International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

ON-THE-FLY DOPPLER BROADENING for MONTE CARLO CODES

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ABSTRACT

A methodology to allow on-the-fly Doppler broadening of neutron cross sections for use in Monte Carlo codes has been developed. The Monte Carlo code only needs to store 0K cross sections for each isotope and the method will broaden the 0K cross sections for any isotope in the library to any temperature in the range 77K-3200K. The methodology is based on a combination of Taylor series expansions and asymptotic series expansions. The type of series representation was determined by investigating the temperature dependence of U238 resonance cross sections in three regions: near the resonance peaks, mid-resonance, and the resonance wings. The coefficients for these series expansions were determined by a regression over the energy and temperature range of interest. Since the resonance parameters are a function of the neutron energy and target nuclide, the ψ and χ functions in the Adler-Adler multi-level resonance model can be represented by series expansions in temperature only, allowing the least number of terms to approximate the temperature dependent cross sections within a given accuracy. The comparison of the broadened cross sections using this methodology with the NJOY cross sections was excellent over the entire temperature range (77K-3200K) and energy range. A Monte Carlo code was implemented to apply the combined regression model and used to estimate the additional computing cost which was found to be less than <1%.

Key Words: On-the-fly Doppler broadening, Monte Carlo particle transport, combined regression model, resonance absorption, temperature dependent cross sections

1. INTRODUCTION

Doppler broadening of nuclear cross sections is one of the most important phenomena during nuclear reactor operation. Resonance capture and fission cross sections change significantly due to the relative motion between the incoming neutron and the target nuclei. As the material temperature increases, the relative energy varies over a wider range due to the increase in the motion of the target nuclides. Summed over all resonance energies, the overall effect of the increased Doppler broadening at higher temperatures is to increase the total resonance absorption (or fission) in the material region, hence giving a strong neutronic feedback as a result of temperature changes.

For realistic, detailed reactor calculations, Monte Carlo codes are part of a multi-physics simulation involving thermal-hydraulic feedback to adjust temperatures and densities. This process can result in 1000s of material temperatures for which broadened cross sections are needed. Existing codes (e.g., MCNP[1]) were not designed to accommodate this need. The objective of this effort is to find a closed form expression in temperature to allow on-the-fly Doppler broadening of the cross sections for an unlimited number of material temperatures while maintaining a modest computing cost and at the same time accounting for interference effects between closely spaced resonances in the keV range.

Current Monte Carlo particle transport codes rely on nuclear data files generated at specific reference temperatures. These files are generated by Nuclear Data Processing (NDP) codes such as NJOY[2] which can produce temperature dependent point-wise and multi-group cross sections and related quantities using evaluated nuclear data in the ENDF format. Doppler broadening of the cross sections in NDP codes can be performed based on either the exact Doppler broadening equation or direct use of the resonance parameters.

The well-known exact Doppler broadening equation developed by Cullen[3] is given in Eq. 1,

$$\sigma(y,T_2)=\frac{1}{y^2}\left(\frac{1}{\pi}\right)^{\frac{1}{2}}\int_0^{\infty}[\sigma(x,T_1)]x^2\left\{\exp\left[-(x-y)^2\right]-\exp\left[-(x+y)^2\right]\right\}dx$$

$$y^2=\alpha E=\beta V^2,\quad x^2=\alpha E_r=\beta V_r^2,\quad \alpha=\frac{A}{k(T_2-T_1)},\quad \beta=\frac{M}{2k(T_2-T_1)} \qquad (1)$$

where $\sigma(y,T_2)$ and $\sigma(y,T_1)$ are the broadened and base cross sections at temperature T_2 and T_1 respectively. The velocity-like terms y and x are related to incoming neutron velocity V and relative velocity V_r, respectively. The relative velocity is defined as $V_r = |V - V_t|$ where V_t is the target nuclide velocity. However, the discretized form of the exact Doppler broadening expression in Eq. 1 requires an unacceptable computing time due to cost to evaluate complementary error functions. Therefore, exact Doppler broadening of the cross sections on-the-fly during the random walk of the neutrons in Monte Carlo codes has been found to be prohibitively expensive.

