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Approximation Error in the Rate Coefficients of Neutral-Ion Interactions

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A study of the error introduced by commonly used approximations of average Maxwellian reaction rate coefficients is presented. Reactions examined are charge exchange and ionization between neutral atoms and ions of a plasma containing hydrogen isotopes and helium. Since some approximations considered have a complementary character, in the sense that one fails in some ranges where the other is successful, it is possible to select in each range the appropriate approximation in order to achieve the required accuracy. A particular combination of methods is suggested which has been tested in Monte Carlo problems with the aim of investigating both its cost and its efficacy. © 1985 Academic Press Inc.

1. INTRODUCTION

In fusion device design, Maxwellian average reaction rate coefficients for neutral-ion interactions are computed for a given injection energy of the neutral particle:

(a) by a straight numerical integration [1, 2], averaging $v_r\sigma(v_r)$ over the ion velocity distribution, v_r being the relative velocity between the interacting particles;

(b) by analytical approximating expressions [3, 4];

(c) by some drastic approximations, substituting the distribution of the plasma ion velocities with an appropriate average velocity [5, 6].

When used in sophisticated computer codes (e.g., Monte Carlo codes) where a wide range of injection neutral energy beside a temperature gradient of the plasma might be considered in the same problem, all of the above methods reveal some weaknesses. For example, Galbraith and Kammash [4] have pointed out numerical difficulties arising in some special cases in their (not simple) analytical approximations. On the other hand, numerical integration becomes troublesome when neutral injection energy is much higher than plasma temperature, whereas, in the same conditions—ion velocity being negligible with respect to that of the neutral—the approximation of an average velocity may be quite satisfactory. In the opposite situation, however, this last approximation will obviously be too rough.

The aim of this work is to study the error induced by these approximations in order to keep it under control. In fact, accurate computation of average rate coefficients, besides avoiding error amplification (cross sections are experimentally

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uncertain, their representation through empirical formulas introduces other errors), may also be a fundamental requirement in order to avoid dangerous inconsistencies in numerical models as, for example, may happen in Monte Carlo methods, a point discussed in the last section.

The above considerations suggest that there is some reason to hope that the average velocity approximation, which offers the obvious advantages of simplicity and praticability, can usefully represent an alternative to other approximations in some ranges. In fact, as will be seen, a strategy combining different methods can be adopted, to obtain a required accuracy.

We shall discuss in Section 3 the error introduced by approximations (a) and (c); Section 4 will be devoted to approximation (b). The reactions considered are charge exchange between hydrogen isotopes, between neutral hydrogen isotopes and alpha particles, and ionization of neutrals by positive ions. Ionization by electrons has not been considered, several simple analytical expressions for rate coefficients being already available [3, 4, 7].

2. Rate Coefficient Approximations

We assume that

(i) cross sections $\sigma(v_r)$ of interactions between neutral particles and plasma ions are given as functions of the relative velocity $v_r = |\mathbf{v} - \mathbf{v}_n|$ between the neutral projectile with injection velocity $\mathbf{v}_n$ and mass m_n, and the plasma ion with velocity $\mathbf{v}$ and mass m_p;

(ii) ions have a Maxwellian distribution of velocities, $M(\mathbf{v})$, with temperature T_p(eV).

To analyze the transport of neutral particles in plasmas one needs $\sigma(v_n)$, and this quantity is usually approximated by an "effective" cross section, $\sigma^*(v_n)$, having the property of preserving the reaction rate between projectile and target. Therefore

$$\sigma^*(v_n) = \frac{\langle \sigma(v_r)\, v_r \rangle}{v_n}, \tag{1}$$

where the average is to be performed over the velocity distribution of the targets. The reaction rate coefficient in Eq. (1) is written thus

$$\langle \sigma(v_r)\, v_r \rangle = \int \sigma(v_r)\, v_r M(\mathbf{v})\, d\mathbf{v},$$

with integration carried out over the whole velocity space. By performing this integration one has [4]

