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THE CALCULATION OF RESONANCE PARAMETERS FOR THE DECART MOC CODE

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ABSTRACT

Accurate resonance parameters can be as important as the multi-group neutron cross sections themselves in the overall accuracy of a multigroup library. The work here describes the generation of resonance parameters for the MOC DeCART which utilizes the subgroup method for its resonance treatment. In this paper, we first introduce a procedure for determining the intermediate resonance parameters for all scattering isotopes, also know as lambda parameters or Goldstein-Cohen parameters which are used in the subgroup method. The lambda factors of scattering isotopes are determined as hydrogen equivalence factors by comparing group average cross sections in the mixture of resonance isotope and hydrogen with the average cross sections in mixtures with the hydrogen which is partly replaced by other isotopes. The NJOY code is used for the calculation of spectra in these mixtures. In addition to U-238, which was used as resonance isotope in previous work on lambda factors, U-235 is also treated as a resonance isotope in the lambda calculation developed here which thus provides lambdas for the groups in which U-238 has no significant resonance. After developing a procedure for generating lambda factors for scattering isotopes, a method is then described for generating subgroup parameters. Again NJOY is used for resonance calculations of a set of mixtures for each resonance isotope at each selected temperature. The group average cross sections instead of the resonance integrals of these mixtures are used to generate subgroup parameters using an optimization algorithm. The generated library is then verified by comparing the solution from DeCART with the solution from MCNP.

Key Words: lambda factor, Goldstein-Cohen parameter, intermediate resonance approximation, subgroup method, subgroup parameters, optimization

1. INTRODUCTION

DeCART (Deterministic Core Analysis based on Ray Tracing)[1], is a 3-dimensional whole core neutron transport code developed as part of an International Nuclear Energy Research Initiative (INERI) project. Currently DeCART is employed within the framework of the Numerical

Nuclear Reactor to perform coupled 3D neutron transport and CFD for practical reactor applications [2]. The objective of the work here is to build a procedure for generating a multi-group neutron cross section library for DeCART directly from basic nuclear data file, such as ENDF. This will provide the capability to generate a multi-group neutron cross section library from the most recent basic nuclear data files and to select suitable group structures for reactors which have neutron spectral significantly different from normal light water reactors.

The subgroup method [3,4,5,6] is used for the resonance treatment in DeCART. In the subgroup method, the group average absorption cross section of each resonance isotope is expressed as

$$\sigma_a = \frac{\sum_n w_n \sigma_n \phi_n}{\sum_n w_n \phi_n + \left(1 - \sum_n w_n\right)\phi_0}, \tag{1}$$

where σ_n and w_n are subgroup level and it's associated weight, which can be determined by optimization while generating a multigroup cross section library with pre-computed resonance integrals. In Eq.(1) ϕ_n is the loss free neutron flux for subgroup level σ_n, and ϕ_0 is the loss free flux between resonances, It is set to 1 hereafter to represent standard 1/E spectrum.

The intermediate resonance parameters or lambda factors, which are also known as Goldstein-Cohen parameters [7] are used for calculating loss free fluxes which are required to determine the subgroup levels and weights for preparing multigroup cross section libraries as well as determining group average cross section of the resonance isotopes with Eqn. (1) in the DeCART calculation. Therefore lambda factors must be generated while determining the multigroup cross section library and then stored in this library along with the multigroup cross sections.

The objective of this work was to use NJOY [8] to calculate the lambda factors and subgroup parameters from any version of ENDF. In section 2, the procedure of generating lambda factors is introduced; in section 3, the method for obtaining subgroup parameters is discussed; and in section 4, the library is validated by comparing DeCART solutions with MCNP solutions. Summary and conclusions are provided in section 4.

2. LAMBDA FACTOR

In this section, the procedure of generating lambda factors is introduced. In subsection 2.1, the algorithm used to determine lambda factor is introduced and in subsection 2.2, the NJOY flux calculator is validated for the resonance integral calculation in an infinite homogenous mixture by comparisons with the MCNP results. An investigation is then performed on the dependences of the lambda factors on three parameters: 1) the temperature of the resonance isotopes, 2) the background cross section, and 3) the fraction of the background cross section from non-hydrogen isotopes. A typical PWR cell is simulated with MCNP to determine the range of applicability of the background cross section for PWR applications. Suitable parameters are then selected for

generating lambda factors for all isotopes as a standard procedure and the results are compared with those in the HELIOS library [11].

2.1 Method for Obtaining Lambda Factor

The intermediate resonance (IR) approximation is based on the traditional narrow (NR) and narrow resonance infinite mass (NRIM) approximations. In the NR approximation, the resonances are considered so narrow such that all neutrons which have energy within range of a resonance and have scattering reactions will lose enough energy to be scattered out of the resonance range. In the NRIM approximation, the resonances are considered as narrow resonances for light scattering isotopes only, the heavy isotopes are assumed to have infinite mass such that the neutron scattering with heavy isotopes will not lose any energy. In the IR approximation, when neutrons within a resonance scatter with a isotope *i*, only a fraction, λ_i, of these neutrons will be scattered out of the resonance range, and the remaining fraction, $1-\lambda_i$, of neutrons are assumed not to lose any energy. The parameter λ_i is called the intermediate resonance (IR) parameter of isotope *i*.

