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ABSTRACT

The charge exchange rate coefficients for hydrogen isotopes are evaluated and the average over a Maxwellian spectrum is carried out analytically. Applications to tokamak calculations are also considered.

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ANALYTICAL SOLUTION; BOLTZMANN STATISTICS; CHARGE EXCHANGE; CHARGE-EXCHANGE REACTIONS; CROSS SECTIONS; ELECTRON LOSS; EV RANGE 10-100; EV RANGE 100-1000; KEV RANGE; HYDROGEN ISOTOPES; PLASMA; REACTION KINETICS

CONTENTS

1. INTRODUCTION

At the AAEC Research Establishment limited effort has been given to evaluating cross sections and rate coefficients relevant to fusion research. A library of data, ADL-1 [Clancy et al. 1981], has been prepared for use with the zero-dimensional transport code SCORCH. In this library, however, the rate coefficients for charge transfer reactions have not been included. The study of this process has a long history, and experimental work has been discussed by Glasstone and Lovberg [1960]. They described how a beam of ions is passed through a neutral gas and the charge exchange, or neutralisation reaction rate, causes a loss term, while the ionisation of neutral atoms by the formed fast neutrals produces a gain term. This second reaction can be neglected in tokamak design calculations since the SCORCH corona model option shows that, from about 100 eV, the approximate neutral-to-ion number density ratio for hydrogen isotope plasmas varies from 10^{-4} to 10^{-8} respectively. The neutral-neutral ionisation rate is therefore entirely negligible.

An excellent compilation of both theoretical and experimental charge transfer cross sections for the hydrogen isotopes has been published by workers at Nagoya University, Japan [Takayanagi and Suzuki 1978]. This process has been investigated to evaluate the rate coefficient required for the ADL-1 temperature scale 10 eV to 1 MeV. It is obvious from the Nagoya plots that there are two distinct energy regions. The first is the electron stripping region from 1 eV to 20 keV; the second is a nuclear charge exchange region extending from about 50 keV to 1 MeV. The latter descends rapidly with increasing energy reaching approx. 10 barns at 1 MeV. The atomic theories of Dalgarno and Yadav [1953] and Smith [1967] do not fit the experiments satisfactorily, nor does the nuclear theory of Cheshire [1964] adequately describe the rapid descent. A great number of references have appeared in the IAEA compilation CIAMBA [1980]. Our approach was to fit the Nagoya experimental information empirically to both regions to make the average of the rate coefficient over a Maxwellian distribution numerically straightforward (see Section 2).

The mathematical theory for computing the rate coefficient may, at first, seem complicated, but for numerical work, analytic solutions are a great deal faster to compute than a direct numerical integration. We even found that LaGuerrre quadrature, although normally quite satisfactory for smoothly varying functions, would not give accurate answers.

In Section 3, applications of the rate coefficients for the hydrogen isotopes are discussed. One example is the interaction of hot plasmas with cold gas blankets; another is the possible application to neutral beam injection theory.

The following reactions are dealt with:

$$H^o + H^+ \rightarrow H^+ + H^o$$

$$D^o + D^+ \rightarrow D^+ + D^o$$

$$D^o + T^+ \rightarrow D^+ + T^o$$

$$T^o + T^+ \rightarrow T^+ + T^o$$

2. RATE COEFFICIENTS

The reaction rate coefficient for a Maxwellian spectrum is defined to be

$$\overline{\sigma v}(T) = \sqrt{\frac{2}{m}} \frac{\int_0^\infty \sigma(E)\, E\, e^{-E/T}\, dE}{\int_0^\infty E^{\frac{1}{2}}\, e^{-E/T}\, dE} \quad (cm^3\ s^{-1}) \quad , \tag{1}$$

where $\sigma(E)$ is the total cross section for the process, E is the energy, and m is the mass of the species involved (or the reduced mass for a mixture of species).

