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On the Fly Doppler Broadening Using Multipole Representation

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1. Introduction

Monte Carlo Simulation allows to design and make analyses of different nuclear reactors in terms of neutron physics. By coupling neutron physics and thermo-hydraulics codes, it is possible to obtain thermo-hydraulic feedback, which currently requires pre-generated cross section data at 10-50 K interval. On the Fly Doppler broadening is the technique to avoid pre-generation of the microscopic cross section, in other words, reduce the amount of storage. Currently, there are different types of formalisms used by NJOY code to generate reaction cross section and accomplish its Doppler broadening. [1] Single-Level Breit-Wigner (SLBW) formalism is limited to well-separated resonances, in other words, it does not consider interference between energy levels. Multi-Level Breit-Wigner formalism (MLBW) was tested as the candidate for the cross section generation in the Monte Carlo code, which is under development in UNIST. According to the results, MLBW method requires huge amount of computational time to produce cross section at certain energy point. [2] Reich-Moore (RM) technique can generate only 0K cross section, which means that it cannot produce broaden cross section directly from resonance parameters. Adler-Adler formalism is used only for s-wave resonances, but most nuclides of the great interest has higher angular momentum states.

In this paper, Multipole representation (MPR) proposed by Dr. Hwang is used as the cross section generation formalism, which allows to apply Doppler broadening using Faddeeva function. This method requires conversion of resonance parameters from nuclear data files to corresponding poles and residues.

2. Methods and Results

In this section multipole representation, conversion of resonance parameters into multipoles, Doppler broadening method, and Hoogenboom benchmark problem specifications are described.

2.1 Multipole Representation

Multipole representation is the alternative to the conventional R-Matrix theory to describe the microscopic cross sections of different nuclides in the resolved resonance region. It is the generalization of rationale suggested by Saussure and Perez, which was limited only to s-wave resonances. Dr. Hwang extended this concept for the higher angular momentums. [3] This formalism is based on the physical condition that collision matrix is single valued and meromorphic in the momentum space. Eqs. (1), (2), and (3) show radiative capture and fission, total, and elastic scattering reaction microscopic cross sections, respectively, in terms of multipole resonance parameters.

$$\sigma_{x=\gamma,f} = \frac{1}{E}\sum_{l,J}\sum_{\lambda}^{N}\sum_{j=1}^{2(l+1)} \mathrm{Re}\left[\frac{\left(-iR_{l,J,\lambda,j}^{(x)}\right)}{p_{l,J,\lambda,j}^{*}-\sqrt{E}}\right], \quad (1)$$

$$\sigma_{t} = \frac{1}{E}\sum_{l,J}\sum_{\lambda}^{N}\sum_{j=1}^{2(l+1)} \mathrm{Re}\left[\frac{\left(-ie^{-i2\phi}R_{l,J,\lambda,j}^{(t)}\right)}{p_{l,J,\lambda,j}^{*}-\sqrt{E}}\right], \quad (2)$$

$$\sigma_{s} = \sigma_{t} - \sigma_{f} - \sigma_{\gamma}, \quad (3)$$

where l, J are relative orbital angular momentum and total spin; λ, N are resonance index and total number of resonances; $R_{l,J,\lambda,j}^{(x)}, p_{l,J,\lambda,j}^{*}, E$ are residue corresponding to the reaction x, complex conjugate of the resonance pole, and energy, respectively.

2.2 Conversion of parameters

The first step to perform multipole representation is generation of poles and residues using resonance parameters, which are given in the nuclear data files. [4] In addition, energy domain should be converted to momentum domain, where the physical condition is satisfied. Currently, in order to construct resolved resonance region cross section there are used two main formalism: MLBW and RM. Therefore, for the each of those methods there are different formats of the given resonance parameters in the nuclear data file. Conversion of parameters for MLBW and RM is different, since different assumptions are done for both methods.

