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CHAIN RULE APPROACH FOR CALCULATING THE TIME-DERIVATIVE OF FLUX

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Abstract:

The reaction history (gamma-flux observable) is mathematically studied by using the chain rule for taking the total-time derivatives. That is, the total time-derivative of flux is written as the product of the ion temperature derivative with respect to time and the derivative of the flux with respect to ion temperature. Some equations are derived using the further simplification that the fusion reactivity is a parametrized function of ion temperature, *T*. Deuterium-tritium (D-T) fusion is used as the application with reactivity calculations from three established reactivity parametrizations.

Introduction

We begin with the definition for alpha as the logarithmic time-derivative of flux:

$$\alpha = \frac{\frac{d\overset{*}{\gamma}}{dt}}{\overset{*}{\gamma}} = \frac{d\ln\overset{*}{\gamma}}{dt} \tag{1}$$

The observable gamma-flux is denoted as γ-dot (or *flux*) for flux of gammas from fusion. All notation listed as "dot" is a derivative with respect to time. All notation listed as "prime" is a derivative with respect to ion temperature *T*. The fusion reactant ion temperature is denoted *T* in keV. In this paper, the chain rule is applied to study the total-time-derivative of flux in Eq. 1. Use of the chain rule gives a simple relationship for flux-change with respect to time: it is the product of the temperature time-derivative, T-dot, and flux change with *T*:

$$\alpha = \frac{\frac{d\overset{*}{\gamma}}{dt}}{\overset{*}{\gamma}} = \frac{\overset{*}{T}}{\overset{*}{\gamma}}\frac{d\overset{*}{\gamma}}{dT} \tag{2}$$

This approach is used for understanding the sensitivity of alpha, α, to temperature regimes and extrema, where

$$\left.\frac{d\alpha}{dt}\right|_{extremum} = 0 \tag{3}$$

The gamma-flux is related to the fusion reactivity, <σν(*T*)>:

$$\dot{\gamma} = n_D n_T < \sigma v(T) > V \tag{4}$$

where n_D and n_T are number densities (cm^{-3}), velocity v (cm/sec), σ cross section (cm^2) and volume V containing the D-T fusion reactants at temperature T.

Alpha Derivatives Development

Substituting Eq. (4) into Eq. (1) produces

$$\alpha(t) = \frac{d\ln(n_D n_T < \sigma v(T) >_{DT} V)}{dt}, \tag{5}$$

or equivalently

$$\alpha(t) = \frac{d\ln(n_D)}{dt} + \frac{d\ln(n_T)}{dt} + \frac{d\ln(\mathrm{V})}{dt} + \frac{d\ln(< \sigma v(T) >)}{dt}. \tag{6}$$

Using the “dot” notation, Eq. (6) becomes:

$$\alpha(t) = \frac{\dot{n}_D}{n_D} + \frac{\dot{n}_T}{n_T} + \frac{\dot{V}}{V} + \frac{d(< \sigma v(T) >)/dt}{< \sigma v(T) >}. \tag{7}$$

Now consider the event that the first three terms in Eq. (7) can be neglected compared to the last term, such that

$$\frac{d(< \sigma v(T) >)/dt}{< \sigma v(T) >} >> \left[\frac{\dot{n}_D}{n_D} + \frac{\dot{n}_T}{n_T} + \frac{\dot{V}}{V}\right]. \tag{8}$$

Eq. (8) is not an unreasonable comparison because of the inverse relationship between volume, V, and total number density. With that inverse relationship, the right side of Eq. (8) is small.

