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ATOMIC AND MOLECULAR DATA NEEDS, PRIORITIES, AND ACCURACIES FOR CTR BEAM INJECTION*

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1. BACKGROUND

The tokamak magnetic geometry processes satisfactory confinement properties[1] and will form the basis for many large, new experiments in the next few years.[2,3] The aim of all of these experiments is to explore the physics of hot, dense plasmas in conditions near to those for which significant thermonuclear energy production is a possibility. Some experiments, such as the Tokamak Fusion Test Reactor, at the Princeton Plasma Physics Laboratory, may even attain breakeven, with energy produced from fusion reactions equalling the energy input needed to sustain the plasma against losses.

It is a common assumption that some sort of external heating mechanism will be required to achieve high plasma temperature. While various forms of radio frequency and other wave heating techniques are being studied, the dominant emphasis is being placed on heating by the injection of energetic beams of neutral hydrogenic particles. We will first discuss the processes which are important to an understanding of the neutral beam injection process in a tokamak, and then discuss those areas for which atomic and molecular data are particularly needed. We conclude with an assessment of the accuracies required and with some estimation of the priorities which ought to be assigned.

2. NEUTRAL BEAM INJECTION: BASIC PROCESSES AND PARAMETERS

To describe the influence of atomic and molecular processes on the plasma physics of neutral beam injection, we will begin with a concise discussion of the injection and thermalization process.

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We will restrict the discussion to events occurring after the accelerated ion beam has been neutralized and enters the plasma chamber. Figure 1 (from Rome et al.[4]) shows the tokamak geometry and a typical incident neutral beam. The neutral particles are trapped in the plasma by charge transfer with plasma ions, by electron impact ionization, or by impact ionization on the plasma ions. Once charged, these energetic injected particles are confined by the tokamak magnetic field. For the case of injection nearly tangential to the magnetic field shown in Fig. 1, the particles follow trajectories which also lie nearly along the fields. However, a projection of their orbits onto a plane perpendicular to the toroidal axis shows that there are important drift motions for these ions: their orbits are displaced outward from the axis of symmetry for particles injected nearly parallel to the plasma current, inward for those particles which are nearly anti-parallel. By calculating this resulting drift after trapping, and averaging the densities of these fast ions near the tokamak radial flux surfaces, the deposition of fast ions is characterized by the function H(r) shown in Fig. 1: the normalized density of deposited fast ions as a function of plasma minor radius. Various radial deposition profiles are shown as a function of a/λ. a is the plasma minor radius, λ the mean free path against trapping by all the processes mentioned.

$$\frac{a}{\lambda} \equiv \int (n_e \langle G_e V_e \rangle + n_H \sigma_X V_o + n_Z \sigma_{XZ} V_o + n_H \sigma_i V_o + n_Z \sigma_{iZ} V_o) dS \qquad (1)$$

$n_{e,H,Z}$: spatial densities of electrons, hydrogenic ions, and other (impurity) species.

V_o: velocity of the injected neutral atoms.

$\langle G_e V_e \rangle$: electron impact ionization rate averaged over the electron distribution.

$\sigma_{X,XZ}$: charge exchange cross section for beam atoms with hydrogenic and other (impurity) species.

$\sigma_{i,iZ}$: ionization cross section for inpact of beam atoms upon hydrogenic and other (impurity) species.

The integral is taken along the path of the beam from entrance to a point on the vacuum chamber wall opposite the injector.

Once deposited, these energetic ions undergo interaction with the background confined plasma. While many possible collective thermalization processes have been considered[5] the model of successive distant binary encounters, as described by the Fokker-Planck drift-kinetic equation[6] is though to be accurate. The injected fast neutrals, now fast ions, thus transfer momentum and energy to the plasma. Calculations with the Fokker-Planck equation yield estimates for these processes which are consistent with the rates observed in a number of present experiments.[7-11] The chief effect of contemporary injection experiments is to transfer energy, to the background plasma, and thus to heat it to temperatures impossible to obtain by ohmic heating alone. The beam particle input is small by comparison with the particle sources on the walls and aperture limiters. The momentum input is minimized by pairing injectors in the directions parallel and anti-parallel to the current, or by injecting nearly perpendicular to the current.

