figure 4 shows U-235 concentration in the fuel assemblies of 1.6% enrichment with burn-up in the first fuel cycle.

Table 6. Specification of spacer grid, guiding channel, central tube, tube for ICID in the reactor core [1]

Parameters	Values
Spacing grid	
number, pcs	15
material	alloy Zr + 1% Nb
Guide channel	
number, pcs	18
material	alloy Zr + 1% Nb
outer diameter, m	13.0×10^{-3}
inside diameter, m	11.0×10^{-3}
Central tube	
number, pcs	1
material	alloy Zr + 1% Nb
outer diameter, m	13.0×10^{-3}
inside diamater, m	11.0×10^{-3}
Tube for ICID	
number, pcs	1
material	alloy Zr + 1% Nb
outer diameter, m	13.0×10^{-3}
inside diamater, m	11.0×10^{-3}

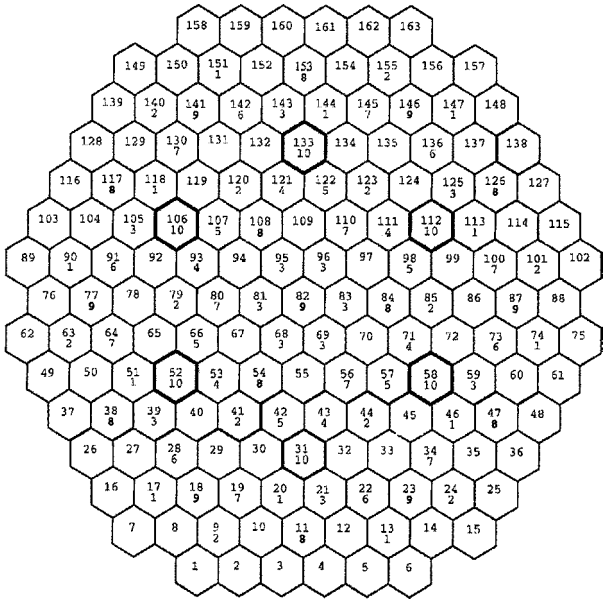

Fig. 3. Arrangement of CPS absorber rods in the core for first fuel cycle [1].

Figure 5 shows U-238 concentration in the fuel assemblies of 1.6% enrichment with burn-up in the first fuel cycle.

Figure 6 shows Pu-239 concentration in the fuel assemblies of 1.6% enrichment with burn-up in the first fuel cycle.

Figure 7 shows Pu-240 concentration in the fuel assemblies of 1.6% enrichment with burn-up in the first fuel cycle.

Figure 8 shows Pu-241 concentration in the fuel assemblies of 1.6% enrichment with burn-up in the first fuel cycle.

Figure 9 shows Pu-242 concentration in the fuel assemblies of 1.6% enrichment with burn-up in the first fuel cycle.

Table 7. Specification of CPS absorber rods in the reactor core [1]

Characterictics	Values
CPS absorber rods	
number of absorbing elements in the COS AR, pcs	18
absorbing material (combined)	$B_4C + (Dy_2O_3 \cdot TiO_2)$
absorber height, cm	
– $Dy_2O_3 \cdot TiO_2$	30
– B_4C	320
absorbing element clad outer diameter, nominal, m	8.2×10^{-3}
absorbing element clad inner diameter, nominal, m	7.2×10^{-3}
absorbing diameter, nominal, m	7.2×10^{-3}
absorbing element clad material	42XHM (42 KhNM)
absorbing material density, g/cm^3, not less than	
– $Dy_2O_3 \cdot TiO_2$	4.9
– B_4C	1.7
service life (including 3 years in the working group), year	10
Nominal CPS AR height, m	4.215
Nominal diameter of absorbing element cladding, m	8.2×10^{-3}
Nominal thickness of absorbing element cladding, m	0.5×10^{-3}
Absorbing material	$B_4C + (Dy_2O_3 \cdot TiO_2)$
absorbing material density, kg/m^3, not less than	
– boron carbide	1.7×10^3
– dysprosium titanate	4.9×10^3
nominal height of absorbing material stack, m	
– boron carbide	3.2
– dysprosium titanate	0.3
– total	3.5
Nominal mass of CPS AR, kg	18.5