$$\langle \sigma(v_r)\, v_r \rangle = \left(\frac{\alpha_p}{\pi}\right)^{1/2} \frac{1}{v_n} e^{-\alpha_p v_n^2} \int_0^\infty v_r^2 e^{-\alpha_p v_r^2} (e^{2\alpha_p v_n v_r} - e^{-2\alpha_p v_n v_r})\, \sigma(v_r)\, dv_r$$
$$\equiv R_{np}(E_n, T_p), \tag{2}$$

where α_p is the parameter characterizing the Maxwellian,

$$\alpha_p = \frac{m_p}{2T_p}, \tag{3}$$

and E_n the injection energy corresponding to v_n.

We shall adopt, as in [4], cross sections for the interactions here considered, written in the form given by Rivière [8]. The approximations to R_{np} represented by the analytical formulas given in [4] will be hereafter referred to as the Galbraith–Kammash approximation and denoted by GK.

For a numerical approach to Eq. (2) we may observe that, since our integrals have the general form

$$R_{np} = \int_0^\infty e^{-x^2} f(x)\, dx,$$

a quadrature formula of the highest algebraic degree of precision is the Gauss–Hermite quadrature formula [9, 10]. The approximation to R_{np} obtained by one of these formulas using n points in the positive semiaxis will be denoted by GH n^+. It can be anticipated that as few points as $n = 2 \div 6$ may provide sufficient precision, so that these formulas can usefully be implemented in computer codes.

Numerical integration by Gauss–Hermite formulas can be improved in all asymptotic cases $E_n \gg T_p$ as follows. By rewriting Eq. (2) in the form

$$R_{np} = A \int_0^\infty v_r^2 \{e^{-\alpha_p (v_r - v_n)^2} - e^{-\alpha_p (v_r + v_n)^2}\}\, \sigma(v_r)\, dv_r,$$

the second exponential can be neglected when, say,

$$\alpha_p v_n^2 = \frac{m_p}{m_n} \frac{E_n}{T_p} \geqslant 4. \tag{4}$$

Moreover, by the substitution

$$x^2 = \alpha_p (v_r - v_n)^2,$$

Equation (2) reduces in these cases to

$$\frac{A}{\sqrt{\alpha_p}}\int_{-v_n\sqrt{\alpha_p}}^{\infty} e^{-x^2}\left(v_n+\frac{x}{\sqrt{\alpha_p}}\right)^2 \sigma\left(v_n+\frac{x}{\sqrt{\alpha_p}}\right) dx = R_{np} \qquad \text{for} \quad \frac{E_n}{T_p} \geqslant 4\frac{m_n}{m_p}. \tag{5}$$

We shall denote by GH n the Gauss–Hermite computation of integral (5) that involves n evaluations of the function. By comparing Eq. (5) with Eq. (2), it is seen that the exponentials in the expression of $f(x)$ have disappeared. As a first consequence, the computation time of GH n reduces by about 40% in our cases, with respect to GH n^+. But there is a second, more important advantage. Namely, the function that has to be evaluated in Eq. (5), acquires a simpler character in all our reactions, so that the number n of points required for a given accuracy is greatly reduced (we recall that Gauss–Hermite formulas with n points in the range $(-\infty, +\infty)$ integrate exactly whenever $f(x)$ is a polynomial of degree not higher than $2n-1$).

Finally, one can avoid the averaging operator and simply replace $\langle\sigma(v_r)\, v_r\rangle$ with $\sigma(v_r^*)\, v_r^*$, where v_r^* is a relative velocity representative in some way of the velocity population of the targets. In particular, one could take, as in [6], an average velocity

$$v_r^* = \langle v_r^2\rangle^{1/2},$$

i.e.,

$$v_r^* = (3T_p/m_p + v_n^2)^{1/2}, \tag{6}$$

or, almost equivalently [5],

$$v_r^* = (\langle v\rangle^2 + v_n^2)^{1/2},$$

yielding

$$v_r^* = (8T_p/\pi m_p + v_n^2)^{1/2}.$$

We shall adopt here definition (6) and denote by AV the approximation to R_{np} obtained through this average velocity.

