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Development of an Isotope-wise Reactivity Module in the Perturbation Code PERT-K

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1. Introduction

PERT-K is a three-dimensional multi-group diffusion perturbation theory code developed by KAERI for use in fast reactor design and analysis [1][2]. It utilizes the eigenvalues, fluxes, and adjoint fluxes from the diffusion theory code, DIF3D [3], for calculating the reactivity effects associated with hexagonal-Z and triangular-Z geometries commonly encountered in fast reactors. By making use of PERT-K, the first-order and exact perturbation theory calculations can be carried out. Thus, it can help to better understand and predict the effects of change on the behaviour of a fast reactor owing to a change in the diffusion equation coefficients.

However, the current version of PERT-K can only provide the global reactivity effects and their reactivity components contributed from the fission, absorption, scattering and leakage processes. In the present study, we developed an isotope-wise reactivity module for the triangular-Z geometry in PERT-K to allow for a finer resolution into the reactivity contributions and components of each specific isotope present in a reactor core region. This information will be useful for a better and safer design of the core. The isotope-wise module will be validated against the global reactivity results calculated by PERT-K through a perturbation analysis in the KALIMER-600 TRU burner core [4].

2. Methods and Results

2.1 Development Method

First, the CCCC standard files, ISOTXS (microscopic group neutron cross sections), ZNATDN (zone atomic densities of nuclides), and NDXSRF (nuclide density, data, cross section referencing) [5], at both the reference and perturbed states were used to make the zone-wise macroscopic group neutron cross sections of each specific isotope in the triangular-Z geometry of a fast spectrum core. In an ISOTXS file, a specific isotope XXAA was classified as a region-wise isotope, XXAHBB, depending on the core region in which it is present; where XX and AA, respectively, represent the symbol and mass number of isotope, A is the last digit of mass number, H indicates the core region, and BB is the region number (01, 02 = inner, outer core; 03, 04 = lower shield; 05, 06 = sodium bond; 07, 08 = gas plenum; 11 = control rods; 12 = control rod tube; 13 = radial shield; 14 = B_4C shield; 15 = reflector; 16 = IVS). For example, the isotope NA3H01 indicates the presence of sodium-23 (NA3) in the inner core (H01).

Second, the isotope-wise reactivity module for the triangular-Z geometry in PERT-K was developed using these above isotope-wise cross sections to calculate the region-wise reactivity of each isotope, which is also composed of reaction-wise terms including fission, absorption, scattering, and leakage components. As a result, the global reactivity and components of each isotope in the whole core can be determined.

Finally, the isotope-wise reactivity module was validated against the global reactivity effect and its components calculated by PERT-K using the macroscopic composition cross sections, COMPXS, which is generated by the cross section processor, HMG4C, in DIF3D through the processing of ISOTXS, ZNATDN, and NDXSRF [3]. An analysis of sodium voiding and fuel temperature change in the KALIMER-600 TRU burner core was performed for this validation.

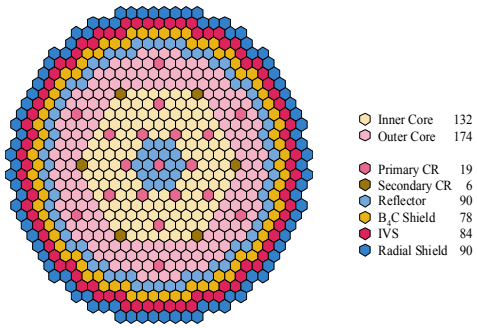

Fig. 1. KALIMER-600 TRU burner core layout

2.2 Validation of the Isotope-wise Reactivity Module

The reference KALIMER-600 TRU burner core configuration is shown in Fig. 1. To validate the isotope-wise reactivity module, the reactivity effects and their components due to sodium voiding and fuel temperature change at the beginning of the equilibrium cycle (BOEC) in the KALIMER-600 TRU burner core (with the triangular-Z geometry) were analyzed for the following cases.

1) Total sodium voiding in the whore active core.
2) Fuel temperature change from 600K to 900K.

A comparison of global reactivity and components caused by sodium voiding and fuel temperature change given in Table I showed that the isotope-wise reactivity module agreed well with the global results calculated by PERT-K using COMPXS within 0.4 pcm. In other words, this module was successfully developed.

Using the isotope-wise module, the resolution into the reaction-wise void reactivity components of each isotope in the whole core was provided in Table II. In the fuel, the uranium-38, plutonium-239, plutonium-240, and zrnat were shown to intensify the void effect of ~134 pcm. The sodium-23, on the whole, mostly enhanced the void reactivity of ~1615 pcm whereas the iron reduced that of ~56 pcm. Also, the leakage through sodium-23 and iron was the key contributor to lessen the void effect. Moreover, the difference between the first-order and exact perturbation results (~320 pcm) was largely contributed by those in predicting the scattering and leakage components of sodium-23 (~280 pcm and ~50pcm, respectively).