Under the condition in Eq. (8) and applying the chain rule, $\alpha(t)$ is expressed as:

$$\alpha(t) = \dot{T} \cdot \frac{d(< \sigma v(T) >)/dT}{< \sigma v(T) >}. \tag{9}$$

The meaning of Eq. (9) is that when the logarithmic time-derivative of the number densities and volume can be neglected, then the alpha, for some temperature domain, depends on the product of the rate of temperature change and the temperature-derivative of the reactivity divided by the reactivity. Comparing right side definition of alpha in Eq. (2) to Eq. (9) gives an expression of the gamma-flux derivative in terms of this product.

$$\frac{d(<\sigma v(T)>)/dT}{<\sigma v(T)>} = \frac{1}{\overset{*}{\gamma}} \frac{d\overset{*}{\gamma}}{dT} \tag{10}$$

The implication of Eq. (10) is that the gamma-flux represents the reactivity under the condition Eq. (8). Even if that condition does not hold, then gamma-flux is at least proportional to the reactivity [1].

A direct measurement of gamma-rays with equipment that exhibits fast temporal response can be used to infer temperature change *T*-dot, if alpha can be measured. If alpha itself can be differentiated, (high signal-to-noise, high bandpass), then the following expressions in terms of function *f*, where *f(T)* represents the reactivity, can be produced. For example, $f_{DT} = <\sigma v(T)>_{DT}$.

The time-derivative of alpha from Eq. (1) is expressed as a function of temperature-derivatives of *f* and Eq. (10) as:

$$\frac{d}{dt}\alpha(t) = \frac{\ddot{T}}{f}\left(\frac{df}{dT}\right) + \frac{\dot{T}^2}{f}\left(\frac{d^2 f}{dT^2}\right) - \frac{\dot{T}^2}{f^2}\left(\frac{df}{dT}\right)^2 \tag{11a}$$

or using the prime notation for designation of temperature-derivatives:

$$\frac{d}{dt}\alpha(t) = \ddot{T}\left(\frac{f'}{f}\right) + \dot{T}^2\left(\frac{f''}{f}\right) - \dot{T}^2\left(\frac{f'}{f}\right)^2 \tag{11b}$$

It can be noted that Eq. (11) can be written in terms of α(*t*) and α(*t*) squared:

$$\frac{d\alpha(t)}{dt} = \alpha\frac{\ddot{T}}{\dot{T}} + \dot{T}^2\left(\frac{f''}{f}\right) - \alpha^2 \tag{12}$$

or

$$\alpha^2 = \alpha\frac{\ddot{T}}{\dot{T}} + \dot{T}^2\left(\frac{f''}{f}\right) - \frac{d\alpha(t)}{dt} \tag{13}$$

Reactivity Parameterizations

Langenbrunner and Makaruk [1] found derivatives with respect to ion temperature, *T*, for D-T fusion reactivity found in the U.S. Naval Research Lab (NRL) [2] formulary. The present work uses the NRL parameterization of reactivity in comparison to two other commonly established parameterizations of reactivity from Caughlan & Fowler (C&F) [3] and Bosch & Hale (B&H) [4]. The D-T fusion reactivity, $f(T) = <\sigma v(T)>$, is a function of *T* at low energy (*T* < 25 keV) and is averaged over a Maxwellian velocity distribution.

The NRL reactivity parameterization [2] is

$$f(T) = A_0 T^{-2/3} \exp(-A T^{-1/3}) \tag{14}$$

For the D-T fusion reaction, the parameters are A=19.94 and A_0=3.68 x 10^{-12}. Reactivity has units of $\mathrm{cm}^3\ \mathrm{sec}^{-1}$. Langenbrunner and Booker verified other fusion parameterizations [5].

The Caughlan & Fowler original parameterization [3] is given as a reaction rate (*RR*):

$$RR = N_A f(T9) \tag{15}$$

where N_A is Avogadro's number, and where temperature $T9$ is in units of a billion degrees Kelvin. This *RR* parameterization and the use of $T9$ are the convention for stellar nucleosynthesis.