The psi-chi method[4,5,6] is the only single level resonance representation where Doppler broadening of cross sections can be performed based on the resonance parameters in NJOY. For large values of neutron energy, the second exponential can be ignored in Eq. 1. However, this approximation overestimates the Doppler-broadened cross sections for lower values of neutron energy. Secondly, since the significant contribution to the remaining integral usually comes from a very narrow range of E_r close to E, $\sqrt{E_r}$ can be expanded in Taylor series about E. Ignoring the higher terms leads to the following equation, where the error introduced increases with decreasing energy:

$$\alpha\left(\sqrt{E_r}-\sqrt{E}\right)^2 \approx \left[(E_r-E)/\Delta\right]^2 \quad \text{where } \Delta=2(E_A/\alpha)^{1/2}=(4k\Delta TE_A/A)^{1/2} \text{ and } \Delta T=T_2-T_1 \qquad (2)$$

The last approximation introduced for the psi-chi method is to change the lower limit of integration to $-\infty$ and assume that the interval $(-\infty,0)$ has negligible contribution to the integral:

$$\sqrt{E}\sigma(E,T_2)=\frac{1}{\Delta\sqrt{\pi}}\int_{-\infty}^{\infty}\sqrt{E_r}\sigma(E_r,T_1)\exp\left\{-\left[\frac{(E_r-E)}{\Delta}\right]^2\right\}dE_r \tag{3}$$

Since the psi-chi method assumes that the 0K cross sections are composed of a series of single-level Breit-Wigner resonances, the Doppler-broadened cross sections become:

$$\sigma_{cap,fis}(E,T)=\left(\frac{2}{\Gamma_T}\right)\left(\frac{E_R}{E}\right)^{1/2}A\psi(x,\xi_R)\qquad \sigma^{scat}(E,T)=\left(\frac{2}{\Gamma_T}\right)\left[A\psi(x,\xi_R)+B\chi(x,\xi_R)\right] \tag{4}$$

The psi-chi method is not as accurate as exact Doppler broadening because the terms important for energies less than about $16kT/A$ are neglected. More importantly, cross sections in current evaluations are not represented as a series of single-level Breit-Wigner resonances. Strong absorber nuclides use resonance formulations that differ from the single-level representations (e.g., multilevel Breit-Wigner, Reich-Moore, Adler-Adler, etc…). In the case of light nuclides, cross sections are usually tabulated functions or do not use resonance parameters.

The line shapes $\psi(x,\xi_R)$ and $\chi(x,\xi_R)$ for are given in terms of the complex functions in MC^2 code[7].

$$\psi(x,\xi_R)=\frac{\xi_R}{2\sqrt{\pi}}\mathrm{Re}\left\{\exp\left(\left[i\frac{(x+i)}{2}\xi_R\right]^2\right)erfc\left(-i\frac{(x+i)}{2}\xi_R\right)\right\} \tag{5}$$

$$\chi(x,\xi_R)=\frac{\xi_R}{2\sqrt{\pi}}\mathrm{Im}\left\{\exp\left(\left[i\frac{(x+i)}{2}\xi_R\right]^2\right)erfc\left(-i\frac{(x+i)}{2}\xi_R\right)\right\} \tag{6}$$

where $\xi_R\approx\Gamma_T/\Delta_R=\Gamma_T(A/4kTE_R)^{1/2}$, $x=2(E_r-E_R)/\Gamma_T$ and $y=2(E-E_R)/\Gamma_T$.

Another approach, proposed by Marable[8] of ORNL in the 1960s, requires resonance parameters in order to Doppler broaden the cross sections and was based on the phi-chi resonance representation. Therefore, this approach inherits all of the approximations inherent in the phi-chi approach mentioned above.

Other methods are based on the interpolation of the cross sections between the nuclear data files generated by NJOY at various reference temperatures. A detailed study was performed by Trumbull[9] from KAPL by applying several different interpolation schemes over various temperature intervals. It was found that small intervals less than 28K were required for nuclides with complex resonance behavior to achieve a target accuracy of 0.1% relative difference in cross sections.

All of methods summarized above to Doppler broaden cross sections for reactor physics applications are not practical and/or do not provide sufficient accuracy. They also require unacceptable amounts of storage, memory space, and computing time for realistic nuclear reactor configurations.

2. THEORY

The combined regression model to perform the Doppler broadening of the cross sections on-the-fly at the energy grid points for Monte Carlo codes is based on the series expansion of multi-level Adler-Adler resonance representation in temperature. The constants of the combined regression model were adjusted for the temperature range of 77K - 3200K to accommodate important fields of study as shown in Table 1.

