

A SIMPLE COMPUTATIONAL FORM FOR MAXWELLIAN REACTIVITIES

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A simple form is given for the evaluation of Maxwellian reactivities for the reactions $T(d,n)^4\text{He}$, $D(d,p)T$, $D(d,n)^3\text{He}$, and $^3\text{He}(d,p)^4\text{He}$, with applications to the analytical treatment of fusion reactor problems.

There are a variety of forms to evaluate Maxwellian fusion reactivities¹⁻⁷ as a function of ion temperature T (keV). In addition to the more convenient computational forms,¹⁻⁵ there are also analytical forms obtained from first principles^{6,7} that are computationally inconvenient.

Brunelli⁵ recently published a simple form for the Maxwellian reactivity of a deuterium-tritium (D-T) plasma:

$$\langle\sigma v\rangle_{D,T}(\text{cm}^3/\text{s}) = 9 \times 10^{-16} \exp[-0.476|\ln(T/69)|^{2.25}] \quad (1)$$

which is accurate to 2% for $10 \leq T \leq 100$ keV and to 10% for $2 \leq T \leq 150$ keV. Equation (1) can be generalized to the form:

$$\langle\sigma v\rangle = \exp[A_1 + A_2|\ln(T/A_3)|^{A_4}] \quad (2)$$

Equation (2) has been fitted to reactivity data by Miley et al.⁸ using the ISML routine ZXSSQ (Ref. 9). The routine ZXSSQ determines the set $\{A_1, \dots, A_4\}$ by minimizing the sum of squares of the differences between the given data and Eq. (2). The results are shown in Table I, together with the curve-fitting errors:

$$\delta = 100(1 - \langle\sigma v\rangle_{\text{calc}}/\langle\sigma v\rangle_{\text{real}}) \quad (3)$$

where $\langle\sigma v\rangle_{\text{calc}}$ is obtained from Eq. (2) and $\langle\sigma v\rangle_{\text{real}}$ is taken from Ref. 8. A comparison of the present results to previous computational forms¹⁻⁵ is shown in Table II. Although the results of Ref. 4 are most accurate, Brunelli⁵ illustrates several advantages in using Eq. (2), which are restated in generalized form here. In particular, the logarithmic derivative of $\langle\sigma v\rangle$ is

TABLE I

Best-Fit Parameters for Eq. (2) in Cubic Centimetres per Second, with Corresponding Curve-Fitting Errors, δ

	$T(d,n)\alpha$	$D(d,p)T$	$D(d,n)^3\text{He}$	$^3\text{He}(d,p)\alpha$
A_1	-34.629731	-37.061587	-36.799066	-35.235392
A_2	-0.57164663	$-3.4503954 \times 10^{-5}$	$-1.0041572 \times 10^{-5}$	-0.15172469
A_3	64.221524	3.0774327×10^5	7.4173511×10^5	802.58671
A_4	2.1373239	5.0816753	5.4366402	2.6497885
$ \delta_{\text{max}} $	3.7	4.6	4.0	9.3
$\delta(T=1)$	2.3	(-10.8)	(-10.8)	(-21.8)
$\delta(T=1.5)$	2.8	-1.9	-2.3	1.9
$\delta(T=5)$	-2.3	2.7	2.7	2.5
$\delta(T=10)$	2.6	-0.5	0.1	-7.1
$\delta(T=20)$	2.8	-3.8	-2.8	-4.7
$\delta(T=40)$	-1.3	-4.3	-3.9	4.7
$\delta(T=60)$	-1.6	-2.4	-2.9	4.3
$\delta(T=80)$	-0.4	0.4	-1.1	-0.5
$\delta(T=100)$	2.7	3.6	1.0	-6.9
Range of T (keV)	1 to 100	1.5 to 100	1.5 to 100	1.5 to 100

TABLE II
Accuracy Comparisons, δ_{max} , for Various Simple Forms for $1.5 \leq T \leq 80$ keV*

Reference	T(d,n) ⁴ He	D(d,p)T	D(d,n) ³ He	³ He(d,p) ⁴ He
Gamow (Ref. 1)	57	12	10	25
Gamow + first-order corrections (Ref. 2)	27	6	4	15
Kozlov (Ref. 3)	8	1	0.6	2
Hively (Ref. 4)	1 ^a	0.052	0.02	0.4
Brunelli (Ref. 5)	10	---	---	---
Present work	4	5	4	9

*See Ref. 4 for details.