Assuming as a reference value for R_{np} the one obtained by a Simpson numerical integration of expression (2) with precision 10^{-5}, the relative difference of the R_{np} value yield by AV or GH approximation with respect to this reference value will be called hereafter "relative error" and denoted by ε. The behaviour of this error will be examined in the next sections, for hydrogen interactions with protons and alpha particles. If interacting particles n, p have the same cross section as n', p', then from Eq. (2) it is seen that the scaling rule for hydrogenic species is

$$R_{np}(E_n, T_p) = R_{n'p'}\left(\frac{E_n}{m_n}, \frac{T_p}{m_p}\right).$$

The hydrogen injection energy ranges in this study from zero to 300 keV, and plasma temperature up to 50 keV. Computations were carried out on the IBM 370/168 computer, double precision arithmetic.

3. Rate Coefficient Errors

3.1. *Charge Exchange Between Hydrogen Isotopes*

Rivière's formula for cross sections of charge exchange between a neutral hydrogen atom and a proton is

$$\sigma_{cx} = \frac{6.937 \times 10^{-15}(1 - 0.155 \log E)^2}{1 + 1.112 \times 10^{-15} E^{3.3}},$$

where E is the relative energy in electron volts.

The absolute value of the error ε in computing the average Maxwellian reaction rate coefficient by AV and GH is given in Fig. 1 for E_n, $T_p \leqslant 5$ keV and in Figs. 2, 3 for higher values of these variables. Injection energy of the neutral is quoted along the lines. We shall first comment on the results of Fig. 1 where AV is compared to GH4$^+$.

If we inject a neutral of a given energy E_n into the plasma and compute the average rate coefficient as the particle penetrates towards increasing plasma temperatures T_p, we see that the AV-error increases, although its maximum value is always less than 10% in the case examined. This first result confirms that AV is a rather good approximation, at least, say, for boundary plasma problems. Another

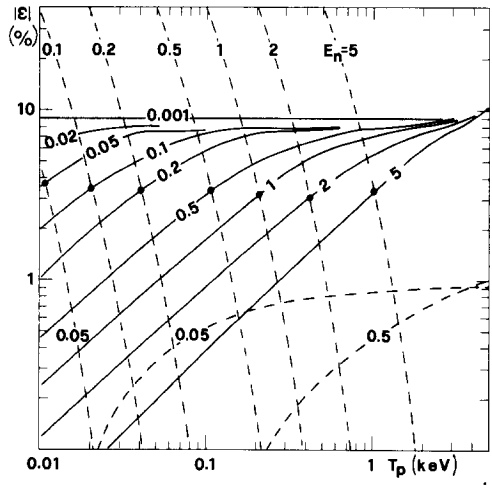

FIG. 1. Hydrogen charge exchange: R_{np} error (%) in AV(—) and GH4$^+$(– – –) vs plasma temperature T_p and neutral injection energy E_n (keV).

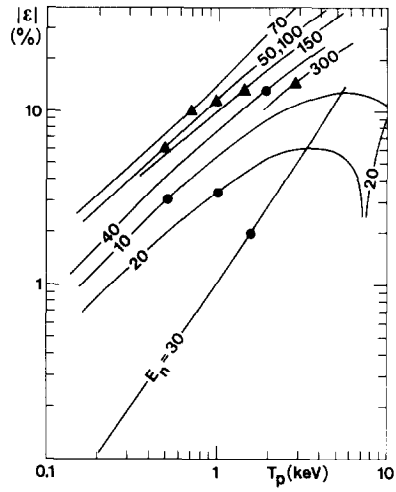

FIG. 2. Hydrogen charge exchange: R_{np} error (%) in AV vs plasma temperature T_p and neutral injection energy E_n (keV). Points corresponding to $\rho = 20$ are marked with circles; those to $\rho = 100$ with triangles.