$$f(T9) = \frac{1}{N_A} \left[\begin{array}{l} B_0/\mathrm{T9}^{2/3} \cdot \exp(B_1/\,\mathrm{T9}^{1/3} \text{-} \{\mathrm{T9}/B_2\}^2) \cdot \\ {[1.0 + B_3 \cdot \mathrm{T9}^{1/3} + B_4 \cdot \mathrm{T9}^{2/3} + B_5 \cdot \mathrm{T9} + B_6 \cdot \mathrm{T9}^{4/3} + B_7 \cdot \mathrm{T9}^{5/3}]} \\ + B_8/\mathrm{T9}^{2/3} \cdot \exp(B_9/\mathrm{T9}) \end{array} \right] \tag{16}$$

For the D-T fusion reaction, the C&F parameters are B_0=8.09x10^{10}, B_1=-4.524, B_2=0.120, B_3=0.092, B_4=1.80, B_5=1.16, B_6=10.52, B_7=17.24, B_8=8.73x10^8 and B_9=-0.523. The conversion between $T9$ and T(keV) is $T9=0.0116T$.

The Bosch & Hale parameterization [4] is their 1992 revision:

$$f(T) = C_1 \theta \sqrt{\xi / (mc^2 T^3)} \exp(-3\xi)$$

$$\text{where } \theta = T \Bigg/ \left(1 - \frac{(C_2 T + C_4 T^2 + C_6 T^3)}{(1 + C_3 T + C_5 T^2 + C_7 T^3)} \right) \text{ and } \xi = \frac{C_0^2}{(4\theta)^{1/3}}. \tag{17}$$

For the D-T fusion reaction, the B&H parameters are C_0=34.3827, C_1=1.17 x 10^{-9}, C_2=1.51 x 10^{-2}, C_3=7.52 x 10^{-2}, C_4=4.61 x 10^{-3}, C_5=1.35 x 10^{-2}, C_6=-1.07 x 10^{-4}, and C_7=1.37 x 10^{-5}. This parameterization was chosen because it was found to provide best reactivity values among the set examined in [5], which included comparison to data. Its major disadvantage is the complicated structure for taking higher order derivatives with respect to T.

The temperature-derivatives for these three reactivity parameterizations, Eq. (14), (16) and (17), are given in the Appendix.

Alpha Derivatives Investigation

Eq. (11) can be rewritten to emphasize the temperature derivatives of reactivity:

$$\frac{d\alpha}{dt}=\ddot{T}\left(\frac{f'}{f}\right)+\dot{T}^{2}\left(\left(\frac{f''}{f}\right)-\left(\frac{f'}{f}\right)^{2}\right). \tag{18}$$

It appears clear that the temperature-derivatives of the fusion reactivity could play an important role in the shape of $\alpha(t)$, as do the time-derivatives of temperature. Graphic exploration of the behavior of the temperature-derivatives in Eq. (18) is provided in the figures below. Three reactivity parameterizations, NRL, B&H, and C&F, are compared in these temperature-derivative terms.

To investigate where $\frac{d\alpha}{dt}=0$, Eq. (18) can be rearranged to give the condition for an extremum as two ratios of derivatives:

$$\frac{\frac{(f')^{2}}{f}-\left(f''\right)}{f'}=\frac{\ddot{T}}{\dot{T}^{2}}. \tag{19}$$

The reactivity temperature-derivatives ratio on the left-hand-side (lhs) of Eq. (19) is known and available for all the fusion reactivity parameterizations, NRL, B&H, and C&F [2, 3, 4]. Understanding this ratio of temperature-derivatives is, in fact, the reason for the investigations done in [1, 5].