It is quite apparent, from the scale of the energy employed in the Nagoya plots, that the data in the atomic region ($0.01\ keV \leq E \leq E_c$), where E_c is the cutoff energy, obey the simple rule

$$\sigma_1(E) = a_0 + a_1 \ell n\, E \quad (cm^2) \quad , \quad E_c = 20\ keV \quad . \tag{2}$$

A least squares fit of $\sigma(E)$ in this region gives

(i) $a_0 = 2.162 \times 10^{-15}\ (cm^2)$,

(ii) $a_1 = -0.565 \times 10^{-15}\ (cm^2)$. (3)

In the second (nuclear) phase, the data correspond to the power law

$$\sigma_2(E) = c_0\ E^{-c_1} \quad . \tag{4}$$

Again, a least squares fit produces the values

(i) $c_0 = 2.077 \times 10^{-10}$,

(ii) $c_1 = 3.849$. (5)

The Maxwellian average (equation 1) can therefore be written

$$\overline{\sigma v}(T) = \frac{2}{\sqrt{\pi}} \sqrt{\frac{2T}{m}}\, T^{-2} \left\{ \int_0^{E_c} \sigma_1(E)\ E\ e^{-E/T} dE + \int_{E_c}^{\infty} \sigma_2(E)\ E\ e^{-E/T}\ dE \right\}$$

$$= \frac{2}{\sqrt{\pi}} \sqrt{\frac{2T}{m}} \left\{ I_1 + I_2 \right\} \tag{6}$$

Let

$$a_2 = a_0 + a_1\ \ln T \quad ; \tag{7}$$

we have

$$I_1 = T^{-2} \int_0^{x_c} (a_2 + a_1\ \ln x) x\ e^{-x}\ dx \quad , \tag{8}$$

where $x = E/T$, $x_c = E_c/T$.

Hence

$$I_1 = a_2 \int_0^{x_c} x\ e^{-x}\ dx + a_1 \int_0^{x_c} \ln (x)\ x\ e^{-x}\ dx$$

$$= a_2\ [1 - e^{-x_c}\ (1+x_c)] + a_1\ \gamma'(2,x_c) \quad , \tag{9}$$

$$\gamma'(2,x_c) = \lim_{\nu\to 2} \frac{d\gamma(\nu,x_c)}{d\nu} \quad , \tag{10}$$

where $\gamma(\nu,x_c)$ is the incomplete gamma function defined as

$$\gamma(\nu,x) = \int_0^x e^{-t}\, t^{\nu-1}\, dt \tag{11}$$

[Gradshteyn and Ryzhik 1965; see appendix for detail]

The second region is obtained from equations (6) and (4), defined by the integral

$$I_2 = T^{-2}\int_{E_c}^{\infty} c_0\, E^{1-c_1}\, e^{-E/T}\, dE$$

$$= c_0\, T^{-c_1}\, \Gamma(1-c_1,x_c) \quad , \tag{12}$$

where $\Gamma(1-c_1,x_c)$ is the associated incomplete gamma function [Gradshteyn and Ryzhik 1965]:

$$\Gamma(\nu,x) = \int_x^{\infty} e^{-t}\, t^{\nu-1}\, dt \quad . \tag{13}$$

The general rate coefficient thus becomes

$$\overline{\sigma v}(T) = \frac{2}{\sqrt{\pi}} \sqrt{\frac{2T}{m}}\; a_2[1-e^{-x_c}(1+x_c)] + a_1\gamma'(2,x_c) \tag{14}$$

$$+ c_0\, T^{-c_1}\, \Gamma(1-c,x_c) \quad .$$

With the fitted laws (2) and (4) for the $H^o + H^+$ curve, a simple rule can be used to obtained the other three cases:

$$\overline{\sigma v}_{m_1(0)m_2(+)}(T) = \frac{1}{\sqrt{2\mu}}\; \overline{\sigma v}_{H^oH^+}(T) \tag{15}$$

in which

$$\mu = \frac{m_1(0)m_2(+)}{m_1(0)+m_2(+)} \quad \text{and} \quad T = \frac{2\mu}{m_H} T_H$$

for the hydrogen plasma at temperature T_H, arbitrary masses m_1, m_2, and hydrogen mass m_H.

The results for the evaluated rate coefficients are listed in Table 1 for the ADL-1 library temperatures. The coefficients are also shown in Figure 1. Particularly surprising is the way in which the lower region law of the cross section contributes at very high temperatures in the integrated average. As there was a mismatch at 4 keV in the 4 to 50 keV range, a simple quadratic interpolation between the lower and upper limits was used.

