Evaluation of a New Group Structure for nTRACER Based on HELIOS 47 Group Structure and Extended Resonance Range for 20w% Uranium and MOX Fuels

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1. Introduction

From the lattice calculations of traditional two-step approach to the recent direct whole core transport calculation codes, less than a thousand groups are used in their calculation with acceptable accuracy. Although there are several practical codes that adopt hundreds groups in their calculations, the simulation results utilizing tens of groups with adequate resonance treatments also have enough accuracy for commercial reactor design such as 69G of WIMS [8], 72G of STREAM [3], and 47G of HELIOS [7]. nTRACER, the direct whole core transport code developed in SNU, has utilized HELIOS 47G and subgroup method as the resonance treatment, which effectively simulates the commercial LEU UO_2 fuels [1]. Recently, the resonance interference factor library method (RIF) [6] and parameterized spectral SPH factor library method (PSSL) [2] was also implemented in the code, which makes great improvement on its accuracy.

However, there are several requests for new fuel types, such as high-assay LEU fuels, a fuel whose enrichment is in between 5w% and 20w%, to overcome the short loading cycle of the current UO_2 fuel of LWR. Especially, for economic refueling program in the naval propulsion reactor, U-Mo alloy fuel with relatively high enrichment about 20w% has been suggested since the alloy fuel has much higher uranium density than oxide fuels due to its chemical structure [5]. For such new types of nuclear fuel, nTRACER whose libraries and methodologies are targeted for UO_2 fuels of commercial LWR could not guarantee the accurate results. In particular, the broad group width of the 11th group (G11) makes large discrepancy of scattering matrix when 47G library is used for high enrichment fuel problem. Moreover, the resonance energy range where the multigroup XSs are treated with the subgroup method is from 1.855eV to 9.119keV in nTRACER, which cannot cover the broad resonances of plutonium isotopes, located near 1eV and 0.3eV. Therefore, the needs for the new group structure and extended resonance range are raised.

Preventing unnecessarily large calculation burdens, it is our goal to find a group structure that consists of tens of groups with adequate resonance treatment. As a preliminary research to find the optimized group structure for general types of nuclear fuels, the extended resonance range from 0.1844eV to 9.1188keV and refined 56G structure based on HELIOS 47G structure have been developed and introduced in this research. All the current resonance treatment methods in nTRACER, such as spectral SPH factor and RIF with the subgroup method, are used in the calculation. The impact of these refinement will be analyzed through 4w% reactor-recycled MOX pin problem, 20w% U-Mo fuel pin problem, and 3.1w% and 20w% UO_2 fuel pins. Although the commercial reactor fuel does not contain the amount of the plutonium isotopes such like mixed oxide fuels, the MOX fuel is selected for the target problem for sufficient accuracy. Note that in the context that 20w% uranium has much more fissile isotope than the commercial fuel in LWR, it is referred as *high enriched fuel* in this research.

2. Problem specification and calculation conditions

All the problems used in this research have the same geometric configuration and temperature condition. The only thing different is the material composition of fuel pellet. The pin cell problem contains 4 regions, fuel pellet, air gap, cladding, and moderator. The rectangular pin cell in which concentric cylindrical fuel pellet, air gap, and cladding are surrounded by moderator of water is solved. The radius of fuel pellet, inner radius of the cladding and outer radius of the cladding are 0.4096cm, 0.4180cm, and 0.4750cm, respectively. The pitch of the pin is 1.260 cm. All the region is 600K except for fuel region whose temperature is 900K. The fuel composition data of MOX problems are from the reactor-recycled MOX of Mosteller benchmark [4], in which the atomic percent of fissile plutonium isotopes is 60 at.%. The U-Mo fuel contains 10% of molybdenum element in its weight as referred in [5].

The ray parameters of a 0.01cm ray spacing and 32 azimuthal and 4 polar angles per the octant sphere are used for nTRACER. The probabilistic code developed in SNU, McCARD, is used as the reference. The McCARD calculations are conducted with 500,000 particles for 50 inactive and 500 active cycles. All the data in this paper are generated based on ENDF/B-VII.1 except for the ultra-fine-group spectra used in GROUPR of NJOY, which are generated with CENTRM or McCARD with ENDF/B-VII.0.