Table I. Temperature Range and Corresponding Field of Study

Temperature Range (K)	Field of Study
77 - 293.6	Cold Neutron Physics
293.6 – 550	Benchmarking Calculations
550 – 1600	Reactor Operation
1600 – 3200	Accident Conditions

2.1. Development of the Regression Model

Adler-Adler[2] is the only multilevel model where cross sections can be Doppler broadened based on resonance parameters in NJOY. The fission and capture cross sections use the following form;

$$\sigma_{cap,fis}(E,\xi_R)=\frac{\pi\sqrt{E}}{k^2}\left\{\sum_R \frac{2}{\Gamma_{R,t}}\left[\left(G_R\psi(x,\xi_R)+H_R\chi(x,\xi_R)\right)\right]+A_1+\frac{A_2}{E}+\frac{A_3}{E^2}+\frac{A_4}{E^3}+B_1E+B_2E^2\right\} \quad (7)$$

where $x=2(E_r-E_R)/\Gamma_T$, $k=\left(2.196771\times10^{-3}\right)\sqrt{E}A/(A+1)$ is the neutron wave number, Φ_l is the phase shift, G_R is the symmetric total parameter, H_R is the asymmetric total parameter, the A_i and B_i are coefficients of the total background correction, and ξ_R represents the resonance parameters, which are fixed once the neutron energy and target nuclide are known. The terms G, H, A_i and B_i appropriate for the desired reaction are used. Interference effects are also taken into account in the keV range. Therefore, Adler-Adler is more accurate than psi-chi.

The quantities ψ and χ are the only temperature dependent functions in the multi-level Adler-Adler resonance representation. Since the resonance parameters are constant for a given neutron energy and nuclide, $\psi(T)$ and $\chi(T)$ may be expressed as expansions in T:

$$\psi_R(T)=\sum_i a_{R,i}\,f_i(T) \qquad \chi_R(T)=\sum_i b_{R,i}h_i(T) \quad (8)$$

where $a_{R,i}$ and $b_{R,i}$ are constants corresponding to the temperature dependent functions f_i and h_i. The multi-level Adler-Adler resonance formulation becomes;

$$\sigma_R^x(T) = A_R + \sum_{R'}\left[B_{R'}\psi(T) + C_{R'}\chi(T)\right]$$

$$\sigma_R^x(T) = A_R + \sum_{R'}\left[B_{R'}\sum_i a_{R',i} f_i(T) + C_{R'}\sum_i b_{R',i} h_i(T)\right]$$

$$\sigma_R^x(T) = A_R + \sum_i f_i(T)\sum_{R'} a'_{R',i} + \sum_i h_i(T)\sum_{R'} b'_{R',i}$$

$$\sigma_R^x(T) = A_R + \sum_i f_i(T) a''_i + \sum_i h_i(T) b''_i \qquad (9)$$

Constants in the above equations are specific to the reaction type for a given neutron energy and nuclide. Once the form of temperature dependence of the functions f_i and h_i is found, the constants in the above regression models can easily be adjusted by applying the real Doppler broadened cross sections over a given range of temperature.

For a given nuclide, cross sections at different resonance energy points show different temperature dependence. Therefore, the temperature dependence of the cross sections must be investigated by dividing the resonance regions into multiple sub-regions.

2.1.1. Doppler-broadened cross sections around the peak of a resonance

In this region, Doppler-broadened cross sections decrease with increasing material temperature. Energy grid points are located very closely to satisfy the given fractional tolerance criteria. For small values of $x = 2(E_r - E_R)/\Gamma_T$, the regression model based on the Taylor series expansion of ψ_R and χ_R in T can calculate the Doppler broadened cross sections ($E_r \cong E_R$ so $|x| \cong 0$) with the least number of terms in the expansion:

$$\psi_R(z) = \frac{\xi_R}{2\sqrt{\pi}}\,\mathrm{Re}\left\{\exp(z^2)\,erfc(-z)\right\} \qquad \chi_R(z) = \frac{\xi_R}{2\sqrt{\pi}}\,\mathrm{Im}\left\{\exp(z^2)\,erfc(-z)\right\} \qquad (10)$$

where $z = i(x+i)\xi_R/2$. Taylor series expansions for the exponential and complementary error function are given by

$$\exp(z^2) = \sum_{n=0}^{\infty}\frac{z^{2n}}{n!} \quad , \quad erfc(-z) = 1 + \frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(-1)^n z^{2n+1}}{n!(2n+1)} \qquad (11)$$

Since $\xi_R = \Gamma_T\left(A/4kE_RT\right)^{1/2}$, z can be written as $z = (a+bi)/\sqrt{T}$ for a given neutron energy and nuclide where a and b are constants. Therefore, we have;

$$\psi_R(T) = \frac{c}{\sqrt{T}} \mathrm{Re}\left\{ \exp\left[\left(\frac{a+bi}{\sqrt{T}} \right)^2 \right] erfc\left(-\frac{a+bi}{\sqrt{T}} \right) \right\} = \sum_{i=1}^{\infty} \frac{a_{R,i}}{T^{i/2}} \tag{12}$$

$$\chi_R(T) = \frac{c}{\sqrt{T}} \mathrm{Im}\left\{ \exp\left[\left(\frac{a+bi}{\sqrt{T}} \right)^2 \right] erfc\left(-\frac{a+bi}{\sqrt{T}} \right) \right\} = \sum_{i=1}^{\infty} \frac{b_{R,i}}{T^{i/2}} \tag{13}$$

