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Neutron Up-Scattering Effect in Refined Energy Group Structure

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ABSTRACT

Aiming at generating a 361-group library, this paper investigated neutron up-scattering effect in the 361-group Santamarina-Hfaiedh Energy Mesh (SHEM). Firstly, the Doppler Broadening Rejection Correction (DBRC) method is implemented to consider the neutron up-scattering effect in Monte Carlo (MC) method. Then the MC method is employed to prepare resonance integral table and scattering matrix for afterward calculation. Numerical results show that the neutron up-scattering affects k_{inf} by ~200 pcm at most for UO_2 pin cell problems in the 361-group SHEM, while the fuel temperature coefficient (FTC) is also influenced by 12~13%. It has also been found that both of the above two influences acts through scattering matrix rather than self-shielded absorption cross sections. In addition, the self-shielding effect of cladding is studied and it's been found that it affects k_{inf} by 30~70 pcm.

KEYWORDS: neutron up-scattering effect; DBRC; 361-group SHEM; multi-group library

INTRODUCTION

Conventionally, neutron elastic scattering in the epithermal energy range is treated by the asymptotic scattering kernel in which the neutron up-scattering caused by thermal agitation of nuclide is underestimated (Lee et al. 2008; ONO et al. 2012). Considering the fact that neutron up-scattering in the left wing of resonance peaks would increase neutron absorption rate, parameters such as multiplication factor (k_{inf} or k_{eff}) and Fuel Temperature Coefficient (FTC) and et al would be influenced also. This is the so-called neutron up-scattering effect (Ghrayeb et al. 2014; Mao and ZMIJAREVIC 2014). The effect can be taken into account by employing different models.

In Monte Carlo (MC) method, the free gas model is employed to consider the thermal agitation together with an assumption of non-resonant elastic scattering cross section at 0 K (X-5 Monte Carlo Team 2003). It is true for non-resonant nuclides, but not for heavy nuclides with elastic resonance peaks in the epithermal energy range (Ouisloumen and Sanchez 1991). For heavy nuclides, the thermal agitation and the resonance of elastic scattering should be considered simultaneously. Consequently, the modified $S(\alpha, \beta)$ method that prepares cross sections for different energies and scattering angles is extended to heavy nuclides (Dagan 2005; Rothenstein 2004). However, it is not easy to perform temperature interpolation on the $S(\alpha, \beta)$ tables. The Doppler Broadening Reject Correction (DBRC) method overcomes this defect by sampling the target velocity on-line which is statistically equivalent to the $S(\alpha, \beta)$ method (Becker et al. 2009). In addition, the Weight Correction (WC) method was developed to save the sampling time of the DBRC method (Lee et al. 2008; Mori and Nagaya 2009). But this method suffers from larger variance of the sampled angle-velocity pairs. Therefore this paper adopts the DBRC method to consider the neutron up-scattering effect.

In contrast, in deterministic methods, the up-scattering effect roots in the target-at-rest assumption during the solution of the neutron Slowing Down (SD) equation when generating the multi-group library by using the GROUPR module of the NJOY code (MacFarlane 2000). The SD solver solves neutron SD problems over a range of background cross sections and generates a Resonance Integral (RI) table for the following resonance treatment. The neutron up-scattering can be eliminated by introducing Doppler broadened scattering kernel into the SD function (ONO et al. 2012) or generate RI table by MC method with Doppler broadened scattering kernel (Lim et al. 2012). Conclusively, this model considers the neutron up-scattering effect through the absorption. The above theory and models are true for continuous energy or 69-group cases. However, it is not the case for refined energy groups. For energy group structures such as WIMS-69 groups, the lethargy widths are large enough to include the entire resonance peaks so that neutrons are up-scattered to the same group. The up-scattering effect mainly influences the multi-group transport calculation through self-shielded absorption cross sections. In contrast, for energy group structures such as 361-group Santamarina-Hfaiedh Energy Mesh (SHEM) (Hebert and Santamarina 2008), it is much more possible to divide a resonance peak into different energy groups. Thus neutrons may be up-scattered to another group. Therefore the transport calculation is influenced by both self-shielded absorption cross sections and the scattering matrix.