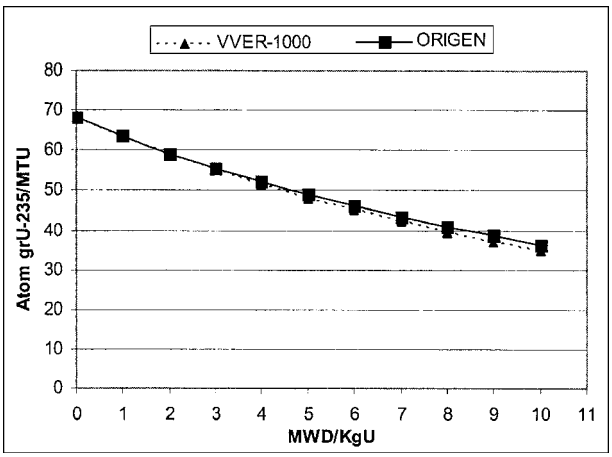

Fig. 4. U-235 concentration changes in the fuel assemblies of 1.6% enrichment with burn-up.

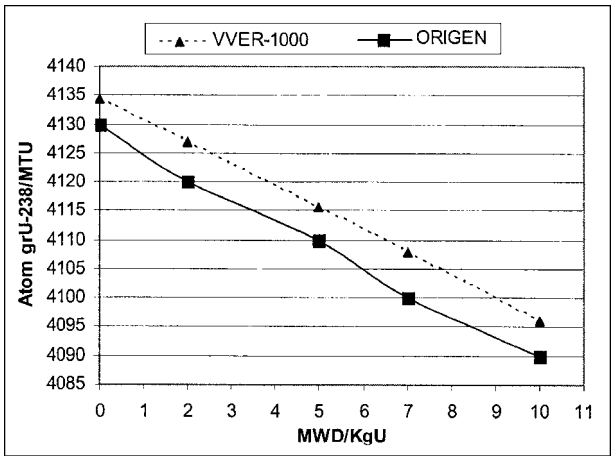

Fig. 5. U-238 concentration changes in the fuel assemblies of 1.6% enrichment with burn-up.

Errors

In accordance with Fig. 4 to Fig. 9, we conclude that the concentration U-235 of changes.

U-238 with burn-up shows a small error, but for Pu-239, Pu-240, Pu-241, Pu-242 errors have been increased. Reasons for the errors are included:

1. Library of ORIGEN code differs from RUSSIAN codes.
2. In few burn-ups RUSSIAN codes consider very small concentration changes (almost zero) for Pu-241, Pu-242, but ORIGEN code gives concentration changes in low burn-ups.

Conclusion

Because solving of chain equations in the nuclear reaction in the reactor core is complex we have used from ORIGEN code for calculations of concentration changes of heavy metals (ORIGEN is a widely used computer code for calculating concentration changes with burn-up). We have simulated materials of the BUSHEHR Nuclear Power Plant (for fuel assemblies with 1.6% enrichment) in the first fuel cycle and then the material masses have been obtained for the input file of ORIGEN code.

Results of ORIGEN code are relatively good for the heavy metals and shows a small error for Pu-239, Pu-240, Pu-241, Pu-242.

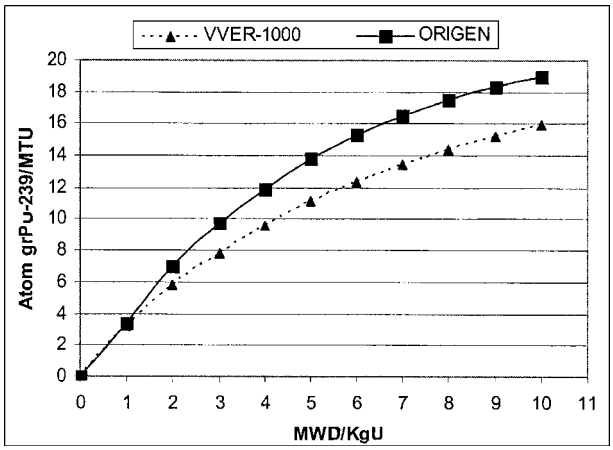

Fig. 6. Pu-239 concentration changes in the fuel assemblies of 1.6% enrichment with burn-up.