With the IR approximation and with the assumption of constant potential (scattering) cross section, the loss free neutron flux $\phi(u)$ which is defined as the true neutron flux $\psi(u)$ divided by resonance escape probability $p(u)$, can be expressed as

$$\phi(u) = \frac{\sigma_b}{\sigma_a(u) + \sigma_b}, \tag{2}$$

where u is the standard definition of lethargy.

The background cross section σ_b is defined as

$$\sigma_b = \lambda_R \sigma_p^R + \frac{1}{N_R} \sum_{i \neq R} \lambda_i N_i \sigma_p^i + \frac{\Sigma_e}{N_R}, \tag{3}$$

where N_i, σ_p^i, and λ_i are the nuclide density, the potential cross section and the IR parameter of isotope *i*, and *R* represents the resonance isotope. The parameter Σ_e is the escape cross section which is used to treat slowing down in the moderator region which does not contain resonance isotopes.

In equation (2), the dependence of the loss free spectrum on lethargy is solely dependent on the absorption cross section at the current lethargy point, so that the loss free neutron flux for a subgroup level can be expressed as,

$$\phi_n = \frac{\sigma_b}{\sigma_n + \sigma_b}. \tag{4}$$

From the definition of the IR parameter, the lambda factor depends on the width of the resonance and the average energy loss due to a single scattering reaction which is related to atomic weight of the scattering isotopes. In practice, all resonances are considered as narrow resonances for Hydrogen, so the lambda factor of Hydrogen is one. The lambda factors of non-hydrogen scattering isotopes have been obtained by comparing solutions in resonance isotope and hydrogen mixtures with mixtures with the hydrogen partly replaced by other isotopes. This transforms λ into a hydrogen-equivalence factor.

Since U-238 is by far the most predominant resonance absorber in most reactors, λ values with respect to U-238 are used for all other resonance isotopes in most of the resonance energy range. As the resonance width varies from one resonance to another, normally the resonances at lower energy regions are wider than these at higher energies. The DeCART library stores lambdas for each resonance groups and the lower energy limits of resonance groups in 47 groups library are listed in Table I.

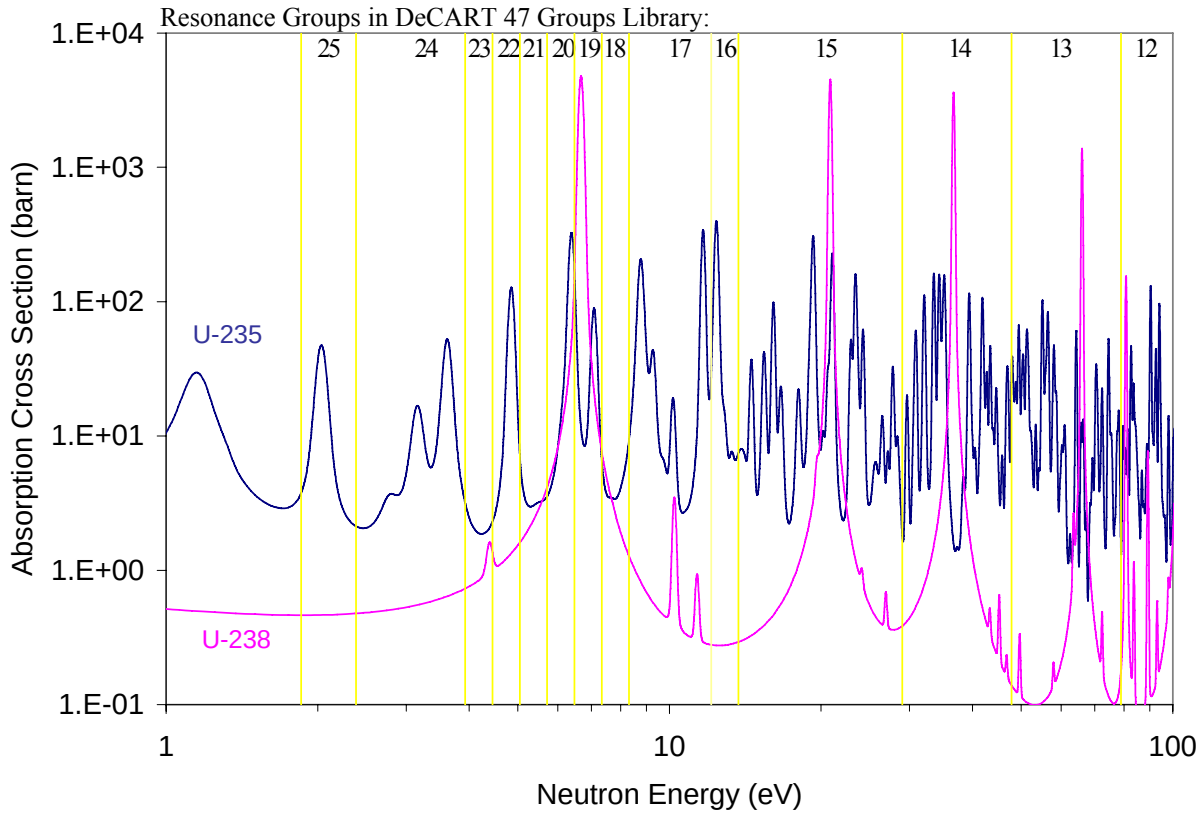

Figure 1. U-238 and U-235 resonances at 800K.