This paper generates the RI tables and scattering matrix by OpenMC (Romano and Forget 2013) which considers neutron up-scattering via the DBRC method. The 361-group SHEM is adopted and NJOY is used to generate other part of the multi-group library. This study is based on a lattice code NECP-CACTI (Li et al. 2015).

The self-shielding of cladding is neglected in old version of NECP-CACTI. However, recent studies revealed the resonance of Zr cannot be ignored in the cladding region (Choi et al. 2015). This paper generates the probability table of Zr for self-shielding calculation by subgroup method. The results show that the self-shielding of cladding affect k_{inf} 30~70 pcm.

The rest of the paper is organized as following. Section 2 detailed the theoretical models, while a series of numerical results are shown in Section 3. Section 4 summarizes the paper and is followed by our acknowledgements.

THEORY AND MODEL

1. Target-at-rest assumption in multi-group library

Multi-group approximation is made in deterministic methods and the effective multi-group cross sections are calculated by

$$\sigma_g = \frac{\int_g F(E)\sigma(E)\phi(E)\mathrm{d}E}{\int_g \phi(E)\mathrm{d}E} \tag{1}$$

where $\sigma(E)$ is cross section with respect to energy E, $\phi(E)$ is flux spectrum and $F(E)$ is the so-called feed function (MacFarlane 2000). A multi-group library has to contain at least total cross section, scattering matrix, absorption cross section, fission cross section, neutron production cross section and fission spectrum for each nuclide. For cross sections, the feed function is set to unity. For matrices, in contrast, the feed function is the l-th Legendre polynomial component of the normalized scattering probability from its initial energy E into secondary energy group g'. The flux spectrum is the typical flux spectrum in reactor in the fast and thermal energy ranges since they are weakly case dependent. In the resonance energy range, however, the flux spectrum is highly dependent on specific problem due to the self-shielding effect. Therefore, resonance integral table is prepared in the resonance energy range for the afterward self-shielding calculation. Resonance integral table is generated by solving the neutron slowing down problems with various background cross sections and temperatures.

In the epithermal energy range, target-at-rest assumption is adopted in two aspects of the multi-group library: the resonance integral table and the scattering matrix.

The neutron slowing down equation is

$$\begin{aligned}&\left[\sigma_0+\sigma_{t,2}(E)\right]\phi(E)\\ &=\int_E^{E/\alpha_1}\sigma_0 f_1(E'\to E)\phi(E')\mathrm{d}E'\\ &+\int_E^{E/\alpha_2}\sigma_{s,2}(E')f_2(E'\to E)\phi(E')\mathrm{d}E'\end{aligned} \tag{2}$$

where σ_0 is dilution cross section, $\sigma_{t,2}(E)$ is total cross section of resonant nuclide, $f(E'\to E)$ is scattering kernel, $\sigma_{s,2}(E')$ is scattering cross section of resonant nuclide, $\alpha=(A-1)^2/(A+1)^2$ and A is the mass ratio of the nuclide to the neutron. Assume that the target is at rest when colliding with neutron, the scattering kernel turns out to be

$$f(E'\to E)=\frac{1}{(1-\alpha)E'} \tag{3}$$

Eq. (3) is the so called asymptotic scattering kernel where only neutron down-scattering shows up. Eq. (2) is solved to obtain the flux spectrum to calculate the resonance integral. Therefore, the neutron up-scattering effect is ignored in the resonance integral table.

The feed function for scattering matrix is

$$F_{l,g'}(E)=\int_{g'}\mathrm{d}E'\int_{-1}^{1}\mathrm{d}\omega f(E\to E',\omega)P_l(\mu[\omega]) \tag{4}$$

where $f(E\to E',\omega)$ is the probability of scattering from E to E' through the cosine of the scattering angle in the center-of-mass coordinate. P_l is Legendre polynomial of order l. Integrating Eq. (4) over the secondary energy gives

$$F_{l,g'}(E)=\int f(E,\omega)P_l(\mu[\omega])\mathrm{d}\omega \tag{5}$$

where the scattering probability is given by

$$f(E,\omega)=\sum_l f_l(E)P_l(\omega) \tag{6}$$

The Legendre coefficients $f_l(E)$ are obtained from ENDF/B File 4. However, the File 4 can only provide the distribution for stationary free targets (Herman and Trkov 2010). Thus, the neutron up-scattering is ignored in generated scattering matrix.