In case of the Single- and Multi-Level Breit-Wigner formalisms, R matrix is represented in terms of the level matrix $A_{\lambda}^{(l)}$ approximations. As it was mentioned, SLBW can be applied only to the well-separated resonances, because level matrix is assumed to consist of the single element. In contrast, in MLBW technique level matrix is assumed to be diagonal matrix, which allows to consider interference between the energy levels of the given (l, J) -state. Hence, there is an interference microscopic cross section term, which is shown in Eqs. (4) and (5).

$$\sigma_{t}^{MLBW} = \sigma_{t}^{SLBW} + \sigma_{\mathrm{int}}, \quad (4)$$

$$\sigma_{\text{int}} = \sum_{l,J} \frac{\pi}{k^2} g_J \,\text{Re}\left\{ \sum_{\lambda}^{N} \sum_{\substack{\mu=1 \\ \mu \neq \lambda}}^{N} \frac{\Gamma_{\lambda n}^{(l)}(u)\Gamma_{\mu n}^{(l)}(u)}{A_{\lambda}(u)A_{\mu}^{*}(u)} \right\}, \qquad (5)$$

where $k = k_0\sqrt{E} = 2.196771\times10^{3} \times \frac{A}{A+1} \times \sqrt{E}$ is wave number in the center-of-mass system; A is the ratio of the particular isotope`s mass to that of a neutron; $u = \sqrt{E}$; g_J is statistical spin factor; $\Gamma_{\lambda n}^{(l)}(u) = \Gamma_{\lambda n} \frac{P_0(u)}{P_0(|E_\lambda|)}$ is the neutron width and $\Gamma_{\lambda n}$ is the neutron width at resonance energy.

In order to find out the resonance poles, it is required to solve the polynomial given in Eq. (6).

$$q_l(u)A_{\lambda}^{(l)}(u) = \sum_{m=0}^{2(l+1)} a_{\lambda,m}^{(l)} u^m = 0 \ , \qquad (6)$$

where $a_{\lambda,m}^{(l)}$ is a polynomial coefficient and $q_l(u)$ is a function defined in Table I.

Eqs. (7) and (8) show level matrix and level shift, respectively.

$$A_{\lambda}^{(l)}(u) = \left[E_\lambda + \Delta_{\lambda}^{l}(u) - (u)^2 \right] - \frac{i}{2}\left[\Gamma_{\lambda n}^{(l)}(u) + \Gamma_{\lambda\gamma} + \Gamma_{\lambda f} \right] , \qquad (7)$$

$$\Delta_{\lambda}^{l}(u) = \Gamma_{\lambda n} \frac{S_l(|E_\lambda|) - S_l(|u|)}{2P_l(|u|)} \ . \qquad (8)$$

where $E_\lambda, \Gamma_{\lambda\gamma}, \Gamma_{\lambda f}$ are resonance energy, capture width, and fission width; $S_l(u), P_l(u)$ are shift and penetration factors, respectively, which are shown in Table II.

Table I: The l - dependent Functions

Angular momentum	s_l	q_l	ϕ_l
0	0	1	ρ
1	1	$1+\rho^2$	$\rho - \tan^{-1}(\rho)$
2	$18+3\rho^2$	$9+3\rho^2+\rho^4$	$\rho - \tan^{-1}\left(\frac{3\rho}{3-\rho^2}\right)$

It can be seen from Eq. (6) that in case of orbital angular momentum l there is polynomial of order $2(l+1)$.

$$\rho = \rho_0 \times u = (k_0 a) \times u = \left(2.196771\times10^{3} \times \frac{A}{A+1} \times a \right) \times u \ , (9)$$

where a is interaction radius (channel radius).