interesting feature which can be read in Fig. 1 is that the error in GH4$^+$ has, fortunately, a complementary behaviour, at least up to certain plasma temperatures: it begins with a decrease as the plasma temperature increases. Its profile shows that it is not convenient to use GH4$^+$ for high values of the ratio

$$\rho = \frac{E_n}{T_p},$$

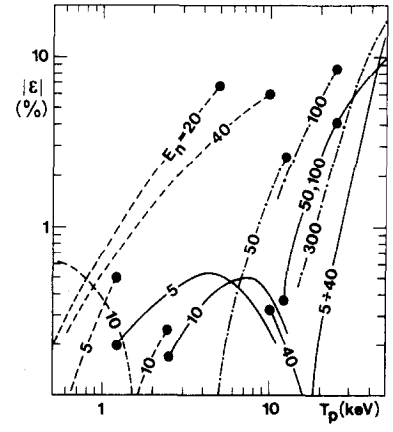

FIG. 3. Hydrogen charge exchange: R_{np} error (%) in GH2 (– – –), GH6 (– · –) and GH6$^+$ (—). Points corresponding to $\rho = 4$ are marked with circles.

whereas results are excellent elsewhere. In fact, the GH4$^+$ error drops, changes sign (twice), and increases again. After the change of sign (appearing as a singularity in the log–log representation) we have represented only two profiles (namely, $E_n = 0.05$, 0.5 keV), the others being almost analogous and remaining, however, below the maximum error of 1% occurring at the extremity $T_p = 5$ keV.

Two lines referring to different approximations but characterized by the same E_n meet in Fig. 1 at a point which can be assumed as a separation point between the two approximations: if we adopt AV for temperatures at the left of this point, and GH4$^+$ at the right, then the maximum error will be halved with respect to AV used alone, reaching a value of about 4%. These points will now be characterized in terms of the ratio ρ, i.e., of the pair (E_n, T_p). Inspection of the results shows that for all these points $\rho \simeq 5$ (a common value, since we have two families of parallel lines). We can conclude that, if we adopt the rule

$$E_n \leqslant 5 \text{ keV} \begin{cases} \rho \geqslant 5 & \text{use AV} \\ \rho < 5 & \text{use GH4}^+, \end{cases}$$

then the error will be limited to 4%. These conclusions, obtained from the errors plotted in the figures given here, will be henceforth collected in Table I. Information about the prevailing sign of the error will also be given, whenever possible, in Table I.

The error analysis proceeded, of course, by finite increments of the two variables E_n, T_p, with a finer step than that plotted in Fig. 1. However, the behaviour of the error is continuous because cross sections are smooth (apart from the apparent singularity introduced by switches of sign).

As regards the left side extremity of our figures (below 100 eV) the above rule still holds, provided Rivière's expression for cross section can be extrapolated at low relative energies.

The high injection energy range described in Figs. 2 and 3 is a little more demanding for a given accuracy. When AV (Fig. 2) becomes insufficient, numerical integration may now require six points if the maximum error is to be kept around 10%. Injection energy (in keV) has here been divided into two regions: $5 < E_n \leqslant 40$, where AV could be applied up to the points marked with a circle (i.e., for $\rho \geqslant 20$), and $40 < E_n \leqslant 300$, where a common limiting value for AV could be $\rho = 100$. (The non-monotonic behaviour of AV as E_n increases from 10 to 40 keV is explained by a change of sign taking place around $E_n = 30$ keV. Note that the worst situation is reached at $E_n = 300$ keV, $T_p = 3$ keV, where the cross section is quite small.) If the above two limiting values for ρ are used, then the numerical integration can be carried out as described in Table I. The separation point between GH and GH$^+$ is $\rho = 4$, derived from Eq. (4) for $m_n = m_p$. Figure 3 shows the error in the numerical integration: in asymptotic conditions GH2 is often sufficient. The points where the application of the asymptotic expression (5) must stop and GH6$^+$ begin are marked with circles lying on the same vertical line. When errors fall below 1%, they oscillate, remaining below this bound, and are no longer faithfully represented.