2. Doppler Broadening Rejection Correction

Conventionally, the free gas model is used to consider the thermal agitation of nucleus in the epithermal energy range, where the "Sampling of the Velocity of the Target nucleus" (SVT) algorithm is adopted (X-5 Monte Carlo Team 2003). The Doppler broadened joint probability density function of the target velocity is

$$P(V,\mu\,|\,v_n)=\frac{\sigma_s(v_r,0)v_rP(V)}{2\sigma_s^{eff}(v_n,T)v_n} \tag{7}$$

where V is speed of target, μ is cosine of scattering angle, v_r is relative speed, T is temperature, $P(V)$ is Maxwell-Boltzmann distribution, $\sigma_s(v_r,0)$ is elastic scattering cross section at zero temperature, $\sigma_s^{eff}(v_n,T)$ is Doppler broadened elastic scatting cross section. In the standard SVT algorithm, the dependence of $\sigma_s(v_r,0)$ on v_r is ignored. This assumption is valid for light nucleus without resonance but not for heavy nucleus such as ^{238}U with elastic scattering resonance (Ouisloumen and Sanchez 1991).

The $S(\alpha, \beta)$ method (Dagan 2005), WC method (Lee et al. 2008; Mori and Nagaya 2009) and DBRC method (Becker et al. 2009) have been proposed to eliminate the assumption. The DBRC method is adopted in this paper. The probability density function can be written as

$$\begin{aligned}&P(V,\mu|v_n)\\ &=C'\left\{\frac{\sigma_s(v_r,0)}{\sigma_s^{\max}(v_\xi,0)}\right\}\left\{\frac{v_r}{v_n+V}\right\}\left\{P_1f_1(V)+P_2f_2(V)\right\}\end{aligned} \tag{8}$$

where

$$C' = \frac{\left(2+\sqrt{\pi}\beta v_n\right)\sigma_s^{\max}\left(v_\xi,0\right)}{2\sigma_s^{\text{eff}}\left(v_n,T\right)\sqrt{\pi}\beta v_n} \tag{9}$$

$$v_\xi \in \left[v_n - \frac{4}{\sqrt{\alpha}}, v_n + \frac{4}{\sqrt{\alpha}}\right] \tag{10}$$

$$\alpha = \frac{M_t}{2kT} \tag{11}$$

$$P_1 = \frac{1}{1+\frac{\sqrt{\pi}\beta v_n}{2}} \tag{12}$$

$$P_2 = 1 - P_1 \tag{13}$$

$$f_1\left(V\right) = 2\beta^4 V^3 e^{-\beta^2 V^2} \tag{14}$$

$$f_2\left(V\right) = \frac{4\beta^3}{\sqrt{\pi}} V^2 e^{-\beta^2 V^2} \tag{15}$$

$$\beta = \sqrt{\frac{AM_n}{2kT}} \tag{16}$$

$\sigma_s^{\max}\left(v_\xi,0\right)$ is the maximum value of elastic scattering cross sections within a range of the dimensionless speed given by Eq.(10). The target velocity is sampled from Eq.(8) with the additional rejection test $\frac{\sigma_s\left(v_r,0\right)}{\sigma_s^{\max}\left(v_\xi,0\right)}$.

The above algorithm is implemented in a MC code named OpenMC (Romano and Forget 2013) in the energy range of 0.4 eV to 210 eV.

3. Group structure and subgroup method

The 361-group SHEM (Hebert and Santamarina 2008) is an adaptation of the 281-group SHEM (Hfaiedh and Santamarina 2005) with refinement of resonance energy groups between 22.5 eV and 11.14 keV. The number of resonance energy groups is increased from 38 to 118 to avoid explicit representation of resonance interference and temperature gradients. Therefore the self-shielding model can be simplified. In this paper, the subgroup method with Narrow Resonance (NR) scattering model is employed for self-shielding calculation.