The U-238 and U-235 resonances at 800K are shown in Figure 1 where it is apparent that U-238 has no resonance in groups 16, 24, and 25, whereas U-235 does have resonances in these groups. As U-235 is often the second most important resonance isotopes in most nuclear reactor, λ values with respect to U-235 are used for the resonance groups in which U-238 has no resonance.

Table I. Lower energy limits of resonance groups in the DeCART 47 groups library

Resonance group	lower energy limit (eV)	Resonance group	Lower energy limit (eV)	Resonance group	lower energy limit (eV)
	9118.8027	15	13.71	21	5.043477
10	2034.6989	16	12.09903	22	4.450895
11	130.07040	17	8.315288	23	3.927901
12	78.89325	18	7.338215	24	2.382392
13	47.85117	19	6.476014	25	1.855391
14	29.02293	20	5.715008		

The procedure used to calculate lambda factors with respect to U-238 is as follows:

1) Calculate a set of spectra with NJOY for infinite homogenous U-238/H mixtures with various density ratio $N_R : N_H^j$ to obtain the absorption cross section tables, $\sigma_{a,g}^{tab}(\sigma_0^j)$, for each resonance group with respect to σ_0 which is defined as

$$\sigma_0 = \frac{1}{N_R}\sum_{i \neq R} N_i \sigma_p^i \,. \tag{5}$$

For the table entry,

$$\sigma_0^j = \frac{N_H^j}{N_R}\sigma_p^H \,. \tag{6}$$

2) For non-hydrogen scattering isotope-*i*, calculate the spectrum with NJOY for infinite homogenous U-238/H/istope-*i* mixtures with density ratio $N_R : N_H : N_i$ to obtain the absorption cross section $\sigma_{a,g}$ for each resonance group.
3) For each resonance group, determine the equivalent $\sigma_{0,g}^{equ}$ by interpolation

$$\sigma_{0,g}^{equ} = \frac{\sigma_{a,g} - \sigma_{a,g}^{tab}(\sigma_0^{j1})}{\sigma_{a,g}^{tab}(\sigma_0^{j2}) - \sigma_{a,g}^{tab}(\sigma_0^{j1})}\sigma_0^{j2} + \frac{\sigma_{a,g} - \sigma_{a,g}^{tab}(\sigma_0^{j2})}{\sigma_{a,g}^{tab}(\sigma_0^{j1}) - \sigma_{a,g}^{tab}(\sigma_0^{j2})}\sigma_0^{j1}, \tag{7}$$

Where σ_0^{j1} and σ_0^{j2} are the two values which have $\sigma_{a,g}^{tab}$ closest to $\sigma_{a,g}$

4) The group *g* lambda for isotop-*i* is then determined as

$$\lambda_{i,g} = \frac{N_R \sigma_{0,g}^{equ} - N_H \sigma_p^H}{N_i \sigma_p^i}, \quad (8)$$

The same procedure can then be applied to calculate lambda factors with respect to other resonance isotopes such as U-235.

2.2 Lambda Factor Calculation with NJOY

Before calculating the lambda factor, the NJOY flux calculator was validated for the resonance integral calculation in an infinite homogenous mixture by comparisons with the MCNP [10] results. Both the NJOY flux calculation and the MCNP calculation use cross section libraries from ENDF/B5 release 8. The reason for selecting ENDF/B5 release 8 instead of most recent ENDF is to provide a consistent comparison with the lambda values in HELIOS library.

Pointwise ENDF (PENDF) were first prepared with the NJOY modules RECONR and BROADR, then the same PENDF were used as input for generating MCNP libraries with the NJOY module ACER and for the NJOY flux calculator in the module GROUPR. Since the scattering isotopes are assumed to have constant potential cross sections, cross section of pseudo-isotopes which contains only constant potential cross sections are also generated for the scattering isotopes in MCNP. For example, the pseudo-hydrogen has constant potential cross sections 20 barn and all other types of cross section are zero.

Table II. Comparison of the average absorption cross sections of U-238 in resonance groups in U-238/H mixture at 800K with $\sigma_0 = 30$ from NJOY and MCNP

Resonance Group	Absorption cross section (barn)		Difference (%)
	NJOY	MCNP	
10	0.78597	0.78935	0.43%
11	1.29657	1.29491	-0.13%
12	2.93175	2.92647	-0.18%
13	1.74240	1.73803	-0.25%
14	4.37252	4.36432	-0.19%
15	3.83435	3.80761	-0.70%
16	0.27975	0.27975	0.00%
17	0.70461	0.70439	-0.03%
18	3.05899	3.05877	-0.01%
19	64.50724	64.65649	0.23%
20	14.88301	14.90176	0.13%
21	2.51127	2.51100	-0.01%
22	1.26796	1.26801	0.00%
23	0.98723	0.98718	0.00%
24	0.55831	0.55815	-0.03%
25	0.46744	0.46751	0.01%

The slowing down spectrum in an infinite homogenous U-238/H mixture at temperature 800K with ratio $N_R : N_H = 1:1.5$, which led to $\sigma_0 = 30$, was calculated by the NJOY flux calculator and MCNP. The average absorption cross sections of U-238 in the resonance groups are compared in Table II. The differences of average absorption cross section are within 1%. These results indicate NJOY flux calculator predicts very accurately the slowing down spectrum in infinite homogenous mixtures.