2.1.2. Doppler-broadened cross sections around the end of the resonance wings

In this region, Doppler-broadened cross sections increase with increasing material temperature. Energy grid points are widely spaced due to slowly varying behavior of the cross sections as a function of energy. For large values of x, the regression model based on the asymptotic expansion of ψ_R and χ_R in T can calculate the Doppler broadened cross sections with the least number of terms in the expansion,

$$erfc(-z) = -\frac{e^{-z^2}}{z\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{n!(2z)^{2n}} \tag{14}$$

This equation can be rewritten as;

$$\exp(z^2) erfc(-z) = -\frac{1}{z\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{n!(2z)^{2n}} \tag{15}$$

where $z = i(x+i)\xi_R/2$. Since $\xi_R = \Gamma_T \left(A/4kE_R T \right)^{1/2}$, z can be written as $z = (a+bi)/\sqrt{T}$ for a given neutron energy and nuclide where a and b are constants. Therefore we have;

$$\psi_R(T) = \frac{c}{\sqrt{T}} \mathrm{Re}\left\{ \exp\left[\left(\frac{a+bi}{\sqrt{T}} \right)^2 \right] erfc\left(-\frac{a+bi}{\sqrt{T}} \right) \right\} = \sum_{i=0}^{\infty} a_{R,i} T^i \tag{16}$$

$$\chi_R(T) = \frac{c}{\sqrt{T}} \mathrm{Im}\left\{ \exp\left[\left(\frac{a+bi}{\sqrt{T}} \right)^2 \right] erfc\left(-\frac{a+bi}{\sqrt{T}} \right) \right\} = \sum_{i=0}^{\infty} b_{R,i} T^i \tag{17}$$

2.1.3. Doppler-broadened cross sections around the middle of the resonance wings

In this region, Doppler-broadened cross sections first increase and then decrease with increasing material temperature. For moderate values of $x = 2(E_r - E_R)/\Gamma_T \approx 1$, it was not easy to find a physical basis to chose a particular series representation in T. Therefore a computational investigation was performed for energy grid points in this region to obtain the best series representation among several models. The SSE (sum of squares error) and RMSE (root mean square error) error terms were monitored to find the best fit for the range of resonance cross sections in this region. The results are presented in Table 2.

As can be seen in Table 2, the second series representation provides the best accuracy among the others for a fixed number of terms. Actually, since $\xi_R \approx \Gamma_T / \Delta_R = \Gamma_T \left(A/4kTE_R\right)^{1/2}$, the width of a given resonance changes proportionally with $\sqrt{T}$ and this is observed around the middle of the resonance wings where the resonance width is defined.

Table II. Comparison of Different 12th–Order Regression Models

	6.630eV		6.619eV		6.609eV	
	SSE	**RMSE**	**SSE**	**RMSE**	**SSE**	**RMSE**
$\sum_{n=0}^{12} a_n (T)^n$	1.23E+04	1.99E+00	8.98E+03	1.70E+00	1.72E+04	2.35E+00
$\sum_{n=0}^{12} a_n (T)^{n/2}$	2.94E+00	3.07E-02	2.66E+01	9.25E-02	2.68E+01	9.29E-02
$\sum_{n=0}^{12} a_n (\ln T)^n$	3.13E+08	3.17E+02	4.12E+08	3.64E+02	4.36E+08	3.75E+02
$\sum_{n=0}^{12} a_n (\ln T)^{n/2}$	2.94E+08	3.07E+02	4.07E+08	3.62E+02	3.70E+08	3.45E+02

2.1.4. Combined Doppler broadening model

Cross sections for the three energy regions (near the peak of the resonance, mid-resonance, and resonance wings) for any resonance based on the Adler-Adler multi-level representation can be summarized as follows:

$$\sigma_{cap,fis}^{\sim peak}(T) = \sum_{i=0}^{\infty} \frac{e_i}{T^{i/2}}, \quad \sigma_{cap,fis}^{mid-res}(T) = \sum_{i=0}^{\infty} f_i T^{i/2}, \quad \sigma_{cap,fis}^{wings}(T) = \sum_{i=0}^{\infty} g_i T^i \tag{18}$$