The subgroup method defines subgroups in magnitude of cross section and the energy range of a subgroup is shown in Figure 1. On each subgroup, the subgroup cross section and subgroup probability are defined as

$$\sigma_{x,g,i} = \frac{\int_{\Delta u_{g,i}} \sigma_x\left(u\right)\phi\left(u\right)\mathrm{d}u}{\int_{\Delta u_{g,i}} \phi\left(u\right)\mathrm{d}u} \tag{17}$$

$$p_{g,i} = \frac{\Delta u_{g,i}}{\Delta u_g} \tag{18}$$

where u is lethargy, $\sigma_x\left(u\right)$ is the "*x*" type cross section, $\phi\left(u\right)$ is the flux spectrum, Δu_g is lethargy width of group *g* and $\Delta u_{g,i}$ is lethargy width of subgroup *i* of group *g*. The subgroup cross section and subgroup probability are obtained by fitting procedure (Cao et al. 2011).

The neutron slowing down equation is

$$\Omega\nabla\phi\left(r,u,\Omega\right) + \Sigma_t\left(r,u\right)\phi\left(r,u,\Omega\right) = \frac{1}{4\pi}\int \mathrm{d}u'\Sigma_{s0}\left(r,u'\to u\right)\phi\left(r,u'\right) \tag{19}$$

where $\Sigma_t\left(r,u\right)$ is total cross section and $\Sigma_{s0}\left(r,u'\to u\right)$ is the zero-th Legendre moment of scattering cross section. Apply the NR approximation and the scattering source can be simplified

$$\Omega\nabla\phi_{g,i}\left(r,\Omega\right) + \Sigma_{t,g,i}\left(r\right)\phi_{g,i}\left(r,\Omega\right) = \Delta u_{g,i}\frac{1}{4\pi}\Sigma_p\left(r\right) \tag{20}$$

where $\Sigma_p\left(r\right)$ is potential scattering cross section.

The Eq. (20) is solved to obtain the subgroup flux $\phi_{g,i}\left(r,\Omega\right)$ and then the effective self-shielded cross sections are computed as

$$\sigma_{x,k,g}^{\text{eff}}\left(r\right) = \frac{\int_{4\pi}\sum_i \sigma_{x,k,g,i}\left(r\right)\phi_{g,i}\left(r,\Omega\right)\mathrm{d}\Omega}{\int_{4\pi}\sum_i \phi_{g,i}\left(r,\Omega\right)\mathrm{d}\Omega} \tag{21}$$

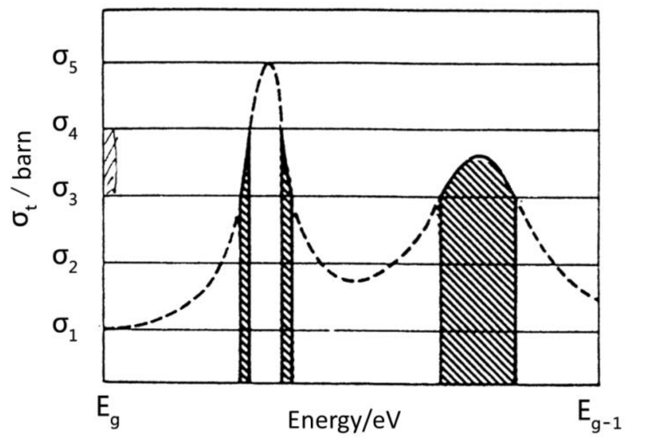

Figure 1. The energy range of subgroup

4. Correction for the 361-group SHEM

The resonance integral table is prepared by OpenMC with conventional SVT algorithm and DBRC algorithm. The physical probability table is generated by a fitting method based on the resonance integral table obtained by SVT algorithm. An up-scattering correction factor table is then prepared by

$$f_{g,k}\left(\sigma_b,T\right) = \frac{\sigma_{g,k}^{\text{DBRC}}\left(\sigma_b,T\right)}{\sigma_{g,k}^{\text{SVT}}\left(\sigma_b,T\right)} \tag{22}$$

where $\sigma_{g,k}^{\text{SVT}}\left(\sigma_b,T\right)$ and $\sigma_{g,k}^{\text{DBRC}}\left(\sigma_b,T\right)$ are self-shielded cross section at background cross section σ_b and temperature *T* with SVT algorithm and DBRC algorithm, respectively. After self-shielding calculation, the self-shielded cross section with SVT algorithm is obtained which is used to interpolate in the SVT resonance integral table to obtain the background cross section. Then the background cross section and the temperature of medium is used to interpolate in the correction factor table to obtain the corresponding correction factor. This factor is applied on the self-shielded cross section with SVT algorithm.

