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Analytic, empirical and delta method temperature derivatives of D-D and D-T fusion reactivity formulations, as a means of verification

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ABSTRACT

We examine the derivatives with respect to temperature, for various deuterium-tritium (D-T) and deuterium-deuterium (D-D) fusion-reactivity formulations. Langenbrunner and Makaruk [1] had studied this as a means of understanding the time and temperature domain of reaction history measured in dynamic fusion experiments. Presently, we consider the temperature derivative dependence of fusion reactivity as a means of exercising and verifying the consistency of the various reactivity formulations.

I. Introduction: Sources of D-D & D-T Reactivity Formulations

A. Beyond the NRL Formulation

Langenbrunner and Makaruk [1] found derivatives with respect to ion temperature (*italicized T*) for formulae of fusion reactivities given in the U.S. Naval Research Lab (NRL) [2] formulary. The present work expands upon the previous by using various other formulations of reactivity, *f*, where $f(T)_{DD} = <\sigma v>_{DD}$ and $f(T)_{DT} = <\sigma v>_{DT}$. These formulations are Hively [3], BUCKY [4], Bosch & Hale [5], T2 LANL [6], DRACO [7], UNC [8] and data [9]. The fusion reactivity, $<\sigma v>$, is averaged over a Maxwellian distribution for velocity [2], as are all of the other formulations. The Maxwellian velocity distribution assumption is $g(v)$ in Eq. (1):

$$<\sigma v> = \int_0^\infty \sigma(v)\cdot v\cdot g(v)dv = \int_0^\infty \sigma(v)\cdot v\cdot 4\pi\cdot\left(\frac{m}{2\pi kT}\right)^{1.5}\cdot v^2\cdot\exp\left(\frac{-mv^2}{2kT}\right)\cdot dv \qquad (1)$$

The NRL fusion reactivity at low energy, below 25 keV, as a function of T is expressed in the following form:

$$<\sigma v> = A_0 T^{-2/3}\exp(-AT^{-1/3}) \qquad (2)$$

with A = 19.94 for the D-T fusion reaction and A = 18.76 for the D-D fusion reaction. The scalar multiplier A_0 is equal to 3.68 x 10^{-12} for D-T fusion and 2.33 x 10^{-14} for D-D fusion, and reactivity has units of $cm^3 sec^{-1}$. The fusion reactivity, as a function of T(keV), is frequently expressed as proportional to a power law of T, [10],

$$<\sigma v> \propto T^a \quad . \tag{3}$$

The temperature derivative of the power law expression, Eq. (3), is found by rearranging terms and assigning the proportionality quantity, *a(T)*, as everything except the ratio of reactivity to T:

$$\frac{d}{dT}<\sigma v> = a(T)\frac{<\sigma v>}{T} \quad . \tag{4}$$

B. The Hively Formulation

A commonly cited formulation in Eq. (5) is from Hively [3]:

$$\begin{aligned}
<\sigma v>_{DT} &= 9.1e-16\cdot\exp\left[-0.572\cdot\left|\ln\left(\frac{T}{64.2}\right)\right|^{2.13}\right] \\
<\sigma v>_{DDp} &= 2e-14\cdot\left[\frac{1+0.00577T^{0.949}}{T^{2/3}}\right]\exp\left(\frac{-19.31}{T^{1/3}}\right) \\
<\sigma v>_{DDn} &= 2.72e-14\cdot\left[\frac{1+0.0039T^{0.917}}{T^{2/3}}\right]\exp\left(\frac{-19.8}{T^{1/3}}\right)
\end{aligned} \tag{5}$$

where the D-D reaction total is the sum of the proton and neutron branches, D-D_p and D-D_n.

The first derivatives with respect to temperature T of the Hively expressions are analytically obtainable as:

$$\begin{aligned}
&\frac{d<\sigma v>_{DT}}{dT} = \frac{2.13\cdot(9.1e-16)\cdot 0.572}{T}\cdot\exp\left[-0.572\cdot\left(-\ln\left(\frac{T}{64.2}\right)\right)^{2.13}\right]\cdot\left[-\ln(\frac{T}{64.2})\right]^{1.13} \\
&\frac{d<\sigma v>_{DDp}}{dT} = 2e-14\cdot(0.00577)\cdot 0.949\left[\frac{1}{T^{(5/3-0.949)}}\right]\exp\left(\frac{-19.31}{T^{1/3}}\right)+2e-14\cdot \\
&(19.31)\cdot\exp\left(\frac{-19.31}{T^{1/3}}\right)\cdot\frac{(1+0.00577\cdot T^{0.949})}{3T^2}-2e-14\cdot(2)\cdot\exp\left(\frac{-19.31}{T^{1/3}}\right)\cdot\frac{(1+0.00577\cdot T^{0.949})}{3T^{5/3}} \\
&\frac{d<\sigma v>_{DDn}}{dT} = 2.72e-14\cdot(0.00539)\cdot 0.917\left[\frac{1}{T^{(5/3-0.917)}}\right]\exp\left(\frac{-19.8}{T^{1/3}}\right)+2.72e-14 \\
&(19.8)\cdot\exp\left(\frac{-19.8}{T^{1/3}}\right)\cdot\frac{(1+0.00539\cdot T^{0.917})}{3T^2}-2.72e-14\cdot(2)\cdot\exp\left(\frac{-19.8}{T^{1/3}}\right)\cdot\frac{(1+0.00539\cdot T^{0.917})}{3T^{5/3}}
\end{aligned} \tag{6}$$

Because the focus is for temperature $T < 30$ keV, the absolute value insides the exponent of D-T derivative in Eq. (6) is replaced with a minus sign outside of the *ln*. All three of these first derivatives can be rearranged for extracting the $a(T)$ factor apart from $<\sigma v>/T$, in Eq. (4).

B. The BUCKY Formulation

MacFarlane, Moses, and Peterson in 1995 [4] and 2002 simulated inertial confinement fusion using 1D hydrodynamics code referred to as BUCKY, with the following formulations of D-D and D-T reactions:

$$f(T) = <\sigma v> = \exp(A_1 T^{-r} + A_2 + A_3 T + A_4 T^2 + A_5 T^3 + A_6 T^4) \quad (7)$$

Parameter	D-T	D-D
r	0.2935	0.3735
A_1	-21.377692	-15.511891
A_2	-25.20405	-35.318711
A_3	-0.071013427	-0.012904737
A_4	1.94E-04	2.68E-04
A_5	4.92E-06	-2.92E-06
A_6	-3.98E-08	1.27E-08

The BUCKY formulation is interesting because it involves various T power-law formulations, involves an exponential function which permits analytical derivatives, and involves computation.