TABLE I

Approximations Suggested for Rate Coefficients

Interaction	Injection energy (keV)	Method	Maximum error (%)	Error sign[a]
$H + H^+ \rightarrow H^+ + H$	$E_n \leqslant 5$ $\rho \geqslant 5$	AV	4	+
	$E_n \leqslant 5$ $\rho < 5$	GH4+[b]	4	− (almost everywhere)
	$\rho \geqslant 20$	AV	13	+ (up to $E_n \simeq 25$)
	$5 < E_n \leqslant 40$ $4 \leqslant \rho < 20$	GH2	7	±
	$\rho < 4$	GH6+	12	±
	$\rho \geqslant 100$	AV	15	−
	$E_n > 40$ $4 \leqslant \rho < 100$	GH6	16	±
	$\rho < 4$	GH6+	10	±
$H + He^{++} \rightarrow H^+ + He^+$	$E_n \leqslant 1$ $T_p \leqslant 1$	AV	5	− for $E_n > 0.05$
	$E_n \leqslant 1$ $T_p > 1$	GH4+[c]	5	±
	$\rho \geqslant 3.5$	AV	8	+ for $E_n > 3$
	$1 < E_n \leqslant 10$ $1 \leqslant \rho < 3.5$	GH2	7	±
	$\rho < 1$	GH4+[c]	4	±
	$\rho \geqslant 20$	AV	15	− for $E_n \geqslant 30$
	$E_n > 10$ $1 \leqslant \rho < 20$	GH2	12	±
	$\rho < 1$	GH3+	2	±
$H + H^+ \rightarrow 2H^+ + e$	$\rho \geqslant 20$	AV	12[d]	±
	$E_n \geqslant 3$ $4 \leqslant \rho < 20$	GH2	5	±
	$\rho < 4$	GH4+	10[d]	±

[a] +, Overestimates; ±, sign changing in the space interval considered.
[b] For $T_p > 20$ keV, GH6+ should substitute GH4+.
[c] If GH3+ is adopted, the maximum error is doubled.
[d] This error is halved for $E_n \geqslant 5$ keV, when the increasing value of the cross section becomes comparable with other reactions.

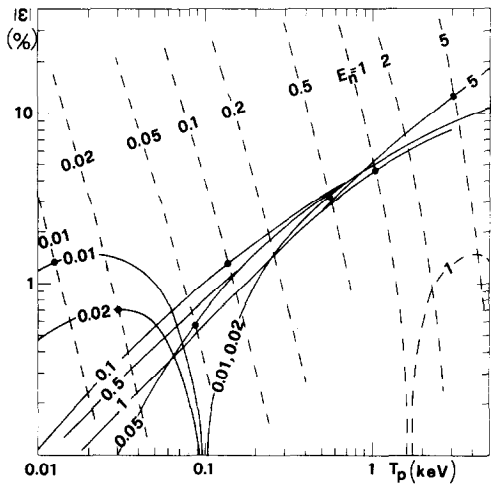

FIG. 4. Hydrogen–helium charge exchange: R_{np} error (%) in AV (—) and GH4$^+$ (----) vs plasma temperature T_p and neutral injection energy E_n (keV).

3.2. *Charge Exchange between Hydrogen and Helium Isotopes*

Rivière's cross sections for charge exchange between hydrogen and alpha particles are

$$\log \sigma_{\alpha x} = -16.54 + 0.09(\log E)^2 \qquad \text{for} \quad E \leqslant 12 \text{ keV}$$
$$= -14.78 - 1.33(4.5 - \log E)^2 \qquad \text{for} \quad E > 12 \text{ keV},$$

where E in electron volts is the relative energy.