The energy input to the plasma is characterized by the ratio of the so-called critical energy of the thermalizing ion, below which energy transfer occurs chiefly to the more massive positive ion species, to the electron temperature. This ratio is:

$$\frac{E_c}{T_e} \equiv 14.6 \frac{A_i}{A^{2/3}} \sum_{k=1}^{N} n_k Zk^2/A_k \qquad (2)$$

where A, A_k: atomic weights of the beam and k^{th} species of positive ion

T_e: electron temperature

E_c: 'critical' energy

n_k: density of kth species of positive ion

Z_k: ionic charge of the kth species of positive ion.

This ratio depends upon the radial distributions of electron temperature, charge, and ion density.

In some present experiments the beam energy transfer to the plasma is degraded by charge exchange of the thermalizing ions with residual low-energy hydrogenic neutrals in the plasma. While the ratio of hydrogenic neutral/hydrogenic ion densities is typically 10^{-5}, the resonance charge exchange cross section is large enough to produce a significant loss of beam ions during the time (of order 10 s of milliseconds) required for thermalization.

Figure 2 shows a typical computed distribution of fast ions in velocity spcae. (This is a solution of the Fokker-Planck equation.) There is a region in the space of particles traveling counter to the current which is empty. This so-called 'loss region' is characterized by particle drift orbits whose trajectories cause them to leave the machine and strike the wall. Perpendicular injection, such as is done on the TFR experiment, also produces such a 'loss region', especially at low plasma current. The rate at which the beam ions are lost through this gap in velocity space is characterized by the rate of diffusion in the angle made by the ion velocity, with the magnetic field. This 'pitch angle diffusion' rate is proportional to the rate of momentum exchange with the background electrons, and is directly proportional to

$$Z_{eff} \equiv \sum_{k=1}^{N} n_k Z_k^2 / n_e \qquad (3)$$

where the other terms have already been defined and n_e is the electron density. Again, the sum is to be taken over the N species of positive ions in the plasma.

Once the energy is transferred to the plasma, the considerations of plasma cooling by impurities to be discussed elsewhere will apply.

In summary, then, the neutral injection process in tokamaks requireds knowledge of the deposition process (and the quantities in Eq. 1), the energy exchange process (quantities in Eq. 2), and momentum exchange (quantities in Eq. 3).

The cross sections and the rate coefficient needed for Eq. (1) are obvious examples of atomic data needs. The charge transfer and impact ionization cross sectionsare needed for quite a large number of species, and over a fairly wide range of energies. (We will discuss specific instances later.) The quantities needed for the critical energy and pitch angle diffusion processes (Eq. 2 and 3) are also needed for plasma diagnostics and for estimates of plasma cooling due to impurity ions. One wishes to ascertain, largely from spectroscopy, the chemical composition (i.e., the n_k) and charge state distribution (i.e., Z_k) for the positive ion species in the plasma. The needs here are typically for identification of strong resonance lines, for transition probabilities and for shifts of K and L lines for highly ionized heavy metals. The plasma cooling processes will require knowledge of the dielectronic and radiative recombination rates for the impurity ions.

Since these latter processes are important to the overall plasma energy balance, and are not unique to the neutral injection process, we will focus on the deposition cross sections in our discussion of atomic data needs.

In Table 1 we list the characteristics of present neutral beam injection experiments which are important to the atomic and molecular physics processes to be discussed.

TABLE 1

Experiment	Injected Species	Plasma + Species	Energy/nucleon*	Minor Radius (cm)
Cleo tokamak[7] (Culham Laboratory)	H^0	H^+,		
ORMAK[8] (ORNL)	H^0, D^0	H^+, D^+, O, Fe	25 keV	~23
Adiabatic toroidal Compressor (ATC)[9] (PPPL)	H^0, D^0, He^0	H^+, D^+, O, Fe	30 keV	17
TFR[10] (Fontenay-aux-Roses)	H^0, D^0	H^+, D^+, O, Fe, H_0	33 keV	20
T-11[11] (Kurchatov Inst.)	H^0	H^+		22

*In present experimental devices the chemical composition is somewhat uncertain. Various devices have reported or suspected significant concentrations of

Table 1 (cont'd)

C, O, Fe, M_o, W, N_i, N, Cr, Hg, P_t, Cu. In additon such gases as He, N_e, Ar, K_r and X_e have been injected as diagnostics and A_g and S_c films have been sublimated by a laser burst and injected into the plasma in a controlled way as a diagnostic.[12,13]

The ATC device employed Ti gettering to reduce the impurity content. While the impurity concentrations were notably diminished[12] some traces of Ti appeared as a result.