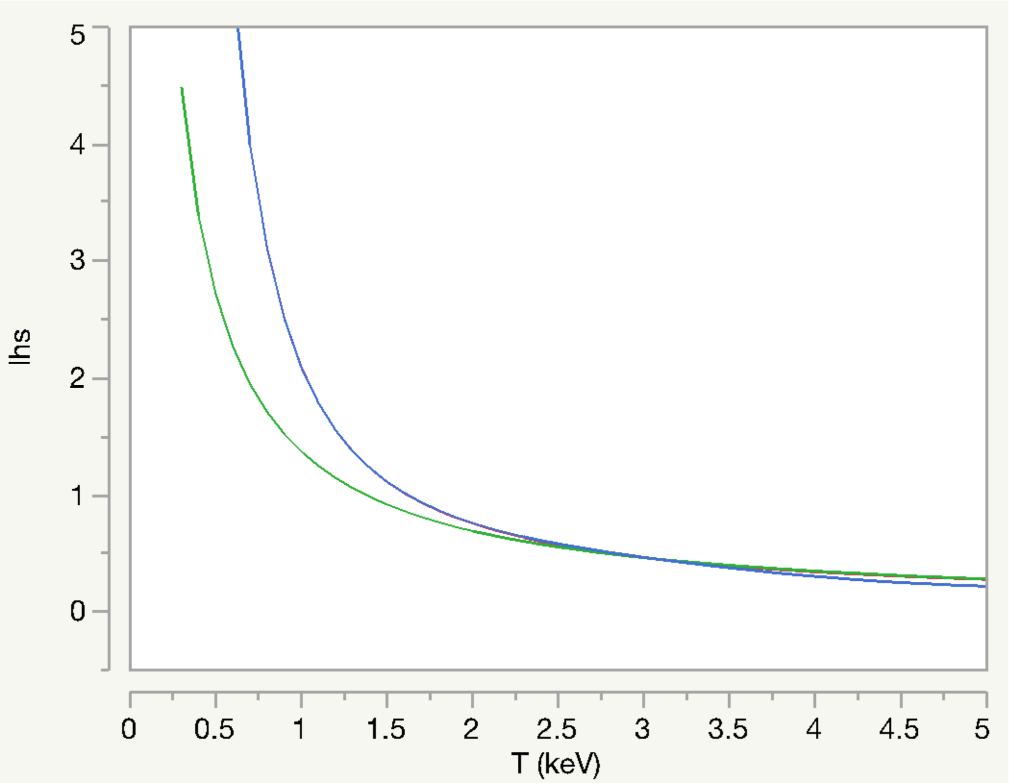

Figure 1. Left-hand-side (lhs) ratio in Eq. (19) with *T* for three D-T reactivity parameterizations— NRL (green), C&F (blue), B&H (red).

Figure 1 shows the behavior of this lhs in Eq. (19) for the NRL (green), C&F (blue), B&H (red) [2, 3, 4] reactivity parameterizations on a low *T* scale $0.2 < T < 5$ keV. The C&F and B&H values are so close that they appear as purple (red plus blue), and are larger than for NRL at $T < 1$ keV. C&F crosses beneath the NRL and B&H at $T = 3$ kev and fluctuates around B&H beyond that. While not shown, the asymptotic trailing off for all three parameterizations continues into larger values of $T < 30$ keV.