It should be noted that the D-D A_3 coefficient appears in later literature, circa 2005, without the minus sign. If this error is propagated through the analytical and empirical derivatives, the extrema temperature value in the 2nd derivative is significantly affected, while the reactivities themselves are not so adversely affected. Figure 1 for the short range of 1-25 keV indicates that the incorrect BUCKY reactivities (as black dots) fall in the middle of those from other sources and the bottom < blue symbols are the verifiable values. It is only when a longer range in temperature is plotted that the incorrect values deviate radically from the others. This result demonstrates how the nonlinearity of Eq. (7) and its derivatives in Eq. (8) can be quite sensitive to seemingly minor changes.

The analytical derivatives for Eq. (7) are:

$$\frac{df(T)}{dT} = \exp(A_1 T^{-r} + A_2 + A_3 T + A_4 T^2 + A_5 T^3 + A_6 T^4) \cdot (-rA_1 T^{-(r+1)} + A_3 + 2A_4 T + 3A_5 T^2 + 4A_6 T^4)$$
$$= <\sigma v> (-rA_1 T^{-(r+1)} + A_3 + 2A_4 T + 3A_5 T^2 + 4A_6 T^4)$$

$$\frac{d^2 f(T)}{dT^2} = <\sigma v> \cdot \left\{ \begin{array}{l} [(r+1) r A_1 T^{-(r+2)} + 2A_4 + 6A_5 T + 12 A_6 T^2] + \\ (-rA_1 T^{-(r+1)} + A_3 + 2A_4 T + 3A_5 T^2 + 4A_6 T^4)^2 \end{array} \right\} \quad (8)$$

$$\frac{d^3 f(T)}{dT^3} = <\sigma v> \left\{ \begin{array}{l} [-(r+1)(r+2) r A_1 T^{-(r+3)} + 6A_5 + 24 A_6 T] + (-rA_1 T^{-(r+1)} + A_3 + 2A_4 T + 3A_5 T^2 + 4A_6 T^4)^3 \\ +3 \cdot (-rA_1 T^{-(r+1)} + A_3 + 2A_4 T + 3A_5 T^2 + 4A_6 T^4) \cdot (r+1) r A_1 T^{-(r+2)} + 2A_4 + 6A_5 T + 12 A_6 T^2 \end{array} \right\}$$

Again, the first derivative can be transformed to factor out $<\sigma v>/T$, from the remaining terms forming $a(T)$ in Eq. (4).

C. The Bosch & Hale Formulation

One of the most prominently cited alternative formulations for reactivity is from Bosch & Hale [5]. Eq. (9) with its coefficient table contain their new, improved, parameterization:

$$\begin{aligned} <\sigma v> &= \frac{C_1 \xi^2 \exp(-3\theta^{1/3}\xi)}{\theta^{5/6}} \\ \theta &= 1 - \frac{(C_2 T + C_4 T^2 + C_6 T^3)}{(1 + C_3 T + C_5 T^2 + C_7 T^3)} \\ \xi &= \frac{C_0}{T^{1/3}} \end{aligned} \quad (9)$$

Parameters	D+D—>3He+n	D+D—>T + p	D-T
C_0	6.2696	6.2696	6.661
C_1	3.57E-16	3.72E-16	6.43E-14
C_2	5.86E-03	3.41E-03	1.51E-02
C_3	7.68E-03	1.99E-03	7.52E-02
C_4	0	0	4.61E-03
C_5	-2.96E-06	1.05E-05	1.35E-02
C_6	0	0	-1.07E-04
C_7	0	0	1.37E-05

Based upon the complexity in Eq. (9), one might expect a high degree of accuracy over a wide range of T, and that is the experience of studies by Langenbrunner and Booker [11] and of Horny' et al. 2011, [12]. However, Eq. (9) is complicated for finding the analytical derivative as demonstrated by the first derivative in Eq. (10). For simplification, the first derivative is expressed in terms of reactivity, θ, ξ, $d\theta/dT$ and $d\xi/dT$:

$$\frac{d<\sigma v>}{dT} = \frac{-5<\sigma v>}{6\theta}\frac{d\theta}{dT} - \frac{2<\sigma v>}{3T} + \frac{<\sigma v>}{T}\left[\frac{-C_1 T^{2/3}}{\theta^{2/3}}\frac{d\theta}{dT} - \xi\theta^{1/3}\right] \quad (10)$$

where

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

The form for determining *a(T)* is accomplished by rearranging the definition of θ in terms of a factor for *T*

$$\theta = T\,\frac{(T^{-1}+C_3-C_2+(C_5-C_4)T+(C_7-C_6)T^2)}{(1+C_3T+C_5T^2+C_7T^3)} \tag{11}$$

and substituting Eq. (11) for θ into the denominator of the first term on the right side of Eq. (10).

D. Additional Formulations

Outputs from complex simulations and hydrodynamics codes are not conducive to an analytical expression for derivatives. Calculations from Los Alamos National Laboratory (T2 LANL) [6], the DRACO code [7] and the University of North Carolina (UNC) [8] have this issue. The same is true of data [9]. Sections II and III present two alternative approaches. Section IV contains the results of determining the extrema temperatures for the 2nd derivatives of D-D and D-T reactions and compares them across this variety of sources, beyond the NRL formulation.

II. Empirical Fitting of D-D and D-T Reactivity Formulations

Derivatives can be obtained for complex reactivity formulations, if these are first fit to a functional form that is conveniently differentiable. Hoffman 1992 [13] suggests fitting such data/outputs to polynomials and then taking the derivatives of those polynomial formulations. These are the empirical derivatives, because the least squares regression procedure of fitting is first applied. Using the JMP software (trademark of SAS corporation), least squares regression fits were made for the calculated reactivities as a function of the powers of *T* from 1 through 7 plus an intercept. To check the viability of the fits, an R^2 value of near 1.000000 was desired, with all the 7 powers of *T* being significant and with all the predicted values being positive. If one or more powers are not significant, it may have been deleted depending upon other criteria. Using the polynomial prediction fit, the first, second and third derivatives were analytically derived from the regression fit, and the values of these empirical derivatives were found. It was expected that the third derivative would have positive values for the lowest *T*'s and then switch to negative values. If this behavior was not evident or if the crossing of the horizontal axis (where the 3rd derivative is zero) was not in the anticipated range of the (2nd derivative) extremum value of *T*, then the fit was not considered appropriate. That is, it was unverified.

In addition to being able to exclude or include powers of *T* terms in the fit, adjustments to the range of values of *T* also was used to determine the best fit. The stepwise procedure in JMP was used for the former, and examination of the predictions and empirical derivatives was used for the latter. The default for the beginning range of *T* was the range published by the developers of the reactivity formulation. However, interest is focused on the lower values of *T*, where the extrema in the 2^{nd} derivative are found. The smallest range of applicability is that of NRL, which runs from 1-25 keV. For formulations with higher ranges, often other problems with fits emerged. Thus, the maximum of 25-30 keV provided good fits for all formulations, code outputs and data. And the minimum of 1 keV or slightly below that applied as the lower range. As shown in Figure 2, for T<1 keV, empirical derivatives do not match their analytical counterparts. Different curvatures and negative values can occur with empirical derivatives.

