SPECIAL TOPIC

CONVENIENT COMPUTATIONAL FORMS FOR MAXWELLIAN REACTIVITIES*

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In the course of our fusion studies, a convenient form was required to calculate reactivities, $S \equiv \langle\sigma v\rangle$, for Maxwellian fusions. Presently available forms include the well-known Gamow equation [1]:

$$S_1 = a_1\, T^{-2/3} \exp\,(-a_2/T^{1/3}) \qquad (1)$$

the Gamow form with first-order corrections [2]:

$$S_2 = a_1(1 + a_3\, T^{1/3})^{5/12}\; T^{-2/3} \exp\,(-a_2/T^{1/3}) \qquad (2)$$

a variation of Eq.(2) due to Kozlov [3] for D-D reactions:

$$S_3 = a_1(1 + a_3\, T^{.75})\, T^{-2/3} \exp\,(-a_2/T^{1/3}) \qquad (3)$$

and a generalization of Eq.(3) also due to Kozlov [3] for D-T and D-^{3}He,

$$S_4 = a_1(1 + a_3\, T^{.75})\, T^{-2/3} \exp\,(-a_2/T^{1/3}) / \sqrt{1 + a_4\, T^{3.25}} \qquad (4)$$

New parametric forms considered in the present work are:

$$S_5 = \exp\,[a_1/T^r + a_2 + a_3 T + a_4 T^2 + a_5 T^3 + a_6 T^4] \qquad (5)$$

$$S_6 = \exp\,[a_1/T^r + a_2 + a_3 T^s] \qquad (6)$$

and a generalization of Eq.[3]:

$$S_7 = a_1(1 + a_3 T^r)\, T^{-2/3} \exp\,(-a_2/T^{1/3}) \qquad (7)$$

There are other analytical forms developed for astrophysics calculations [4] which are inconvenient for rapid computations. The purpose of this work is to compare (1)–(7) for several reactions and to propose accurate, convenient computational forms for $\langle\sigma v\rangle$.

The reactions considered here are:

$t \equiv {}^3\mathrm{H}(d,n)^4\mathrm{He}$; $\quad g \equiv {}^3\mathrm{He}(d,p)^4\mathrm{He}$

$p \equiv {}^2\mathrm{H}(d,p)^3\mathrm{H}$; $\quad n \equiv {}^2\mathrm{H}(d,n)^3\mathrm{He}$

The reactivity data used here have been calculated accurate to 0.01% by Miley et al. [5–6], based on cross-section curve fits by Duane [7]. The basic cross-sections themselves contain a larger uncertainty, perhaps as much as 5%. From the tabulated reactivities, S_{calc}, the parameters $a_1, \ldots, a_6$, r, s were found by using the IMSL routine ZXSSQ [8] on the PDP 10 and Cyber 175 computers at the University of Illinois. The routine ZXSSQ calculates the set $\{a_i, r, s\}$ by minimizing the sum of squares of the difference between the given data and the parametric function. In all cases, the temperature is measured in keV over a curve-fitting range, $1 \leqslant T \leqslant 80$ keV; $S \equiv \langle\sigma v\rangle$ is measured in $\mathrm{cm}^3 \cdot \mathrm{s}^{-1}$.

The best-fit parameters for the various reactions and the corresponding fitting errors are given in Tables I–IV. Fits for Eqs (3) and (7) are excluded for reactions t and g because these forms provide little improvement over Eq.(2). Also, for the reactions t and g, Tables I and II show a comparison of Eq.(5), using all the polynomial terms, with the same form using fewer terms in the polynomial. For reactions p and n, fits for Eq.(4), and

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for Eq.(5) with fewer terms than T^4, are excluded because Eqs (5) and (7) provide adequate fits. Tables I–IV indicate that Eqs (1) and (2) yield poor fits, with maximum errors of 25–57%, 15–25%, 6–12% and 4–10% for reactions t, g, p and n, respectively. Reactivities for reaction t can be fitted within 8% by Eq.(4); peak errors for Eq.(3) are 1.5%, 0.9% and 0.6% for reactions g, p and n, respectively. Unfortunately, as noted above, the error in fitting Eq.(3) to reaction t remains large, of the order of 30%. However, Eq.(5) provides excellent fits in all cases with maximum errors of 1.2%, 0.4%, 0.1% and 0.1% for reactions t, g, p and n, respectively. Peak errors for fits to Eq.(6) are 4.5%, 2.5%, 0.9%, and 0.4% for the four reactions, t, g, p and n. If only D-D reactions are of interest, then Eq.(7) provides excellent fits, having peak errors of 0.05% and 0.02% for reactions p and n, respectively.