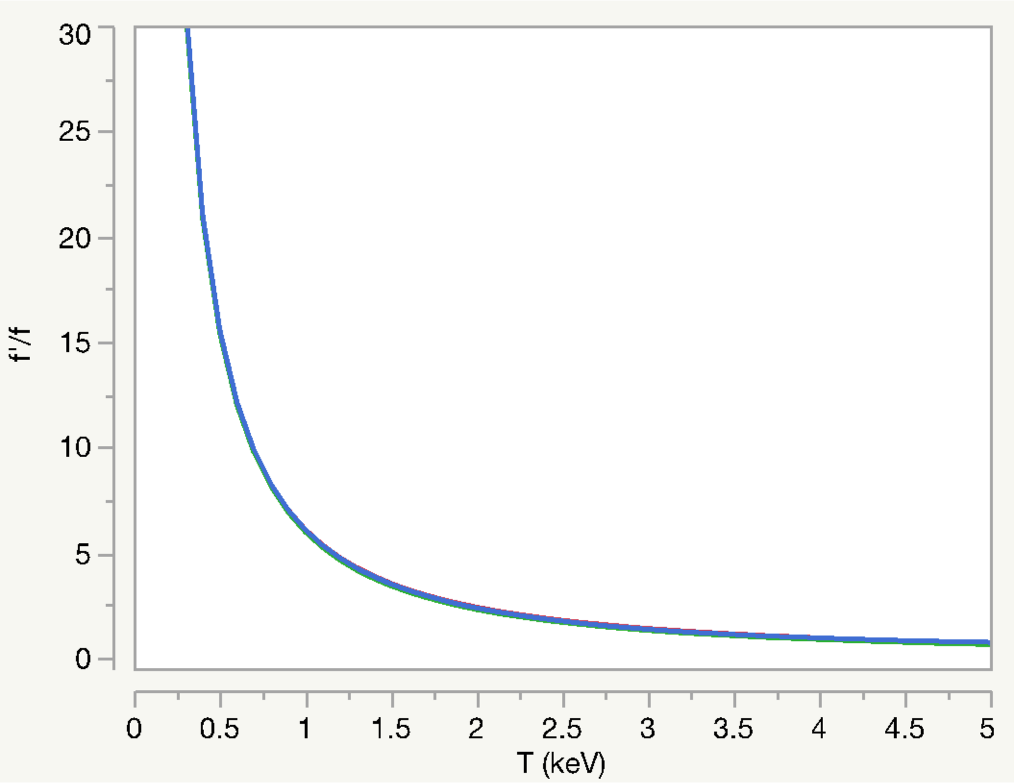

Figure 2. f'/f with T, the $\ddot{T}$ term in Eq. (19)—NRL (green), B&H (red), and C&F (blue).

The term multiplying the $\ddot{T}$ term in Eq. (18) is the ratio of the first temperature-derivative to the reactivity and is shown in Figure 2 for the three parameterizations. Again, NRL (green), B&H (red), and C&F (blue) reactivity f parameterizations are illustrated on a low T scale $0.2 < T < 5$ keV. All three parameterizations appear to be identical; however, there are differences in the first decimal place which cannot be resolved in the figure. This alignment is not unexpected because this term acts like a standardization of the first derivative scaled by the reactivity, minimizing any difference in reactivity parameterization. We intend to take up this point in a future publication.