Another issue is determining the ranges of *T* where these calculations (and even the data) are applicable. Again, this is a sensitivity issue which shows up in derivatives looking suspicious and not something one would worry about if they were not considering derivatives for analytical analysis and verification. The developers of the formulations have published what they determined as an operational/ applicable range for their calculation/code based on just the reactivities themselves (and their physics expertise). The *T* ranges were sometimes altered (*e.g.*, deleting *T*'s < 1 keV, and *T*'s > 25 keV) in order to obtain the derivatives (either analytical ones or empirical ones) to be well behaved—and verified in that sense.

To test the accuracy and feasibility of this empirical derivative method (in other words, to verify), analytical derivatives for NRL and BUCKY were compared to the empirical derivatives from polynomial fits. Figure 2 displays this comparison for the Bosch & Hale derivatives and Figure 3 for the BUCKY derivative. Note that only the first derivatives for Bosch & Hale were compared to the first derivative from polynomial fits because the analytical second and third derivatives were too complex and cumbersome.

To judge the best polynomial fits using least squares regression, the R^2 values approaching 1.000000 were desired and the significance of the power terms was desired. While fits with no significant terms can (statistically) produce the highest R^2 values, lack of significance results in poor predictability from the fitted models. Therefore, this trade-off must be balanced in determining the best fit. Additional issues regarding the fits were discussed above.

A. NRL Empirical Fitting and Derivatives

The following least squares polynomial fits were obtained for the NRL reactivity values, $f\,(T)_{DD} = <\sigma v>_{DD}$ and $f\,(T)_{DT} = <\sigma v>_{DT}$:

$$
\begin{aligned}
f\,(T)_{DD} &= 2.79\text{e-}21 - 5.10\text{e-}21 \cdot T^2 + 3.38\text{e-}21 \cdot T^3 - 3.25\text{e-}22 \cdot T^4 + 1.55\text{e-}23 \cdot T^5 \\
&\quad - 3.81\text{e-}25 \cdot T^6 + 3.81\text{e-}27 \cdot T^7 \\
f\,(T)_{DT} &= -1.80\text{e-}20 + 4.84\text{e-}19 \cdot T - 6.96\text{e-}19 \cdot T^2 + 3.12\text{e-}19 \cdot T^3 - 2.59\text{e-}20 \cdot T^4 + \\
&\quad 1.10\text{e-}21 \cdot T^5 - 2.42\text{e-}23 \cdot T^6 + 2.21\text{e-}25 \cdot T^7
\end{aligned}
\tag{12}
$$

It should be noted that the $f\,(T)_{DD}$ fit has no linear T term because it was not significant (to even the 10% level). Comparing the fits with and without that linear term indicates that the better fit is the one shown above with an R^2=0.999999. The $f\,(T)_{DT}$ fit has all terms as highly significant with an R^2=1.0000000.

Determining empirical derivatives by fitting a polynomial of powers of T relates to some previous formulary studies and papers, *e.g*. [11]. In those studies, predictability of the NRL reactivity formulation was investigated over discrete ranges of T. The results indicated that higher powers of T (up to and including 6) were the best predictors of reactivity for the lower values of T, and lower powers (*e.g*. cubic terms) were best for the higher values of T. In light of those results, having a non-significant linear term for the D-D fit is not unexpected nor detrimental.

As previously noted in [1], the analytical third derivative crosses the horizontal axis at 4.4 keV for D-D and 5.29 keV for D-T. The empirical third derivative crosses the horizontal axis at 4.6 keV or D-D and 5.50 keV for D-T. In close examination of the polynomial fits reveals that the nonlinearities and lack of fit is greatest in the small values of T near to these extrema regions. However, those differences smooth out over the higher values of T.

B. Bosch & Hale Empirical Fitting and Derivatives

While the published range of applicability for Bosch & Hale formulation is 0.2-100 keV, using that range for the polynomial fits to determine empirical derivatives produces negative predicted reactivities around the 0.2-2 keV range and produces a crossing of the horizontal axis of the third derivative at unexpectedly high (~100 keV) values of T. Restricting the upper range to the NRL limit of 25 or 30 keV removes this problem, and restricting the lower range to 0.9 keV smooths the fluctuations to a monotone function. Figure 2 illustrates the mismatch of analytical and empirical first derivatives at small T values. These two problems in determining the empirical derivatives are not unique to Bosch & Hale and are an artifact of the nonlinear relationships of the power fits and the reactivity formulations. Thus, careful monitoring of all empirical derivatives is required. Because of such issues it is recommended that, where possible, empirical derivatives should be compared to analytical ones.

The following power fits for T were obtained for the Bosch & Hale reactivity values from Eq. (9), $f(T)_{DD} = \langle\sigma v\rangle_{DD}$ and $f(T)_{DT} = \langle\sigma v\rangle_{DT}$:

$$
\begin{aligned}
f(T)_{DD} &= 1.08e\text{-}21 + 1.66e\text{-}21\cdot T - 6.79e\text{-}21\cdot T^2 + 4.17e\text{-}21\cdot T^3 - 3.55e\text{-}22\cdot T^4 + \\
&\quad 1.53e\text{-}23\cdot T^5 - 3.39e\text{-}25\cdot T^6 + 3.06e\text{-}27\cdot T^7 \\
f(T)_{DT} &= -1.10e\text{-}18 + 2.98e\text{-}18\cdot T - 2.22e\text{-}18\cdot T^2 + 6.40e\text{-}19\cdot T^3 - 4.69e\text{-}20\cdot T^4 + \\
&\quad 1.60e\text{-}21\cdot T^5 - 2.67e\text{-}23\cdot T^6 + 1.72e\text{-}25\cdot T^7
\end{aligned}
\tag{13}
$$

For D-D, all 7 powers of T are included in the fit, and all powers are significant, except the T linear term which is significant at the 0.13 level. The fit has an impressive R^2 =0.999999. For D-T, all 7 powers are significant and are used in the fit with an excellent R^2 =0.999998.

The third empirical derivative crosses the horizontal axis at 5.34 keV for D-D and 5.69 keV for D-T. These (2nd derivative) extrema are somewhat higher than the NRL values of 4.4 and 5.3 keV. These extrema are not sensitive to changes in the T ranges. The use of empirical derivatives does not appear to be responsible either for the shift from NRL values as evidenced by comparing the analytical first derivative to its empirical counterpart and by comparing all analytical derivatives to their empirical counterparts wherever available. The differences in the extrema values are apparently due to the different formulations of reactivity—Eq. (2) versus Eq. (9).

C. BUCKY Empirical Fitting and Derivatives

The analytical derivatives for the BUCKY formulation in Eq. (7) are given in Eq. (8); however, the powers of T fits for empirical derivatives were also determined for comparison. The D-D T range is from 0.5-30 keV without any difficulties at the small T values. The D-T range is from 0.2-20 keV with a few negative reactivity predictions at T<1 keV. Changing the lower range moves the negative values to higher temperatures.

