TREATMENT OF NEUTRON CROSS-SECTION WITH INTERPOLATION

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Abstract

Using NJOY to generate the temperature dependent neutron cross-section is too time-consuming in practice, especially for many nuclides. So an approach involving interpolation between nuclear data libraries at different temperatures is investigated.
Based on the ACE data at different temperatures, we used ITND – an neutron cross-section interpolation program, to generate the target temperature ACE data, then we compared it with the ACE data which generated by NJOY at the same temperature. We focused on the interpolation result of 238U、235U、232Th、Zr、16O、10B and 1H at the temperature of 575K. To that nuclides, several interpolate schemes were studied, and we demonstrated the relative differences, and explain their reasons. Finally we applied these ACE data to benchmark calculation, and good agreement was observed with the benchmark results.

Keywords: ACE, Interpolation, temperature dependent

I. Introduction
For the modern simulation of neutron transport problems, Monte Carlo method plays a significant role and with famous codes such as MCNP (A General Monte Carlo N-Particle Transport Code)[1] enables us to perform model calculations more conveniently. However, as in the case of temperature changing problem, MCNP treats the relevant cross-sections by Doppler broadening which is inadequate in unresolved resonance range (URR). As a result, MCNP can not solve temperature based calculations properly.
In order to perform the temperature based MCNP simulation, we have to generate a group of cross-sections at the desired temperature. Usually, this task is accomplished by NJOY. But in practice, NJOY calculation is too time-consuming. An additional complication to this approach is that we may not know the finial temperature distribution in prior, especially for a thermal-hydrologic feedback problem as it is.
Another way of generating the temperature dependent cross-sections is to employ a scheme of interpolation among several given cross-sections at different temperatures. We dealt with the cross-sections interpolation in ACE format and the basic process is showed in Figure 1.

The accuracy of interpolation is dependent not only on the size of the interval but also on the interpolation scheme used, the temperature range for specific problems, and the behavior of the cross-section in the resolved resonance region [2]. As relative error is largely caused by the loss of points in energy grid, multiple reference ACEs (more than two) can make compensation and hence reduce the relative error significantly.

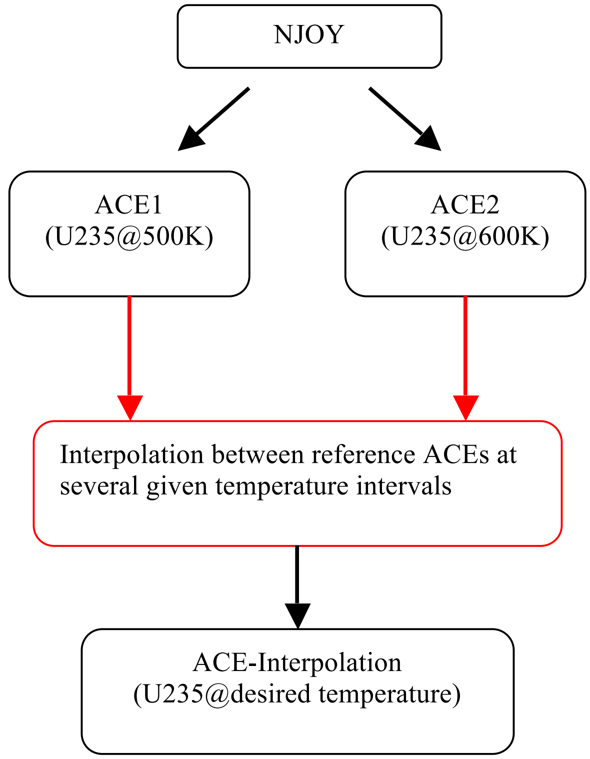

Figure 1. An example of interpolation between several given reference ACEs at some temperature intervals.

II.A. Interpolation Scheme for Reference ACEs

The famous Doppler broadening equation implies that the cross-section (σ) relies on both neutron energy and temperature of the target nuclide. Eq. (1)[3] listed below shows this dependency:

$$\sqrt{E}\sigma(E,T)=\frac{1}{2}\left(\frac{\alpha}{\pi E}\right)^{\frac{1}{2}}\cdot\int_{0}^{\infty}\sqrt{E_r}\cdot\sigma(E_r,0)\cdot\left\{e^{[-\alpha(\sqrt{E}-\sqrt{E_r})^2]}-e^{[-\alpha(\sqrt{E}+\sqrt{E_r})^2]}\right\}dE_r \qquad (1)$$

where[3]

$$\alpha=\frac{A}{KT}$$

A = atomic weight ratio of the target mass to the projectile mass
K = Boltzmann's constant
T = temperature of the target nuclei (K)
E = energy of the projectile (eV)
E_r = relative energy of the neutron as "seen" by the target nuclei
$\sigma(E,T)$ = Doppler broaden cross-section at energy E for target nuclei temperature T
$\sigma(E_r,0)$ = cross-section at energy E_r for target nuclei temperature of 0 K.