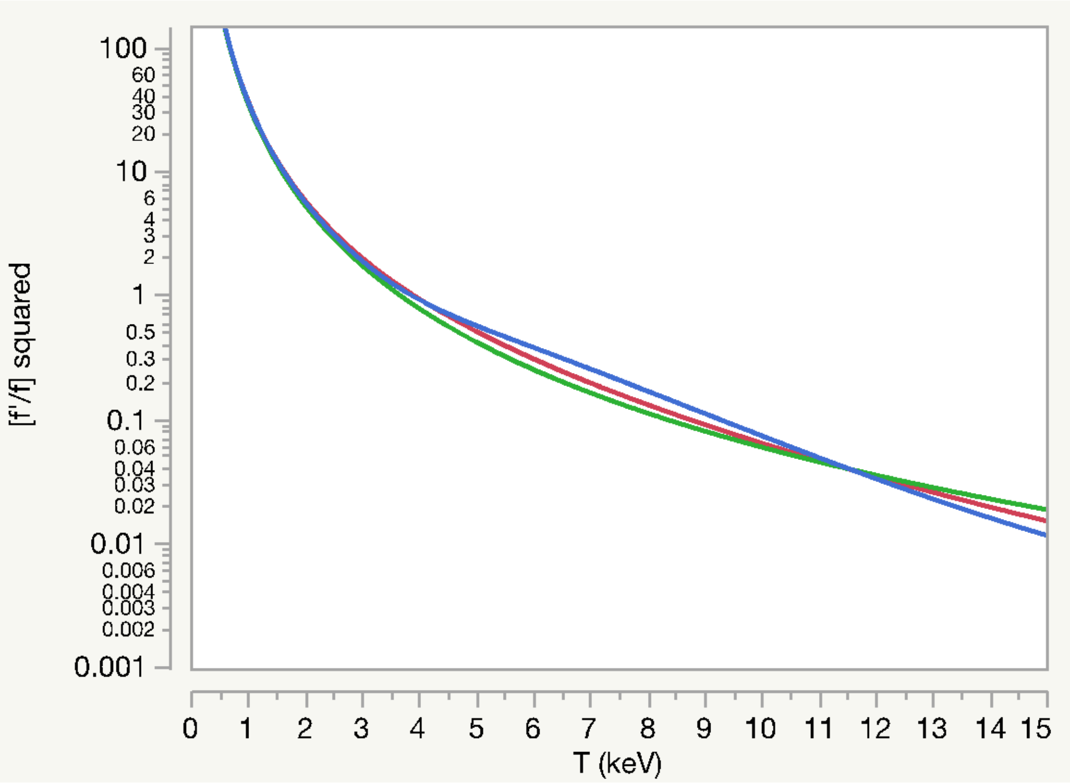

Figure 3. [f'/f]^2 on a log scale with longer T scale and log vertical scale to display differences—NRL (green), B&H (red), and C&F (blue).

Figure 3 shows the squared values plotted in Figure 2, which corresponds to the negative portion of the $\dot{T}^2$ term in Eq. (18). It is also the first term in the lhs of Eq. (19). This term also behaves as a standardization, resulting in all three parameterizations aligning at $T < 5$ keV. Note that the vertical scale is on a logarithmic scale. While not shown in Figure 3, the larger T values show some separation of the three reactivity parameterizations.

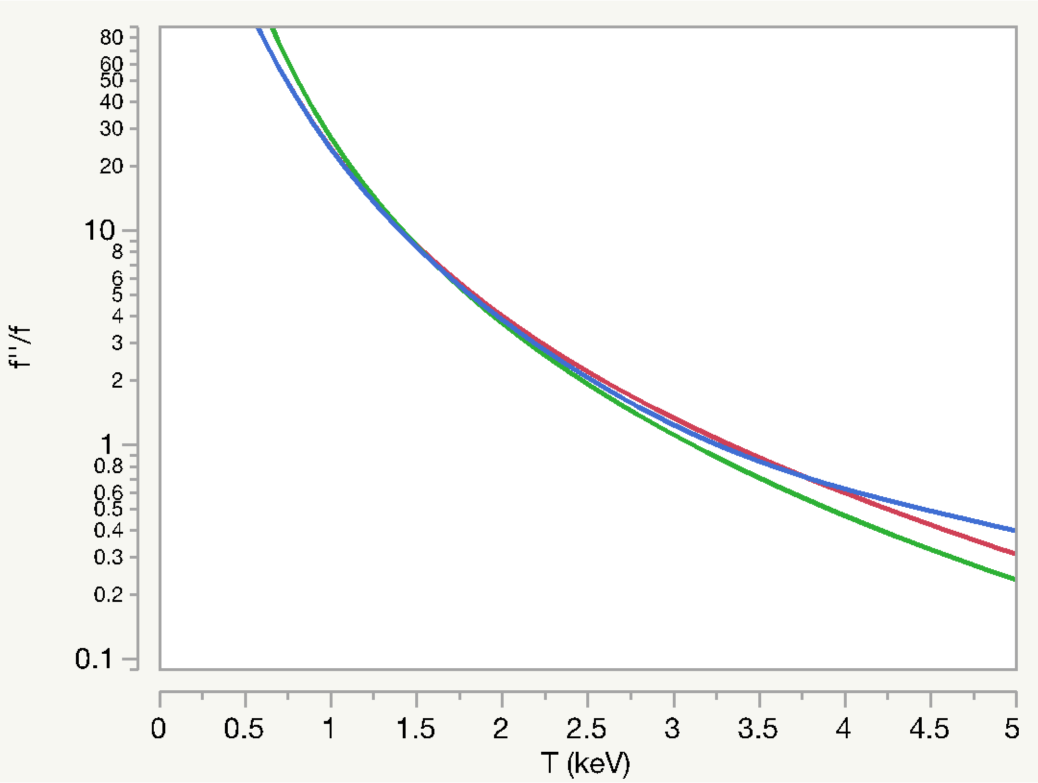

Figure 4. *f* ″/*f* on a log scale with *T* shows separation of NRL—NRL (green), B&H (red), and C&F (blue).