Because the neutron up-scattering effect becomes more significant with the increase in temperature as proved by previous studies (Ghrayeb et al. 2014; Zoia et al. 2013), the scattering matrices are obtained by OpenMC with SVT and DBRC below 212.11 eV (upper boundary of 100-th group in 361-group SHEM) at several temperature points. However, the multi-group library of NECP-CACTI is based on WIMS format which assumes that scattering matrix is independent of temperature in resonance and fast energy range. There is only one set of scattering matrix in the fast and resonance energy range at all temperature points. Therefore the library of NECP-CACTI is extended to incorporate this effect between 22.5 eV and 212.11 eV in 361-group SHEM.

NUMERICAL RESULTS

The ACE format library for OpenMC and the multi-group library for NECP-CACTI are both based on combined ENDF/B- Ⅵ .8 and ENDF/B- Ⅶ .0. The self-shielding method of NECP-CACTI is subgroup method is based on NR scattering model and its transport solver is a modular Method of Characteristics (MOC) (Li et al. 2015). The self-shielding of cladding is studied firstly to eliminate errors other than neutron up-scattering effect. The Mosteller Doppler defect benchmark (Mosteller 2006) is used to verify the correction method.

1. Self-shielding of cladding

Self-shielding of cladding is ignored in old version of NECP-CACTI. However, the resonance of total cross section is explicit in the energy range between 1E-4 MeV and 0.1 MeV as shown in Figure 2. The cross section in this energy range is given at a dilution of 800 barn. In this paper, the resonance of Zr is explicitly represented by the subgroup method. The UO_2 pin cell problems of Mosteller benchmark are calculated by NECP-CACTI and OpenMC which provides the reference results. The neutron up-scattering effect is not considered in these calculations. For the 5% enriched UO_2 pin cell problem at Hot Zero Power (HZP) condition, the errors of self-shielded cross sections with and without self-shielding calculation are shown in Figure 3. It can be found that the errors of self-shielded cross section are -20% at most. On the contrary, the errors are within 5% if Zr resonance is represented by subgroup method. The k_{inf} errors of UO_2 pin cell problems at Hot Full Power (HFP) of Mosteller benchmark with and without self-shielding calculation of cladding are compared in Table 1. The NECP-CACTI code predicts k_{inf} within 100 pcm of errors with self-shielding calculation of Zr. The resonance of Zr affects k_{inf} 30~70 pcm.

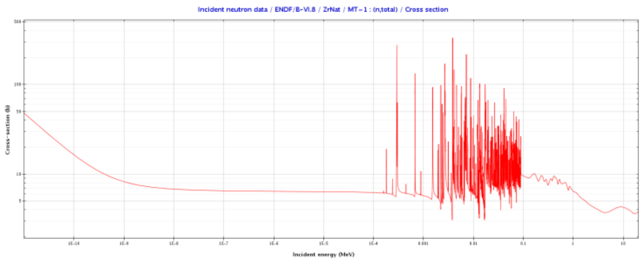

Figure 2. Continuous total cross section of Zr-natrual

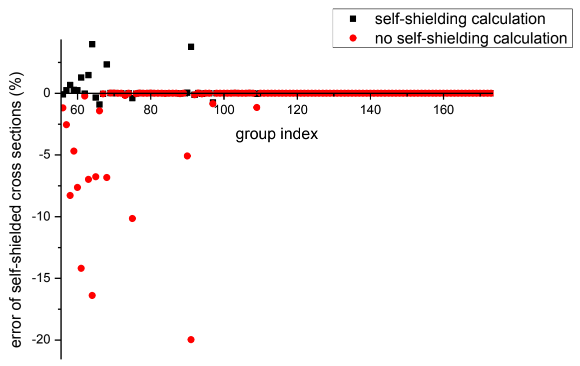

Figure 3. Self-shielded cross section errors of Zr-natural with and without self-shielding calculation