The nature of Doppler-broaden equation (Eq. (1)) does not suggest a simple interpolation scheme to calculate $\sigma(E,T)$ at the desired temperature T from the given reference cross-sections $\sigma(E,T_1)$ and $\sigma(E,T_2)$ [2]. So we have tried six interpolation schemes to see which one is the best. All of these six schemes adopt Lagrangian Interpolation Polynomial in order to get an easy expansion to higher degrees. The use of 2nd degree Lagrangian interpolation polynomials are listed below:

"lin-lin":

$$\sigma(E,T)=\sigma(E,T_1)\cdot\frac{T-T_2}{T_1-T_2}+\sigma(E,T_2)\cdot\frac{T-T_1}{T_2-T_1} \tag{2}$$

"log-log":

$$\ln[\sigma(E,T)]=\ln[\sigma(E,T_1)]\cdot\frac{\ln[T]-\ln[T_2]}{\ln[T_1]-\ln[T_2]}+\ln[\sigma(E,T_2)]\cdot\frac{[T]-[T_1]}{[T_2]-[T_1]} \tag{3}$$

"lin-log":

$$\ln[\sigma(E,T)]=\ln[\sigma(E,T_1)]\cdot\frac{T-T_2}{T_1-T_2}+\ln[\sigma(E,T_2)]\cdot\frac{T-T_1}{T_2-T_1} \tag{4}$$

"sqrt-lin":

$$\sigma(E,T)=\sigma(E,T_1)\cdot\frac{\sqrt{T}-\sqrt{T_2}}{\sqrt{T}_1-\sqrt{T}_2}+\sigma(E,T_2)\cdot\frac{\sqrt{T}-\sqrt{T_1}}{\sqrt{T}_2-\sqrt{T}_1} \tag{5}$$

"sqrt-log":

$$\ln[\sigma(E,T)]=\ln[\sigma(E,T_1)]\cdot\frac{\sqrt{T}-\sqrt{T_2}}{\sqrt{T}_1-\sqrt{T}_2}+\sigma(E,T_2)\cdot\frac{\sqrt{T}-\sqrt{T_1}}{\sqrt{T}_2-\sqrt{T}_1} \tag{6}$$

"insqrt-lin":

$$\sigma(E,T)=\sigma(E,T_1)\cdot\frac{\frac{1}{\sqrt{T}}-\frac{1}{\sqrt{T_2}}}{\frac{1}{\sqrt{T_1}}-\frac{1}{\sqrt{T_2}}}+\sigma(E,T_2)\cdot\frac{\frac{1}{\sqrt{T}}-\frac{1}{\sqrt{T_1}}}{\frac{1}{\sqrt{T_2}}-\frac{1}{\sqrt{T_1}}} \tag{7}$$

II.B. Treatment of Energy Grid

As indicated before, the cross-section is also a function of neutron energy. ACE format solves this problem by dividing the continuous neutron energy into a large number of discrete energy points which together form an energy grid. The quantity of points in energy gird, however, varies not only with the type of the material but also with its temperature. Table I shows the quantities of energy points of U235 at different temperatures.

TABLE I
Quantities of energy points of U235 at different temperatures

Temperature(K)	700	600	500	400
Quantity of energy points	31704	32732	34055	36024

The variety in quantity of energy points leads us to select a reference ACE, copy its energy grid and regard it to be the energy grid of target ACE. Energy grids in other reference ACEs should be normalized to fit the selected one by liner interpolation. For example, we want to generate the ACE of U235 at 575K by doing interpolation between ACE-U235@500K and ACE-

U235@600K. We could firstly choose energy grid of ACE-U235@600K as the standard and then normalized ACE-U235@500K to fit it.
The problem is that energy grid of ACE-U235@600K is more or less different from the ACE-U235@575K. Although the difference isn't very significant, the loss of energy points does contribute to the inaccuracy dominatingly.
In order to reduce interpolation error, we expanded the 2nd degree Lagrangian Interpolation polynomial to 3rd or 4th degree. The 4th degree Lagrangian Interpolation polynomial is described below ("log-log" interpolative scheme):

$$\begin{aligned}\ln[\sigma(E,T)] = {} & \ln[\sigma(E,T_1)]\cdot\frac{\ln[T]-\ln[T_2]}{\ln[T_1]-\ln[T_2]}\cdot\frac{\ln[T]-\ln[T_3]}{\ln[T_1]-\ln[T_3]}\cdot\frac{\ln[T]-\ln[T_4]}{\ln[T_1]-\ln[T_4]} \\ & +\ln[\sigma(E,T_2)]\cdot\frac{\ln[T]-\ln[T_1]}{\ln[T_2]-\ln[T_1]}\cdot\frac{\ln[T]-\ln[T_3]}{\ln[T_2]-\ln[T_3]}\cdot\frac{\ln[T]-\ln[T_4]}{\ln[T_2]-\ln[T_4]} \\ & +\ln[\sigma(E,T_3)]\cdot\frac{\ln[T]-\ln[T_1]}{\ln[T_3]-\ln[T_1]}\cdot\frac{\ln[T]-\ln[T_2]}{\ln[T_3]-\ln[T_2]}\cdot\frac{\ln[T]-\ln[T_4]}{\ln[T_3]-\ln[T_4]} \\ & +\ln[\sigma(E,T_4)]\cdot\frac{\ln[T]-\ln[T_1]}{\ln[T_4]-\ln[T_1]}\cdot\frac{\ln[T]-\ln[T_2]}{\ln[T_4]-\ln[T_2]}\cdot\frac{\ln[T]-\ln[T_3]}{\ln[T_4]-\ln[T_3]}\end{aligned} \tag{8}$$

III.A. Software Development
The interpolation software was written in C programming language and entitled as ITND – an acronym for Interpolation of Temperature dependent Neutron Data. The program processes ACE data step by step. Four major steps are listed below:
Step 1:
Read in the reference ACEs. Crack a group of structures in the computer memory to store and organize these ACEs data.