The absorption and nu-fission reactivity error of group g and region k is defined as:

$$\Delta\rho_{gk}^{\Sigma_a} = \left(\Sigma_{a,gk}\phi_{g,k}V_k\right)^{ref} - \left(\Sigma_{a,gk}\phi_{g,k}V_k\right)^{nTRAER} \quad (1)$$

$$\Delta\rho_{gk}^{\nu\Sigma_f} = \frac{1}{k^{ref}}\left(1+\frac{1}{\left(\nu\Sigma_{f,gk}\phi_{g,k}V_k\right)^{nTRACER} - \left(\nu\Sigma_{f,gk}\phi_{g,k}V_k\right)^{ref}}\right)^{-1} \quad (2)$$

where $\Sigma_{a,gk}$ is the absorption XS of group g and region k, $\nu\Sigma_{f,gk}$ is the nu-fission XS of group g and region k, $\phi_{g,k}$ is the multigroup flux at group g and region k, V_k is the volume of the region k. As fission reactivity errors are normalized making the summation of all the reactivity errors to be zero, only the absorption reactivity error defined as Eq. (1) is used in this paper. Normally the behavior of absorption and nu-fission reactivity errors are reverse and can be cancelled each other in an energy group, however, the level of the absorption reactivity error can be regarded as the measurement of the reactivity error contribution of each group. It is because most of fission reaction occurs by thermal neutrons which is beyond the topic of this research and they have similar behaviors in their magnitudes. Also, note that in this paper, the N^{th} group in a group structure is referred as '*GN*' and the group structure containing M groups is referred as '*M*G'.

3. The necessity of refined group structure and extended resonance range

The current 47G library of nTRACER has high accuracy for the LEU fuel as the results of 3.1w% in Fig. 1 has no significant error. However, for the nuclear fuels with high enrichment, large flux error occurs in the G11, the energy group between 0.1301keV and 2.0347keV, and the groups below G11 as shown in Fig. 1. The flux error of G11 is about -2%, which makes about 236pcm of reactivity error. However, there is no distinctive error in multigroup XS for those groups. In other words, there is another source of the error rather than the multigroup XS of fuel.

In the nTRACER library, the scattering matrix of hydrogen in moderator is generated with NJOY or McCARD using a representative problem of LEU fuel pin, the 3.1w% APR1400 fuel pin. The error of moderator scattering matrix is mainly from the spectrum change between the high enriched fuel pin and the representative pin of nTRACER library. Fig. 2 shows the difference of the scattering matrix of moderator between 3.1w% and 20w% tallied from McCARD, which is defined as:

$$\Delta_{g'g} = \frac{\Sigma_{g'g}^{3.1w\%} - \Sigma_{g'g}^{20w\%}}{\Sigma_{g'g}^{20w\%}} \times 100 \quad [\%] \qquad (3)$$

where $\Sigma_{g'g}^{Xw\%}$ is the scattering matrix element which indicate the scattering kernel from g' to g when the fuel enrichment is X w%.

As shown in Fig. 2, the 47G scattering matrix significantly changes with the enrichment especially in the G11. Particularly, in the G11, the self-scattering element of 3.1w% is -1.4% lower than that of 20w% while the down-scattering elements are 3% higher. Therefore, when the scattering matrix generated with 3.1w% is used for 20w% problem, the flux of G11 is underestimated whereas those of the groups below G11 are overestimated. These flux errors of 20w% fuel problem generate the large reactivity error of G11.

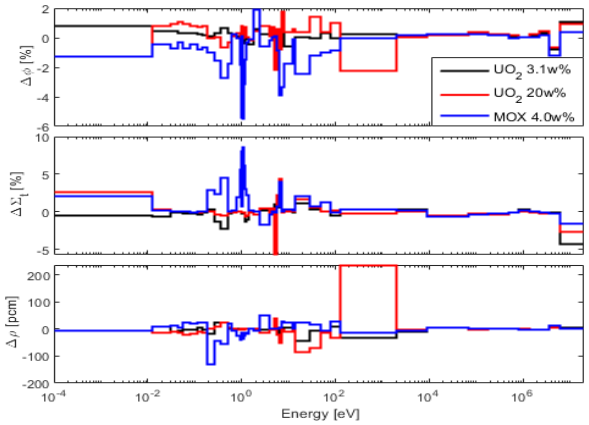

Fig. 1 Multigroup flux error [%] (top), macroscopic XS error [%] (middle), and reactivity error [pcm] (Bottom) of various fuels (black: UO_2 3.1w%, red: UO_2 20w%, blue:MOX 4w%) with 47G structure and current resonance range