The dependencies of the lambda factors on temperature of resonance isotopes, the background cross sections, and the fraction of background cross sections from non-hydrogen isotopes were then investigated with the NJOY flux calculator. The spectra of a U-238/H mixture at 300K and 800K with various ratios were calculated with NJOY and all average absorption cross sections of U-238 at resonance groups were condensed. Figure 2 shows the 19th group absorption cross sections which depends on σ_0. The lambdas for O-16 are then calculated with the procedure described in section 2. The lambda values for group 19 are given in Table III.

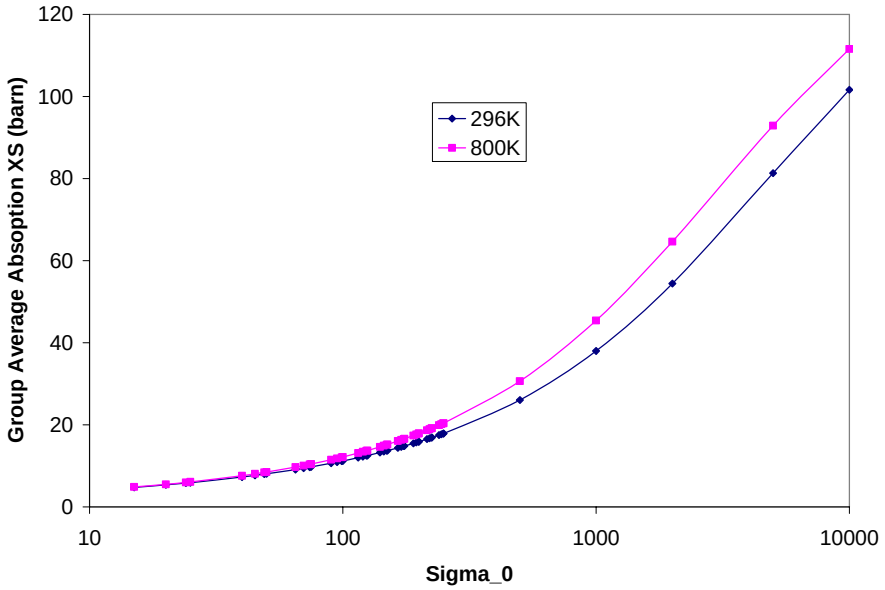

Figure 2. U-238 Group 19 Average Absorption Cross Section in U-238/H mixtures

The results indicate that the lambda factors are reasonably insensitive to the temperature of the resonance isotopes and the fraction of the background cross section from non-hydrogen isotopes. However, the lambda factors do depend on the background cross sections. The lambdas of O-16 at other resonance groups are also shown in Figure 3 which shows that the lambdas of O-16 are close to 1 in groups 10 to 15 for any σ_0. The computed lambdas for groups 16 and groups 20 to 25 except 23 are outside a reasonable range due to lack of resonances in these groups. As indicated the lambdas are sensitive to σ_0 in groups 19, 18 and 23.

Table III. Lambdas of O-16 at group 19

Temperature	300K				800K			
σ_0 \ γ*	2%	4%	10%	20%	2%	4%	10%	20%
5	0.511	0.509	0.503	0.491	0.504	0.502	0.495	0.484
10	0.611	0.609	0.605	0.597	0.605	0.604	0.600	0.592
15	0.666	0.665	0.662	0.656	0.662	0.661	0.658	0.652
20	0.703	0.702	0.699	0.695	0.698	0.697	0.695	0.691
25	0.729	0.728	0.726	0.722	0.724	0.723	0.721	0.717
50	0.795	0.794	0.793	0.790	0.787	0.787	0.786	0.783
100	0.845	0.845	0.844	0.843	0.833	0.833	0.832	0.831
200	0.881	0.881	0.880	0.879	0.864	0.864	0.863	0.862
500	0.928	0.928	0.928	0.927	0.911	0.911	0.910	0.910