Table 1 k_{inf} errors of UO_2 pin cell problems of Mosteller benchmark at HFP condition with and without self-shielding calculation of Zr

Enrich--ment/ %	Error of NECP-CACTI/pcm	
	no self-shielding calculation of cladding	self-shielding calculation of cladding
0.771	124	91
1.6	106	57
2.4	97	40
3.1	91	30
3.9	66	2
4.5	59	-6
5	47	-20

2. Resonance up-scattering effect

Different neutron up-scattering correction schemes are compared. Scheme 1 only corrects the self-shielded cross sections by the up-scattering correction factor. Scheme 2 both corrects the self-shielded cross sections and scattering matrices. Scheme 3 only corrects the scattering matrix. All schemes consider self-shielding of cladding. Figure 4 and Figure 5 summarize the influence of neutron up-scattering effect on k_{inf} by scheme 1, scheme 2 and scheme 3 at HZP and HFP, respectively.

The results show that for 361-group SHEM, the neutron up-scattering effect influence criticality calculation mainly via scattering matrices rather than the self-shielded cross sections. With only self-shielded cross section correction, the k_{inf} is slightly influenced. Because the 361-group SHEM refines the energy groups to explicitly represent the correlated slowing down effects, resonance interference effect and temperature gradient effect. The first three resonance peaks of ^{238}U, which contribute most to the neutron up-scattering effect, are divided into several energy groups. Therefore, flux spectrum and self-shielded cross sections will not change much due to neutron up-scattering. However, neutron may up-scattered to another energy group if neutron up-scattering is considered. The neutron up-scattering affects k_{inf} 40~80 pcm at HZP condition and 100~200 pcm at HFP condition as shown in Figure 4 and Figure 5.

The Fuel Temperature Coefficient (FTC) is calculated by

$$\mathrm{FTC}=\left(\frac{1}{k_{\mathrm{HZP}}}-\frac{1}{k_{\mathrm{HFP}}}\right)\frac{1\times10^{5}}{\Delta T} \tag{23}$$

Figure 6 summarizes the influence of neutron up-scattering on FTC calculation. The neutron up-scattering is considered through both self-shielded cross sections and scattering matrices. As the thermal agitation of target becomes fiercer with increase in temperature, the up-scattering effect becomes more explicit. Therefore FTCs are 12~13% more negative with neutron up-scattering correction.

When both the self-shielding of cladding and neutron up-scattering effect are considered, the errors of k_{inf} calculated by NECP-CACTI compared with OpenMC are summarized in Figure 7 and Figure 8. Both codes consider these two effects in the calculations. It's shown that NECP-CACTI code predicts k_{inf} within 100 pcm of errors.

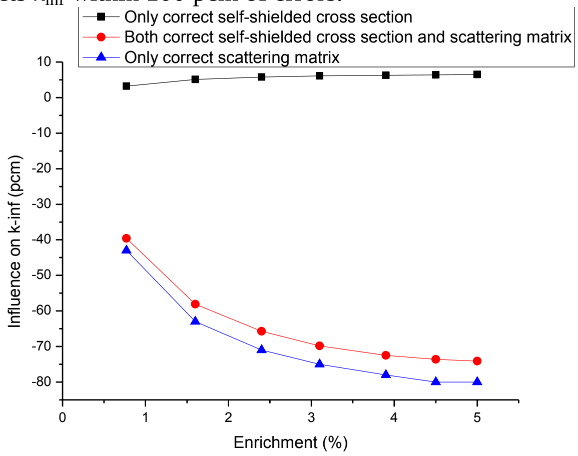

Figure 4. Influence of neutron up-scattering on k_{inf} of UO_2 pin cell problems at HZP with different correction schemes

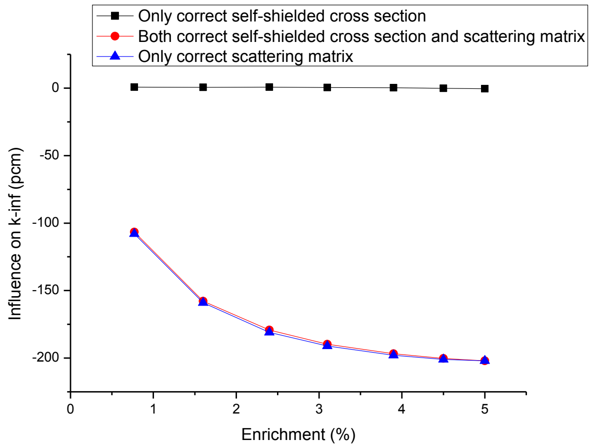

Figure 5. Influence of neutron up-scattering on k_{inf} of UO_2 pin cell problems at HFP with different correction schemes