Several important resonances of U^{238} were analyzed to decide the number of terms to be for each of the series expansions in Eq. (18). The best form of the combined regression model for the resonances of U^{238} was found to be:

$$\sigma_{cap,fis}(T) = \sum_{i=1}^{6} \frac{a_i}{T^{i/2}} + \sum_{i=1}^{6} b_i T^{i/2} + c \tag{19}$$

where a_i, b_i, c are the constants of the above regression model and appropriate for a given type of reaction. The combined regression model requires the pre-generated temperature dependent cross sections at every 1K to adjust the constants in Eq. 19. However, NJOY cannot generate Doppler-broadened cross sections based on the 0K cross sections while at the same time keeping the 77K energy grid points the same for the temperature range of interest [77K-3200K]. Therefore, an Auxiliary Doppler Code (ADC) was implemented to perform the required task. ADC was tested against NJOY at different reference temperature points for several resonance absorbers and it was found that ADC is exactly the same as NJOY. ADC is required to preprocess the 0K cross

section data for the temperature range of interest. Once the cross sections at the energy grid points are calculated correctly by the regression model, linear interpolation can be performed to find the cross section for the given incoming neutron energy. In addition, scattering cross sections are broadened with the same methodology as the capture and fission cross sections.

3. RESULTS

The combined Doppler broadening regression model equation developed in the previous section was applied to the discrete temperature dependent U238 absorption cross section data generated by ADC at every 1K interval between 77K and 3200K. Constants of the model equation were adjusted by least squares linear regression.

3.1. Maximum Relative Error Analysis

After applying our regression model equation to the discrete temperature dependent U238 absorption cross section data at every energy grid point, the maximum relative differences (%) in cross sections were calculated:

$$\text{Max. Relative Diff. (\%)} = \frac{\sigma_a^{Exact}(T) - \sigma_a^{Model}(T)}{\sigma_a^{Exact}(T)} x100 \qquad (20)$$

Results were compared with the equivalent simple polynomial regression model of degree N-1 as shown in Figure 1.

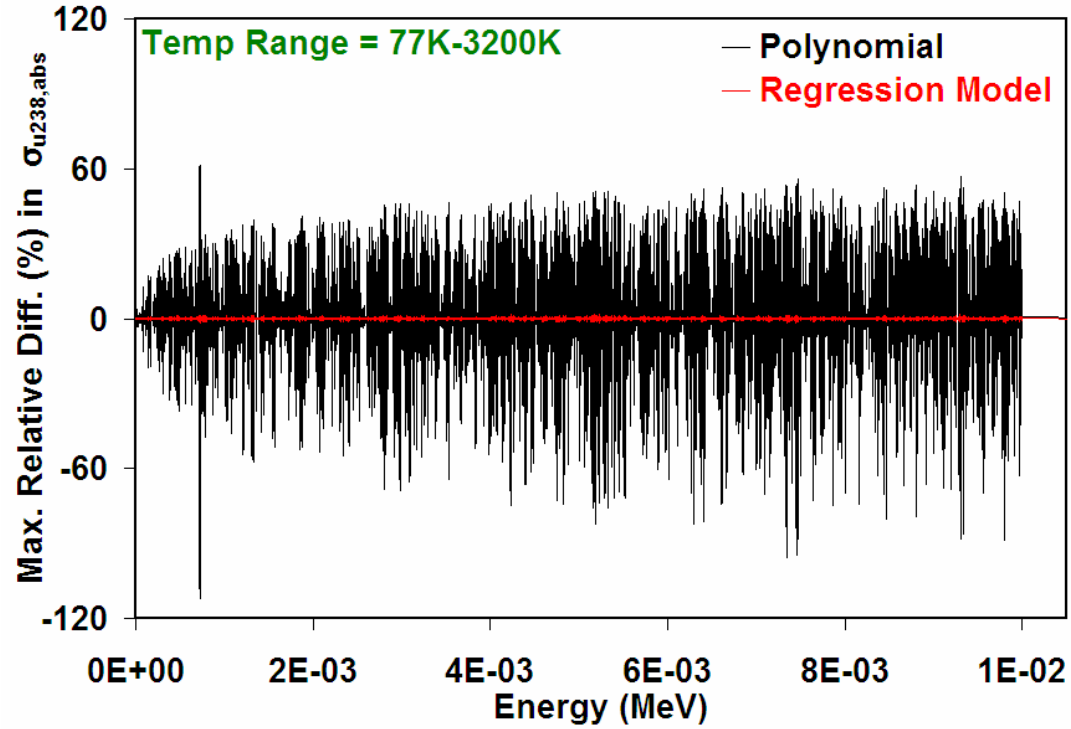

Figure 1. σ_a^{U238} as a function of energy

It was found that our regression model equation can accurately calculate the temperature dependent cross section using N=13 constants adjusted by least squares linear regression. For comparison, an equivalent polynomial regression model of degree N-1 was used resulting in maximum relative differences around 3-4% for the resonances in eV region and up to 100% in the keV region as shown in Figure 1.