Step 2:
Select a reference ACE, copy its energy grid and regard it to be the energy grid of target ACE. Normalize other reference ACEs' energy grids to fit the selected one by liner interpolation.

Step 3:
After energy grid normalization, program executes the Lagrangian Interpolation point by point according to the union energy grid.

Step 4:
Output the result cross-sections in ACE format. Output the relevant xsdir file for MCNP use.

III.B. Generating the Intermediate Cross-Section
A group of materials includes U238, U235, Th232, natural Zr, O16, B10 and H1 were used in this study. These materials were chosen to represent typical light water reactor applications. Doppler-broadened cross-section libraries were generated over these materials using NJOY code at the following temperatures: 294, 400, 500, 550, 575, 600, 650, 700, and 800K. The ENDF/B-6.8 files were downloaded from the National Nuclear Data Center website. Pointwise cross sections were reconstructed from resonance parameters using a tolerance of 0.1% in the

RECONR[4] module and no thinning was used in the BROADR[4] module. Total, elastic scattering, fission, and radiative capture cross-sections were examined in this study.
Seven different temperature intervals were investigated. They were: 294 to 800K, 400 to 700K, 500 to 650K, 550 to 600K, 500 to 600 to 700K, 400 to 500 to 600 to 700K, and 500 to 550 to 600 to 650K. The desired temperature was set to 575K. Interpolation results were then compared to NJOY Doppler-broadened cross-sections. Relative error and the number of energy point losses were counted. At last, two MCNP calculations were performed to test the validity of these interpolated cross-sections.

IV. Result

To the nuclides with complex resonance behavior such as U238 and U235, they are most challenging to accuracy represent using an interpolation method. This is because such nuclides contain much more energy points than others; and also because their resonance energy points are very sensitive to the change of temperature. Nuclides having many resonance areas and sharp resonance peaks require more narrow temperature intervals to achieve the same error tolerance compared to nuclides with fewer resonance points.

IV. A. U238 Cross-Sections

Table II shows the results of six interpolation schemes for four different temperature intervals for the total cross-sections of U238 at 575K. As we expected, such nuclide seems to be more “resistible” to interpolation. In spite of this resistance, log-log proved to be more effective than other schemes and relatively good results are obtained by using thin temperature interval.

TABLE II[5]

Results of Various Interpolation Methods over Various Temperature Intervals for the Total Cross-Section of U238 at 575K

Interpolation Method	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Temperature Interval: 294 to 800K						
Insqrt – lin	81.83	2.76	11941	4897	6707	18051
Lin – lin	49.80	2.31	9046	3828	5885	22867
Lin – log	32.56	2.38	9060	3817	5880	22839
Log – log	40.48	1.73	10677	5150	8002	17767
Sqrt – lin	71.48	2.37	10106	4755	6937	19798
Sqrt – log	31.16	1.93	9467	4376	6453	21300
Temperature Interval: 400 to 700K						
Insqrt – lin	29.00	0.96	19699	4981	5801	11115
Lin – lin	18.33	0.79	15297	4690	6511	15098
Lin – log	12.62	0.83	15325	4735	6639	14897
Log – log	14.01	0.58	19207	6516	5492	10381
Sqrt – lin	25.45	0.82	17874	5284	6936	11502
Sqrt – log	11.30	0.67	16697	5058	7008	12833
Temperature Interval: 500 to 650K						
Insqrt – lin	7.90	0.25	29088	4056	4173	4279
Lin – lin	5.25	0.20	24902	5041	7542	4111
Lin – log	3.22	0.21	25118	5093	7040	4345
Log – log	3.90	0.15	29982	3725	4463	3426
Sqrt – lin	7.02	0.21	28372	5500	4270	3454
Sqrt – log	3.19	0.17	26946	6737	4050	3863
Temperature Interval: 550 to 600K						
Insqrt – lin	1.795	0.029	38577	1420	1218	381
Lin – lin	1.677	0.024	39888	1107	543	58
Lin – log	1.613	0.024	39085	1673	804	34
Log – log	1.691	0.018	39848	1389	321	38
Sqrt – lin	1.755	0.025	39173	1183	1002	238
Sqrt – log	1.652	0.020	39533	1655	372	36

Interpolation results of other reaction types are provide in Table III. These results are reported at the smallest temperature interval (550 to 600K) with log-log interpolation scheme. Owning the largest average and maximum relative difference, radiative capture cross-section is the toughest one for interpolation.

