Development of a Burnup Program based on the Krylov Subspace Method

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1. Introduction

The depletion calculation of the DeCART code [1] has been performed by the support of the ORIGEN code. Recently, a burnup program based on the Krylov subspace method [2] is developed and implemented to the DeCART code. Numerical solution for the burnup equation by the Krylov subspace method is well described in Reference 2. Therefore, this paper describes the Krylov subspace method for a burnup equation briefly in Section 2, and focuses on the DeCART solution for a pin cell problem by comparing it with the HELIOS solution.

2. Methods

2.1. Krylov Subspace Method for Burnup Equation

General solution for the burnup equation can be written as:

$$\vec{N}(t+\Delta t) = \exp(\mathbf{A}\Delta t)\vec{N}(t), \quad (1)$$

where

$\vec{N}(t)$ = nuclide vector at time t,
$\mathbf{A}$ = the burnup matrix,
Δt = burnup step size.

In the Krylov subspace method, the isotope vector $\vec{N}(t+\Delta t)$ can be approximated by the Krylov subspace of dimension m as:

$$K_m\left(\mathbf{A}\Delta t, \vec{N}(t)\right) = Span\{\vec{N}(t), (\mathbf{A}\Delta t)^1 \vec{N}(t), \cdots, (\mathbf{A}\Delta t)^{m-1} \vec{N}(t)\} \quad (2)$$

In the Krylove subspace method, the approximate solution of Eq. (1) can be written as:

$$\vec{N}_{app}(t+\Delta t) = \beta \mathbf{V_m} \exp(\mathbf{H_m}\Delta t)\vec{e}_1, \quad (3)$$

where

β = L2-norm of $\vec{N}(t)$,
$\mathbf{V_m} = [\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_1] \in \mathbf{R}^{nxm}$ = orthogonal basis matrix for the Krylov subspace method,
$\mathbf{H_m} \in \mathbf{R}^{nxm}$ = a Hessenberg (upper triangular with an extra sub-diagonal) matrix,
$\vec{e}_m$ = m-th unit vector whose m-th element is one and the other elements are zero.

By introducing the Arnoldi procedure, β, $\mathbf{V_m}$ and $\mathbf{H_m}$ can be obtained. The generated $\mathbf{V_m}$ and $\mathbf{H_m}$ have the following features.

$$\mathbf{H_m} = \mathbf{V_m^T A V_m}, \quad (4)$$

$$\mathbf{V_m^T V_m} = \mathbf{I}, \quad (5)$$

In the calculation of the exponential value of $\mathbf{H_m}\Delta t$, the conventional scaling and squaring scheme is used.

2.2 Development of DECBURN program

DECBURN program is developed based on the Krylov subspace method and examined for a 4.5 % enriched UO_2 fuel by comparing it with the ORIGEN solutions. ORIGEN solves the burnup equation by introducing the matrix exponential method for the long-lived isotopes and the asymptotic Bateman solution for the short-lived isotopes. Therefore, in the ORIGEN calculation, the burnup step is minimized to obtain an absolute solution by removing the asymptotic solution for the short-lived isotopes. In the depletion calculation of the DECBURN program, a consistent depletion library with the ORIGEN code is used. The computational solution shows that DECBURN estimates the same number densities for all the isotopes with the ORIGEN code. This result means that the burnup calculation based on the Krylov subspace method is programmed correctly in the DECBURN program and it works soundly.

3. Benchmark Calculation

DECBURN progrom is implemented to the DeCART code that performs a radial MOC and an axial SP_N transport calculation and examined for a pin cell problem that contains a 4.5 % enriched UO_2 fuel. The depletion calculation is performed up to 50 MWD/kgHM and compared with the HELIOS solution. The HELIOS calculation is performed by using the '0' interface current option which means a full collision probability calculation.

Fig. 1 shows three k-infinites of HELIOS and their differences. The first k-infinite is obtained by performing the depletion calculation with the infinite spectrum. The second k-infinite is obtained by performing the depletion and k-infinite calculation with the critical spectrum. The third k-infinite is obtained by performing the depletion calculation with the critical spectrum, but the k-infinite calculation with the infinite spectrum. The first and the third k-infinites are similar showing less than 200 pcm differences, but the second k-infinite is quite different from the others showing a maximum 1,000 pcm difference.

Fig. 2 shows the same three k-infinites of the DeCART code. DeCART code shows a very similar behavior to Fig. 1 of the HELIOS code. Fig. 3 shows the k-infinite differences between the HELIOS and the DeCART codes for the three k-infinites. The k-infinites of the DeCART code agree very well with those of the HELIOS code showing less than 100 pcm k-infinites than the HELIOS code and the difference shapes of the

three k-infinites are very similar. These results mean that the DECBURN program implemented in the DeCART code works soundly and produces a very consistent solution with the HELIOS code. Also, it is proven that the criticality calculation is performed very consistently with the HELIOS code.

