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Monte Carlo Simulation of the Charge-Transfer Reaction in a Plasma

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The Monte Carlo simulation of the charge-transfer process between a single-charged plasma ion and a neutral atom is considered. The main point examined is the sampling of the velocity of the emerging neutralized particle when a shifted Maxwellian velocity distribution is assumed for the plasma ions. An algorithm based on a rejection game is given in order to sample from the velocity distribution of those ions which undergo the reaction. The motion of the targets makes the study of this process by no means easy: The possibility is pointed out that a sampling technique, combined with approximations introduced to compute average cross sections, may destroy the internal consistency of the stochastic model.

1. INTRODUCTION

In the Monte Carlo approach to neutral-atom transport in magnetically confined fusion plasmas, as for example in studies of neutral-beam injection or plasma recycling, one is faced with the problem of simulating the charge-transfer reaction between single-charged ions and neutrals. It may be assumed that the ionized atom undergoing this type of process loses its charge, becoming itself a neutral, but retains its velocity [1]. The main purpose of this work is to discuss the sampling of this velocity assuming that the plasma ion velocities are distributed according to a shifted Maxwellian. An approximation which is frequently made is that of selecting the velocity of the emerging neutral from the distribution of the plasma ions [2, 3]. This does not take into account that, although the individual velocities of the collided ions remain unchanged immediately after neutralization, the velocity distribution of these collided ions is generally not the same as that of the plasma.

To introduce all the terms of the problem, the determination of the cross sections in the form needed for the simulation is first discussed in Section 2. This matter is by no means trivial, due to the motion of the target ions. In Section 3, velocity slection is discussed and a rejection algorithm is given in order to sample from the correct distribution. In this way, besides avoiding large probability tables, statistical weights originated by certain sampling techniques are not needed either. As will be pointed out, these weights, if combined with approximations introduced to compute average cross sections, could make the mathematical model inconsistent. In Section 4, numerical examples are discussed.

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2. Computing The Cross Sections

To track histories of neutral particles in a plasma, a medium of moving targets, one needs the cross sections of all possible interactions to be given as local functions only of the velocity $\mathbf{v}_0$ of the tracked particle. From these cross sections, the collision point and the type of reaction can be selected in standard ways [4, 5]. Cross sections are instead usually given as functions of the relative projectile–target velocity $v_r = |\mathbf{v} - \mathbf{v}_0|$, where $\mathbf{v}$ is the ion velocity. Therefore we shall first discuss the problem of obtaining the cross sections in the form required by the mathematical method used.

Assume for the sake of simplicity that the plasma contains only one species of ion, with mass m and absolute temperature T, and that the projectile can undergo just one type of reaction, characterized by the cross section $\sigma(v_r)$. Then one defines an "effective" cross section $\sigma^*(v_0)$ so as to preserve the reaction rate between projectile and target as follows:

$$\sigma^*(v_0) = \frac{\langle \sigma(v_r)\, v_r \rangle}{v_0}, \tag{1}$$

where the average is to be performed over the velocity distribution of the targets. We consider the case where the plasma, whose ions have a background Maxwellian distribution $M(\mathbf{v}')$, flows with a constant drift velocity $\mathbf{a}$. Then the velocity distribution of the target ions is a shifted Maxwellian $M_s(\mathbf{a}, \mathbf{v})$ given by

$$M_s(\mathbf{a}, \mathbf{v}) = M(\mathbf{v} - \mathbf{a}). \tag{2}$$

In fact, with $\mathbf{v} = \mathbf{v}' + \mathbf{a}$,

$$M_s(\mathbf{a}, \mathbf{v})\, d\mathbf{v} = M(\mathbf{v}')\, d\mathbf{v}' = M(\mathbf{v} - \mathbf{a})\, d\mathbf{v}.$$

Making use of Eq. (2), the rate coefficient in Eq. (1) can be written as

$$\langle \sigma(v_r)\, v_r \rangle = \int \sigma(v_r)\, v_r M(\mathbf{v} - \mathbf{a})\, d\mathbf{v}, \tag{3}$$

where integration is to be carried out over the whole velocity space.