TABLE III[5]

Results for Interpolating the Elastic Scatter, Fission, and Radiative Capture Cross-Sections over the Temperature Interval 550 to 600K for U238 at 575K

Interpolation Method	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Elastic Scatter						
Insqrt – lin	2.711	0.029	38849	1154	1101	492
Lin – lin	2.534	0.022	39919	1001	502	174
Lin – log	2.391	0.022	39256	1379	927	34
Log – log	2.509	0.016	39885	1325	351	35
Sqrt – lin	2.652	0.025	39367	956	892	381
Sqrt – log	2.450	0.018	39608	1409	545	34
Fission						
Insqrt – lin	12.92	0.021	40075	342	701	478
Lin – lin	12.38	0.014	40318	620	451	207
Lin – log	11.11	0.012	40129	681	694	92
Log – log	11.47	0.011	40337	758	412	89
Sqrt – lin	12.74	0.018	40222	351	654	396
Sqrt – log	11.29	0.011	40174	859	497	66
Radiative Capture						
Insqrt – lin	12.56	0.155	29779	3433	5019	3365
Lin – lin	12.35	0.122	31354	6121	2809	1312
Lin – log	12.22	0.130	26984	7011	7208	393
Log – log	12.34	0.095	31453	7523	2100	520
Sqrt – lin	12.48	0.137	31596	3105	4306	2589
Sqrt – log	12.28	0.109	28774	7861	4549	412

Table IV shows the effectiveness of high degree Lagrangian Interpolation for U238 using log-log scheme. Compared to 2nd degree Lagrangian Interpolation, the 4th degree interpolation method significantly improved the accuracy. Only 3.02% of radiative capture cross-sections exceeding the 0.1% relative difference target, compared to 24.38% using 2nd degree interpolation.

TABLE IV[5]

Results for interpolating the Total, Elastic Scatter, Fission, and Radiative Capture Cross-Sections for U238 at 575K using high degree Lagrangian Interpolation (log-log)

N-th* degree Lagrangian Interpolation	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Total						
II	1.69	0.0178	39848	1389	321	38
III	0.85	0.0099	40904	425	194	73
IV-1	0.85	0.0056	41196	167	174	59
IV-2	1.65	0.0030	41249	140	176	31
Elastic Scatter						
II	2.51	0.0162	39885	1325	351	35
III	0.89	0.0089	40934	380	187	95
IV-1	0.89	0.0050	41243	149	115	89
IV-2	2.47	0.0027	41305	95	162	34
Fission						
II	11.47	0.0105	40337	758	412	89
III	10.61	0.0062	40966	364	208	58
IV-1	10.36	0.0038	41353	123	71	49
IV-2	10.68	0.0027	41491	19	48	38
Radiative Capture						
II	12.34	0.0952	31453	7523	2100	530
III	10.65	0.0629	37153	2279	1289	875
IV-1	10.61	0.0503	39451	847	376	922
IV-2	11.88	0.0404	40338	210	559	489

* N-th degree Lagrangian Interpolation: II (500 to 600K), III (500 to 600 to 700K), IV-1 (400 to 500 to 600 to 700K), IV-2 (500 to 550 to 600 to 650K).

As showed in Table V, the choice of standard energy grid also affects the accuracy. All reactions turn to have a better result with the "temperature adjacent strategy". This strategy suggests us to select the standard energy grid from one of reference ACEs as whose temperature most closes to the desired one.

TABLE V[5]

Results for interpolating the Total, Elastic Scatter, Fission, and Radiative Capture Cross-Sections for U238 at 575K with different choice of energy gird (log-log, IV-2)

Temperature	Maximum	Average	Number of Pointwise Cross-Sections (total = 41596)

for standard Energy grid	Relative Difference (%)	Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Total						
500K	1.65	0.0054	41010	212	255	119
550k	1.65	0.0030	41249	140	1761	31
600k	0.85	0.0039	41208	119	201	68
650k	1.00	0.0096	40578	285	422	311
Elastic Scatter						
500K	2.47	0.0048	41104	149	218	125
550k	2.47	0.0027	41305	95	162	34
600k	1.19	0.0033	41280	87	120	109
650k	1.19	0.0081	40792	190	266	348
Fission						
500K	18.20	0.0060	41424	26	56	90
550k	10.68	0.0027	41491	19	48	38
600k	10.41	0.0024	41485	25	43	43
650k	12.15	0.0050	41382	44	71	99
Radiative Capture						
500K	19.06	0.1051	40115	158	370	953
550k	11.88	0.0404	40338	210	559	489
600k	10.64	0.0386	40331	185	437	643
650k	13.00	0.0847	39658	88	484	1366

Note: the quantity of points in each energy grid: 500K (NXS[3] = 42621); 550K (NXS[3] = 41895); 600K (NXS[3] = 41329); 650K (NXS[3] = 40786).

Of the points exceeding the 0.1% relative difference target, their distribution versus cross-section value is described in Table VI. These results were generated under the typical interpolation scheme that is: log-log, IV-2, and the standard energy grid at 550K. To total and elastic scatter cross-sections, their values all exceeded 0.1b; 83% points have the value >10 b. To the fission reaction, of the 105 points exceeding the 0.1% relative difference target, 103 points have cross-section values <0.1 b. Radiative capture, however, has 1258 points over the 0.1% limitation, most of which owns a value less than 10b. Figures 2 to 5 show the relative difference for the interpolated total, elastic scatter, fission, and radiative capture cross-sections as a function of neutron energy using typical interpolation scheme for U238 at 575K. These relative differences are all dominated in the resonance area (neutron energy range from 10eV to 10KeV).