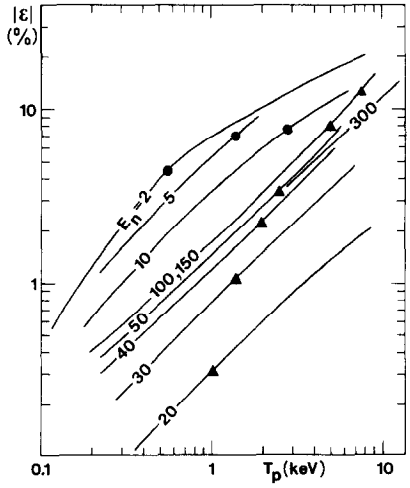

FIG. 5. Hydrogen–helium charge exchange: R_{np} error (%) in AV vs plasma temperature T_p and neutral injection energy E_n (keV). Points corresponding to $\rho = 3.5$ are marked with circles, those to $\rho = 20$ with triangles.

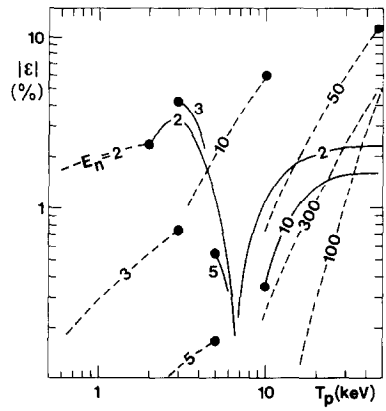

FIG. 6. Hydrogen–helium charge exchange: R_{np} error (%) in GH2 (---) and GH4$^+$ (—) vs plasma temperature T_p and neutral injection energy E_n (keV). Points corresponding to $\rho = 1$ are marked with circles.

The plots of AV and GH-errors in Figs. 4–6 are given with the same conventions as before. In particular, with some exceptions, errors ε are no longer represented when they tend to increase above 10% or when they oscillate below 1%.

From Fig. 4 it is seen that for both E_n and T_p less than 1 keV, (including very low values not represented in the figure) AV can be safely used—the error being less than 5% and this maximum being reached only at one point. The GH4$^+$ curve corresponding to $E_n = 1$ keV is truncated at $T_p = 5$ keV where $\varepsilon = 1.5\%$; however, at 10 keV we have $\varepsilon = 1.2\%$. Therefore the alternative method to AV, when T_p

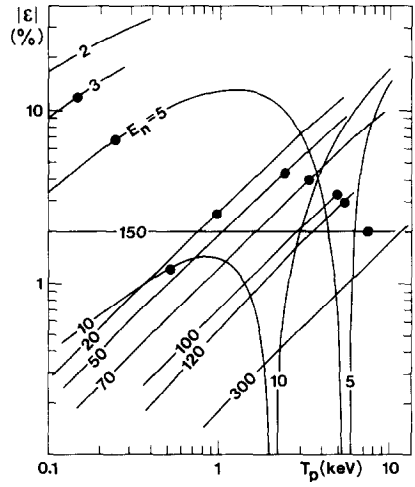

FIG. 7. Hydrogen ion ionization: R_{np} error (%) in AV vs plasma temperature T_p and neutral injection energy E_n (keV). Points corresponding to $\rho = 20$ are marked with circles.

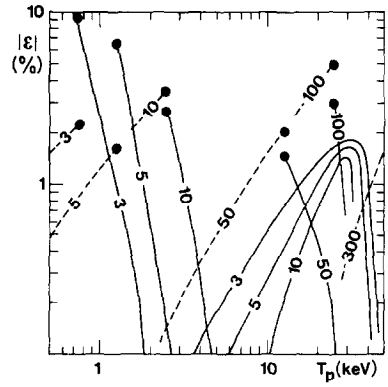

FIG. 8. Hydrogen ion ionization: R_{np} error (%) in GH2 (---) and GH4$^+$ (—) vs plasma temperature T_p and neutral injection energy E_n (keV). Points corresponding to $\rho = 4$ are marked with circles.

increases, also has a maximum of about 5%, and only at one point. (Local perturbations due to change of sign in AV hide the substantial complementarity of the two methods here.)

Figures 5 and 6 give the error behaviour at higher injection energies. For numerical integration (see Table I) these energies are divided into two groups, one below 10 keV, where GH2 and GH4$^+$ have been used, and another above 10 keV, where GH2 and GH3$^+$ have been used. The separation point between GH and GH$^+$ is now $\rho = 1$ (Eq. (4)).