* γ is the fraction of non-hydrogen potential cross section in σ_0

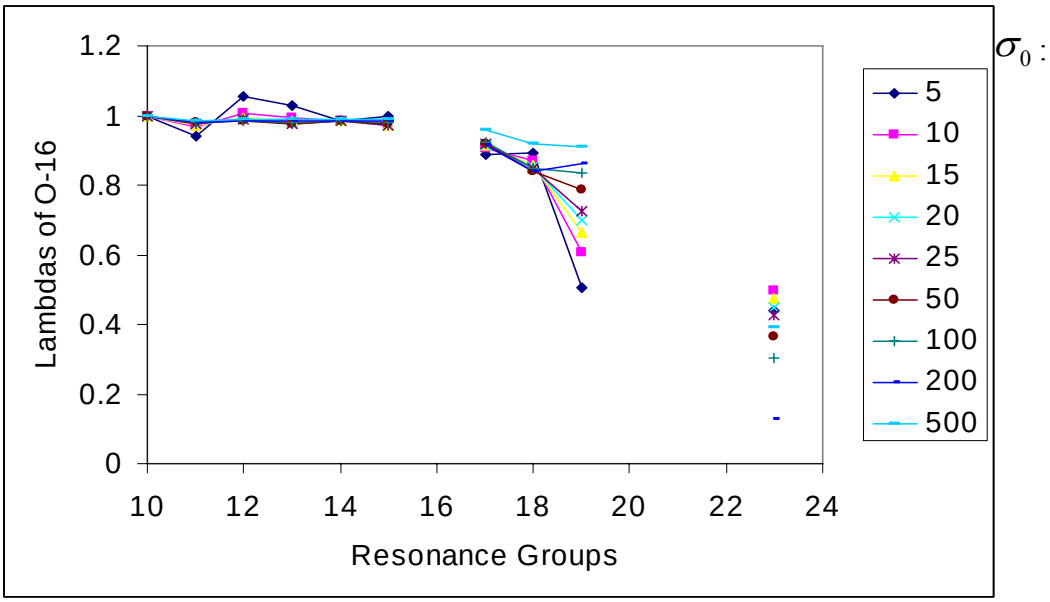

Figure 3. Lambdas of O-16 computed with different σ_0

A typical PWR pin cell was then simulated with MCNP to determine the range of background cross sections for light water reactor applications. From the U-238 average absorption cross section of all resonance groups, the equivalent $\sigma_{0,g}^{equ}$ was determined using Eq. (6). The results are shown in Table IV.

Table IV. Equivalent background cross section for U-238 in a typical PWR pincell

Resonance group	$\sigma_{0,g}^{equ}$ (barn)	Resonance group	$\sigma_{0,g}^{equ}$ (barn)	Resonance group	$\sigma_{0,g}^{equ}$ (barn)
10	40.88	15	33.19	20	26.80
11	36.81	16	-	21	13.84
12	34.92	17	35.01	22	3.994
13	36.08	18	40.87	23	14.49
14	32.90	19	28.32	24-25	-

Since the lambdas are only sensitive to σ_0 in groups 19, 18 and 23, and the U-238 has a very small resonance in group 23, the most important groups to determine σ_0 for the lambda calculation are group 19 then group 18. Using this reasoning, 30 barn was selected as σ_0 for the lambda calculation.

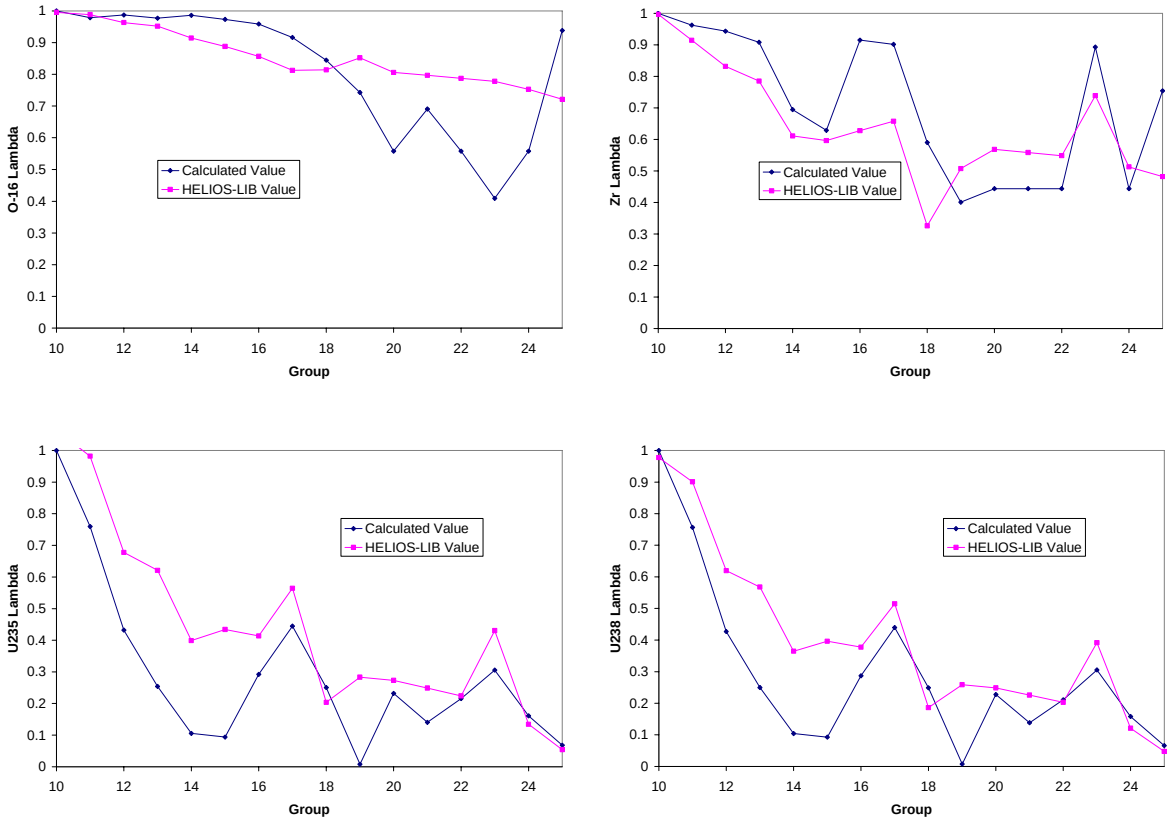

Figure 4. Lambda Values for O16, Zr, U235 and U238

A code was developed to calculate lambdas for all resonance groups of any scattering isotopes with average absorption cross section in U-238/H, U-235/H mixtures with different density ratios and in mixtures in which part of the H has been replaced by other scattering isotopes. The lambdas with respect to U-238 will be used for all resonance groups if these lambdas are in the range of [0,1]. If the lambda with respect to U-238 is not in this range, then lambdas with respect to U-235 in this range will be used. 1000 barn was selected as σ_0 for calculating lambdas with respect to U-235 using the same study of a PWR pin cell.