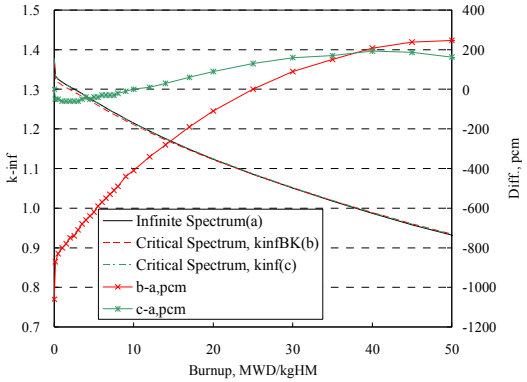

Fig.1 Different k-infinites and Their Differences on HELIOS

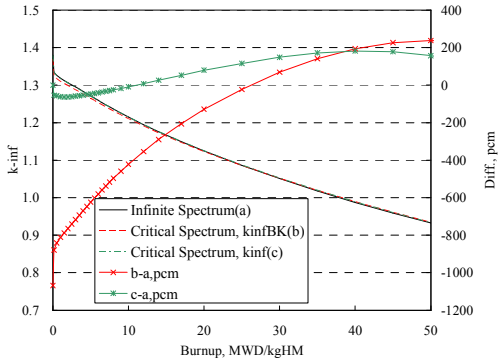

Fig.2 Different k-infinites and Their Differences on DeCART

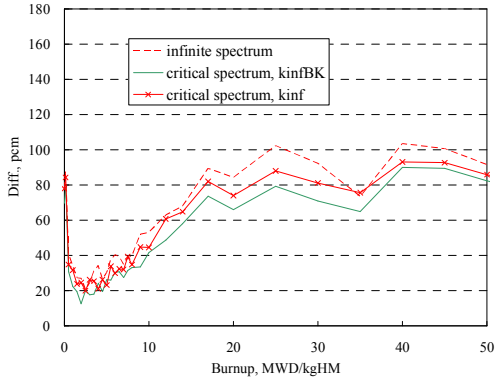

Fig.3 kinf Difference between DeCART and HELIOS

Table 1 shows the isotope number density comparison between the HELIOS and DeCART codes. At a burnup of 50 MWD/kgHM, DeCART shows less than 1 %, 2 % and 4 % differences for the U-235, Pu-238 and Xe-135 number densities, respectively. The differences for the U-235 and Pu-239 number densities are not much because these differences introduce a trivial difference in the k-infinites. However, 4 % difference in the Xe-135 number density is not small and introduces about less than 100 pcm in the k-infinite. This lower Xe-135 number density results from the inaccurate fission yield data in the DECBURN program. Current depletion data of the DECBURN program contains the fission yield data for the limited fission isotopes, which results in the lower fission product number densities. Therefore, the fission yield data for more fission isotopes needs to be supplemented in the future.

Table 1. Isotope Number Density Comparison

	Bu	U-235	U-238	Pu-239	Xe-135
HELIOS, #/barn/cm	10	2.53E-04	6.87E-03	2.71E-05	3.83E-09
	20	1.92E-04	6.82E-03	4.11E-05	3.77E-09
	30	1.43E-04	6.76E-03	4.82E-05	3.65E-09
	40	1.04E-04	6.71E-03	5.17E-05	3.47E-09
	50	7.36E-05	6.65E-03	5.30E-05	3.28E-09
DeCART, Diff., %	10	-0.06	-0.01	-1.16	-0.42
	20	-0.16	0.00	-1.36	-1.29
	30	-0.32	0.01	-1.56	-2.42
	40	-0.54	0.01	-1.73	-2.95
	50	-0.84	0.02	-1.86	-3.31

4. Conclusion

In this paper, a DECBURN burnup program based on the Krylov subspace method wass developed and implemented to the DeCART code. The DECBURN program produces the same isotope number densities as the ORIGEN code. The DeCART code performing the depletion calculation by the DECBURN program shows very consistent k-infinite behaviors with the HELIOS code. Therefore, it is concluded that the DECBURN program solves the depletion equation very accurately and the DeCART code performs the depletion calculation consistently with the HELIOS code. Also, it is concluded that the fission yield data in the depletion library of the DECBURN program needs to be supplemented in the future.

Acknowledgement

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REFERENCES

[1] J. Y. Cho, et al., "DeCART Benchmark Calculation for LWR Next Generation Fuels," '2005 KNS Spring Mtg., May 27, 2005, Jeju.
[2] Akio Yamamoto, et al., "Numerical Solution of Stiff Burnup Equation with Short Half Lived Nuclides by the Krylov Subspace Method," Journal of Nuclear Science and Technology, Vol. 44, p 147, 2007.