The positive portion of the $\dot{T}^2$ term in Eq. (18) is shown in Figure 4. While one might expect the standardization effect seen in Figure 2, the second derivative exhibits more nonlinear behavior even when divided by reactivity. The vertical scale is on a logarithmic scale. As with Figure 1, NRL separates somewhat from the others. As with Figure 3, there is some separation among the three parameterizations with higher *T* values. That separation becomes more prominent at higher values of *T* than shown.

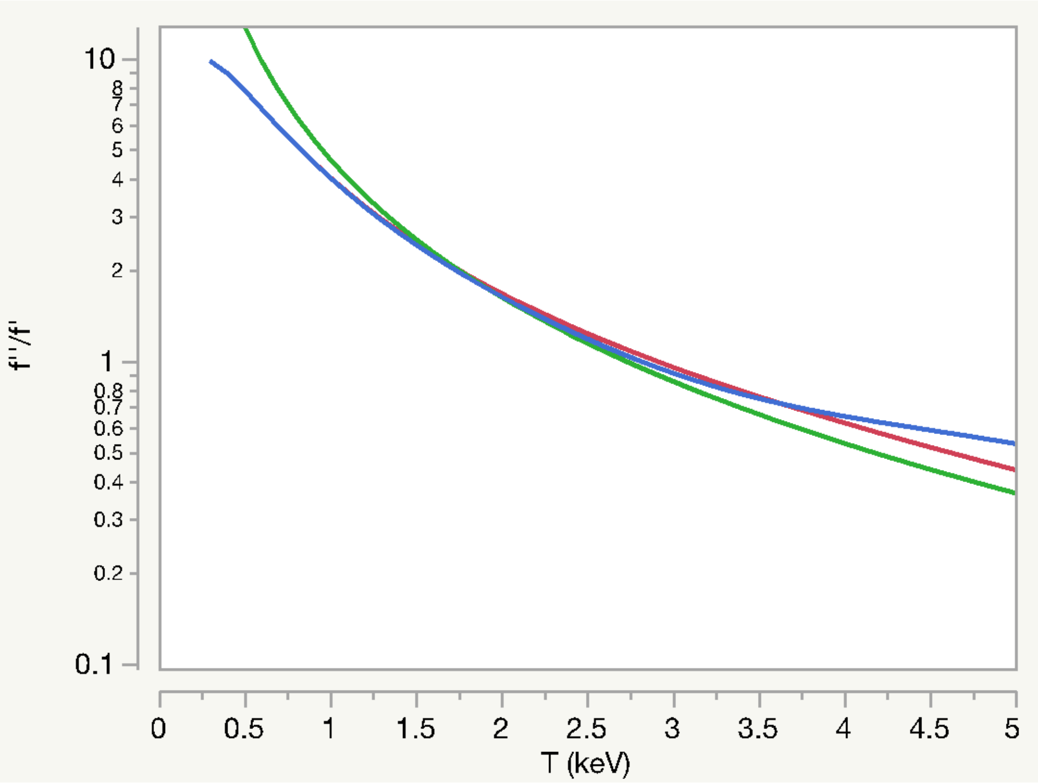

Figure 5. *f'' / f'* on a log scale with *T*—NRL (green), B&H (red), and C&F (blue).

Figure 5 is the second term (negative term) in the lhs of Eq. (19). Because it is the ratio of the second derivative to the first derivative, one might expect this to behave like the ratio of the first derivative to the reactivity—like a standardization. However, NRL separates out, being higher for $T < 1$ and lower for $T > 2$ keV. In addition, Figure 5 looks similar to Figure 4, with the second derivative dominating. The vertical scale is on a logarithmic scale.