The powers of T fits have all terms significant. The D-D R^2=1.000000 and the D-T R^2=0.999999.

$$f(T)_{DD} = 1.03e\text{-}21 + 9.92e\text{-}22\cdot T - 3.78e\text{-}21\cdot T^2 + 2.14e\text{-}21\cdot T^3 - 1.80e\text{-}22\cdot T^4 + 7.60e\text{-}24\cdot T^5 - 1.65e\text{-}25\cdot T^6 + 1.45e\text{-}27\cdot T^7$$

$$f(T)_{DT} = -8.173e\text{-}19 + 2.35e\text{-}18\cdot T - 1.87e\text{-}18\cdot T^2 + 5.62e\text{-}19\cdot T^3 - 4.08e\text{-}20\cdot T^4 + 1.41e\text{-}21\cdot T^5 - 2.46e\text{-}23\cdot T^6 + 1.74e\text{-}25\cdot T^7 \quad (14)$$

Figure 4 illustrates how the D-D empirical first, second and third derivatives compare to their analytical counterparts for T <10 keV. The D-T plots are similar and are not shown. There is good matching of both derivative methods, especially in the region of T extrema (~4-6 keV).

The third empirical derivative crosses the horizontal axis at 5.32 keV or D-D and 5.81 keV for D-T. The third analytical derivative crosses the horizontal axis at 5.03 keV or D-D and 5.87 keV for D-T. As with the Bosch & Hale values, these extrema are somewhat higher than the NRL values of 4.4 and 5.3 keV.

D. Hively Empirical Fitting and Derivatives

The Hively formulation is given in Eq. (5) and the analytical first derivative is given in Eq. (6). The D-D T range is from 0.5-30 keV without any difficulties at the small T values. The D-T range is from 0.2-20 keV with a few negative reactivity predictions at T<1 keV. Changing the lower range moves the negative values to higher temperatures.

The powers of T fits have all terms significant for both D-D and D-T fits. Both fits have a perfect R^2=1.000000:

$$f(T)_{DD} = -1.18e\text{-}21 + 7.12e\text{-}21\cdot T - 1.01e\text{-}20\cdot T^2 + 4.78e\text{-}21\cdot T^3 - 3.96e\text{-}22\cdot T^4 + 1.66e\text{-}23\cdot T^5 - 3.57e\text{-}25\cdot T^6 + 3.12e\text{-}27\cdot T^7$$

$$f(T)_{DT} = -7.31e\text{-}19 + 2.23e\text{-}18\cdot T - 1.88e\text{-}18\cdot T^2 + 5.95e\text{-}19\cdot T^3 - 4.72e\text{-}20\cdot T^4 + 1.82e\text{-}21\cdot T^5 - 3.61e\text{-}23\cdot T^6 + 2.91e\text{-}25\cdot T^7 \quad (15)$$

The third empirical derivative crosses the horizontal axis at 5.48 keV or D-D and 5.48 keV for D-T. This is the only formulation with the D-D and D-T extrema T's so close together. As with the Bosch & Hale formulation, the higher derivatives are too complicated for analytical evaluation.

E. Data Empirical Fitting and Derivatives

The $<\sigma v>$ data source comes from the Brookhaven National Laboratory Nuclear Data Center—Experimental Nuclear Reaction Data, available online at:
http://www.nndc.bnl.gov/exfor/exfor.htm.

Unfortunately, the various sources from available reports and publications do not consistently use the term "data" as that which is not from a calculation, computation/simulation or formula. Three screening methods were used to determine if values listed as "data" were likely experimentally obtained values or from calculations.

1) The reactivity values at posted values of [keV] were all not identical to another set of values known to be calculations.
2) Plots of the reactivity values with T did not precisely fall on a smooth curve; that is, some variability expected in experimental science is detectible.
3) The values of [keV] were listed with decimal places and not integer values. This was only rarely used because it is a less reliable experimental signature.

These so-determined data fell into the range of less than 1 keV up to 1000 keV. There were 60 such values found. The range from 1-30 keV was selected to avoid problems with the shapes of the third derivatives for higher T's. There were only 28 values in that range.

Because there are no formulations, only empirical derivatives can be used on these 28 data reactivity values. With so few data points, it is not surprising that the fits are not as impressive and the polynomial terms are not all significant. With an R^2 =0.991975 and no significant terms, the D-D fit is:

$$f(T)_{DD} = 4.29e\text{-}19 - 6.27e\text{-}19 \cdot T + 2.87e\text{-}19 \cdot T^2 - 5.65e\text{-}20 \cdot T^3 + 5.93e\text{-}21 \cdot T^4 - 3.22e\text{-}22 \cdot T^5 + 8.61e\text{-}24 \cdot T^6 - 8.95e\text{-}26 \cdot T^7 \qquad (16)$$

With a better R^2 =0.999988, but with only the third and fourth powers significant[1], the D-T fit is:

$$f(T)_{DT} = -1.76e\text{-}18 + 3.376e\text{-}18 \cdot T - 2.24e\text{-}18 \cdot T^2 + 6.19e\text{-}19 \cdot T^3 - 4.45e\text{-}20 \cdot T^4 + 1.49e\text{-}21 \cdot T^5 - 2.41e\text{-}23 \cdot T^6 + 1.48e\text{-}25 \cdot T^7 \qquad (17)$$

In spite of these issues less than ideal fits, the third empirical derivative crosses the horizontal axis at reasonable values of 4.66 keV for D-D and 5.81 keV for D-T.

F. T2 LANL and DRACO Empirical Fitting and Derivatives

[1] The T squared term is significant at the 8% level.

The calculations from the DRACO code include only 3 points in range of interest, 1-30 keV. Therefore, it was combined with another source. By examining plots of these values and by using ANOVA, it was determined that these 3 values were in line with those from the LANL T2 calculations. The LANL T2 plus DRACO calculations fit has an R^2 =0.999924, but with no significant terms:

$$f\,(T)_{DD} = 2.97e\text{-}20 \;-3.43e\text{-}20\cdot T + 7.52e\text{-}21\cdot T^2 + 1.69e\text{-}21\cdot T^3 - 1.40e\text{-}22\cdot T^4 + 5.50e\text{-}24\cdot T^5 - 1.17e\text{-}25\cdot T^6 + 1.07e\text{-}27\cdot T^7 \qquad (18)$$

This fit was the best possible having attempted range changes and elimination of terms. However, reactivity predictions from this fit still produce negative values in the T=1-2 keV range.