3. APPLICATIONS

The corona model, when applied to tokamak calculations, predicts that the neutral hydrogen isotopes should cluster mostly near the wall or limiter. In some machines, cold gas blankets are actually part of the design. In these circumstances, charge exchange collisions may well be important number density and power density losses. If a semi-heuristic argument is used, the number density loss could be described by the rate equation [Spitzer 1956]

$$\frac{dn_+}{dt} = f(T) + \frac{n_0 - n_+}{\tau_{cxe}} \quad , \tag{16}$$

where

$\tau_{cxe} = \frac{1}{2}\left(\frac{m_+}{m_0}\right)\tau_{cx+}$ = the equilibration time,

$\tau_{cx+} = \frac{1}{\nu_{cx+}}$, ν_{cx+} = the charged species collision frequency with neutrals,

n_+ = the number density of the charged species,

n_0 = the number density of the neutral species,

t = time, and

$f(T)$ = the balance of other losses and gains.

The collision frequency would then be

$$\nu_{cx+} = n_0 \; \overline{\sigma v}_{cx} \quad . \tag{17}$$

Similarly, the power loss could be described by the relationship

$$\frac{dT}{dt} = \frac{T_0 - T_+}{\tau_{cxe}} + g(T) \quad , \tag{18}$$

where g(T) is the balance of other losses and gains to the power.

For a combination of two species, the ADL-1 table can be looked up in such a way that the appropriate temperature is

$$\overline{\sigma v}\,(T_{eff}) = \overline{\sigma v}\,(T_1,T_2) \times N(T_1,T_2);\; N = \left(\frac{4\mu}{T_{eff}\left(\frac{m_1}{T_1} + \frac{m_2}{T_2}\right)}\right)^{\frac{1}{2}} \quad ,$$

for species temperatures T_1 and T_2, and where

$$T_{eff} = \left\{ \frac{1}{M} \left(\frac{m_1}{T_1} + \frac{m_2}{T_2}\right) + \frac{\mu\left(\frac{1}{T_1} - \frac{1}{T_2}\right)^2}{\frac{m_1}{T_1} + \frac{m_2}{T_2}} \right\} , \tag{19}$$

where μ is the net reduced mass, $M = m_1 + m_2$, for masses m_1 and m_2.

The second possible application is far more complicated. In neutral beam injection, the evolution of the beam heating would require calculations on the way in which fast neutrals interact with a charged particle plasma with ions at a much lower energy than the beam. The desired cross section can be acquired by using the theorem of detailed balance, i.e.

$$k_+^2 \, \sigma_{+0}(k_+) = k_0^2 \sigma_{0+}(k_0) \quad , \tag{20}$$

where k_+ is the centre-of-mass momentum of the ion, and k_0 is the centre-of-mass momentum of the neutral.

4. CONCLUSION

The rate coefficients for the hydrogen isotope charge exchange collisions have been evaluated and added to the ADL-1 library. Possible applications to tokamak calculations have also been discussed. This library is available either from the Australian Atomic Energy Commission, or from the Fusion Data Section, IAEA, Vienna.