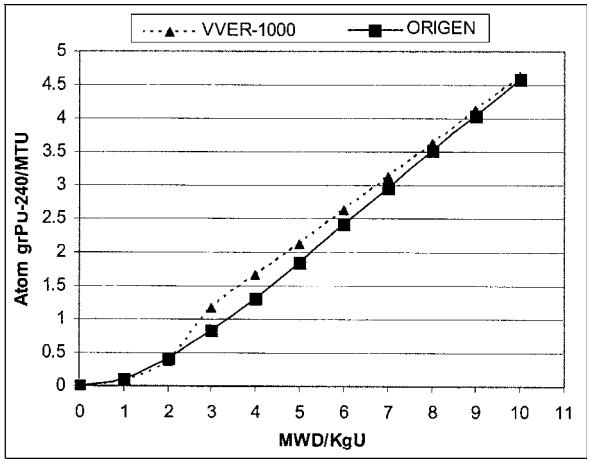

Fig. 7. Pu-240 concentration changing in the fuel assemblies of 1.6% enrichment with burn-up.

Because the library of ORIGEN code differs from the RUSSIAN codes, errors have occurred. From Ref. [1], we know that in few burn-ups RUSSIAN codes very small concentration changes for Pu-241, Pu-242 are considered, but ORIGEN code gives concentration changes in low burn-ups. Because calculations of concentration changes are time dependent (concentration changes in "t + dt" time is dependence on concentration changes in "t" time, where "t" is "a few time"), therefore results differ.

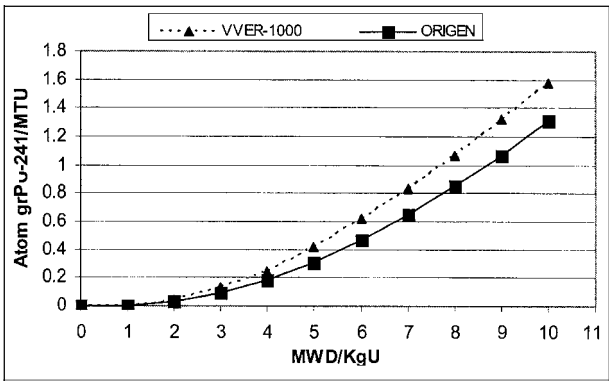

Fig. 8. Pu-241 concentration changing in the fuel assemblies of 1.6% enrichment with burn-up.

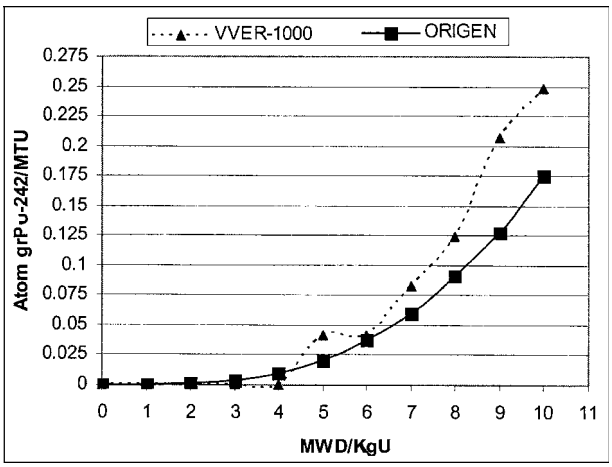

Fig. 9. Pu-242 concentration changing in the fuel assemblies of 1.6% enrichment with burn-up.

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