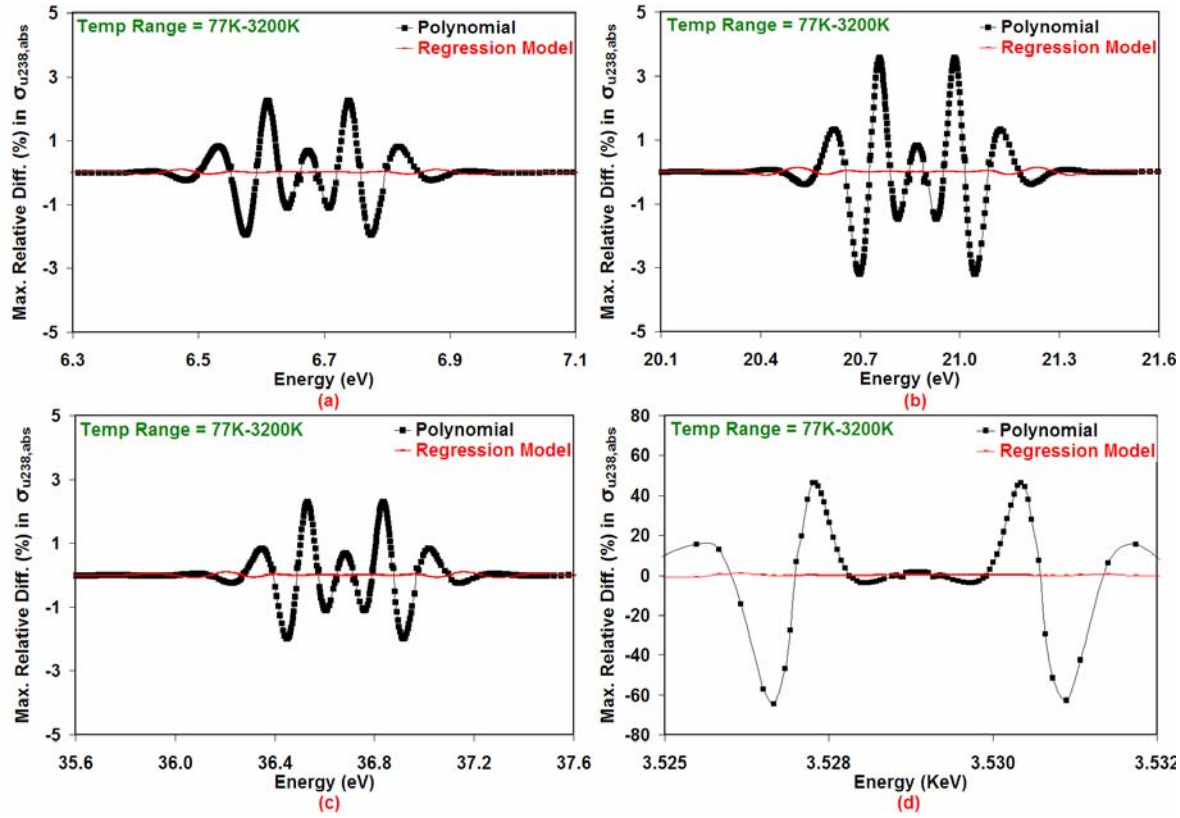

Figure 2. Maximum relative difference (%) for σ_a^{U238} at selected resonance energy grid points

3.2. Residual Error Analysis

Residuals for U238 absorption cross sections at selected energy grid points of important resonances were calculated between 77K and 3200K by applying our linear regression model equation. Results were compared with the equivalent simple polynomial regression model of degree N-1 as shown in Figure 3. The residual error is defined as follows:

$$\text{Residual error} = \sigma_a^{Exact}(T) - \sigma_a^{Model}(T) \tag{21}$$

As seen in Figure 3a, the maximum residual in σ_a^{U238} was calculated as 6E-7 barns with our regression model equation at 77K. Residuals in σ_a^{U238} decrease down to 1E-9 barns as the temperature increases. With the equivalent polynomial model, the residuals change from 5 to 35 barns for those selected energy grid points of important resonances as shown in Figures 3b, 3c and 3d.