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TABLE 1

CHARGE TRANSFER RATE COEFFICIENT vs. TEMPERATURE

T(KEV)	H0 + H+	D0 + D+	D+ + T0	T0 + T+
0.01	3.494D-08	1.892D-08	1.609D-08	1.319D-08
0.02	4.514D-08	2.463D-08	2.059D-08	1.724D-08
0.03	5.222D-08	2.864D-08	2.443D-08	2.019D-08
0.04	5.779D-08	3.182D-08	2.717D-08	2.237D-08
0.05	6.244D-08	3.449D-08	2.947D-08	2.429D-08
0.06	6.645D-08	3.681D-08	3.147D-08	2.596D-08
0.07	6.999D-08	3.887D-08	3.326D-08	2.745D-08
0.08	7.318D-08	4.073D-08	3.487D-08	2.880D-08
0.09	7.608D-08	4.244D-08	3.634D-08	3.003D-08
0.10	7.874D-08	4.401D-08	3.771D-08	3.118D-08
0.20	9.783D-08	5.549D-08	4.771D-08	3.960D-08
0.30	1.101D-07	6.314D-08	5.441D-08	4.528D-08
0.40	1.192D-07	6.895D-08	5.953D-08	4.965D-08
0.50	1.264D-07	7.366D-08	6.370D-08	5.323D-08
0.60	1.323D-07	7.762D-08	6.722D-08	5.626D-08
0.70	1.373D-07	8.103D-08	7.027D-08	5.890D-08
0.80	1.416D-07	8.403D-08	7.296D-08	6.124D-08
0.90	1.453D-07	8.670D-08	7.537D-08	6.334D-08
1.00	1.486D-07	8.910D-08	7.753D-08	6.524D-08
2.00	1.673D-07	1.047D-07	9.190D-08	7.806D-08
3.00	1.740D-07	1.130D-07	9.983D-08	8.544D-08
4.00	1.752D-07	1.179D-07	1.048D-07	9.032D-08
5.00	1.771D-07	1.209D-07	1.082D-07	9.375D-08
6.00	1.768D-07	1.226D-07	1.104D-07	9.622D-08
7.00	1.759D-07	1.234D-07	1.117D-07	9.801D-08
8.00	1.747D-07	1.243D-07	1.125D-07	9.926D-08
9.00	1.733D-07	1.246D-07	1.127D-07	1.001D-07
10.00	1.718D-07	1.248D-07	1.136D-07	1.006D-07
12.00	1.686D-07	1.246D-07	1.139D-07	1.007D-07
14.00	1.654D-07	1.239D-07	1.137D-07	1.018D-07
16.00	1.622D-07	1.231D-07	1.133D-07	1.018D-07
18.00	1.592D-07	1.221D-07	1.128D-07	1.017D-07
20.00	1.563D-07	1.210D-07	1.121D-07	1.013D-07
30.00	1.435D-07	1.154D-07	1.079D-07	9.879D-08
40.00	1.333D-07	1.101D-07	1.037D-07	9.573D-08
50.00	1.265D-07	1.053D-07	9.973D-08	9.271D-08
60.00	1.182D-07	1.011D-07	9.615D-08	8.987D-08
70.00	1.115D-07	9.732D-08	9.290D-08	8.723D-08
80.00	1.059D-07	9.391D-08	8.994D-08	8.479D-08
90.00	1.012D-07	9.083D-08	8.724D-08	8.254D-08
100.00	9.712D-08	8.911D-08	8.476D-08	8.044D-08
250.00	6.599D-08	6.254D-08	6.144D-08	5.998D-08
500.00	4.802D-08	4.648D-08	4.599D-08	4.528D-08
750.00	3.960D-08	3.867D-08	3.838D-08	3.795D-08
1000.00	3.447D-08	3.382D-08	3.362D-08	3.333D-08