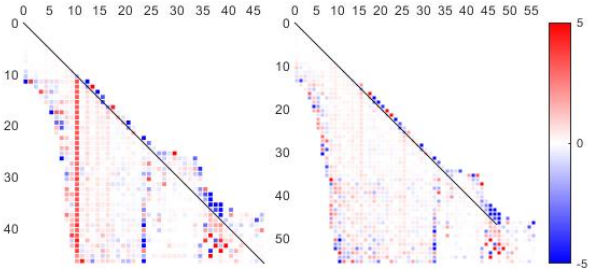

Fig. 2 Moderator scattering matrix difference between 3.1w% and 20w% UO_2 problems [%] for 47G (left) and 56G (right)

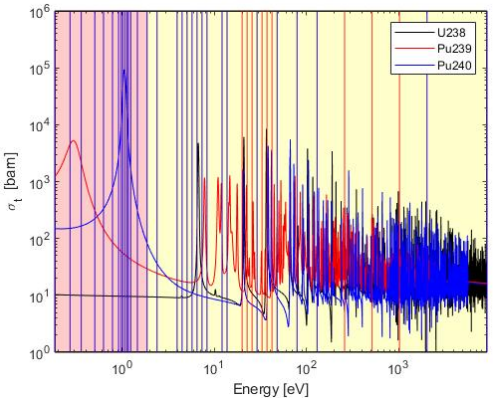

Fig. 3 Group structure between 0.1844eV and 9.118keV of 56G, red vertical lines are added group boundaries from 47G HELIOS group structure. The yellow zone is the current resonance energy range(1.855eV to 9.118keV) and the red zone is the extending energy range (0.1844eV to 1.855eV)

Moreover, there are relatively large XS errors at the groups containing broad resonances of U238 in Fig. 1, near 6.67eV(G19), 20.3eV(G15), and 36.2eV(G14). These errors are not noticeable in commercial LWR problems, but they make relatively large reactivity errors in the high enriched fuels. Although the groups near 6.67eV also have the XS error, the contribution of reactivity error in these groups are not significant due to small group widths. However, the G14 and G15 that contains the second and third resonances of U238 have non-negligible errors of XS and corresponding reactivity

error about -87pcm and -69pcm in 20w% UO_2 problem, respectively. To resolve such XS errors near U238 resonances, the G14 and G15 also divided in 56G. Considering the scattering matrix distortion in G11 and XS error in the G14 and G15, a refined group structure having 56 groups depicted in Fig. 3 is tested for nTRACER library.

On top of that, the XS errors near the resonances of Pu isotopes make significant error in flux and reactivity as shown in Fig. 1. The XS error near 1eV and 0.3eV are mainly from the broadest resonances of Pu240 and Pu239, respectively. In particular, the energy group between 0.1844eV and 0.2705eV, G39 for 47G, shows 132pcm of reactivity error due to its large XS error. Note that the current library does not imply the spectral SPH factor beyond the 1.855eV, which makes large flux errror near the resonance. To resolve these XS errors due to the resonances of the Pu isotopes, the energy range of resonance treatment should be extended. In this research, the effect of the extended resonance range of (0.1844eV, 9.1188keV) depicted in Fig. 3 will be tested with 47G and 56G.

4. Calculation results and analysis

As mentioned above, the two group structures, 47G and 56G, and two resonance ranges for each group structure are used to generate library. Therefore, there are four libraries which are named as OR47G, ER47G, OR56G, and ER56G in the legend of the following figures. The first 2 characters in the library name, 'OR' and 'ER' means the original resonance range and the extended resonance range, respectively. The calculation results of MOX, UO2, Mo-U fuels with various group structures are shown in this chapter via Fig. 4 to Fig. 7. In those figures the black lines indicate 47G and the red lines indicates 56G. With respect to the resonance range, the solid lines mean the original resonance range while the dotted lines are for the extended one.