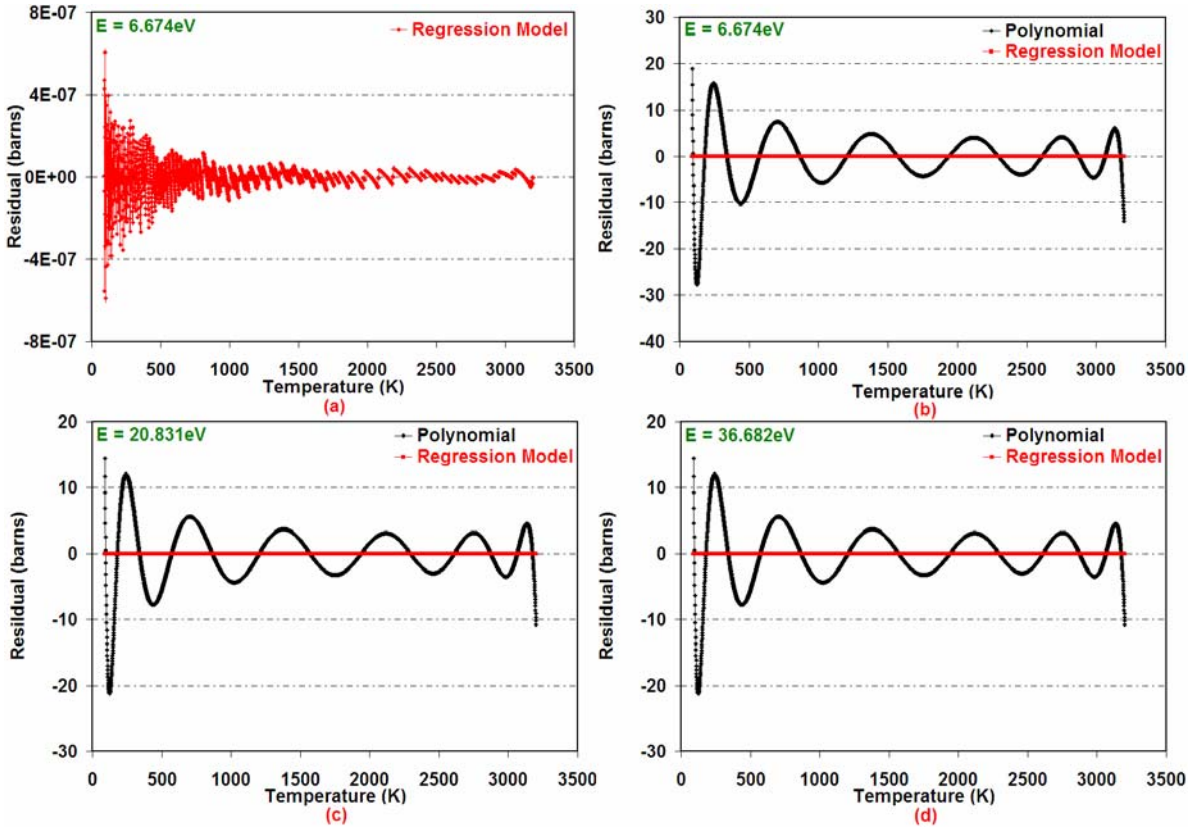

Figure 3. Residual scatter for σ_a^{U238} at selected resonance energy grid points

3.3. Goodness of the Linear Regression Model

Another way to look at the goodness of the proposed combined regression model is to calculate the SSE and RMSE over a given temperature range. The SSE statistic measures the total deviation of the response values from the fit to the response values. It is also called the summed square of residuals. The RMSE statistic is also known as the fit standard error or the standard error of the regression. The SSE and RMSE statistics are defined in Eq. 22:

$$\text{SSE} = \sum_{T=77}^{3200}\left[\sigma_a^{Exact}(T) - \sigma_a^{Model}(T)\right]^2 \qquad \text{RMSE} = \sqrt{\frac{SSE}{\nu}} \tag{22}$$

where $\nu = n - m$ is the residual degrees of freedom is defined as the number of response values n minus the number of fitted coefficients m estimated from the response values. The quantity ν indicates the number of independent pieces of information involving the n data points that are required to calculate the sum of squares. For a given temperature range of 77K-3200K and 13 constants in the model equation, ν=(3200-77+1)-13=3111.

Plots of SSE and RMSE near selected important resonances of σ_a^{U238} are shown in Figure 4. It can be seen that both SSE (~1E-11) and RMSE (~6E-8) are very close to zero indicating an outstanding fit of the data to the combined regression model.