Table II: Shift and Penetration Factors

Angular momentum	Shift Factor	Penetration Factor
0	0	ρ
1	$-\frac{1}{1+\rho^2}$	$\frac{\rho^3}{1+\rho^2}$
2	$-\frac{18+3\rho^2}{9+3\rho^2+\rho^4}$	$\frac{\rho^5}{9+3\rho^2+\rho^4}$

By using Eq. (6) and definition of the level matrix with respect to the formalism type it is possible to find out the coefficients of the polynomial. In this study, polynomial solver based on Laguerre`s method was used in order to calculate poles. Table III show poles of the s-wave resonance at energy 2810 eV for ^{23}Na:

Table III: ^{23}Na poles for $l=0, J=1$ (ENDF/B-VII.1)

Energy (eV)	$\text{Re}(p^*)$	$\text{Im}(p^*)$
2.810E+03	5.2979765E+01	1.7749350E+00
2.810E+03	-5.2979765E+01	1.7716036E+00

After finding the poles, it is possible to calculate residues with respect to every cross section type such as total, capture, fission, and interference. Eqs. (10), (11), and (12) show derived reaction residues.

$$R_{l,J,\lambda,j}^{(t)} = \frac{2\pi}{k_0^2} g_J \times \frac{q_l(p_{l,J,\lambda,j}^{*}) \times \Gamma_{\lambda n}^{(l)}(p_{l,J,\lambda,j}^{*})}{-\rho_0^{2l} \prod_{\substack{k=1 \\ k\neq j}}^{2(l+1)} (p_{l,J,\lambda,j}^{*} - p_{l,J,\lambda,k}^{*})} \ , \qquad (10)$$

$$R_{l,J,\lambda,j}^{(x=\gamma,f)} = R_{l,J,\lambda,j}^{(t)} \times \frac{\Gamma_{\lambda n}}{\Gamma_{\lambda n}^{(l)}(p_{l,J,\lambda,j}^{*}) + \Gamma_{\gamma n} + \Gamma_{fn}} \ , \qquad (11)$$

$$R_{l,J,\lambda,j}^{(\text{int})} = R_{l,J,\lambda,j}^{(t)} \times i\left[\sum_{\substack{\mu=1 \\ \mu\neq\lambda}}^{N} \frac{\Gamma_{\mu n}^{(l)}(p_{l,J,\lambda,j}^{*})}{A_{\mu}^{r}(p_{l,J,\lambda,j}^{*}) + iA_{\mu}^{i}(p_{l,J,\lambda,j}^{*})} \right] . (12)$$

2.3 Doppler broadening

There are different ways of performing Doppler broadening. In case of the most nuclides of great interest NJOY code pre-generate 0K cross section using RECONR module, which further is broadened by different module, called BROADR.

On the other hand, MPR allows to produce cross section at certain temperature directly from resonance poles and residues, which are generated as shown in previous section. Doppler-Broadened line-shape functions are used to modify cross section with respect to the temperature, while MPR is generating it. [5] It is based on the Faddeeva function as shown in Eq. (13).

$$W(z) = \frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}dt}{z-t}\ , \qquad (13)$$

where z is the complex variable.

2.4 Hoogenboom benchmark

Benchmark specifications: pin cell dimension 1.26 cm, fuel pin outer radius 0.41 cm, and cladding outer radius 0.475 cm; fuel is UOX, which consist of 16 fission products and oxygen, cladding is made of natural zirconium. Additionally, there is no gap in between fuel and cladding. Borated water is taken as moderator with concentration satisfying reactor to be near criticality. [6]

This problem was simulated using Monte Carlo code, which is under development in UNIST. There were used 10 inactive, 1000 active cycles, and 10000 neutron histories. The given problem was computed using 16 cores and the multiplication factor and computational time results are given in the following section.

3. Results

After implementation of the on-the-fly Doppler broadening module into MCS for the resolved resonance region (RRR), there was tested Hoogenboom benchmark pin cell problem. This module was applied only for U^{238} isotope for energy above 4.4eV and up to 20keV, the upper limit of the RRR. In order to perform this calculation nuclear data from MC^2-3 code was used, since in this transport code RM formalism is substituted by multipole representation method. [7]

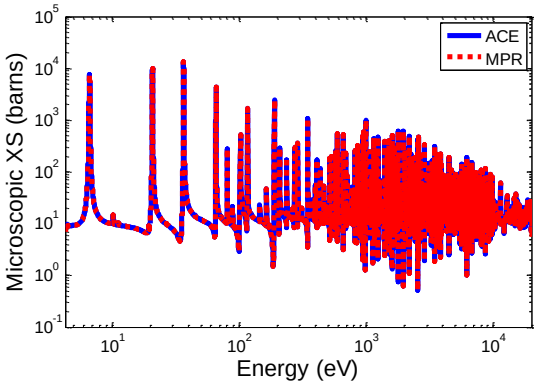

Fig.1. ACE format and MPR generated total reaction cross sections of the U^{238} at temperature 293.6 K.