Fig. 4 and Fig. 5 show the calculation results of oxide and Mo alloy high enriched fuels. In both the problems, the impact of extended resonance range is negligible since there is no nuclide that has significant resonance under 1.8eV. The implementation of the 56G group structure resolves the flux error in G11 of 47G group structure and corresponding reactivity error in both high enriched fuels. As U-Mo fuel has higher uranium number density than UO_2 fuel by its structure, the improvement in U-Mo fuel by the 56G is much greater than that in the oxide fuel. About 711pcm of reactivity error and -2.97% of flux error in G11 of 47G is corrected by 56G. The flux errors of the groups below G11 also decrease according to the resolution of scattering matrix error of the moderator. Although G19 of 47G and other groups near 6.67eV, the broadest resonance of U238, show large cross section errors, the reactivity error from those groups are small due to narrow group widths. Also, despite of the existence of larger XS errors in the divided groups of G14 and G15, the narrower widths give smaller reactivity errors. Therefore, for the high enriched fuel, the implementation of 56G successfully reduces the reactivity errors. For the U-Mo fuel, although there are several multigroup XS errors and corresponding low thermal fluxes due to the resonance interference effect of Mo isotopes, they do not give severe reactivity errors.

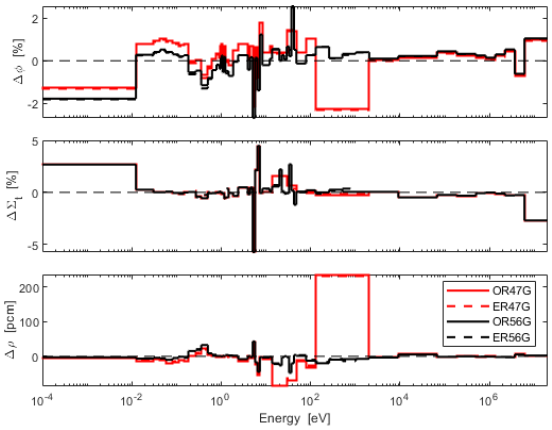

Fig. 4 Flux (top), total XS (middle), and absorption reactivity error (bottom) of 20w% UO_2 fuel pin with various group structures

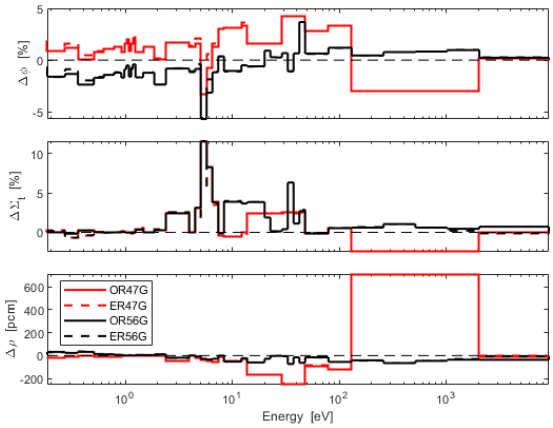

Fig. 5 Flux (top), total XS (middle), and absorption reactivity error (bottom) of 20w% U-Mo fuel pin with various group structures

As shown in Fig. 6, there is no significant difference in the MOX problem between 47G and 56G if they use the same resonance energy range. There are remaining errors near the resonances of U238, 6.67eV, 20.3eV, and 36.2eV, in MOX fuel. However, these errors are out of scope in this research because such the XS errors are due to the resonance interference of nuclides and U238 which is already considered with the current library. By the optimization of resonance parameters in further research, there errors would be resolved. Fig. 7 shows the errors of groups between 0.1844eV and 1.855eV, in which the resonance treatment is conducted only for ER47G and ER56G.

As shown in Fig. 7, the extended energy range of resonance treatment improves the XS near 1eV and 0.3eV except for the group between 0.1844eV and 0.2705eV, G39 for 47G and G48 for 56G, which still has large XS error about 2.86%. Particularly, the XS errors

between 0.2705eV and 0.3577eV are improved with the extended resonance range. Also, the XS error between 0.7821eV and 1.457eV are reduced in both the ER47G and ER56G except for the groups between 1.014eV and 1.125eV where there are remaining errors for ER56G.