^aThere is a typographical error in Table I of Ref. 4: The coefficient a_5 of s_5^2 for the reaction T(d,n)⁴He should be negative; the magnitude is correct.

$$\mu(T) \equiv \frac{d \ln \langle \sigma v \rangle}{d \ln T} = A_2 A_4 |\ln(T/A_3)|^\alpha, \quad (4)$$

where $\alpha = A_4 - 1$. In addition, the maximum value y_m of the function $y = \langle \sigma v \rangle / T^m$ (which arises frequently in reactor power balances) occurs at temperature T_m by solving $\mu(T) = m$. The value of T_m can be found explicitly as

$$T_m = A_3 \exp[\pm(m/A_2 A_4)^{1/\alpha}], \quad \pm \text{ for } m \leq 0. \quad (5)$$

Thirdly, a truncated expansion of $\ln y$, near T_m , can be obtained in powers of $\ln(T/T_m)$:

$$\begin{aligned} \ln(y/y_m) &= \frac{1}{2} \left(\frac{d\mu}{d \ln T} \right)_{T_m} \ln^2(T/T_m) \\ &= A_2 A_4 (A_4 - 1) (m/A_2 A_4)^\beta \ln^2(T/T_m), \end{aligned} \quad (6)$$

where $\beta = (A_4 - 2)/(A_4 - 1)$. Following Brunelli, Eq. (6) can be rewritten as

$$\langle \sigma v \rangle = y_m T^m,$$

which is a local approximation to Eq. (2) with a relative error given by the right side of Eq. (6). The remainder of Brunelli's results can be trivially generalized and will not be repeated here. It is concluded that Eq. (2) provides a good computational form for Maxwellian reactivities, with applications to the analytical treatment of fusion reactor problems.

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REFERENCES

1. G. GAMOW and C. L. CRITCHFIELD, *Theory of the Atomic Nucleus and Nuclear Energy Sources*, Chap. 10, Oxford University Press, Oxford, U.K. (1949).
2. C. L. CRITCHFIELD, "Analytic Forms of the Thermonuclear Functions," *Cosmology Fusion and Other Matters*, p. 186, F. REINES, Ed., Colorado Associated University Press, Boulder (1972).
3. B. N. KOZLOV, "Thermonuclear Reaction Rates," *At. Energy*, **12**, 238 (1962).
4. L. M. HIVELY, "Convenient Computational Forms for Maxwellian Reactivities," *Nucl. Fusion*, **17**, 873 (1977).
5. B. BRUNELLI, "An Empirical Formula for the (D,T) Reaction Rate Parameter $\langle \sigma v \rangle$," *Nuovo Cimento*, **55B**, 264 (1980).
6. J. N. BAHCALL, "Non-Resonant Nuclear Reactions at Stellar Temperatures," *Astrophys. J.*, **143**, 259 (1966).
7. H. J. HAUBOLD and R. W. JOHN, "Analytical Representation of the Thermonuclear Reaction Rate . . .," *Plasma Phys.*, **23**, 399 (1981).
8. G. H. MILEY et al., "Fusion Cross Sections and Reactivities," COO-2218-17, University of Illinois (June 17, 1974).
9. International Mathematical and Statistical Libraries, Inc., Sixth Floor, GNB Building, 7500 Bellaire Boulevard, Houston, Texas 77036 (Library 3, Edition 8.1).