In conclusion, Eq.(5) is an accurate, convenient computation form for all four reactions. If only reactivities for D-D reactions are required, Eq.(7) provides outstanding fits.

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TABLE I. BEST-FIT PARAMETERS FOR $\langle\sigma v\rangle_t$ AND CURVE-FITTING ERRORS, $\delta = 100\,(S_t/S_{calc} - 1)$

	S_1	S_2	S_4	S_5	S_5*	S_5**	S_5+	S_6
a_1	2.3521091×10^{-12}	1.0312800×10^{-11}	3.3729298×10^{-12}	-21.377692	-22.711874	-20.779964	-17.226965	-71.293084
a_2	19.424262	21.138726	20.407142	-25.204054	-23.836412	-25.813871	-29.497319	61.931426
a_3	-	-0.23487447	0.20293722	-7.1013427×10^{-2}	-9.3925317×10^{-2}	-6.6251351×10^{-2}	-2.6326812×10^{-2}	-37.304761
a_4	-	-	8.8829520×10^{-5}	1.9375451×10^{-4}	7.9944173×10^{-4}	3.0934551×10^{-4}	0.0	-
a_5	-	-	-	4.9246592×10^{-6}	3.1438516×10^{-6}	0.0	0.0	-
a_6	-	-	-	-3.9836572×10^{-8}	0.0	0.0	0.0	-
r	-	-	-	.2935	.27472414	.30366647	.38691539	.13963366
s	-	-	-	-	-	-	-	.10059041
$\lvert\delta_{max}\rvert$	57.2	26.7	8.1	1.16	1.5	3.0	10.3	4.5
δ(T=1)	57.2	11.0	1.5	.001	1.1	-0.72	-9.34	-1.38
δ(T=5)	-27.2	-5.5	-2.2	0.69	0.77	0.61	1.92	1.71
δ(T=10)	-43.5	-16.6	2.2	-0.96	-0.74	-1.60	-6.95	-3.03
δ(T=20)	-41.3	-10.3	8.1	0.85	0.26	1.40	-3.26	-1.85
δ(T=40)	-14.4	15.4	-0.5	-0.29	-0.06	1.11	7.75	3.20
δ(T=60)	19.7	18.6	-2.6	-0.07	-0.07	-2.14	3.73	1.38
δ(T=80)	57.0	-26.7	-1.6	-0.70	-0.22	3.00	-10.3	-4.53

* T^4 term excluded
** T^3 and T^4 terms excluded
\+ T^2, T^3 and T^4 terms excluded

TABLE II. BEST-FIT PARAMETERS FOR $\langle\sigma v\rangle_g$ AND CURVE-FITTING ERRORS, $\delta = 100\ (S_g/S_{calc} - 1)$

	S_1	S_2	S_4	S_5	S_5*	S_5**	S_5†	S_6
a_1	5.2689838×10^{-12}	4.0045517×10^{-13}	-4.2145988×10^{-14}	-27.764468	-27.731978	-28.863682	-30.478894	-29.264460
a_2	33.083882	32.189295	28.415670	-31.023898	-31.058052	-29.888864	-28.215862	-29.452283
a_3	-	76.788536	-2.5739067	2.7809999×10^{-2}	2.7991287×10^{-2}	5.865272×10^{-3}	-1.1277343×10^{-2}	-2.1114609×10^{-5}
a_4	-	-	-1.3007516×10^{-6}	-5.5321633×10^{-4}	-5.3895197×10^{-4}	-1.3084623×10^{-4}	0.0	-
a_5	-	-	-	3.0293927×10^{-6}	2.6589549×10^{-6}	0.0	0.0	-
a_6	-	-	-	-2.5233325×10^{-9}	0.0	0.0	0.0	-
r	-	-	-	.3597	.36031698	.34389314	.32063812	.33768389
s	-	-	-	-	-	-	-	2.3106701
$\lvert\delta_{max}\rvert$	25.3	14.8	1.58	0.36	0.36	2.4	5.7	2.5
δ(T=1)	-25.3	-14.8	0.13	0.0003	-0.15	1.43	5.65	2.45
δ(T=5)	7.09	5.14	-0.11	-0.18	-0.15	0.03	-0.61	-0.11
δ(T=10)	7.02	3.78	0.58	0.29	0.22	0.95	3.35	1.46
δ(T=20)	-3.99	-5.95	-0.99	-0.14	-0.19	-1.24	0.87	-0.86
δ(T=40)	-12.2	-11.5	-0.07	0.07	0.15	-0.83	-3.31	-1.23
δ(T=60)	-6.06	-3.17	1.07	0.03	-0.02	1.84	-0.62	1.54
δ(T=80)	6.15	11.5	-1.58	0.23	0.34	-2.42	3.26	-1.90