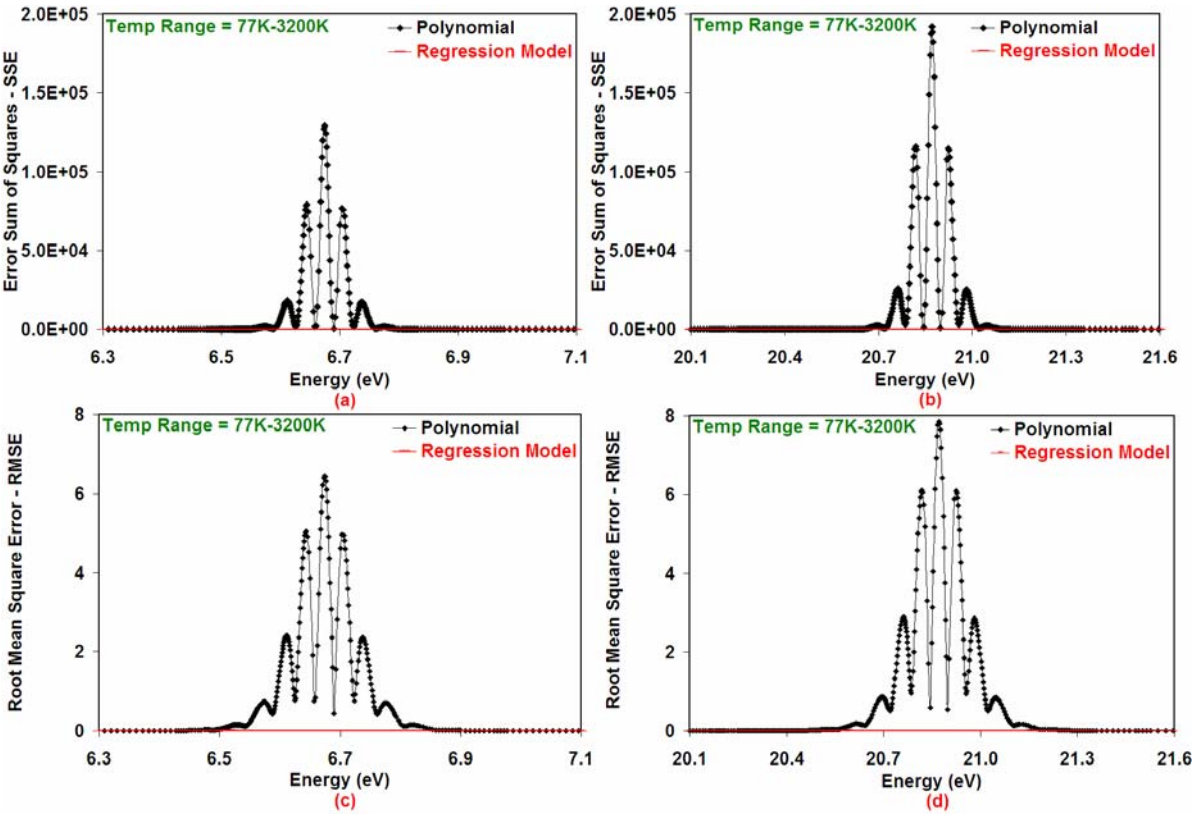

Figure 4. SSE and RMSE around selected important resonances of σ_a^{U238}

3.4. Timing

A Monte Carlo Code was implemented in C++ to determine the computing cost of our regression model equation to calculate the cross sections at the energy grid points with on-the-fly Doppler broadening. It was observed that the additional computing cost to evaluate the three sets of cross sections (σ_t, σ_a and σ_f) at a collision site by the combined regression model Eq. 19 is less than 1% of the conventional approach where cross sections are linearly interpolated between the energy grid points.

4. CONCLUSIONS

A combined regression model was derived based on the multi-level Adler-Adler resonance representation. The proposed model can broaden the cross sections at the energy grid points of a given nuclide accurately over the energy range and temperature range of interest (77K-3200K). The maximum errors compared to the NJOY approach is less than 1E-6% over the peak and mid-resonance regions for U-238. For the wings of the U238 resonances, the cross section difference was less than 0.01% or so but the absolute difference was negligible because the cross sections are so small in this range. This should be compared with a maximum relative difference of up to 100% for all regions with the equivalent polynomial regression model.

Existing Monte Carlo codes store one NJOY-processed cross section dataset for every temperature. This severely inhibits the use of Monte Carlo in multiphysics calculations (e.g., coupling MC to T/H codes), since many 1000s of temperatures may be required, resulting in prohibitive amounts of memory storage. On-the-fly Doppler broadening removes these issues (minimal storage and essentially no increase in computer time), and will be a key enabler for more realistic multiphysics calculations.

Since there is no need to store the Doppler broadened cross sections, one can analyze an unlimited number of temperature regions as will occur for realistic, detailed reactor calculations involving thermal-hydraulic feedback.

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