The lambdas of O-16, Zr-40, U-235 and U-238 are calculated and compared with these values in HELIOS library in Figure 4. As indicated, the lambdas agree well with the values in the HELIOS library for the resonance groups in which there exists important resonances.

3. SUBGROUP PARAMETERS

3.1 Optimization method for Subgroup Parameters

The subgroup levels σ_n s and their associated weights w_n are referred to as the subgroup parameters. In the DeCART library, there are a set of subgroup weights for each isotope, each reaction type (absorption or fission), each resonance group, and each temperature. However, all temperatures share the same set of subgroup levels.

In reference [11], the subgroup weights are determined by minimizing

$$\min_w f(w) = \sum_{k=1}^{K} \left(\frac{1}{R_k} \sum_{n=1}^{N} \frac{w_n \sigma_n \sigma_{bnk}}{\sigma_{bnk} + \sigma_n} - 1 \right)^2 \tag{9}$$

$$\text{Subject to } g(w) = \frac{1}{R_\infty} \sum_{n=1}^{N} w_n \sigma_n - 1 = 0$$

Where ΔuR_∞ is the infinite diluted resonance integral, and ΔuR_k s are resonance integrals in K different configurations. For a homogeneous mixture, the background cross section is independent from σ_n, $\sigma_{bnk} = \sigma_{bk}$. The relation between resonance integral and group average cross section is then simply,

$$R_k = \frac{\sigma_{ak}}{1 + \sigma_{ak} / \sigma_{bk}} \tag{10}$$

The subgroup levels are obtained by trial-and-error to minimize the objective functions (9) for all temperatures.

In the work here, the subgroup levels are taken directly from reference [11], but the optimization problem is modified for determining the optimum subgroup weights,

$$\min_{w} f(w) = \sum_{k=1}^{K}\left(\sum_{n=1}^{N} \frac{w_n \sigma_n \left(\sigma_{bnk} + \sigma_{ak}\right)}{\sigma_{ak}\left(\sigma_{bnk} + \sigma_n\right)} - 1 \right)^2 \qquad (11)$$

$$\text{Subject to } g(w) = \frac{1}{\sigma_{a\infty}} \sum_{n=1}^{N} w_n \sigma_n - 1 = 0$$

If all configurations are homogeneous mixtures, then optimization problem (11) is mathematically equivalent to problem (9). However, for the heterogeneous cases, the approximation for R_k are avoided by using group average cross sections which are already defined. After obtaining the subgroup parameters, the resonance integral can be approximated as,

$$R_k \approx \sum_{n=1}^{N} \frac{w_n \sigma_n \sigma_{bnk}}{\sigma_{bnk} + \sigma_n} \qquad (12)$$

This problem can be solved using the penalty function method:

$$\min_{w} f(w) = \frac{1}{2}\sum_{k=1}^{K}\left(\sum_{n=1}^{N} \frac{w_n \sigma_n \left(\sigma_{bnk} + \sigma_{ak}\right)}{\sigma_{ak}\left(\sigma_{bnk} + \sigma_n\right)} - 1 \right)^2 + \frac{1}{2} P \left(\frac{1}{\sigma_{a\infty}} \sum_{n=1}^{N} w_n \sigma_n - 1 \right)^2 \qquad (13)$$

Where penalty factor P can be selected such that the constraint is satisfied to a desired level of accuracy. The objective function is in quadratic form with respect to an unknown vector $w = [w_{1t}, ...w_{Nt}]^T$. This optimization problem is equivalent to solve the following over-determined linear system with least square method.

$$\begin{aligned} &\sum_{n=1}^{N} \frac{w_n \sigma_n \left(\sigma_{bnk} + \sigma_{ak}\right)}{\sigma_{ak}\left(\sigma_{bnk} + \sigma_n\right)} = 1, \qquad k = 1, ..., K \\ &\frac{P}{\sigma_{a\infty}} \sum_{n=1}^{N} w_n \sigma_n = P \end{aligned} \qquad (14)$$

In matrix form: $Aw = b$

Where A is $(K+1) \times N$ matrix, and $b = [b_1, ...b_K, b_{K+1}]^T$

For $k \le K$, $A_{(k,n)} = \dfrac{\sigma_n \left(\sigma_{bnk} + \sigma_{atk}\right)}{\sigma_{atk}\left(\sigma_{bnk} + \sigma_n\right)}$, $b_k = 1$. And $A_{(K+1,n)} = \dfrac{P\sigma_n}{\sigma_{at\infty}}$, $b_{K+1} = P$

This linear system can be solved efficiently by the CGNR Krylov method.

$$Hw = A^T A w = A^T b = -f_w \qquad (15)$$

3.2 Subgroup Parameters Calculation with NJOY

A total of 16 homogeneous mixtures of resonance isotopes (U-235 or U-238) and hydrogen with different ratios were calculated with NJOY for 5 different temperatures. The last case was performed with a very high H/U ratio representing the infinite diluted case. A total of 16 cross sections of each resonance isotopes for each reaction type were obtained for each resonance group at each temperature from these 16 mixtures and were then used for determining the subgroup weights. As an example, Table V shows the 16 absorption cross sections of U-238 in group 19 at 296K which were calculated by NJOY for 16 mixtures. The subgroup levels and optimal weights are given in Table VI. The cross sections are calculated again with subgroup expression (1) with these subgroup parameters are then compared with the cross sections from the NJOY calculation in Table V.