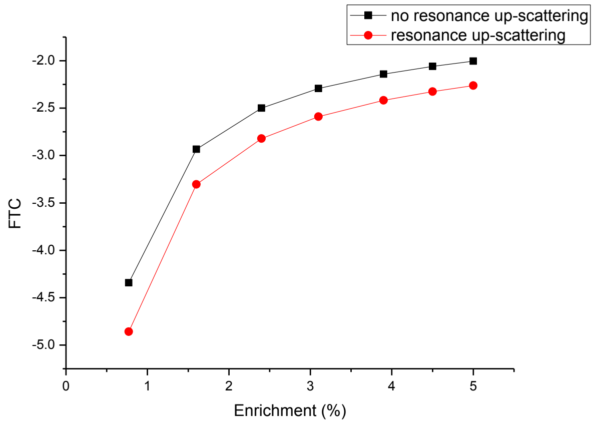

Figure 6. Influence of neutron up-scattering effect on FTC

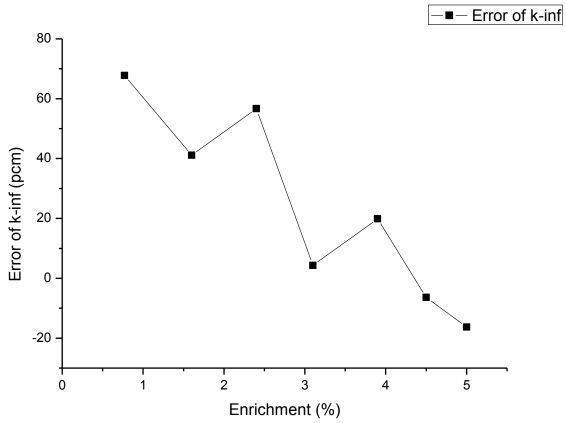

Figure 7. Error of k_{inf} of UO_2 pin cell problems at HZP

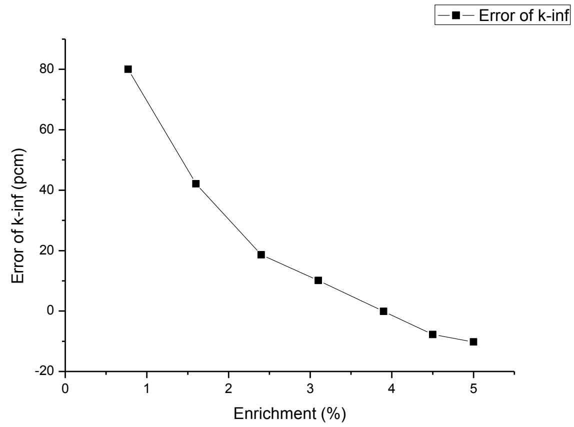

Figure 8. Error of k_{inf} of UO_2 pin cell problems at HFP

CONCLUSIONS

The neutron up-scattering effect and self-shielding effect of cladding are studied. The DBRC method is implemented in MC code OpenMC to considering both the thermal agitation of target and resonance elastic cross sections. The modified OpenMC is used to prepare neutron up-scattering correction factor table and scattering matrices in the multi-group library of lattice code NECP-CACTI. Numerical results have shown that the neutron up-scattering affect criticality calculation mainly through scattering matrices rather than self-shielded cross sections for 361-group SHEM. This effect influence k_{inf} 200 pcm at most for LWR pin cell problems at HFP. The FTC is 12~13% more negative when the neutron up-scattering is considered. Besides, the self-shielding of cladding is studied based on the subgroup method in NECP-CACTI. It's found that self-shielding of cladding affects k_{inf} 30~70 pcm. When these two effects are considered, NECP-CACTI predicts k_{inf} within 100 pcm of errors compared to OpenMC.

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