Since numerical integration of Eq. (3) at each flight of the tracked particle is out of the question, one must have recourse to many-dimensional fittings, or to interpolation in large precomputed many-entry tables, or must introduce a drastic approximation to solve Eq. (3). For instance, one can substitute the relative velocity v_r with an average velocity v_r^* which is in some way representative of the velocity population. In particular, to simplify the calculations, we can take

$$v_r^* = \langle v_r^2 \rangle^{1/2} \tag{4}$$

with

$$\langle v_r^2 \rangle = \int v_r^2 M(\mathbf{v} - \mathbf{a})\, d\mathbf{v}.$$

Since the explicit form of $M(\mathbf{v}')$ is

$$M(\mathbf{v}') = M(v_x')\, M(v_y')\, M(v_z'),$$

with

$$M(w) \propto \exp(-mw^2/2kT),$$

then the integral above becomes

$$\langle v_r^2 \rangle = \int \{[v_x' + (a_x - v_{0x})]^2 + \cdots\}\, M(v_x')\, M(v_y')\, M(v_z')\, d\mathbf{v}'$$
$$= \langle v^2 \rangle_b + |\mathbf{a} - \mathbf{v}_0|^2 = 3kT/m + |\mathbf{a} - \mathbf{v}_0|^2,$$

where $\langle \cdot \rangle_b$ denotes the average over the background Maxwellian M. Note that cross terms of the type

$$\int_{-\infty}^{+\infty} 2v_x'(a_x - v_{0x})\, M(v_x')\, dv_x'$$

vanish, being averages of the odd function v_x' over the even function $M(v_x')$.

Another possible choice could be

$$v_r^* = (\langle v \rangle^2 + v_0^2)^{1/2},$$

as in [2] where, however, no drift velocity $\mathbf{a}$ is considered.

In any case, given a representative velocity v_r^*, Eq. (1) reads

$$\sigma^*(v_0) = \sigma(v_r^*)\, \frac{v_r^*}{v_0}, \tag{5}$$

and finally yields the required cross sections in a form suitable for the Monte Carlo simulation.

3. Charge-Transfer Simulation

Let us now assume that a charge-transfer reaction between a neutral with velocity $\mathbf{v}_0$ and a single-charged ion has been chosen by taking into account the probabilities of all possible reactions, i.e., on the basis of their respective cross sections computed as shown in the previous section. Furthermore, let σ_{cx} be the charage-transfer cross section for the selected ion species. To simulate the charge-exchange mechanism, one takes into account the assumption (see Section 1) that the velocity $\mathbf{v}$ of the emerging neutral after the reaction is that of the collided ion. Let us also denote by $q(v_r)$ the rate coefficient of this reaction,

$$q(v_r) = \sigma_{cx}(v_r)\, v_r.$$

Since the number of charge exchanges due to the travelling neutral per unit time and unit volume in the velocity element $d\mathbf{v}$ about $\mathbf{v}$ is $n_i q(v_r)\, M_s(\mathbf{a}, \mathbf{v})\, d\mathbf{v}$, with n_i the density of the ion species chosen, then $\mathbf{v}$ is to be selected from the probability density function (pdf)

$$d(\mathbf{v}) = \frac{q(v_r)\, M_s(\mathbf{a}, \mathbf{v})}{\int q(v_r)\, M_s(\mathbf{a}, \mathbf{v})\, d\mathbf{v}}.$$

Using Eqs. (2), (3), and (1), we have

$$d(\mathbf{v}) = \frac{q(v_r)\, M_s(\mathbf{a}, \mathbf{v})}{q^*(v_0)}, \tag{6}$$

where $q^*(v_0) = \sigma_{cx}^*(v_0)\, v_0$.

Equation (6) shows that the selection of $\mathbf{v}$ simply from the pdf of the ions before the collision (as in [2, 3]) does not take into account the fact that the rate coefficient operates as a selective filter. Only if $\sigma_{cx}(v)$ has a $1/v$-behavior would the choice from M_s not introduce any approximation.

Velocities could be sampled from pdf (6) by storing large tables in the computer memory, these depending on the local ion-temperature, on the velocity of the neutral relative to the plasma drift and on the ion species.

A correct choice of $\mathbf{v}$ from density (6) could also be performed by an "importance sampling" [4]. For example, choose $\mathbf{v}$ from M_s and apply the statistical weight

$$w = q(v_r)/q^*(v_0) \tag{7}$$

to this choice (a scaling factor of this type is used in [6]). This method requires highly accurate knowledge of the normalization factor. Indeed, if the normalization integral $q^*(v_0)$ is not accurately computed (for example, if the Maxwellian population has been substituted by a unique representative velocity for computation of the average cross section, as in the numerical samples of the next section), then the function $d(\mathbf{v})$ is no longer normalized to unity and the internal consistency of the simulation is lost. By using in this case the weight (7), particles are erroneously created or destroyed during the history according to whether the normalization constant adopted is less or greater than the true one, and the balance between the physical events considered no longer closes, making *inter alia* impossible control of the correctness of the calculation (whereas an assumption like Eq. (5), when used to determine free paths or the reaction type, makes the mathematical model approximate but not inconsistent).

