Thermochemical Equilibrium in a Kernel of a UN-TRISO Coated Fuel Particle

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1. Introduction

A coated fuel particle (CFP) with a uranium mononitride (UN) kernel has been recently considered as an advanced fuel option, such as in fully ceramic micro-encapsulated (FCM) replacement fuel for light water reactors (LWRs). In FCM fuel, a large number of tri-isotropic coated fuel particles (TRISOs) are embedded in a silicon carbide (SiC) matrix.

Thermochemical equilibrium calculations can predict the chemical behaviors of a kernel in a TRISO of FCM fuel during irradiation. They give information on the kind and quantity of gases generated in a kernel during irradiation. This study treats the quantitative analysis of thermochemical equilibrium in a UN-TRISO of FCM LWR fuel using HSC software [1].

2. Thermochemical Equilibrium in a kernel of a TRISO

A TRISO in FCM fuel consists of a kernel at its central region and four coating layers surrounding the kernel. The kernel material is a UN, the diameter of which is 700 μm. Many fission products and gases, nitrogen gas, transuranic radionuclides, and UN exist in a kernel during irradiation. It can be assumed that the above species instantly attain their chemical equilibrium. The possible phases in the UN fuel kernel are gases, iodides, nitrides, carbides, and the remaining condensed compounds.

3. Calculation Results

The enrichment of the UN kernel is 11.8 atom %. It was assumed that the fuel temperature was 600, 700, 800, 900, and 1000 ^{o}C. The McCARD code [2] was used to generate neutronic data and nuclide inventory according to the fuel burnup. At 600 EFPD, the fuel burnup and fast fluence are 60.5 GWd/tHM and 10.7×10^{25} n/m^2 (E > 0.18 MeV), respectively. The following 43 nuclides were generated as a result of the inventory calculation using McCARD: H, B, C, N, Se, Br, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Cs, Ba, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, U, Np, Pu, Am, Cm, Bk, and Cf. The HSC software, however, did not succeed in calculating the thermochemical equilibrium for all of the above nuclides. For a simpler equilibrium calculation, the radionuclides of an element were summed, and were classified into groups of similar chemical behavior, as shown in Table 1.

It was revealed though the thermochemical equilibrium calculation that the generation of iodides and carbides was negligible under the irradiation range. The produced nitrides are $(U_{0.8}Pu_{0.2})N$, LaN, ZrN, U_2N_3, NpN, NbN, UN_2, BN, Sr_3N_2, Nb_2N, Mo_2N, PuN, and MoN. The generated condensed compounds excluding nitrides are Mo, Sr, Cs, UPd_3, Cs_2Te, MoB, Cd, SrTe, U, Nb, La, LaTe, B, and Pd. The gases such as Cs(g), CsI(g), Cd(g), Sr(g), Cs2I2(g), and SrI(g) are significantly generated above 910 ^{o}C. Fig. 1 presents the material balance in a kernel under irradiation. The gases are generated after 15 GWd/MTHM. The nitride generation does not depend on the temperature in the range of 600 to 1000 ^{o}C.

Table 1 Element Groups Used in a Thermochemical Equilibrium Calculation

Groups	Elements	Chemical states
B	B	BN, element
C	C	Element
N	N	Gas
Sr	Sr, Ba	[a] $(AE)_3N_2$
Te	Te, Se	Volatile
I	I, Br	Volatile
Cs	Cs, Rb	Volatile
La	Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Ho, Er	[b] (RE)N
Zr	Zr	ZrN
Nb	Nb	Nb_2N
Mo	Mo	Mo_2N
Pd	Tc, Ru, Rh, Pd, Ag	Metal phase
Cd	Cd, In, Sn, Sb	Metal phases
U		UN, U_2N_3
Np		NpN
Pu		PuN
Am		
Cm		

[a] AE means alkali earth metal.
[b] RE means rare earth.

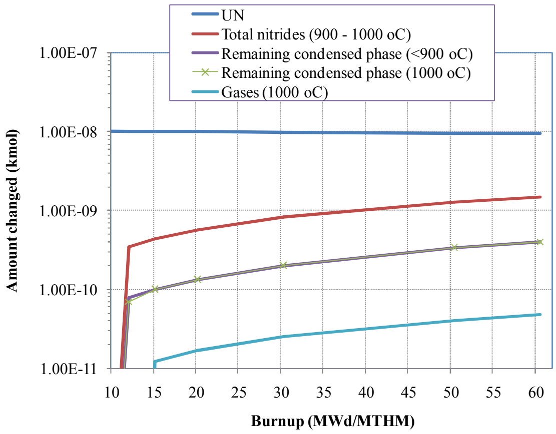

Fig. 1 Variation in Material Amount in a kernel of FCM TRISO

4. Conclusions

The thermochemical equilibrium calculation for a UN kernel of FCM LWR fuel, which is irradiated until a fuel burnup of 60.5 GWd/tHM, has been performed. The following conclusions have been obtained:

- The generation of iodides and carbides was negligible.
- The significantly produced nitrides are $(U_{0.8}Pu_{0.2})N$, LaN, ZrN, U_2N_3, NpN, NbN, UN_2, BN, Sr_3N_2, Nb_2N, Mo_2N, PuN, and MoN.
- The generated condensed compounds are Mo, Sr, Cs, UPd_3, Cs_2Te, MoB, Cd, SrTe, U, Nb, La, LaTe, B, and Pd.
- The gases, Cs(g), CsI(g), Cd(g), Sr(g), Cs2I2(g), and SrI(g), are significantly generated above 910 ^{o}C after 15 GWd/MTHM.

REFERENCES

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