* T^4 term excluded
** T^3 and T^4 terms excluded
† T^2, T^3 and T^4 terms excluded

TABLE III. BEST-FIT PARAMETERS FOR $\langle\sigma v\rangle_p$ AND CURVE-FITTING ERRORS, $\delta = 100\ (S_p/S_{calc} - 1)$

	S_1	S_2	S_3	S_5	S_6	S_7
a_1	2.6948677×10^{-14}	2.4321393×10^{-15}	1.8742387×10^{-14}	-15.511891	-14.879261	2.0018602×10^{-14}
a_2	19.727318	18.872238	19.244282	-35.318711	-36.019495	19.307336
a_3	-	52.886985	1.6109164×10^{-2}	-1.2904737×10^{-2}	5.5964022×10^{-2}	5.7756259×10^{-3}
a_4	-	-	-	2.6797766×10^{-4}	-	-
a_5	-	-	-	-2.9198685×10^{-6}	-	-
a_6	-	-	-	1.2748415×10^{-8}	-	-
r	-	-	-	.3735	.39648171	.94955669
s	-	-	-	-	-3.1005261	-
$\lvert\delta_{max}\rvert$	12.1	5.7	0.85	0.11	0.92	0.052
δ(T=1)	-12.1	-1.77	0.69	0.003	0.042	-0.048
δ(T=5)	2.58	0.19	-0.27	0.054	0.023	0.009
δ(T=10)	5.34	2.08	-0.02	0.084	-0.263	-0.015
δ(T=20)	4.87	3.03	0.42	-0.049	0.094	-0.027
δ(T=40)	-0.09	1.21	0.54	0.010	0.543	0.013
δ(T=60)	-5.64	-2.06	0.02	0.021	0.111	0.024
δ(T=80)	-10.9	-5.70	-0.85	0.085	-0.921	-0.052

TABLE IV. BEST-FIT PARAMETERS FOR $\langle\sigma v\rangle_n$ AND CURVE-FITTING ERRORS, $\delta = 100\ (S_n/S_{calc} - 1)$

	S_1	S_2	S_3	S_5	S_6	S_7
a_1	$3.4920841 \times 10^{-14}$	$3.9853533 \times 10^{-15}$	$2.6001260 \times 10^{-14}$	-15.993842	-15.314707	$2.7219425 \times 10^{-14}$
a_2	20.144728	19.297132	19.751844	-35.017640	-35.903973	19.795543
a_3	-	30.099091	1.2703127×10^{-2}	$-1.3689787 \times 10^{-2}$	.19465321	5.3891144×10^{-3}
a_4	-	-	-	2.7089621×10^{-4}	-	-
a_5	-	-	-	$-2.9441547 \times 10^{-6}$	-	-
a_6	-	-	-	1.2841202×10^{-8}	-	-
r	-	-	-	.3725	.40568858	.91723383
s	-	-	-	-	-1.5743113	-
$\lvert\delta_{max}\rvert$	10.0	3.7	0.56	0.11	0.44	0.018
δ(T=1)	-10.0	0.37	0.500	0.006	0.081	0.0175
δ(T=5)	2.19	-0.31	-0.195	-0.055	0.088	-0.0010
δ(T=10)	4.44	-1.12	-0.010	0.084	-0.175	-0.0018
δ(T=20)	4.05	2.14	0.298	-0.048	-0.079	-0.0025
δ(T=40)	-0.036	1.20	0.361	0.010	0.252	0.0013
δ(T=60)	-4.62	-1.05	0.015	0.022	0.104	0.0070
δ(T=80)	-9.01	-3.71	-0.561	0.086	-0.443	-0.0158

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