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Fission Product Inventory Calculation by a CASMO/ORIGEN Coupling Program

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Abstract

A CASMO/ORIGEN coupling utility program was developed to predict the composition of all the fission products in spent PWR fuels. The coupling program reads the CASMO output file, modifies the ORIGEN cross section library and reconstructs the ORIGEN input file at each depletion step. In ORIGEN, the burnup equation is solved for actinides and fission products based on the fission reaction rates and depletion flux of CASMO. A sample calculation has been performed using a 14×14 PWR fuel assembly and the results are given in this paper.

1. Introduction

In the DUPIC fuel cycle, spent PWR fuel is fabricated as CANDU fuel without any wet chemical process. Therefore, all the actinides and fission products are contained in the DUPIC fuel from the beginning. Such a complexity in fuel composition causes a difficulty in predicting the neutronics property and material performance as well. Therefore, it is necessary to calculate the composition of all actinides and fission products accurately in order to reduce the uncertainties in nuclear design and performance of DUPIC fuel. For the lattice cell and burnup calculation of a PWR fuel assembly, the multi-group transport code CASMO-3[1] is widely used. The cross section library of CASMO-3 contains 17 heavy nuclides, 24 separate fission products and 2 pseudo fission products.

ORIGEN2[2] is a flexible reactor physics code that provides compositions of various nuclear material. ORIGEN2 has 130 actinides, 850 fission products and 720 activation products (a total 1700 nuclides) and provides details of the burnup chains which are not available in CASMO.

ORIGEN2 has two drawbacks, however, such as a point-reactor-depletion module (no spatial dependence) and one group flux (one group effective cross section). The accuracy of calculating the composition of fission products depends largely on the composition of actinides and

nuclear fission rates, which are used for the fission product generation. Therefore, an attempt to combine CASMO and ORIGEN was made to provide accurate composition of actinides and nuclear fission rate for ORIGEN2, and the burnup calculation for fission products was performed by ORIGEN2.

2. Calculation Method and Related Programs

2.1. Code Descriptions

CASMO-3

CASMO-3 is a multi-group transport code used for lattice and burnup calculations in reactor physics design. It is used here to generate burnup-dependent number densities of actinides and fission reaction rates for the PWR fuel assembly. The cross section library used by CASMO is limited to isotopes of primary importance to the calculation of reactor neutronic parameters. For the sake of computational economy, many nuclides are not modelled and decay chains are simplified accordingly. Two pseudo fission products are included to offset errors introduced by these artificial modifications.

ORIGEN2

ORIGEN2 is a versatile point depletion and radioactive decay calculation code used to simulate nuclear fuel cycles and calculate nuclide compositions and characteristics of materials contained therein. However, because of the spatial independence of the code, it is required that the effects, which affect the prediction of isotopic concentrations, are incorporated into the cross section library prior to performing a burnup calculation. In addition, variations in the cross section with time, caused by the changing neutron energy spectrum and fuel isotopic concentrations, must also be taken into account.

2.2 CASMO/ORIGEN Coupling Method

After a CASMO-3 depletion calculation, the CASMO-3 standard output and Card Image file are read by a CASMO-3 Post-Processor (CASMO-POST) to generate an interface file, which contains the time-dependent CASMO absolute fluxes, number densities of actinides, and fission cross sections. The ORIGEN2 library and input file are processed by the ORIGEN2 Pre-Processor (ORIGEN-PRE), which updates absolute fluxes, number densities of actinides, and fission cross sections contained therein. The updated ORIGEN2 library and input file are then used to generate new compositions following an irradiation time step. The ORIGEN-PRE subsequently reads and processes the fuel compositions of the next step and writes a new material composition file. The

sequence proceeds until the desired burnup is achieved. The data flow is shown diagrammatically in Figure 1 and the functions of each processor are described as follows:

CASMO-POST

The CASMO-POST takes input from two sources: the CASMO-3 standard output and Card Image file. It provides the average number densities of actinides, time-dependent absolute fluxes, and fission cross sections for the ORIGEN2 calculation through an interface file which is referred to as a CASMO-POST output. The average number densities and absolute fluxes are from the standard output file and the one-group microscopic fission cross sections of the actinides are from the Card Image file.