Table V. U-238 group 19 absoption cross sections

Case	Back ground XS (barn)	Group average absorption XS from NJOY(barn)	Absorption XS from Subgroup formula (barn)	Difference (%)
1	1.9924E+01	49.81925	49.78786	-0.063
2	2.1824E+01	51.37510	51.37664	0.003
3	2.8084E+01	56.19061	56.22601	0.063
4	3.5124E+01	61.16083	61.18713	0.043
5	5.2024E+01	71.77349	71.76344	-0.014
6	8.5724E+01	89.56017	89.51987	-0.045
7	1.5772E+02	119.9025	119.8713	-0.026
8	3.2372E+02	172.6190	172.7157	0.056
9	7.3672E+02	264.2267	264.2663	0.015
10	1.8377E+03	413.6375	413.2818	-0.086
11	5.1777E+03	624.5229	625.0163	0.079
12	1.6098E+04	826.4993	826.6067	0.013
13	5.5600E+04	946.3275	945.6651	-0.07
14	2.1200E+05	992.5742	992.2169	-0.036
15	8.9200E+05	1006.202	1006.101	-0.01
16	1.0000E+10	1010.555	1010.555	0

Table VI. Subgroup parameters for U-238 group 19 absoption cross sections

n	σ_n (barn)	w_n
1	4.8	3.052980E-01
2	40	3.336865E-01
3	250	2.133614E-01
4	750	-6.081921E-03
5	2000	1.466291E-01
6	7000	9.717065E-02
7	20000	-1.324474E-03

4. VALIDATION

We first validate the resonance parameter generation procedure with infinite homogenous mixtures which consists with H-1 and U-235 only. These configurations are most close to those used in NJOY spectrum calculation for generating resonance group constants of U-235. The only difference is that real H-1 instead of the pseudo scatter is used. DeCART and MCNP codes are applied to these cases with libraries generated from same ENDF. There are 30,000X1,000 neutrons simulated in each MCNP run. The infinite multiplication factors from both codes are compared in Table VII to IX. Table VII contains the results for mixture with H/U-235ratio 40.46 at 6 temperatures from 296K to 1000K. Table VIII and IX contain results for 9 mixtures with H/U-235 ratio from 8.6195 to 102.43 at 296K and 800K temperatures respectively. The maximum difference between infinite multiplication factors from DeCART and MCNP for all of these cases is 131 pcm.

Table VII. Comparison for mixture with ratio H/U-235=40.45

Temperature (K)	MCNP K-inf	MCNP Standard Deviation	Difference(pcm) DeCART-MCNP	Difference(pcm) Due to Resonance
296	1.89133	0.00008	-43	-9
400	1.88889	0.00008	-1	6
500	1.88648	0.00008	28	6
600	1.88414	0.00008	46	-6
800	1.88003	0.00008	82	-6
1000	1.87664	0.00008	131	-11

Table VIII. Comparison for mixtures at 296K temperature

H/U235 Ratio	MCNP K-inf	MCNP Standard Deviation	Difference(pcm) DeCART-MCNP	Difference(pcm) Due to Resonance
8.6195	1.80826	0.00009	-103	16
17.7337	1.83749	0.00009	-45	-14
40.46	1.89133	0.00008	-43	-9
50	1.90116	0.00008	-33	-1
60	1.90688	0.00008	-18	0
70	1.90969	0.00007	-34	0
80	1.90994	0.00007	-23	2
90	1.90872	0.00007	-32	1
102.43	1.90541	0.00006	-34	2

Table IX. Comparison for mixtures at 800K temperature

H/U235 Ratio	MCNP K-inf	MCNP Standard Deviation	Difference(pcm) DeCART-MCNP	Difference(pcm) Due to Resonance
8.6195	1.79486	0.00009	3	15
17.7337	1.82502	0.00010	83	-13
40.46	1.88003	0.00008	82	-6
50	1.88974	0.00008	91	-1
60	1.89534	0.00008	90	-1
70	1.89765	0.00007	89	0
80	1.89760	0.00007	91	0
90	1.89622	0.00007	57	2
102.43	1.89225	0.00007	66	-3

In order to isolate the differences attributable to the resonance treatment, group constants from DeCART were used to evaluate the infinite multiplication factor with the absorption and fission cross sections for resonance groups replaced by those edited from the flux and reaction rate

tallies of MCNP. The results are also listed in the last column of Tables VII-IX. As expected the differences caused by resonance treatment are small. The maximum difference caused by resonance treatment appeared in the mixture with a H/U-235 ratio 8.6195 at 296K. Detailed comparisons of cross sections from DeCART, MCNP, and NJOY for this case are shown in Table X. Except for the 0.63% difference in group 10 which is caused by the unresolved resonance treatment, the maximum difference in cross sections between DeCART and MCNP is 0.14% and the maximum difference in the cross sections between DeCART and NJOY is 0.12%. The differences in the cross sections between DeCART and NJOY results in about a 10 pcm difference in the infinite multiplication factor. These differences are attributable to the subgroup representation of resonance cross sections.