3.3. *Ionization by Positive Ions (Hydrogen Isotopes)*

With the relative energy E in electron volts, Rivière's cross section for $E \leqslant 150$ keV is written

$$\log \sigma_{ii} = -0.8712(\log E)^2 + 8.156 \log E - 34.833.$$

For $E < 3$ keV, σ_{ii} is negligible with respect to other interactions occurring in the plasma. The AV error is large just when σ_{ii} is negligible (Fig. 7); otherwise AV can largely satisfy at least those problems not requiring too high accuracy. However, a possible alternative to AV is GH2 or GH4$^+$ (see Table I) whose errors are shown in Fig. 8.

4. COMPARISON BETWEEN GH AND GK

Up to now we have examined the behavior of the AV approximation, the simplest and most economic one, finding for each reaction the range of E_n and T_p where its error is acceptable, and switching to the numerical integration formulas only when AV was no longer usable. At the boundary of the AV validity range one could also

switch to the explicit analytical formulas GK. The errors introduced by these formulas, as pointed out in [4], are of the order of 10%. Therefore, as far as accuracy is concerned, numerical integration and GK seem largely equivalent. The choice between the two methods then depends upon which of the two is faster and, also, which is more numerically stable. The decision about these two requirements, velocity and stability, depends in its turn on the problem one has to solve (i.e., on the range of energies and temperatures) and the computer one is going to use. Unfortunately, application of the GK approximation is not always straightforward, in the sense that in some energy ranges it gives rise to numerical troubles [4, p. 1056]. For this reason we were unable to carry out a systematic analysis of the GK error, similar to the GH analysis, scanning all the energy–temperature space considered. However, in ranges where no numerical instabilities occur, one can make use of the following conclusions to decide between GH and GK.

For charge exchange, the velocity ratio between $GH4^+$ and GK is 5/4 at low injection energy and almost 1 at high energy. For ionization the same ratio is 6/7. Thus GK is competitive with $GH4^+$. Of course, $GH2^+$ requires half the time of $GH4^+$ and, as pointed out in Section 2, a further 40% reduction is offered by the asymptotic formulas GH2.

5. Discussion and Conclusions

The problem of controlling the size of the error in R_{np} estimates for neutral-ion interactions has been answered by the error profiles given. With these results one may design a strategy of approximations suited to one's particular problem: when the average velocity approximation produces "effective" cross sections σ^* significantly different from the properly averaged ones, more precise approximations have to be used. These may be numerical quadratures or also analytical expressions.

The strategy epitomized in Table I bounds the error to around 5% in boundary plasma problems and around 10% in supplementary heating and fuelling problems. This strategy has been implemented and tested in the low energy range for a boundary plasma problem solved by a Monte Carlo code [11] in a realistic situation including complex geometry and wall interactions. Cross sections were computed according to Eq. (1) whenever the neutrals changed their relative energy during their histories. With respect to the use of the AV approximation alone, it gave rise to an increment of 7% in computation time. In this problem energies and temperatures were typically well below 1 keV, so that besides AV, only $GH4^+$ was used for charge exchange.

Finally, it may be interesting to comment on the influence of the strategy proposed here in a problem which arose in the Monte Carlo choice of the neutral energy after a charge exchange with plasma ions, discussed in [6]. It was shown there that a highly accurate knowledge of rate coefficients was required when a special sampling technique was used. If this requirement was not satisfied, in fact, the simulated model became inconsistent in the following sense: after a charge exchange the number of

injected neutrals increased or decreased. This bias was numerically evaluated in two typical cases of low and high injection energy when rate coefficients were approximated through v_r^*. A uniform decrease of the number of neutrals was observed at the rate of about 6% at each charge exchange collision after the first. By applying in these two examples the more accurate evaluation of the rate coefficients proposed in Table I, the bias was still present, but was reduced to about 1% and, what is more important, its sign was no longer constant, so that the error was no longer amplified along the collision cascade. This severe test confirms that the approximations used in both the low and high energy range considered seem to behave reasonably well.

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