Similarly, the best D-T fit has some of the same negative predictions for $f\,(T)_{DT}$ in the T<0.5 keV range. However the R^2=0.999971, and all power terms except T^7 are significant. T^7 was significant at the 8% level and was included in the fit:

$$f\,(T)_{DT} = -7.65e\text{-}19 + 2.51e\text{-}18\cdot T - 2.04e\text{-}18\cdot T^2 + 6.08e\text{-}19\cdot T^3 - 4.41e\text{-}20\cdot T^4 + 1.47e\text{-}21\cdot T^5 - 2.36e\text{-}23\cdot T^6 + 1.44e\text{-}25\cdot T^7 \qquad (19)$$

The quality of the above fits was unchanged by eliminating the DRACO 3 points.

The third empirical derivative crosses the horizontal axis at 5.03 keV for D-D and 5.69 keV for D-T—within the range of values from other formulations.

G. UNC Empirical Fitting and Derivatives

The calculations from UNC form a relatively small data set of 37 values, with 10 of those at T<1 keV. Those low values were included without adversely affecting the results even though such low values were not included in other fits. The range used is T=0.09 -25.86 keV. The following D-D fit has R^2 = 1.000000, and all terms are significant:

$$f\,(T)_{DD} = -1.16e\text{-}21 + 6.81e\text{-}21\,T - 9.94e\text{-}21\cdot T^2 + 4.97e\text{-}21\cdot T^3 - 4.52e\text{-}22\cdot T^4 + 2.15e\text{-}23\cdot T^5 - 5.37e\text{-}25\cdot T^6 + 5.50e\text{-}27\cdot T^7 \qquad (20)$$

The following D-T fit has R^2 =0.999998, and T^5 and T^6 are not significant but are included:

$$f\,(T)_{DT} = -3.92e\text{-}19 + 1.54e\text{-}18\cdot T - 1.47e\text{-}18\cdot T^2 + 4.64e\text{-}19\cdot T^3 - 2.69e\text{-}20\cdot T^4 +$$

$$3.98e\text{-}22 \cdot T^5 \ +9.74e\text{-}24 \cdot T^6 \ \text{-}2.61e\text{-}25 \cdot T^7 \qquad (21)$$

The third empirical derivative crosses the horizontal axis at 5.22 keV for D-D and 5.84 keV for D-T—within the range of values from other formulations.

III. Derivatives Using the Delta (Finite Differencing) Method

The empirical derivatives, from least squares polynomial fits, were good by statistical modeling criteria and by visual inspection, compared to their analytical derivatives. Figure 3 shows how well the second derivatives matched using the BUCKY formulation. However, as noted previously, there were some discrepancies at the small *T* values, as shown in Figure 2 for the Bosch & Hale first derivatives. In addition, the unusual result of identical *T* extrema for D-D and D-T from the Hively empirical derivatives, warranted another approach. A third derivative method was implemented, especially to address the difficulty in determining the extrema values from analytical derivatives for Bosch & Hale and Hively. This is called the delta method and utilizes a finite differencing method in place of the analytical or empirical derivative.

Using the first analytical derivative of any formulation, the second derivative is obtained by taking the difference between the first derivative values divided by the difference between their *T* values—$\Delta\{d<\sigma v>/dT\}/\Delta T$. For convenience, the denominator is fixed as ΔT=0.1 keV for values from *T*=1-10- keV. Then the numerator is the difference in adjacent reactivities separated by ΔT=0.1 keV.

Figure 3 shows that the delta method is a better match to the analytical derivative than the empirical derivative for the BUCKY formulation. This same result holds for NRL and Bosch & Hale, not shown. It should be noted that determining the extrema using a second derivative can be done by determining the maximum value when there is assurance that the third derivative will cross the horizontal axis. This short-cut was implemented for the Bosch & Hale formulation to verify the extrema *T* to avoid the complicated analytical higher order derivatives and avoid the less accurate empirical derivatives. It was implemented for the Hively formulation to determine if the *T* extrema for D-D was at a lower temperature than for D-T, as was seen with the other formulations but not with the Hively empirical derivative. For Bosch & Hale, the delta method derivative resulted in a lower *T* extremum for D-D, at 5.05 keV, than for the empirical derivative, at 5.34 keV, and resulted in a higher T extremum for D-D, at 6.00 keV, than for the empirical derivative, at 5.69 keV. The same was true for the Hively delta derivative method, with T extremum for D-D lowered to 5.25 keV and raised to 5.55 keV for D-T. This D-D D-T separation is more inconsistent with other extrema, as seen in Table 1 below. This separation from the delta method over the empirical derivative method demonstrates the utility of the delta method, where possible.

IV. Extrema of Reactivity-derivative Formulations

Table 1 contains the extrema T (keV) values in the 2nd derivatives, and reactivities (cm^3/sec) at those temperatures for D-D and D-T reactions. These are found using various methods for the derivatives and over the different sources and formulations, including data. The last two columns contain the predicted $\langle\sigma v\rangle$ values from the polynomial fits using the empirical derivatives, and the calculated $\langle\sigma v\rangle$ values using analytical and delta-method derivatives.

Table 1. Extrema Temperatures & Reactivities (cm^3/sec) for D-D and D-T

Source	Method	T (keV) D-D	T (keV) D-T	$\langle\sigma v\rangle$DD	$\langle\sigma v\rangle$DT
BUCKY	Empirical Derivative	5.32	5.81	1.07E-19	2.19E-17
BUCKY	Delta on 1st analytical	5.01	5.90	9.33E-20	2.30E-17
BUCKY	Analytical Derivative	5.03	5.87	8.93E-20	2.25E-17
NRL	Empirical Derivative	4.60	5.50	1.06E-19	1.47E-17
NRL	Analytical Derivative	4.40	5.29	9.25E-20	1.30E-17
NRL	Delta on 1st analytical	4.45	5.35	9.55E-20	1.34E-17
Bosch & Hale	Empirical Derivative	5.34	5.69	2.22E-19	2.15E-17
Bosch & Hale	Delta on 1st analytical	5.05	6.00	1.85E-19	2.55E-17
Hively	Empirical Derivative	5.48	5.48	2.38E-19	1.88E-17
Hively	Delta on 1st analytical	5.25	5.55	2.06E-19	1.93E-17
UNC	Empirical Derivative	5.22	5.84	2.07E-19	2.28E-17
T2 LANL + Draco	Empirical Derivative	5.03	5.69	1.89E-19	2.14E-17
Data	Empirical Derivative	4.66	5.81	1.86E-19	2.20E-17

Table 2 provides some statistics for the above 2nd derivative extrema temperatures and their corresponding reactivities.

Table 2. 2nd derivative Extrema Temperature & Reactivity Statistics

Statistic	T (keV) D-D	T (keV) D-T	$\langle\sigma v\rangle$DD	$\langle\sigma v\rangle$DT
Mean	4.99	5.69	1.55E-19	2.00E-17
Standard deviation	0.355	0.223	5.77E-20	3.96E-18

There are no significant differences in the extrema T values for D-D or for D-T based upon the method used for their determination. However, there are significant differences due to the source, that is, the formulation used. For D-D, the Hively, UNC, Bosch & Hale and BUCKY-T 2^{nd} derivative extrema are significantly larger than the corresponding NRL formulation values. For D-T, the BUCKY and B&H 2^{nd} derivative T extrema are significantly larger than the NRL 2^{nd} derivative T extrema.