ORIGEN-PRE

The ORIGEN-PRE takes the fluxes and fission cross sections from the CASMO-POST output file and the burnup data from another data file. It merges them into the skeletal ORIGEN2 input files and ORIGEN2 cross section libraries for each burnup step. A modified ORIGEN2 input file and revised cross section library for each time step are then generated by ORIGEN-PRE. At the same time, a new ORIGEN2 composition input file for the next time step is prepared.

The ORIGEN2 skeletal input file contains the basic depletion information required by ORIGEN2. This input file must instruct ORIGEN2 to retrieve the nuclide compositions from file unit 4 and must specify the density units as grams. The "IRF" entries for the desired burnup steps are required, even though the coupling program will replace the fluxes given in these entries. Any nuclides that are time-dependent and require fission cross section information must have a complete cross section specification. The ORIGEN2 is then executed for one time step, each ORIGEN2 run creates its own composition file on unit 7 and these compositions are read in unit 4 for the next time step. It should be noted that there have been no modifications to either CASMO-3 or ORIGEN2, so any version of these two codes will work with the coupling program.

3. Sample Calculation

A sample calculation was performed for a 14×14 PWR fuel assembly of 3.5 wt% UO_2 fuel. The CASMO-3 and ORIGEN2 burnup calculations were performed to obtain the number densities of fission products and actinides, and the results were compared with those of a coupling calculation. Table 1 shows the number densities of the major fission products with fuel burnup. According to the results, for fission products having relatively large contents, such as Kr-83 and Rh-103, the above three calculations show similar results. For fission products having relatively small contents, such as Xe-135 and Sm-149 however, the coupling calculation gives similar values

to the ORIGEN2 calculation but gives somewhat different values from the CASMO-3 calculation. Therefore, the results of the coupling program must be proved by exact benchmark calculations.

4. Summary and Recommendation

A CASMO/ORIGEN coupling program was developed to predict the composition of all actinides and fission products in spent PWR fuels. The coupling program is aimed at combining the exactness of CASMO-3 multi-group transport calculations and the ability of calculating all the fission products in ORIGEN2. However, the results of a sample calculation by CASMO-3, ORIGEN2, and the coupling program tend to show large discrepancies for some of the fission products. Therefore, it is recommended to perform a benchmark test using either the experimental results or another code system like HELIOS[3]. The benchmarking work is currently underway to verify the applicability of the coupling program for the calculation of fission product inventory.

References

1. M. Edenius and B.H. Forssen, "CASMO-3: A Fuel Assembly Burnup Program User's Manual Version 4.4," STUDSVIK/NFA-89/3, Studsvik of America, Inc., 1989.
2. A.G. Croff, "ORIGEN2.1: Isotope Generation and Depletion Code Matrix Exponential Method," CCC-371, Oak Ridge National Laboratory, 1991.
3. E.A. Villarino, "HELIOS: Angularly Dependent Collision Probabilities," *Nucl. Sci. Eng.*, **112**, 16 (1992).