TABLE VI[5]

Distribution for Total, Elastic Scatter, Fission, and Radiative Capture Cross-Section values over the 0.1% relative difference target using typical interpolation scheme for U238 at 575K

Reaction type	Quantity of points over the relative difference target	Distribution of Cross-Section values				
		[0, 0.1b]	(0.1, 1b]	(1, 10b]	(10, 100b]	(100b, ∞)
Total	347	0	1	52	259	35
Elastic Scatter	291	0	1	47	217	26
Fission	105	103	2	0	0	0
Radiative Capture	1258	454	486	265	43	10

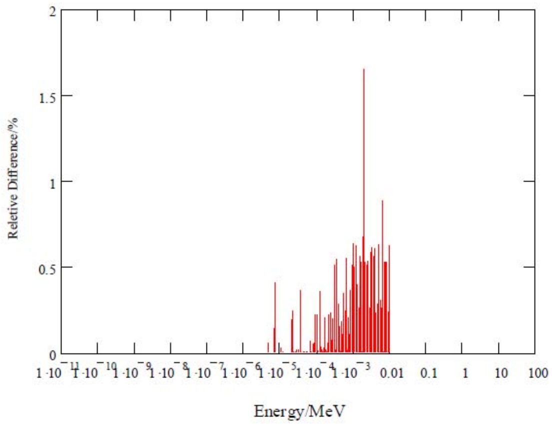

Fig. 2. Relative differences value in the interpolated U238 Total cross-section as a function of neutron energy by using typical interpolation scheme.

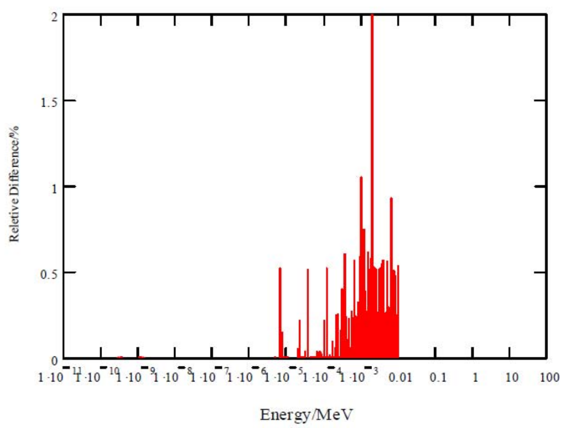

Fig. 3. Relative differences value in the interpolated U238 Elastic Scatter cross-section as a function of neutron energy by using typical interpolation scheme.

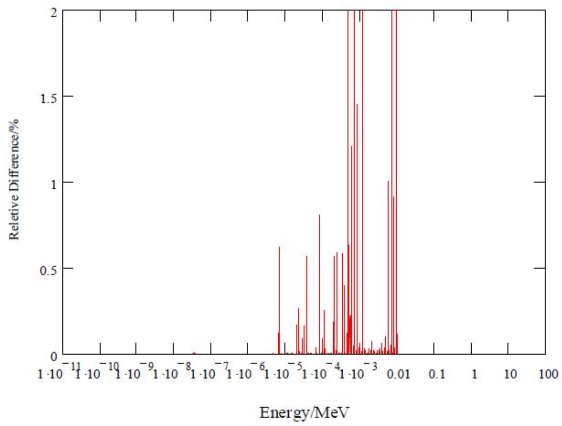

Fig. 4. Relative differences value in the interpolated U238 Fission cross-section as a function of neutron energy by using typical interpolation scheme.

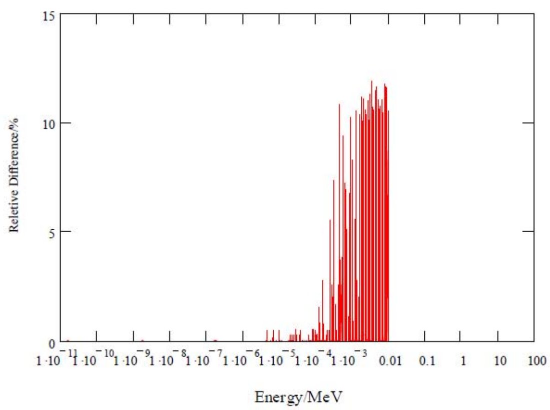

Fig. 5. Relative differences value in the interpolated U238 Radiative Capture cross-section as a function of neutron energy by using typical interpolation scheme.

IV.B. U235 Cross-Sections

Interpolation results of U235 for total, elastic scatter, fission, and radiative capture cross-sections for six different interpolation schemes over the smallest temperature range from 550 to 600K are provide in Table VII. As Table IV, Table VIII tells the effectiveness of high degree Lagrangian Interpolation for U235 using log-log scheme.

All average relative differences were less than 0.1%. Although high degree Lagrangian Interpolation did not largely increase the number of points under the 0.1% relative difference target, it indeed reduced the average relative difference.

TABLE VII[5]

Results for Interpolating the Total, Elastic Scatter, Fission, and Radiative Capture Cross-Sections over the Temperature Interval 550 to 600K for U235 at 575K