The extrema reactivities in Table 1 are also significantly different depending upon the source but not depending on the derivative method. On average, the D-D BUCKY and NRL reactivities are significantly smaller than all the other formulations analyzed. For D-T, the NRL extrema reactivities stand out as significantly smaller than all others. This result partially explains why so much effort has been invested to find tractable, accurate expressions for (1), improving upon the historical NRL formulation.

The 28 data points fall in line with the other sources for both D-D and D-T. We wish to explore the details under which the data were reduced. We wish to explore if the velocity-distribution choice affects the values for the 2^{nd} derivative T extrema. Horny' et al., [12] found some differences in reactivities with a few non-Maxwellian distributions. A future study would be to determine if there are any differences in the extrema T's due to the choice of $g(v)$ in Eq. (1).

Figure 5 shows that there is a very weak (at 6% level of significance) correlation between the 2^{nd} derivative T extrema and the reactivity for D-D; however, there is a highly significant correlation (<0.01%) between 2^{nd} derivative T extrema and the reactivity for D-T. For D-D, the three values at the bottom right are BUCKY, and the single value in the upper left is the data.

A measure of uncertainty for the D-D and D-T T extrema can be determined from their standard deviations in Table 2 or from the root mean square errors (RMSE) in the linear fits of the T's to their reactivity as shown in Table 3. From Table 2, the D-T 2^{nd} derivative T extrema percent error is 4%, while that for D-D is nearly twice at 7%. The last row shows the RMSE values using $<\sigma v>$ and the source as predictors, producing a much-reduced uncertainty for D-D because the source explains much of the variability in the extrema for D-D. In that last row, which accounts for variability due to reactivity and source, the percent error for D-T is reduced to 0.4% but that of D-D is only down to 1%.

Table 3. 2^{nd} derivative Extrema Temperature Uncertainties

Statistic	*T* (keV) D-D	*T* (keV) D-T
Standard deviation	0.355	0.223
RMSE using <σv>	0.299	0.072
RMSE using <σv> & source	0.055	0.025

V. Conclusions

The temperature derivative dependence of fusion cross-section reactivity is considered as a means of exercising and verifying the consistency of the various sources of reactivity expressions. This work also enhances the scope of Langenbrunner and Makaruk [1], which focused on the NRL formulation but introduced the <σv> derivatives for determining the *T* at the extremum of the 2^{nd} derivative.

In detail, we have found that there are no significant differences in temperature *T* at the extremum for D-D and for D-T fusion, based upon the three methods used for their derivative determination. However, there are significant differences due to the source, that is, the formulation used to conveniently represent Eq. (1). Three derivative methods were used to determine temperature at the 2^{nd} derivative extrema—analytical, empirical and delta methods. While the delta method derivatives match analytical ones slightly better than empirical, there is no significant difference due to the choice of method for taking temperature derivatives.

Source (meaning formulation choice) affects extrema *T*'s, especially for the D-D reaction. The NRL formulation produces significantly smaller extrema for D-D and D-T than other methods.

A distance metric for verification and validation, D_n [11], can be used to make additional comparisons between the *T* extrema, including determinations of formulations matching to data. This is the topic of another paper.

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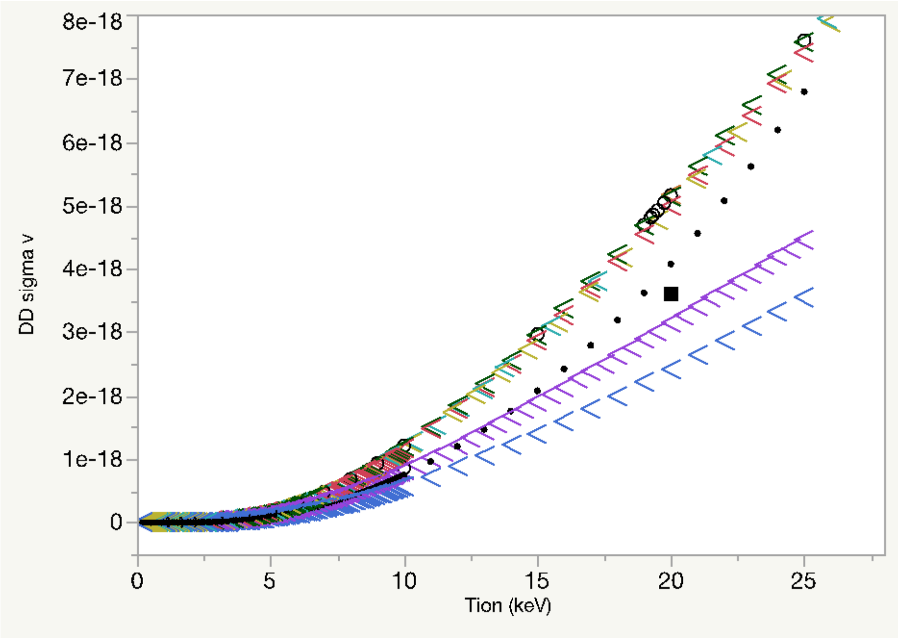

Figure 1. D-D reactivities from all sources including incorrect coefficient A_3 values as black dots, with corrected values as blue < at the bottom.