Table I: Global reactivity and components (pcm)

100% whole core void at BOEC					
Reactivity	ρ_{fiss}	ρ_{abso}	ρ_{scat}	ρ_{leak}	ρ_{total}
First-order PERT-K					
Isotope-wise	72.2	182.2	3511.7	-2372.0	1394.1
COMPXS	72.4	182.2	3511.9	-2372.0	1394.4
Diff.	-0.2	0.0	-0.1	0.0	-0.3
Exact PERT-K					
Isotope-wise	67.1	151.4	3810.5	-2316.6	1712.4
COMPXS	67.3	151.4	3810.6	-2316.6	1712.8
Diff.	-0.2	0.0	-0.2	0.0	-0.4
Fuel temperature change from 600K to 900K at BOEC					
First-order PERT-K					
Isotope-wise	27.8	-167.2	-1.5	2.1	-138.9
COMPXS	27.7	-167.2	-1.5	2.1	-139.0
Diff.	0.1	0.0	0.0	0.0	0.1
Exact PERT-K					
Isotope-wise	27.1	-164.3	-1.5	2.1	-136.7
COMPXS	27.0	-164.3	-1.5	2.1	-136.7
Diff.	0.1	0.0	0.0	0.0	0.1

Table II: Resolution into the global isotope- and reaction-wise void reactivity components (pcm)

100% whole core void at BOEC (Exact PERT-K)					
Reactivity	ρ_{fiss}	ρ_{abso}	ρ_{scat}	ρ_{leak}	ρ_{total}
U-234	0.4	-0.4	0.1	0.0	0.1
U-235	0.1	0.0	0.0	0.0	0.1
U-236	0.0	0.0	0.0	0.0	0.0
U-238	2.4	44.2	30.1	-0.8	75.9
PU238	2.6	-0.8	0.1	0.0	1.9
PU239	18.6	-1.3	1.1	-0.1	18.3
PU240	29.7	-8.6	1.7	0.0	22.8
PU241	1.1	-0.3	0.3	0.0	1.1
PU242	5.2	-1.8	0.6	0.0	4.0
MA	7.0	-2.6	0.3	-0.1	4.7
FP	0.0	0.0	0.0	0.0	0.0
ZRNAT	0.0	6.4	11.8	-1.5	16.7
FE	0.0	20.5	95.6	-172.1	-56.0
CR	0.0	0.2	11.2	-7.3	4.1
MONAT	0.0	0.5	0.5	-0.1	0.9
SINAT	0.0	0.0	1.6	-0.1	1.5
MN55	0.0	1.2	-0.6	0.6	1.3
NI	0.0	0.1	0.3	-0.4	0.0
NA23	0.0	93.9	3655.3	-2134.5	1614.6
B10	0.0	0.1	0.0	0.0	0.1
B11	0.0	0.0	0.4	-0.1	0.3
CNAT	0.0	0.0	0.1	0.0	0.1
SUM	67.1	151.4	3810.5	-2316.6	1712.4

The resolution into the region-wise void reactivity components of sodium-23 was illustrated in Table III. Through such resolution, it was found that the change in the global reactivity was mostly contributed from the reactivity change of isotopes present in the sodium voiding regions (inner, outer core: H01, H02; sodium bond: H05, H06; gas plenum: H07, H08). In addition, it allows for calculating the local reactivity of each region in the core, e.g., inner and outer cores, lower shield, etc.

Table III: Illustration of region-wise void components (pcm)

100% whole core void at BOEC (Exact PERT-K)					
Reactivity	ρ_{fiss}	ρ_{abso}	ρ_{scat}	ρ_{leak}	ρ_{total}
NA3H01	0.0	43.6	1799.9	-469.4	1374.1
NA3H02	0.0	43.7	1622.8	-987.9	678.6
NA3H03	0.0	0.0	0.3	0.2	0.5
NA3H04	0.0	0.0	0.2	0.2	0.5
NA3H05	0.0	2.6	77.4	-187.2	-107.2
NA3H06	0.0	2.3	61.9	-219.7	-155.5
NA3H07	0.0	0.9	50.4	-139.0	-87.7
NA3H08	0.0	0.9	40.9	-135.1	-93.2
NA3H011	0.0	0.0	0.0	0.0	0.0
NA3H012	0.0	-0.1	1.4	3.0	4.3
NA3H013	0.0	0.0	0.0	0.0	0.0
NA3H014	0.0	0.0	0.0	0.0	0.0
NA3H015	0.0	0.0	0.0	0.3	0.3
NA3H016	0.0	0.0	0.0	0.0	0.0
NA23	0.0	93.9	3655.3	-2134.5	1614.6

3. Conclusions

An isotope-wise reactivity module was newly developed in this study for the triangular-Z geometry in PERT-K, and agreed well with the global results calculated by PERT-K using COMPXS in analyzing the reactivity change caused by sodium voiding and fuel temperature change in the KALIMER-600 TRU burner core. This module provided a resolution into the global, region- and reaction-wise reactivity changes of each specific isotope in the core. Hence, it would be important for a better core design against severe accidents, particularly the sodium void effect.

In future work, a further perturbation analysis in the KALIMER-600 TRU burner core will be conducted using this isotope-wise reactivity module.

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