Interpolation Method	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Total						
Insqrt – lin	0.470	0.012	32476	232	41	0
Lin – lin	0.390	0.014	32619	113	17	0
Lin – log	0.363	0.014	32608	119	22	0
Log – log	0.414	0.010	32558	126	29	0
Sqrt – lin	0.443	0.010	32558	159	32	0
Sqrt – log	0.387	0.011	32608	117	24	0
Elastic Scatter						
Insqrt – lin	0.529	0.003	32707	29	12	1
Lin – lin	0.511	0.005	32714	26	8	1
Lin – log	0.510	0.005	32714	26	8	1
Log – log	0.522	0.003	32710	27	11	1
Sqrt – lin	0.523	0.003	32170	27	11	1
Sqrt – log	0.516	0.004	32713	26	9	1
Fission						
Insqrt – lin	0.730	0.022	31743	718	275	13
Lin – lin	0.607	0.023	32444	194	100	11
Lin – log	0.540	0.026	32027	620	91	11
Log – log	0.617	0.017	32406	183	148	12
Sqrt – lin	0.689	0.019	32132	414	190	13
Sqrt – log	0.576	0.020	32359	271	107	12
Radiative Capture						
Insqrt – lin	0.826	0.028	30734	1460	528	27
Lin – lin	0.704	0.028	32243	348	133	25
Lin – log	0.634	0.032	32109	1415	101	24
Log – log	0.715	0.021	32190	353	180	26
Sqrt – lin	0.785	0.024	31510	884	329	26
Sqrt – log	0.675	0.024	32025	562	137	25

TABLE VIII[5]

Results for interpolating the Total, Elastic Scatter, Fission, and Radiative Capture Cross-Sections for U235 at 575K using high degree Lagrangian Interpolation (log-log)

N-th* degree Lagrangian Interpolation	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Total						
II	0.4136	0.0096	32594	126	29	0
III	0.4876	0.0058	32448	115	186	0
IV-1	0.4871	0.0035	32447	118	184	0
IV-2	0.3435	0.0017	32552	161	36	0
Elastic Scatter						
II	0.5216	0.0030	32710	27	11	1
III	0.5168	0.0019	32658	51	36	4
IV-1	0.5153	0.0012	32600	51	34	4
IV-2	0.5034	0.0006	32707	29	12	1
Fission						
II	0.6173	0.0166	32406	183	148	12
III	0.5671	0.0099	32444	34	141	130
IV-1	0.5730	0.0059	32431	49	135	134
IV-2	0.5291	0.0028	32452	92	196	9
Radiative Capture						
II	0.7153	0.0206	32190	352	180	26
III	0.6076	0.0125	32414	12	106	217
IV-1	0.6100	0.0074	32384	42	108	215
IV-2	0.6158	0.0035	32396	50	280	23

* N-th degree Lagrangian Interpolation: II (500 to 600K), III (500 to 600 to 700K), IV-1 (400 to 500 to 600 to 700K), IV-2 (500 to 550 to 600 to 650K).

IV.C. Th232 and Nature Zr Cross-Sections

Table IX provides the results for Th232 and nature Zr under the typical interpolation scheme. Because the total 146 fission points of Th232 are unrelated to temperature, they have the same cross-section values in ACE-Th232 at any temperature. In radiative capture cross-section of Th232, the maximum relative difference 3.09% has its corresponding neutron energy 1.067381KeV which is not found in ACE-Th232's energy grid both at 550K and 500K. Meanwhile, the maximum relative difference 10.97% in radiative capture cross-section of nature Zr also has its corresponding neutron energy 16.69554KeV not found in the energy grid in ACE-Zr@550K.

Although the value of maximum relative difference is very large, interpolation accuracy is balanced by its small cross-section value (as showed in Figure 6). Of the 205 points exceeding the 0.1% relative difference target, 190 have cross-section values less than 0.1b; the remaining 15 points also limit their cross-section values within 10b.

TABLE IX[5]

Results for Interpolating the Total, Elastic Scatter, Fission, and Radiative Capture Cross-Sections under typical interpolation scheme for Th232 and nature Zr at 575K

Reaction type	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596)			
			Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Th232 (Quantity of points in energy grid = 21274)						
Total	0.63	0.0036	21033	119	117	5
Elastic Scatter	0.63	0.0030	21090	78	95	11
Fission	0	0	146	0	0	0
Radiative Capture	3.09	0.0193	20701	114	244	215
Nature Zr (Quantity of points in energy grid = 10102)						
Total	1.00	0.0031	10017	17	58	10
Elastic Scatter	0.99	0.0029	10023	13	56	10
Radiative Capture	10.97	0.0332	9897	37	81	87

Note: The quantity of Fission points for Th232 = 146

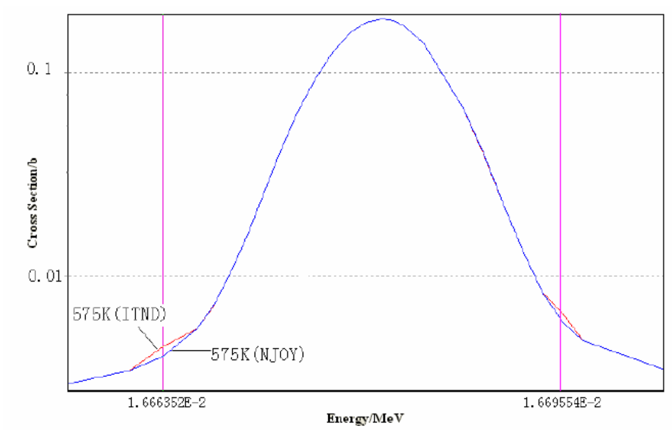

Fig. 6. Nature Zr Radiative Capture cross-section as a function of neutron energy by using typical interpolation scheme.

