LA-UR-13-21233

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Intended for: Technical Report
Report

ANALYSIS REPORT ON NRL PLASMA FORMULARY DT REACTION-RATE FORMULA

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Introduction

The thermonuclear fusion section of the 2011 NRL Plasma Formulary (Huba, 2011) provides the reaction rate for DT fusion as a function of temperature, on pages 44-45. We describe a statistical analysis based on finding alternative functions for the ***DT reaction rate*** in a gaseous mixture (averaged over a Maxwellian ion distribution parametrized as a function of ion temperature). The purpose of these alternative fits is to determine the validity of reaction rate expressed as a power of the parameter T_{ion}, when compared to the NRL Plasma Formulary.

Formulary Reaction Rate Calculation

The reaction of interest is the DT reaction rate listed as reaction (2) in the 2011 NRL Plasma Formulary (Huba) on page 44:

$$D + T \rightarrow 4He\,(3.5\text{ MeV}) + n(14.1\text{ MeV}).$$

Reaction rate, $\sigma\nu$ ($cm^3\ sec^{-1}$), averaged over Maxwellian distributions is given by

$$(\sigma\nu)_{DT} = 3.68 \times 10^{-12}\, T^{-2/3} \exp(-19.94 T^{-1/3})\ cm^3\ sec^{-1} \qquad (1)$$

where $T = T_{\text{ion}}$ is measured in keV.

In this investigation, Equation (1) is used to produce values for reaction rate at temperatures in 0.1 keV increments. These values compose samples in temperature intervals which are fit using least-squares regression functions that are *powers of T_{ion}*. This is possible at the cost of dividing the applicable physical regime, 1-10 keV into small parts: 1 keV intervals. The T_{ion} values thus split define regimes and the results are shown in Table 1.

The ***reaction rate*** is in a gaseous mixture wherein the (assumed) Maxwellian distribution of ion velocities introduces a factor exp(-E/kT). Interior to a star, light-nuclear-ion kinetic energies are of the order of 1 keV. The fastest (hottest) ions in the Maxwellian distribution react (fuse) preferentially. The number of particles in a given energy interval is a strongly decreasing function of energy, and the result is that the reactions in a Maxwellian gas occur in a narrow energy interval, below about 25 keV. We chose 1 keV intervals up to 10 keV.

TABLE 1. Reaction Rate Fits with Powers of T_{ion} by Interval

Region 1: 0.1 keV < $T_{ion} \leq$ 1 keV, can be fit with T^6_{ion}

R^2	0.9997	RMSE=5.08e-23	Mean=1.55e-21
Predictor	Estimate	Std error	Significance prob
Intercept	-6.26e-22	3.31e-22	0.0758
T^6_{ion}	9.999e-21	3.86e-23	<0.0004

Region 2: 1. keV < $T_{ion} \leq$ 2. keV, can be fit with no intercept and T^5_{ion}

R^2		RMSE=2.53e-21	Mean=1.09e-19
Predictor	Estimate	Std error	Significance prob
Intercept			
T^5_{ion}	9.849e-21	5.15e-23	<0.0001

Region 3: 2.0 keV $\leq T_{ion} \leq$ 3 keV, can be fit with T^4_{ion}

R^2	0.9999	RMSE=4.9e-21	Mean=8.93e-19
Predictor	Estimate	Std error	Significance prob
Intercept	-4.15e-20	3.5e-21	<0.0001
T^4_{ion}	2.226e-20	7.54e-23	<0.0001

Region 4: 3 keV $\leq T_{ion} \leq$ 4 keV, can be fit with T^3_{ion}

R^2	0.9998	RMSE=1.46e-20	Mean=3.27e-18
Predictor	Estimate	Std error	Significance prob
Intercept	-7.33e-19	1.7e-20	<0.0001
T^3_{ion}	9.112e-20	3.75e-22	<0.0001

Region 5: 4 keV $\leq T_{ion} \leq$ 5 keV, can be fit with T^3_{ion}

R^2	0.9999	RMSE=3.06e-21	Mean=7.8e-18
Predictor	Estimate	Std error	Significance prob
Intercept	-9.02 e-19	4.51e-21	<0.0001
T^3_{ion}	9.409e-20	4.78e-23	<0.0001

Region 6: 5 keV $\leq T_{ion} \leq$ 6 keV, can be fit with T^3_{ion}

R^2	0.9994	RMSE=2.24e-20	Mean=1.48e-17
Predictor	Estimate	Std error	Significance prob
Intercept	-4.69e-19	4.e-20	<0.0001
T^3_{ion}	9.08e-20	2.35e-22	<0.0001

Region 7: 6 keV $\leq T_{ion} \leq$ 7 keV, can be fit with T^3_{ion}

R^2	0.9999	RMSE=4.15e-20	Mean=2.43e-17
Predictor	Estimate	Std error	Significance prob
Intercept	8.578e-19	8.71e-20	<0.0001
T^3_{ion}	8.48e-20	3.12e-22	<0.0001

Region 8: 7 keV $\leq T_{ion} \leq$ 8 keV, can be fit with T^3_{ion}

R^2	0.9998	RMSE=5.86e-20	Mean=3.63e-17
Predictor	Estimate	Std error	Significance prob
Intercept	3.272e-18	1.41e-19	<0.0001
T^3_{ion}	7.785e-20	3.3e-20	<0.0001

Region 9: 8 keV $\leq T_{ion} \leq$ 9 keV, can be fit with T^3_{ion}

R^2	0.999	RMSE=7.3e-20	Mean=5.06e-17
Predictor	Estimate	Std error	Significance prob
Intercept	6.89e-18	1.99e-19	<0.0001
T^3_{ion}	7.082e-20	3.21e-22	<0.0001

Region 10: 9 keV $\leq T_{ion} \leq$ 10 keV, can be fit with T^3_{ion}

R^2	0.9998	RMSE=8.49e-20	Mean=6.7e-17
Predictor	Estimate	Std error	Significance prob
Intercept	1.177e-17	2.58e-19	<0.0001
T^3_{ion}	6.416e-20	2.99e-20	<0.0001

Evaluating the goodness-of-fit of the various regression formulae examined (both reported and not reported) relies on the following diagnostics:

Small RMSE value indicating a small "noise" value,
Large R^2 (percentage of cross section variability explained by the fit),
Plot of the fit compares in form and shape to the original function,
Residual plot shows a lack of pattern,
Strength of significance of predictors is 1% or less,
Alternative powers of T_{ion} match common-usage knowledge.