Table X. Comparison for mixtures at 800K temperature

Group	XS from DeCART (barn)		XS difference DeCART - MCNP		XS difference DeCART - NJOY	
	σ_a	$\nu\sigma_f$	σ_a	$\nu\sigma_f$	σ_a	$\nu\sigma_f$
10	5.952197E+00	1.050709E+01	0.61%	0.63%	0.00%	0.00%
11	1.757828E+01	2.902727E+01	0.11%	0.12%	0.00%	0.01%
12	3.142937E+01	4.912849E+01	-0.10%	-0.05%	-0.06%	-0.05%
13	4.388277E+01	7.474680E+01	-0.09%	-0.07%	-0.06%	-0.05%
14	4.853681E+01	7.316408E+01	-0.01%	-0.02%	-0.02%	-0.02%
15	5.255721E+01	8.277858E+01	-0.07%	-0.08%	-0.05%	-0.05%
16	7.538939E+01	9.936917E+01	-0.14%	-0.09%	-0.02%	-0.01%
17	6.873864E+01	1.053317E+02	-0.09%	-0.08%	-0.03%	-0.02%
18	9.329700E+00	1.207749E+01	0.02%	0.02%	0.00%	0.00%
19	4.372854E+01	4.186620E+01	-0.02%	-0.05%	-0.04%	-0.05%
20	7.576493E+01	8.278819E+01	-0.01%	-0.06%	0.01%	-0.01%
21	1.564084E+01	2.988850E+01	0.04%	0.03%	0.03%	0.02%
22	3.390630E+01	1.678937E+01	0.07%	0.09%	-0.06%	0.04%
23	5.393027E+00	8.005022E+00	-0.13%	-0.13%	-0.12%	-0.12%
24	2.957963E+01	5.110235E+01	-0.03%	-0.03%	-0.04%	-0.03%
25	2.656379E+01	3.566709E+01	-0.14%	-0.03%	-0.07%	0.00%

After validating the procedure for generating resonance parameters with H/U-235 mixtures, the resonance interference effect was examined for a H/U-235/U-238 mixture with isotopic ratios of

1.2/0.03/0.97 at 800K. With 30,000 X 1,000 neutron histories, the MCNP infinite multiplication factor was 1.08629 with a standard deviation of 0.00012. DeCART predicts 1.08796 as an infinite multiplication factor for this case which is 167 pcm higher than MCNP results. The resonance cross sections from DeCART and MCNP are compared in Table XI. The maximum difference is about 37.7%. These differences in resonance cross sections contribute about a -305 pcm difference in the infinite multiplication factor.

Table XI. Resonance XS Comparison for H/U-235/U-238 mixture

Group	XS from DeCART (barn)			XS difference from MCNP		
	U-235 σ_a	U-235 $\nu\sigma_f$	U-238 σ_a	U-235 σ_a	U-235 $\nu\sigma_f$	U-238 σ_a
10	5.9426E+00	1.0483E+01	7.7434E-01	0.28%	0.24%	0.18%
11	1.9399E+01	3.1791E+01	1.2462E+00	2.17%	1.54%	0.51%
12	3.5038E+01	5.3545E+01	2.8033E+00	-0.86%	0.07%	0.13%
13	5.2806E+01	8.9374E+01	1.6661E+00	-3.01%	-3.51%	-2.73%
14	6.5474E+01	9.6846E+01	4.2083E+00	-4.11%	-3.12%	0.30%
15	6.7563E+01	1.0289E+02	3.6774E+00	6.78%	2.34%	0.51%
16	1.1738E+02	1.4130E+02	2.8008E-01	0.04%	0.05%	0.00%
17	1.0243E+02	1.5372E+02	7.0528E-01	1.36%	1.78%	0.58%
18	9.6673E+00	1.2577E+01	3.0492E+00	-0.77%	-1.03%	-0.16%
19	5.8206E+01	5.4190E+01	6.1806E+01	-21.25%	-30.54%	-0.46%
20	1.0781E+02	9.9579E+01	1.4772E+01	37.70%	18.35%	4.96%
21	1.5792E+01	3.0026E+01	2.5103E+00	0.55%	0.74%	0.12%
22	4.2448E+01	1.8687E+01	1.2692E+00	-0.12%	-0.03%	0.26%
23	5.4359E+00	8.0384E+00	9.8774E-01	0.10%	0.16%	0.11%
24	3.2261E+01	5.5246E+01	5.5893E-01	0.12%	0.10%	0.19%
25	2.8122E+01	3.6446E+01	4.6796E-01	-0.05%	-0.02%	0.09%

5. CONCLUSIONS

Procedures were developed for generating resonance parameters, including lambda factors and subgroup parameters for the DeCART library. The lambda factors generated with this procedure agree well with the HELIOS library values. A new optimization process was introduced to generate the subgroup parameters and results were validated using MCNP calculations. The results indicate that the subgroup method can very accurately represent resonance cross section

effects. The study here also indicates that large errors can be introduced if resonance interference effects between resonance isotopes are not properly treated. An improvement in the treatment of resonance interference effect treatment will be the focus of future work.

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