IV.D. O16 Cross-Section

Table X lists the result of O16 interpolation for the total, elastic scatter and radiative capture cross-sections for six different interpolation schemes over a temperature range of 500 to 600K. We selected the energy grid from ACE-O16@600K as the standard. At this interval, it is possible to achieve an average relative difference of less than 0.05% for all kinds of reactions. One maximum relative difference in radiative capture exceeds the 0.1% relative difference target due to the lack of corresponding point in standard energy grid.

TABLE X[5]

Results for Interpolating the Total, Elastic Scatter, and Radiative Capture Cross-Sections over the Temperature Interval 500 to 600K for O16 at 575K

Interpolation Method	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596) Relative Difference [0, 0.1%]	Relative Difference (0.1, 0.2%]	Relative Difference (0.2, 0.5%]	Relative Difference (0.5%, ∞)
Total (Elastic Scatter)						
Insqrt – lin	0.145	0.0050	2148	82	0	0
Lin – lin	0.074	0.0020	2500	0	0	0
Lin – log	0.150	0.0042	2435	65	0	0
Log – log	0.064	0.0006	2500	0	0	0
Sqrt – lin	0.089	0.0027	2500	0	0	0
Sqrt – log	0.075	0.0019	2500	0	0	0
Radiative Capture						
Insqrt – lin	0.348	0.0002	2499	0	1	0
Lin – lin	0.386	0.0002	2499	0	1	0
Lin – log	0.384	0.0002	2499	0	1	0
Log – log	0.359	0.0002	2499	0	1	0
Sqrt – lin	0.361	0.0002	2499	0	1	0
Sqrt – log	0.371	0.0002	2499	0	1	0

Note: The results of Elastic Scatter are exactly the same with Total cross-section.

IV.E. B10 and H1 Cross-Section

Wide temperature interval can also be applied to B10 and H1. Showed in Table XI, the maximum relative difference is < 0.05%. To such light nuclide, elastic scatter cross-section interpolation doesn't perform as well as radiative capture for its value is more sensitive to temperature change within the neutron energy range 0 to1eV (showed in Figure 7 and 8).

TABLE XI[5]

Results for Interpolating the Total, Elastic Scatter, and Radiative Capture Cross-Sections over the Temperature Interval 500 to 600K for B10 and H1 at 575K using log-log scheme

Reaction Type	Maximum Relative Difference (%)	Average Relative Difference (%)	Number of Pointwise Cross-Sections (total = 41596) Relative Difference [0, 0.1%]	Relative Difference (0.1%, ∞)
B10 (Quantity of points in energy grid = 687)				
Total	0.0001	<0.0001	687	0
Elastic Scatter	0.0412	0.0030	687	0
Radiative Capture	0.0001	<0.0001	687	0
H1 (Quantity of points in energy grid = 404)				
Total	0.0411	0.0050	404	0
Elastic Scatter	0.0413	0.0049	404	0
Radiative Capture	0.0001	<0.0001	404	0

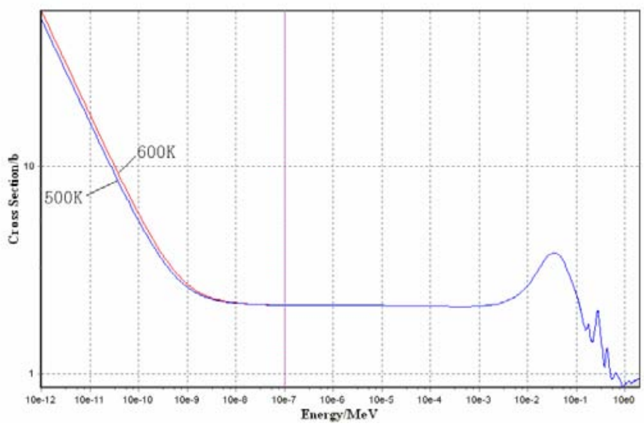

Fig. 7. B10 Elastic Scatter cross-section as a function of neutron energy at two temperatures, generated by NJOY.

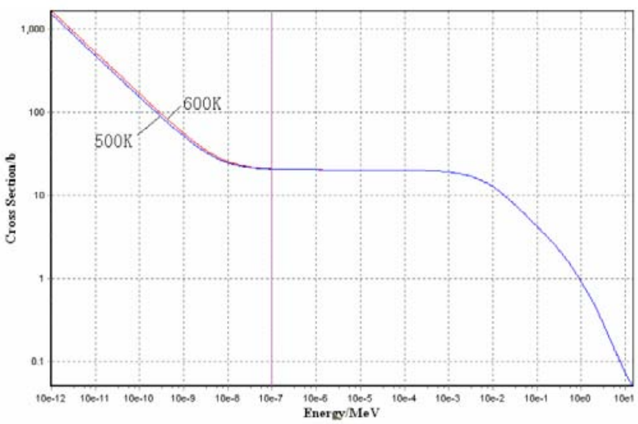

Fig. 8. H1 Elastic Scatter cross-section as a function of neutron energy at two temperatures, generated by NJOY.

IV.F. The Major Cause to Interpolating Error

Together with table I, figures 2 to 5 suggest the interpolating error is dominated in resonance area where energy points vary very much with the temperature changes. Listed in table VI, of the 1258 points exceeding 0.1% relative difference target for U238 radiative capture reaction, all their corresponding energy values are not found in the standard energy grid. Figure 9 tells the detail.