The residual plots of all these fits do not strictly meet the criterion stated. Because of the nonlinear nature of Equation (1) and the nonlinear nature of fitting powers of T_{ion}, one would expect to see some regular patterns in the residuals with the fits weaving around the formulary values. Therefore meeting this criterion is better stated as not finding any *unexpected* patterns in the residuals.

It should be noted that for regions 7-10 (6 keV through 10 keV, in 1 keV intervals), T^2_{ion} works equally as well as T^3_{ion} and is the first choice for a fit using standard procedure for stepwise regression. The entire range (all regions) can be fit using T^3_{ion}, and even slightly better using cubed with sixth powers of T_{ion}, but the residuals at low energies were judged by JRL to be too great in comparison to their absolute value. Therefore, those fits are not reported herein.
Fits were analyzed using JMP software, a trademark of SAS Corporation, and the statistical-error analysis diagnostics are provided.

Formulary Reaction Rate Validation

The NRL Plasma Formulary provides Observation-based values for reaction rates averaged over Maxwellian distributions in the table so designated in Huba, page 45. These values are reproduced in Table 2 below, in the second column, and denoted as "*O*." We compare values *calculated* from Equation 1, in the third column, denoted as "*C*."

TABLE 2. Reaction Rate Fits with Powers of T_{ion} by Region

T_{ion}	Reaction Rate (cm^3/s), *O*	Reaction Rate Equation 1 (cm^3/s), *C*
1	5.5e-21	8.0541e-21
2	2.6e-19	3.1035e-19
5	1.3e-17	1.0853e-17
10	1.1e-16	7.5795e-16
Mean	3.08e-17	1.92e-16
Standard deviation	5.31e-17	3.77e-16

It is of interest to determine how well the experimentally-based reaction rates (second column) match those calculated with Eq. (1) (third column). This is a validation exercise which can be accomplished using the Langenbrunner D_n metric (Langenbrunner et al. 2007). We report the following as a statistical example, not as a physics-based uncertainty analysis.

As the last two rows of Table 2 show, the standard deviation for the formula values (calculated, *C*) is almost an order of magnitude larger than for the experimental values (observed, O). This disparity is taken into account in the D_n metric, in equation (2), which permits the specification of two different variances. The precision variance, s^2_n, is specified as the square of the standard deviation from the observations, *O*'s. The second variance of (*O*-*C*), $\sigma^2_{(O\text{-}C)}$, is specified as the variance of the differences in the second and third columns of Table 2. That standard deviation is 3.24e-16, which is aligned with the larger calculation variance using the values "*C*'s" in the third column.

$$D_n = \left[\sum^n_{i=1} \{(O_i\text{-}C_i)^2/s^2_n\}\right] / (n\text{-}k). \qquad (2)$$

D_n is a statistic whose distribution is a two-parameter Gamma Function with parameters $a = n/2$ and

$$b = \Sigma^n_{i=1}\{2a_i\sigma^2_{(O\text{-}C)}\} / \{a(n\text{-}k)s^2_n\}.$$

The resulting analysis used $n=4,\ k=1,\ a_i=0.5,\ a=2$, b=7384.28, and D_n =14,736.81. The 90th percentile of the Gamma distribution with parameters a and b as above is 28,723; therefore D_n =14,737 indicates a match at the "10% and below" levels-of-significance. Visual examination of the values in Table 2 confirms this validation.

Conclusion

The empirical formula (Equation 1) for deuterium and tritium thermonuclear fusion averaged over Maxwellian distributions is widely used for beam-physics and plasma-physics research. It is published in the NRL PLASMA FORMULARY, supported for publication and dissemination by the Office of Naval Research. Often though, *authors* *want an even simpler representation of this formula, for back-of-the envelope estimates of DT fusion. The sole purpose of this analysis is to report and document power-law estimates and goodness-of-fit of those estimates in small, one keV intervals for* T_{ion} *from 1 to 10 keV.* In the interval shown the power functions are:

0.1 keV < T_{ion} ≤ 1 keV, reaction rate can be fit with T^6_{ion};

1. keV < T_{ion} ≤ 2. keV, reaction rate be fit with no intercept and T^5_{ion};

2.0 keV ≤ T_{ion} ≤ 3.0 keV, can be fit with T^4_{ion};

3.0 keV ≤ T_{ion} ≤ 10. keV, can be fit with T^3_{ion} in 1 keV intervals;
6.0 keV ≤ T_{ion} ≤ 10. keV, can be fit with T^3_{ion} or with T^2_{ion}.

The goodness-of-fit between the "tabular Observation values" in Huba and Equation (1) is about +/- 10%. This was not expected by one of the authors (JRL). That author expected Equation (1) to be a more accurate representation of the observational data. Apparently, the statistical fits determined and documented in Table 1 herein fit Equation (1) better than Equation (1) fits the data. This is cause for further investigation, both of the cross section data, the formulary fits and the Maxwellian-average assumption.

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(Unclassified.)