*We quote the highest energy components. The presence of various molecular species in the ion source causes the appearance of lower energy injected atoms at fractions of the full energy. These are a characteristic of the source used on each experiment.

In Table 2 we list the relevant injection parameters and some of the nearer term planned injection experiments.

Table 2

Experiment	Injected Species*	Plasma Species+	Energy Nucleon	Minor Radius (cm)‡
PLT (PPPL)	H^o, D^o	H^o D^o	45 keV	45
ORMAK Upgrade (ORNL)	"	"		30
Doublet III (General Atomic)	"	"		45**
DITE (Culham)	"	"		
TFR 600 (Fontenay-aux-Roses)				
PDX (PPPL)				***

*Others, such as He, may be tried.

+The same impurities as noted in Table 1 are likely to be present.

‡Again, as with Table 1, some distribution of lower energies is expected, depending on the source.

**Doublet III has a vertical dimensions (cm).

***PDX has a vertical dimension (cm).

In Table 3 we note the injection parameters planned for large tokamak experiments, to be operating circa 1980.[7]

TABLE 3

Device	Injected Species*	Plasma Species+	Energy/ Nucleon	Minor Radius (cm)‡
TFTR (PPPL)	H^0, D^0 (H_c^0?, T^0?)	H^0, D^0, T^0	60 keV	85
JET (EURATOM)	"	"	80 keV	125
JT-60 (JAERI)	"	"	50 keV	100
T-10M (Kurchatov)	"	"	?	75

*Proposals for a counterstreaming ion torus[13] employ to injection.

+The impurity concentrations noted in Table 1 may be expected.

‡The designers hope to optimize the beams in these large systems, so that most of the beam current is carried in the highest energy component.

Finally, we note that studies of fusion reactor power plants have been made[14] and that neutral beam energies of 180-200 keV D^0 are foreseen for D-T reactor operation. We note also that these reactor systems will contour an appreciable alpha particle residue from D-T reactions, so that there is an inevitable 'impurity' for these systems. The minor radii of these devices are typically foreseen to be $\sim$ 2 m.

3. BEAM TRAPPING

Making reference once more to Fig. 1 we note that beam deposition may be characterized by the ratio a/λ. Further, the depositon profile becomes flat for $a/\lambda \sim 4$. In present tokamaks the energy confinement is better in the center of the device than at the edge; thus, the peaked profiles in Fig. 1 will produce an efficient plasma heating, while those peaked outwardly will produce poor heating. Not only that, but such profiles will also produce a stronger

interaction with the wall, as we will discuss. Thus we choose $a/\lambda \sim 4$ as representing the lower limit of adequate beam penetration.

The cross sections needed in Eq. (1) are not known for the impurities and energies of interest. Since many large experiments with injection energy/nucleon $\gtrsim$ 40 keV were predicted on the assumption that hydrogenic ion impact ionization was the dominant process, we will consider the consequences suggested by Girard et al.[15] of a different assumption. Assuming that the Born approximation is valid at these relatively low energies and that the impurity ion impact ionization cross section simply scales as Z^2 times the hydrogenic cross section, then

$$\left.\frac{a}{\lambda}\right)_{\substack{\text{impact}\\ \text{ionization}}} = \int ds\, (n_H + n_Z Z^2)\, \sigma_H$$