Final Thoughts

The figures demonstrate that the C&F and B&H reactivity parameterizations behave similarly for the terms in Eqs. (18-19). The differences in some terms for NRL at low temperatures makes its less viable because of the low temperature regimes typically found in experiments. The next step is to utilize experimental data to study the temperature with time function and corresponding derivatives. This will complete the exploration of the alpha derivative and its extremum values.

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[4] H.S. Bosch, G.M. Hale “Improved Formulas for Fusion Cross-sections and Thermal Reactivities” *Nuclear Fusion,* Vol. 32 No. 4, 1992, pp. 611-631

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APPENDIX
Temperature-derivatives for the three parameterizations

The analytical derivatives of reactivity with temperature for the NRL parameterization, Eq. (14), are relatively easy to determine. The first derivative is:

$$\frac{df}{dT} = f' = \frac{A_0(A - 2T^{1/3})\exp(-AT^{-1/3})}{3T^2}$$

and the second derivative is:

$$\frac{d^2f}{dT^2} = f'' = \frac{A_0(A^2 - 8T^{1/3} + 10T^{2/3})\exp(-AT^{-1/3})}{9T^{10/3}}$$

The B&H parameterization, Eq. (17), is complicated for finding first and second analytical derivatives with *T*. For simplification, the first derivative is expressed in terms of reactivity, θ, ξ, dθ/d*T* and dξ/d*T*:

$$f' = \frac{-5f}{6\theta}\frac{d\theta}{dT} - \frac{2f}{3T} + \frac{f}{T}\left[\frac{-C_1T^{2/3}}{\theta^{2/3}}\frac{d\theta}{dT} - \xi\theta^{1/3}\right]$$

where

$$\frac{d\theta}{dT} = \frac{-[(\theta-1)(C_3 + 2C_5T + 3C_7T^2) + (C_2 + 2C_4T + 3C_6T^2)]}{(1 + C_3T + C_5T^2 + C_7T^3)} \text{ and } \frac{d\xi}{dT} = \frac{-\xi}{3T}.$$

Because the first derivative is so complicated, making the second derivative even more difficult, the second derivative is obtained by taking the difference between the first derivative values divided by the difference between their *T* values—$\Delta\{df/dT\}/\Delta T$. This was shown to be a good approximation of the second derivative in [5].

The C&F *f* parameterization is also difficult for determining its analytical second derivative. The difference method used for B&H was also employed here. The first derivative of the reaction rate, *RR*, and *T*9 in Eq. (15) and Eq. (16) is:

$$
\begin{aligned}
\frac{dRR}{dT9} &= -\frac{C_8 C_9 \exp(C_9 / T)}{T^{8/3}} - \frac{2RR}{3T} \\
&+ \frac{C_0 \exp(C_1 / T^{1/3} - T^2 / C_2^2)(\frac{C_3}{3T^{2/3}} + \frac{2C_4}{3T^{1/3}} + C_5 + \frac{4}{3}C_6 T^{1/3} + \frac{5}{3}C_7 T^{2/3})}{T^{2/3}} \\
&+ \frac{C_0 \exp(C_1 / T^{1/3} - T^2 / C_2^2)(-C_1 / 3T^{4/3} - 2T / C_2^2)(1 + C_3 T^{1/3} + C_4 T^{2/3} + C_5 T + C_6 T^{4/3} + C_7 T^{5/3})}{T^{2/3}}
\end{aligned}
$$

To calculate d*f*/d*T* from d*RR*/d*T*9 requires the following transformation and chain rule:

$$\frac{1}{N_A}\frac{df}{dT9} = \frac{dRR}{dT9}$$

and

$$f' = \frac{dT9}{dT} \cdot \frac{df}{dT9}$$

where d*T*9/d*T* =0.0116. Thus the analytical derivative above is divided by N_A and multiplied by 0.01106.