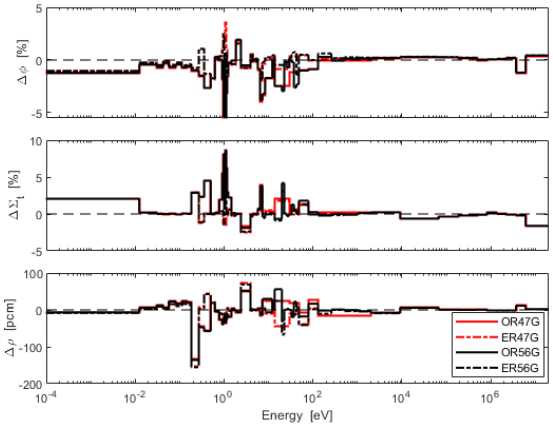

Fig. 6 Flux (top), total XS (middle), and absorption reactivity error (bottom) of 4w% MOX fuel pin with various group structures

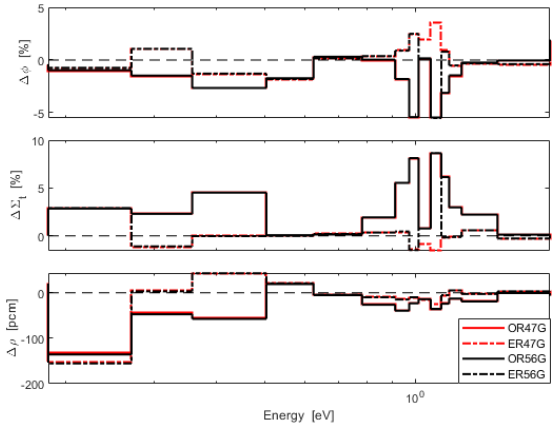

Fig. 7 Flux (top), total XS (middle), and absorption reactivity error (bottom) of 4w% MOX fuel pin with various group structures between 0.1844eV and 1.855eV.

5. Conclusion

One of the most important findings of this work is that using the scattering matrix of moderator generated from the representative pin cell makes significant distortion of scattering kernel in the broad group, G11 of 47G, for high enrichment fuels. This distorted scattering kernel incurs the flux error at the G11 and the groups below G11. Especially, U-Mo alloy fuel pin, the new type of fuel suggested for naval propulsion reactor, has higher density of uranium isotopes than oxide fuel due to its chemical structure, in which the reactivity error is much more severe than oxide fuel. The error in G11 makes large reactivity errors about 236pcm for 20w% UO_2 problem and 711pcm for 20w% U-Mo problem. The refined group structure of 56G tested in this research resolves the problem of scattering kernel of moderator, which is verified with 20w% UO_2 and U-Mo fuel pin cell problem. Moreover, the broad resonances of plutonium isotopes, especially the resonance of Pu239 near 0.3eV and that of Pu241 near 1eV, make large XS error without proper resonance treatment. Although the groups near 1eV have very fine energy widths, the groups near 0.3eV are relatively broad. Therefore, the extended group structure by spanning the low boundary of resonance energy region from 1.855eV to 0.1844eV has been tested in this research, showing there are mitigation of XS error near the resonances of plutonium isotopes.

In this research, it is implied that the scattering matrix of moderator can be one of the parameters determining group structure. Dividing broad energy groups whose scattering kernel extremely changes, 56G can be chosen as the substitute of current HELIOS 47G structure. Moreover, the extended resonance range reduces the XS errors near the resonances of plutonium isotopes. However, there are still remaining errors for several groups even with extended resonance treatment. Since the resonance parameters in this research are generated with the same procedure for commercial UO_2 pin, investigation on the optimal parameters for general fuels is needed in further research. Although the MOX fuel is tested in this research, in which large amount of Pu exists compared with the LEU pins during reactor cycle, the impact on the fission products is remaining task. Therefore, impact of the refined group structure and extended resonance range in the depleted fuel pins should be analyzed in further research.

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