Knowledge of the normalization constant in Eq. (6) and the use of large tables can be avoided by a "rejection technique," as follows. Assume that $q(v_r)$ is bounded and let

$$G = \max_{v_r} q(v_r)$$

with v_r ranging over the velocity space of the problem. Equation (6) can now be written as

$$d(\mathbf{v}) \propto \frac{q(v_r)}{G} M_s(\mathbf{a}, \mathbf{v}),$$

and $d(\mathbf{v})$ can be regarded as proportional to the product of a pdf (M_s) by a probability ($q/G < 1$). One then selects $\mathbf{v}$ out of M_s by choosing a velocity $\mathbf{v}'$ isotropically from $M(\mathbf{v}')$ (see, e.g., [7] for a Maxwellian energy), and by adding $\mathbf{a}$; this velocity $\mathbf{v} = \mathbf{v}' + \mathbf{a}$ is accepted only if a number c, chosen uniformly in (0, 1), is such that $c < q/G$, otherwise the whole procedure is repeated by selecting a new velocity from M_s.

Thus, the probability of accepting a velocity in the element $d\mathbf{v}$ about $\mathbf{v}$ is $M_s \, d\mathbf{v}$ multiplied by the probability q/G, as required.

Any number $G' > G$ could be used in the rejection game, but efficiency (ratio between accepted and sampled velocities) would decrease.

If $q(v_r)$ is unbounded, then a suitable velocity cut-off is needed. In this case G could be computed as the maximum of q for $0 < E_r < \alpha T$, E_r being the neutral kinetic-energy corresponding to v_r, T the local plasma temperature and α a numerical coefficient. Note that if the plasma can be subdivided into piecewise homogeneous regions, the value of G in each region depends only on the interacting particle species. The choice $\alpha = 30$ (ensuring a fair game for practically all velocities), together with definition (4) and a piecewise homogeneous plasma subdivision, was adopted for hydrogen isotopes in computations of neutral transport in poloidal divertors [8] where the efficiency of the rejection game turned out to be about 0.5.

4. Numerical Examples

We now compare the performance of the rejection technique (RT) proposed in this paper with the Maxwellian sampling approximation (MSA) and an importance sampling technique (IST) which uses the weight (7) together with the crude approximation of the representative relative velocity (4).

As a first example, let us consider the injection of a monoenergetic beam of neutrals at 3 eV into a Maxwellian plasma at temperature 25 eV, a typical situation of particle recycling in diverted plasmas. It is assumed that the properties of the plasma do not change in time, that no drift velocity is present and that both the beam and the plasma are composed of equal parts of deuterium and tritium, modelled as a single hydrogenic species with mass 2.5. Charge-transfer cross sections are computed according to empirical formulas proposed in [9]. To isolate the effect of the charge-transfer process an infinite medium is considered so that effects of wall interactions are avoided. Finally, ionization will not, for the moment, be considered.

The distributions of the energy E of the neutrals after one or more charge-transfer collisions computed by RT are given in Fig. 1. The Maxwellian is represented in the

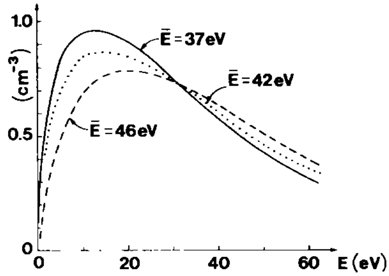

FIG. 1. RT-computed energy distributions of the neutrals after charge-transfer process. Plasma at 25 eV, neutrals injected at 3 eV (——, Maxwellian; – – –, after the first collision; ···, after $n = 2 \div 10$ collisions).

same figure to show the difference from the plasma ions distributions. Of course, method MSA reproduces this Maxwellian at each collision. A measure of the distance of the distribution (6) from the Maxwellian is given in terms of the mean value $\bar{E}$ quoted for each distribution. Histories were followed up to $n = 10$ collisions, but no appreciable difference was observed between the distribution corresponding to $n = 2$ and $n = 3 \div 10$. The efficiency of the rejection game was 0.37 at the first collision and 0.45 for $n = 2 \div 10$.

Profiles obtained by IST were the same as those obtained by RT, but the approximate computation of the normalization factor $q^*(v_0)$ introduced a bias which, in this case, was equivalent to an absorption of particles. Figure 2 shows the devastating effect of this approximation on the beam intensity, I, whose initial value was $I_0 = 1$: about 6 % of the travelling neutrals "disappear" from the balance at each charge-transfer collision, although no ionization has been considered.