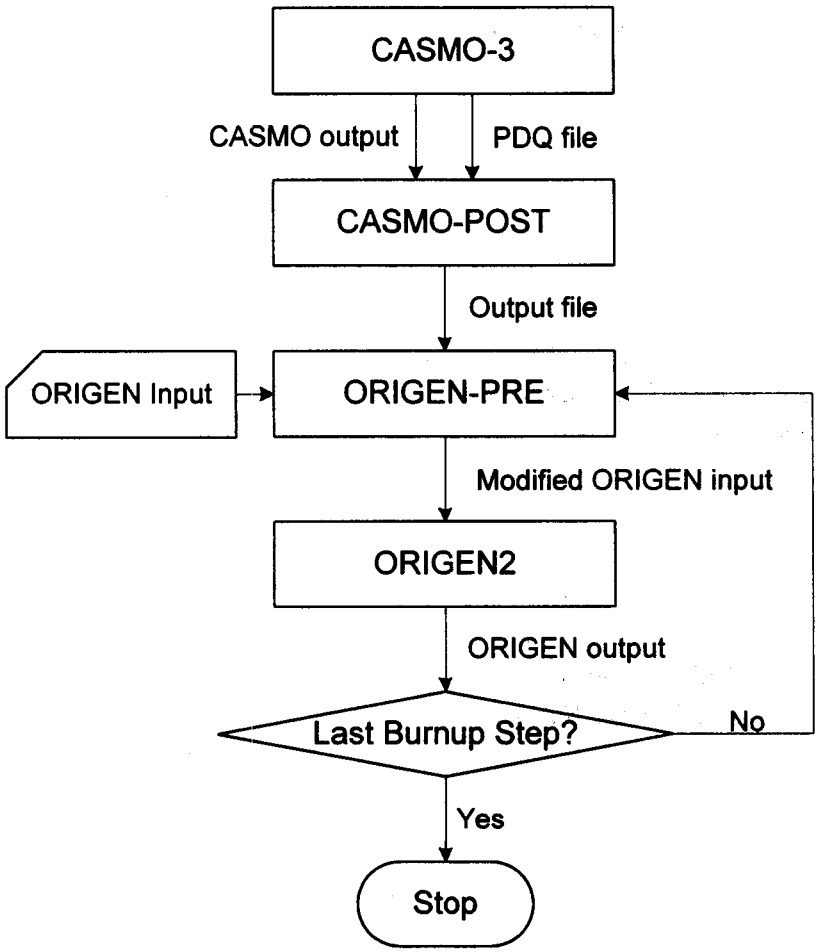

Figure 1. Data Flow Diagram for the CASMO/ORIGEN Coupling Program

Table 1. Comparison of PWR Inventory for Fission Products

Burnup (MWD/TU)	Kr83/U238			Rh103/U238		
	CASMO-3	ORIGEN2	Coupling	CASMO-3	ORIGEN2	Coupling
0	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
150	8.39058E-07	8.33436E-07	8.31360E-07	5.01879E-06	2.19350E-07	2.20872E-07
1500	8.23615E-06	8.62087E-06	8.58063E-06	5.03318E-05	1.76241E-05	1.77197E-05
3000	1.61452E-05	1.69675E-05	1.68778E-05	1.00854E-04	5.64571E-05	5.69670E-05
6000	3.10960E-05	3.27698E-05	3.24500E-05	2.01430E-04	1.57087E-04	1.58480E-04
10000	4.94219E-05	5.21499E-05	5.12954E-05	3.32785E-04	3.02419E-04	3.03982E-04
14000	6.60718E-05	6.97145E-05	6.81399E-05	4.59491E-04	4.46249E-04	4.46111E-04
20000	8.81167E-05	9.27904E-05	8.99700E-05	6.38720E-04	6.51508E-04	6.45582E-04
30000	1.17555E-04	1.22871E-04	1.18200E-04	9.03628E-04	9.49941E-04	9.31575E-04
40000	1.38484E-04	1.43314E-04	1.37982E-04	1.12302E-03	1.17780E-03	1.15504E-03
50000	1.51987E-04	1.55481E-04	1.50361E-04	1.29331E-03	1.33506E-03	1.31492E-03

Burnup (MWD/TU)	Xe135/U238			Sm149/U238		
	CASMO-3	ORIGEN2	Coupling	CASMO-3	ORIGEN2	Coupling
0	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
150	3.92635E-07	3.73825E-07	3.44384E-07	7.12977E-07	6.98986E-07	6.84796E-07
1500	4.01101E-07	3.75997E-07	3.40658E-07	3.27533E-06	2.89428E-06	2.71183E-06
3000	4.05799E-07	3.76875E-07	3.39133E-07	3.49229E-06	3.07918E-06	2.85132E-06
6000	4.10089E-07	3.75096E-07	3.35769E-07	3.81812E-06	3.58067E-06	2.90470E-06
10000	4.10739E-07	3.68838E-07	3.30063E-07	4.13088E-06	3.83451E-06	3.41762E-06
14000	4.07142E-07	3.60760E-07	3.23908E-07	4.33815E-06	3.96727E-06	3.57043E-06
20000	3.98241E-07	3.45520E-07	3.15670E-07	4.50042E-06	4.04031E-06	3.72891E-06
30000	3.78297E-07	3.17838E-07	3.01035E-07	4.51352E-06	3.96725E-06	3.77007E-06
40000	3.52093E-07	2.93715E-07	2.88010E-07	4.30581E-06	3.80409E-06	3.72918E-06
50000	3.36310E-07	2.75024E-07	2.71243E-07	4.13576E-06	3.64037E-06	3.60149E-06