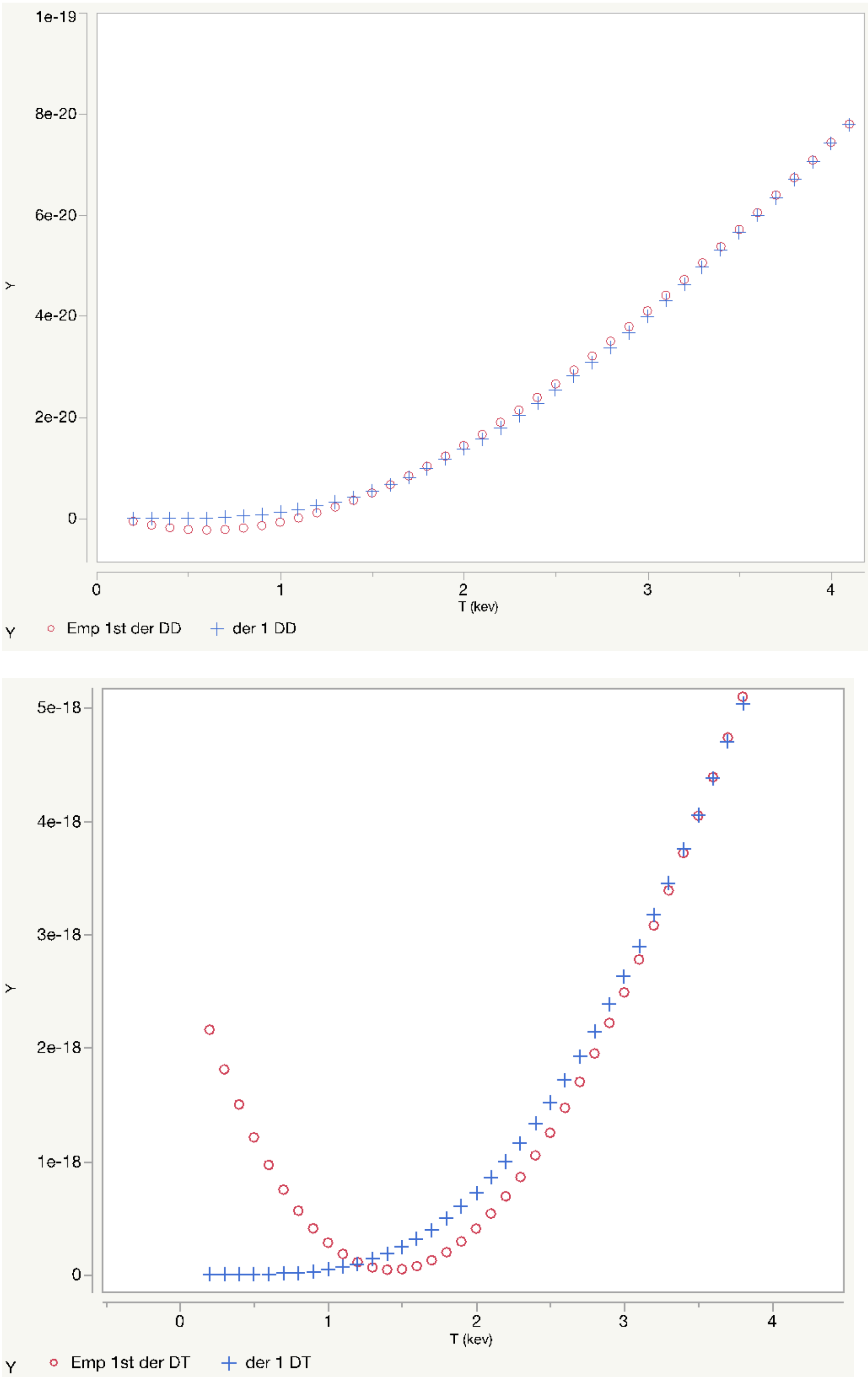

Figure 2. Bosch & Hale empirical first derivatives (red circles) with analytical first derivatives (blue pluses); D-D (top) and D-T (bottom)

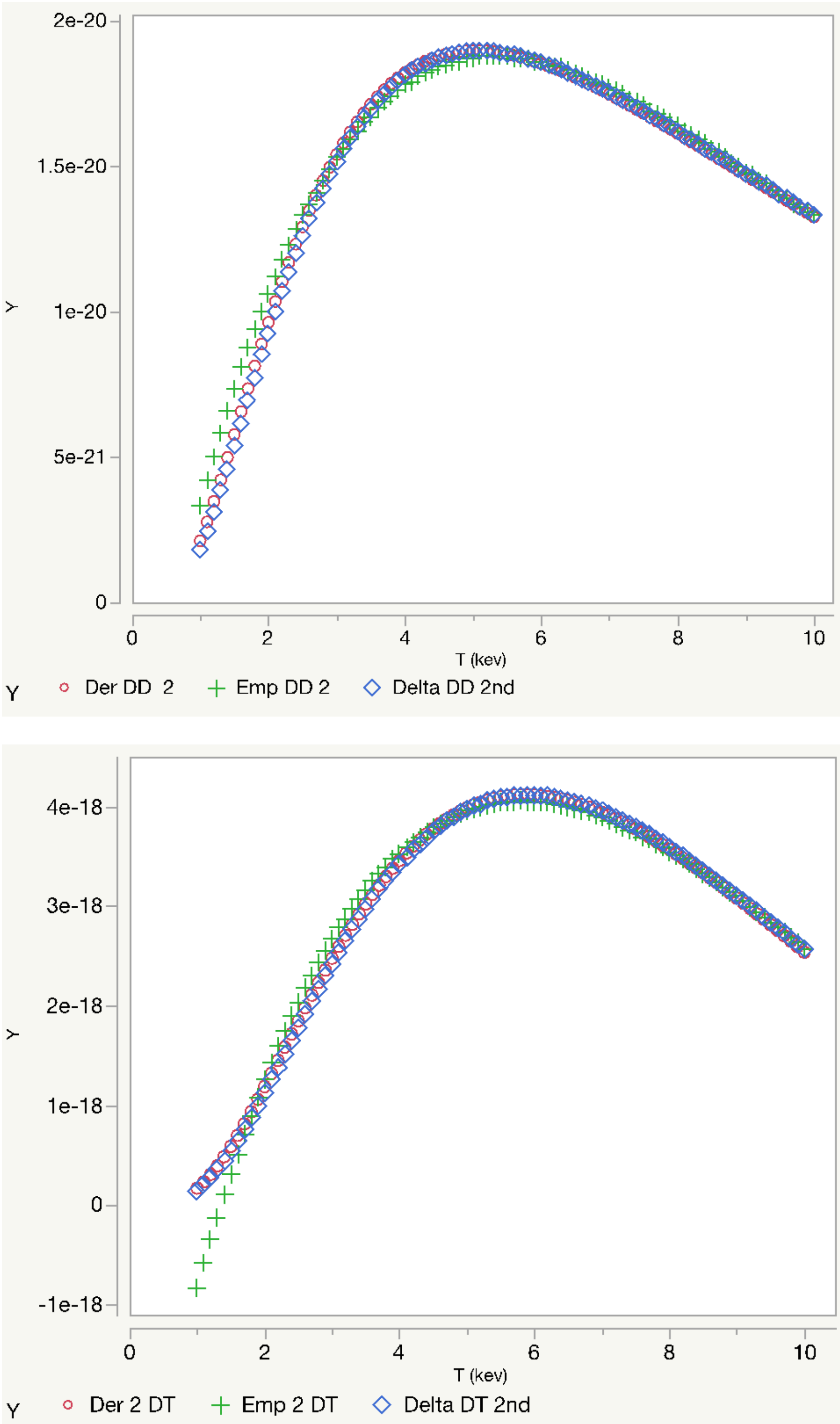

Figure 3. BUCKY D-D (top) and D-T (bottom) second derivatives using three methods: analytical (red circles), empirical (green pluses) and finite differences (blue diamonds). The finite difference method more closely tracks the analytical derivatives.