where the conventions are the same as for Eq. (1). Using the definition of Eq. (3), the local trapping rate is proportional to $n_e Z_{eff} \sigma_H$. In Fig. 3 we see a 'universal curve' prepared by H. C. Howe, Jr., which embodies these assumptions. The figure shows the locus of points which satisfy $\frac{a}{\lambda} = 4$ as a function of $a \cdot \bar{n}_e \cdot Z_{eff}$ and the energy/nucleon. (a is the plasma minor radius.) For all the experiments in Table 1 the range of average electron density ($\bar{n}_e$) is $2 \cdot 10^{13}\ cm^{-3} \leq \bar{n}_e \leq 10^{14}\ cm^{-3}$ while $Z \leq Z_{eff} \leq 12$. Thus, most of the points for present experiments would lie above the curve, indicating adequate penetration. The near term experiments listed in Table 2 become marginal, however, and the 1980-era experiments very clearly lack adquate penetration if the Born approximation assumptions are valid. The status of the present and near-term experiments relies on assumptions made about the hitherto unknown charge transfer cross sections. They are assumed <u>not</u> to depend on impurities in Fig. 3 (the dotted line shows the locus of $a/\lambda = 4$ if this cross section is to be enhanced).

As an example of the consequences of having $a/\lambda > 4$, we present a computational study of the FTR device. The computer model has been described in Refs. 16-18. We assume that $\sigma_{iZ} \propto Z^2 \sigma_i$. The initial plasma state is shown in Fig. 4a, $T_{e,i} = 4$ keV, plasma isolated from the wall. We suppose that 12 MW of D^0 neutrals are injected, with 25% of the particles at 120 keV, 50% at 60 keV and 25% at 40 keV. The plasma is assumed to have 2% oxygen impurity relative to the proton density, distributed uniformly in radius. The hydrogenic plasma ions are initially assumed to be T^+. As the beam injection proceeds the plasma becomes a D-T mixture. As the 120 keV D^+ ions thermalize, they produce direct thermonuclear reactions by interacting with the background fuel ions.[19] Thus, a 'breakeven' experiment may be envisaged in which the thermonuclear energy production is derived only from reactions between the beam and the background plasma. Such an experiment would be relatively insensitive to the deleterious effects of impurities on the plasma energy balance in general, providing only that the beam ions can be deposited in the center of the plasma. In Figs. 4a-d we see the interrelation of impurity trapping of the beam and the subsequent dynamics. As the beam energy thermalizes the plasma is heated and produces some impurities by sputtering. As these impurities (assumed to be Fe, as seen in Fig. 4c) enter the plasma, they enhance the impact ionization cross section. This, in turn, traps the beam farther to the outside, in a region of higher neutral density. The combination of edge heating and high neutral density at the edge produces an even stronger charge exchange bombardment of the wall, more sputtering, and a cascade in which the beam is effectively excluded from the plasma (Fig. 4d). The ratio of fusion energy production to beam energy input is $\sim$ 0.35 in this case, and roughly 2 MJ of neutron energy are produced.

This beam deposition instability has been examined by a number of workers[20-23] and serves as an excellent example of the need for atomic data. To assess the

likelihood of this cascade are needs the cross sections for charge transfer and impact ionization for the injection of H^0, D^0 (and perhaps T^0) into a hydrogenic plasma (electrons, H^+, T^+, D^+ and impurity ions). The energy ranges of interest are given in the Table.

4. ACCURACY AND PRIORITIES

We first of all note that the beam density deposited along the chord s in Fig. 1 is proportional to $e^{-\int ds/\lambda}$. Thus, all the relevant cross sections appear in an exponent. We note also that the calculations we have employed to suggest the importance of the beam deposition instability are model-dependent. If the dielectronic recombination rates were known we might as well as have concluded that photon emission carried the energy from the plasma, not charge exchange. Then the sputtering rates would be much lower.

Thus we may rather arbitrarily assign an overall estimate of 20% to the accuracy with which these charge transfer and impact ionization cross sections should be known. We must know the magnitude as well as the dependence on energy and charge.

The tables list quite a number of possible impurity ions to study for the relevant energy ranges. We should order them by the following remarks.

1. The wall material of all the experiments is stainless steel; the limiter which all (except PDX) use, or will use, is M_o or W.
2. Ubiquitous light elements are C, O.
3. Novel wall or limiter materials are now being tried, or are planned for the future. Pyrolytic C, SiC, B_4C have all been mentioned.

Cross section measurements are needed for this problem to asses the impact of this cascade process on large machine designs.

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