Fig.2. shows that the U^{238} ACE format and MPR generated total reaction cross sections have maximum relative difference smaller than 1%, for the given energy region.

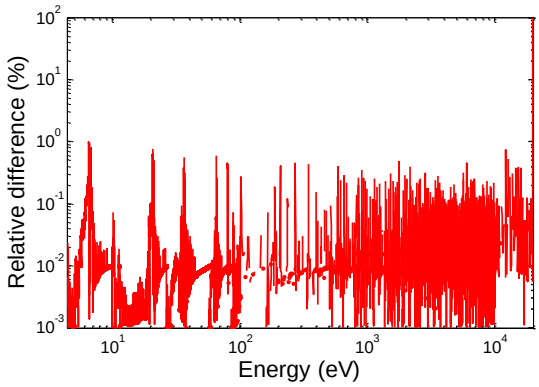

Fig.2. Absolute relative difference (%) between ACE format and MPR generated total cross sections.

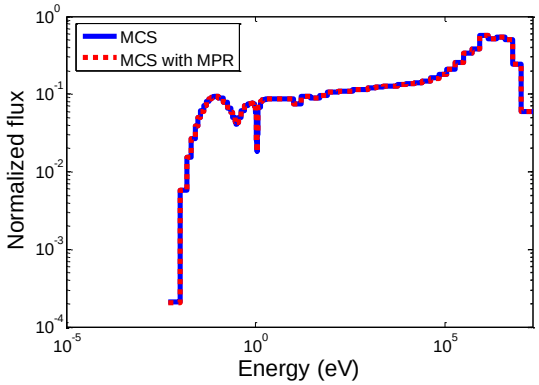

Fig.3. Fuel region energy spectrum generated by original MCS, and MPR implemented MCS.

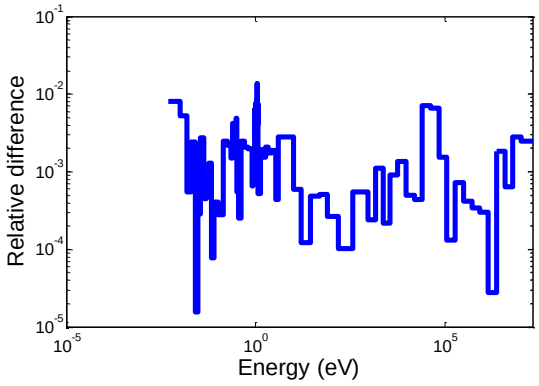

Fig.4. Absolute relative difference of the energy spectrums generated by original MCS, and MPR implemented MCS.

In Figs. 3 to 4, energy spectrums and absolute relative difference are shown. The maximum relative difference of energy spectrum is around 1%.

According to the results of the simulations, k-eff values for reference and MPR applied MCS show good agreement.

Table IV: Multiplication Factor Comparison

	k-eff (STD)	Time Ratio
MCS	1.01942 (0.00020)	1
MCS with MPR	1.01887 (0.00021)	20

From Table IV, there can be seen multiplication factor difference of 55 pcm, and the relative time ratio. Application of the MPR as the part of on-the-fly Doppler Broadening module, caused increase in computational time.

4. Conclusions

Multipole representation and Doppler-broadened line shape functions were used to construct microscopic cross section of ^{238}U at different temperatures. The first step was to convert resonance parameters given in nuclear data file into multipoles.

MPR shows very high potential to be used as the formalism in the on-the-fly Doppler broadening module of MCS. One of the main reasons is that comparison of the time cost shown in Table IV supports application of multipole representation.

Further improvements in terms of computational time decrease, and cross section accuracy can be achieved through implementation of the energy window concept and more detailed studies of the conversion of resonance parameters.

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