Introduction of ionization does not produce any effect on the energy distribution, because hydrogenic species have a $1/v$ electron ionization cross section. In our example, this new process would only reduce the neutral population by about 1/3 at each collision.

As a second example we consider the somewhat opposite situation encountered in problems of plasma heating by neutral injection: a neutral beam at 160 keV is

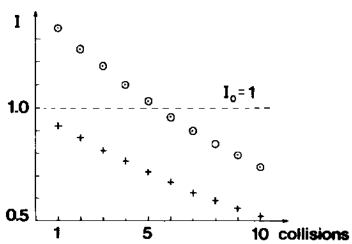

FIG. 2. Bias induced in the intensity of the neutral beam by IST vs collisions undergone (+, first example; ⊙, second example).

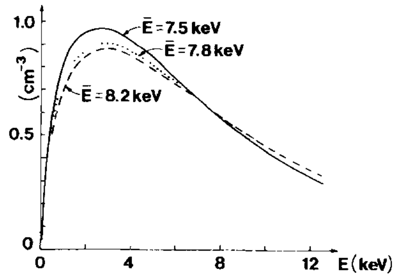

FIG. 3. RT-computed energy distributions of the neutrals after charge-transfer processes. Plasma at 5 keV, neutrals injected at 160 keV (——, Maxwellian; – – –, after the first collision; ···, after $n = 2 \div 10$ collisions).

injected into a Maxwellian plasma at the temperature of 5 keV, all other conditions being the same as in the previous example.

The RT-computed energy distributions are shown in Fig. 3 and are compared to the MSA represented by the Maxwellian. A smaller distortion is observed in this case. The RT efficiency was 0.14 for the first and 0.81 for further collisions.

The bias introduced by IST is given in Fig. 2 and this time it appears as an initial "creation" of particles, with I_0 multiplied by the factor 1.34 after the first collision, followed by a "disappearance" of neutrals at the rate of about 7 % at each collision (we recall that for $E > 15$ keV, σ_{cx} drops rapidly and so, although in our case the beam energy prevails on the average Maxwellian energy, w is sensitive even to small variations of v_r).

Ionisation (both by electrons and by ions) does not change the distributions in this case either, and its introduction produces an attenuation of the beam by about 1/6 at each collision.

From the examples above we may conclude that the energy of neutrals emerging from the charge-transfer collision may be rather different from that of plasma ions, due to a non-$1/v_r$ trend of $\sigma_{cx}(v_r)$. Both RT and importance sampling allow selection of the new energy from the correct distribution. However, the use of weights in importance sampling techniques may be dangerous when the average reaction rates are not correctly calculated. Recourse to tabulation could ensure better knowledge of the reaction rates and avoid the inconsistency, provided the interpolation error be negligible.

5. CONCLUSIONS

Monte Carlo simulation of particle transport in a medium of moving targets like that examined in this work often requires drastic approximations for the determination of cross sections necessary to sample free paths, reaction types, and motion parameters after a reaction. For determination of the energy and direction of the neutral originated by a charge transfer from a plasma ion to a neutral atom, we have seen that some of these approximations could destroy the internal consistency of the mathematical model. It has been shown that this undesirable feature may be avoided by having recourse to a rejection algorithm.

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References

1. E. W. McDaniel, "Collision Phenomena in Ionized Gases," Wiley, New York, 1964.
2. M. H. Hughes and D. E. Post, *J. Comput. Phys.* **28** (1978), 43.
3. Y. Seki *et al.*, *Nuclear Fusion* **20** (1980), 1213.
4. J. M. Hammersley and D. C. Handscomb, "Monte Carlo Methods," Methuen, London, 1964.
5. L. L. Carter and E. D. Cashwell, "Particle Transport Simulation with the Monte Carlo Method," ERDA Critical Review Series, 1975.
6. D. Heifetz, *et al.*, *J. Comput. Phys.* **46** (1982), 309.
7. E. J. McGrath and D. C. Irving, "Techniques for Efficient Monte Carlo Simulation," Vol. II, p. 38, ORNL-RSIC-38, April 1975.
8. E. Cupini, A. De Matteis, R. Simonini and E. S. Hotston, *in* "International Tokamak Reactor, European Contributions to the INTOR Phase 2 — A Workshop," Commission of the European Communities, Brussels, Vol. II, Chap. VI.4, App. 2, EUR FU BRU/XII-132/82/EDV30, December 1982.
9. A. C. Rivière, *Nuclear Fusion* **11** (1971), 363.