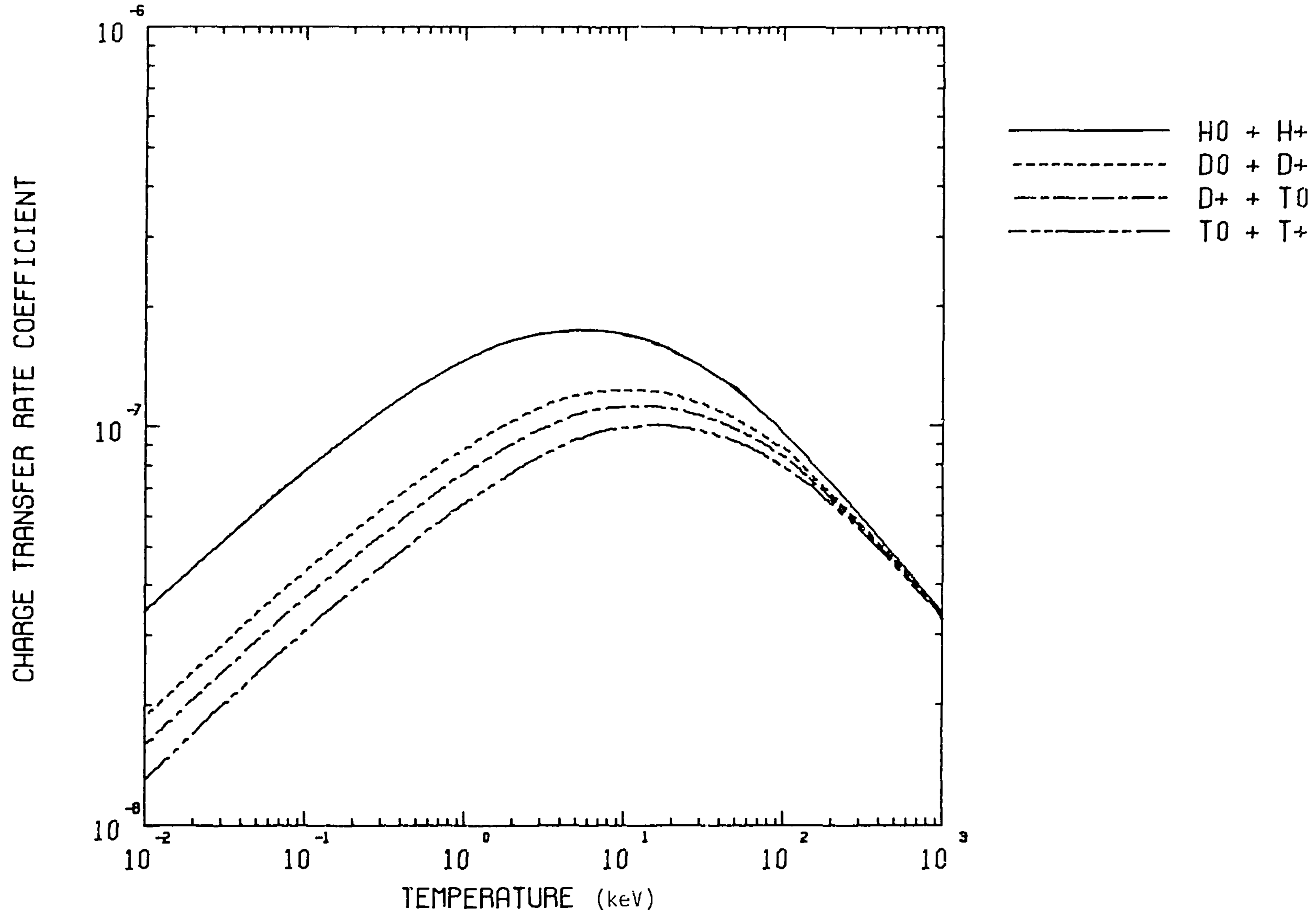

FIGURE 1. CHARGE TRANSFER RATE COEFFICIENT vs. TEMPERATURE

APPENDIX A
EVALUATION OF THE INCOMPLETE GAMMA FUNCTIONS

Using standard formulae [Erdélyi et al. 1953; Gradshteyn and Ryzhik 1965], we found the following results

$$\gamma'(2,x) = x^2 \ln x \;\; (2,x) - x^2 \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!(n+2)^2} \tag{A1}$$

$$\gamma(2,x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!(n+2)} \tag{A2}$$

For large values of x, say x > 10, the following relationship is used:

$$\gamma'(2,x) = \psi(2) - \Gamma'(2,x) \quad , \tag{A3}$$

where $\psi(2) = 1-\gamma = 0.422784335$, and γ = Euler's constant, to obtain the aysmptotic series

$$\Gamma'(2,x) = x\, e^{-x} \left[\left(1 + \frac{1}{x}\right) \ln x + \frac{1}{x} S(x) \right] \tag{A4}$$

in which

$$S(x) = 1 + \frac{1}{x} - \frac{1}{x^2} + \frac{2}{x^3} - \frac{6}{x^4} + \frac{24}{x^5} \quad . \tag{A5}$$

In the computation of the gamma functions, the relationships

$$\begin{aligned} &\text{(i)} \quad \Gamma(\nu,x) = \Gamma(\nu) - \gamma(\nu,x), \text{ and} \\ &\text{(ii)} \quad \Gamma(-\nu)\Gamma(\nu) = \frac{-\pi}{\nu \sin \nu\pi} \end{aligned} \tag{A6}$$

are used. For large values of x, the continuous fraction

$$\Gamma(\nu,x) = \cfrac{x^{\nu} e^{-x}}{x + \cfrac{1-\nu}{1 + \cfrac{1}{x + \cfrac{2-\nu}{1+\ldots}}}} \tag{A7}$$

can also be employed.