Showed in Fig 9, maximum relative difference for U238 radiative capture cross-section happened in the lowest point of the red line. Its corresponding energy value 0.003394801 MeV was definitely not found in energy grid of ACE-U238@550K (the black line). ITND program treated energy gird in ACE-U238@550K as the standard and mistook it to be the energy grid of ACE-U238@575K. This inaccurate simulation is unavoidable, because the energy grid of ACE at desired temperature was unknown in prior.

The loss of energy points is the major cause to interpolating error. The maximum relative difference 10.97% in radiative capture reaction for nature Zr also approves this trace.

As light nuclide, such as H1, contains no resonance energy range, the point loss phenomenon is so little that it could be neglected. Such advantage provides light nuclide a good candidate for interpolation.

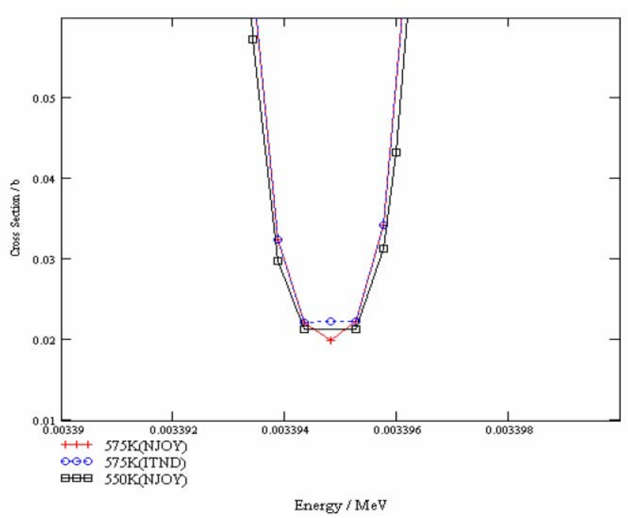

Fig. 9. The maximum relative difference for U238 radiative capture cross-section using typical interpolation scheme.

IV.G. Interpolated Cross-Section Tests

a. Simple PWR fuel cell calculation

Model of this fuel cell is briefly showed in Figure 10. Its parameters are listed in table XII. ITND interpolating schemes are also listed in table XII. We performed the test under two kinds of temperature intervals, results are listed in table XIII.

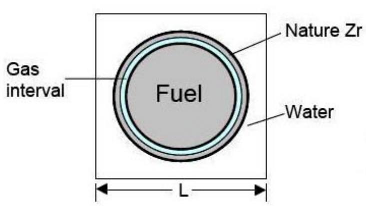

Fig. 10. Model figure for PWR fuel cell.

TABLE XII

Parameters for PWR fuel cell using in this test

Parameter	Value
Material of this model	H1,N14,O16, Nature Zr,U235,U238
Diameter for fuel	8.43 mm
Diameter for fuel cladding's inner circle	8.6 mm
Diameter for fuel cladding's outer circle	10.0 mm
L	12.6 mm
Density of fuel	10.41 g/cm^3
Fuel enrichment	3.1%
Density of zirconium cladding	6.57 g/cm^3
Material temperature	568 K
Temperature interval 1	500 to 600K
Temperature interval 2	400 to 500 to 600 to 700K
Standard energy grid comes from	ACEs at 600K
Interpolation scheme	Log-log

TABLE XIII

Results for this PWR model test using MCNP (Version 4C)

ACEs generated by	Keff for this PWR model
NJOY	1.35726±0.00058
ITND (Temperature interval 1)	1.35788±0.00063
ITND (Temperature interval 2)	1.35725±0.0006

b. Simple fast reactor fuel cell calculation

We conducted this model test to examine the validity of interpolated cross-sections within high neutron energy range. Geometric structure of simple fast reactor fuel cell is identical to the PWR fuel cell as showed in figure 10. Detail parameters are deleted in this paper to avoid redundancy. To all nuclides, we used 4th degree Lagrangian Interpolation and log-log scheme, fuel materials are set to 600K. Results are showed in Table XIV.

TABLE XIV

Results for this fast reactor model test using MCNP (Version 4C)

ACEs generated by	Keff for this PWR model
NJOY	1.0780 ± 0.0003
ITND (Temperature interval*)	1.0778 ± 0.0003

* Temperature interval: 400 to 500 to 700 to 800K.

V. Conclusion

Interpolation of cross-sections provides an alternative and convenient way to generate ACE, especially for temperature changing problem without prior knowledge of the final temperature distribution. By now, ITND program can finish 2nd degree Lagrangian Interpolation for U235 within 1.5s, and it costs no more than 3s to accomplish the 4th degree Lagrangian Interpolation. By inserting this interpolation program into MCNP codes, we can really perform temperature based Monte Carlo calculations without extra preparation of specific ACE files. Cross-sections can be calculated "on the fly" for any temperature.

The loss of points in standard energy grid significantly increased interpolation error. For such a reason, materials with complex resonance behavior, such as U238, require narrow temperature intervals and high degree Lagrangian Interpolation polynomial to reduce the relative differences. Of the six interpolation schemes examined, the log-log interpolation scheme performed the best. This scheme generally resulted in lower average and maximum relative differences and a greater number of points under the 0.1% target. All interpolation cases turn to have a better result with the use of "temperature adjacent strategy".

Two MCNP simulation tests approved the validity of interpolated cross-sections. Keff values stay the same for three digits below decimal point for both PWR and fast reactor cell model.

VI. Reference

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