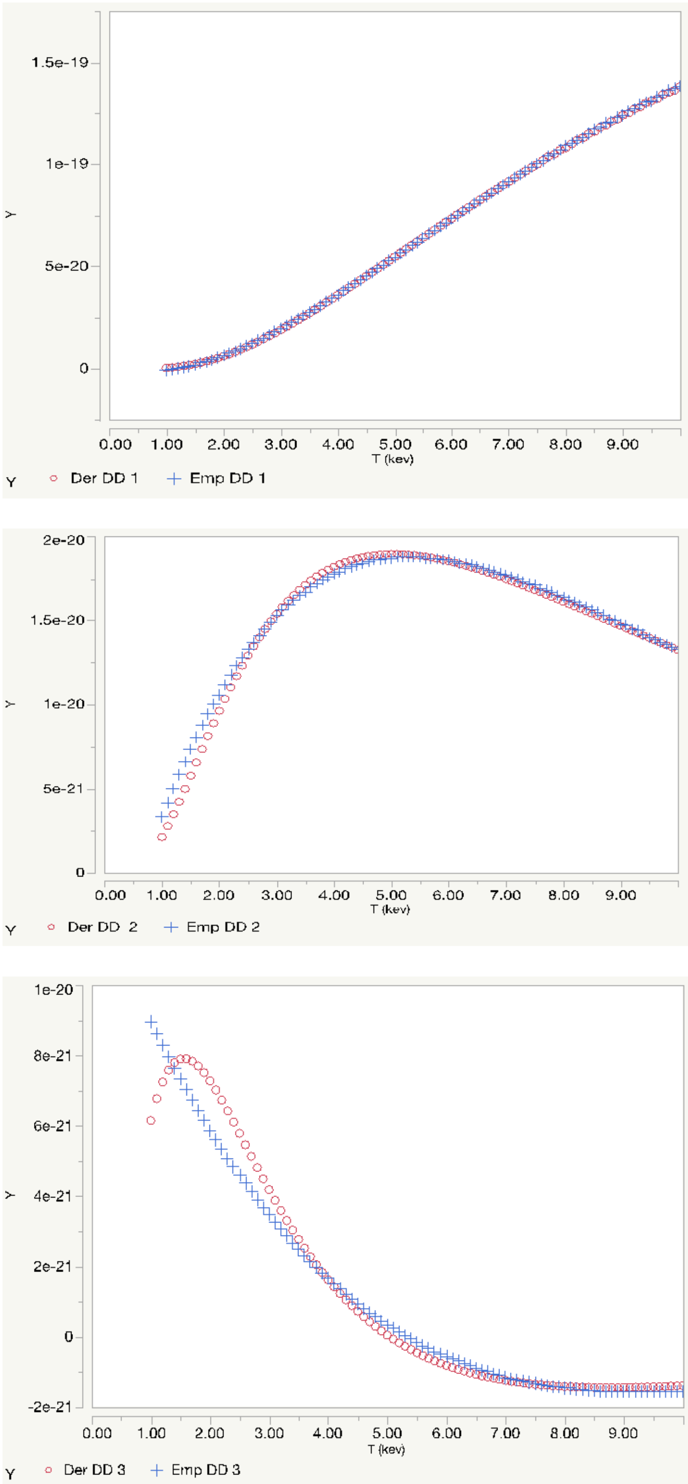

Figure 4. BUCKY DD empirical derivatives (red circles) with analytical derivatives (blue pluses); first derivatives (top), second (middle), and third (bottom).

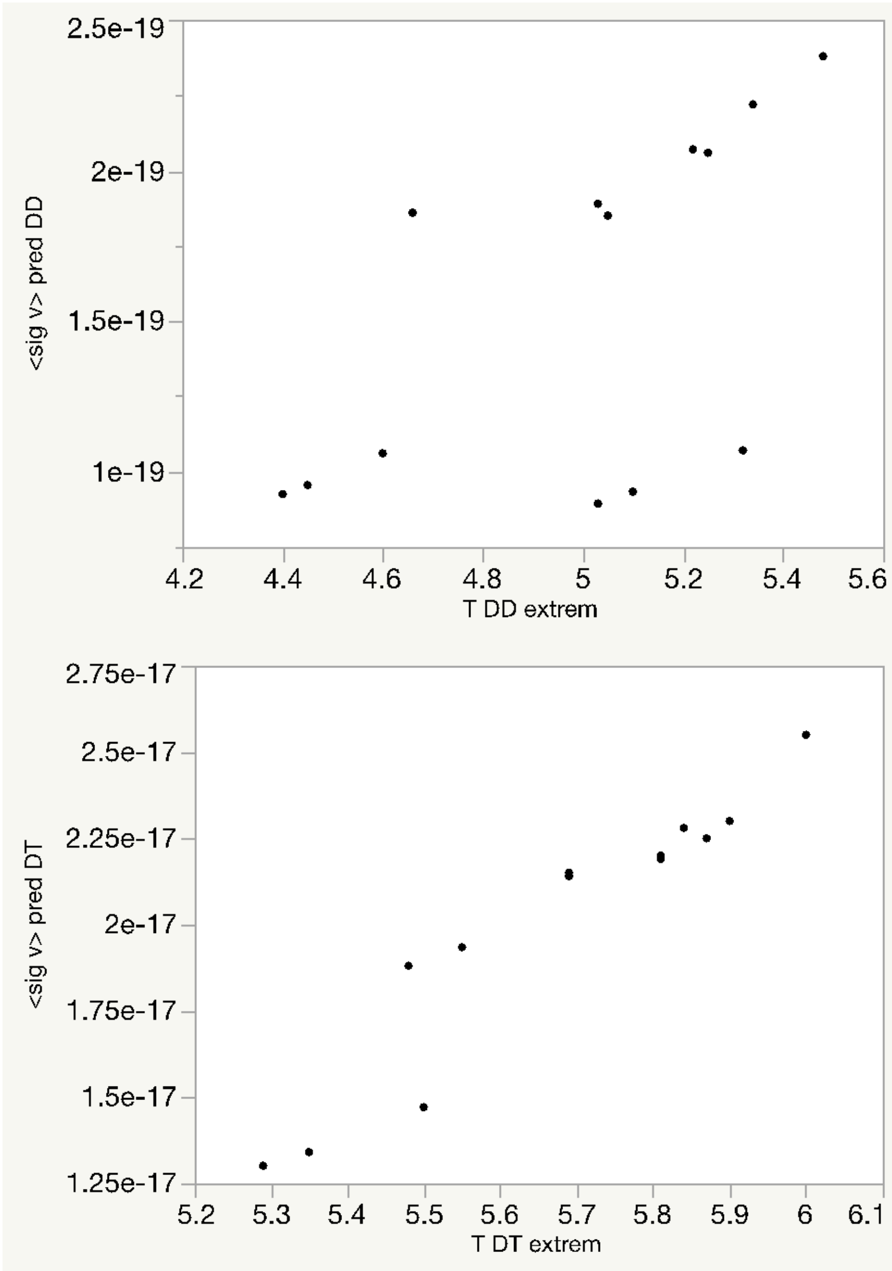

Figure 5. 2nd derivative extrema *T* with reactivity, <σv>,for DD (top) and DT (bottom)