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O-H CHARGE EXCHANGE IN COLD,
DENSE, HYDROGEN PLASMAS

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DENSE, HYDROGEN PLASMAS

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ABSTRACT

We point out that the accidentally resonant charge exchange reaction, $O^+ + H^0 \rightleftharpoons O^0 + H^+$, is an important mechanism for causing the loss of singly charged oxygen ions from oxygen contaminated hydrogen plasmas. Results of a Monte Carlo simulation are presented which show that the fraction of oxygen lost because of charge exchange exceeds 1/3 when the parameters $n_e \sim 10^{13} \text{ cm}^{-3}$, $n_{H^0} \sim 10^{11} \text{ cm}^{-3}$ and $T_e \sim 3 \text{ eV}$ are attained.

Recent studies of atomic processes in plasmas have focused on the highly ionized species that exist in the high temperature plasma core [1]. Conditions in the edge region of plasma devices are quite different. There the electron temperature may be sufficiently low and the neutral atomic and molecular densities sufficiently high that ion-molecule scattering, dissociative neutralization, mass transfer or charge transfer by low energy (chemical) processes can occur at rates competitive with electron impact ionization and plasma transport. Under appropriate conditions, chemical processes can be the dominate mechanisms for hydrogen, impurity, or energy losses at the edge.

Resonant $H^0 - H^+$ charge exchange, one low energy process, has already been discussed as a mechanism contributing to appreciable cross-field hydrogen transport in tokamaks [2]. To illustrate another example of important low energy processes, we present results of a numerical simulation of oxygen transport in a cold, dense, hydrogen plasma. The only chemical effect included in the simulation is charge exchange between oxygen and hydrogen. Charge exchange between the pairs

is accidentally resonant [3], because the ionization potentials of ground state O and H atoms are nearly equal,

$$I_H \approx I_O \approx 13.6 \pm .02 \text{ eV}.$$

The rate for this process, $\sim 10^{-9} \text{ cm}^3/\text{s}$, is as large as for $\text{H}^+ + \text{H}^0$ charge exchange in the energy range 0.1 - 100 eV. In the following description of our model we specialize the discussion to tokamak plasmas because of the importance of impurities to their operation.

Neutral oxygen enters a tokamak from the wall by H^0 , H^+ , e^- , photon or impurity impact, chemical erosion, or thermal desorption. Neutral oxygen may also be formed on limiters, possibly by the recycling of oxygen ions. Although the velocity and spatial distributions and the molecular form of the incoming oxygen are not known, it is reasonable to expect an isotropic influx of atomic oxygen with energies near 1 eV. These atoms penetrate the plasma (Fig. 1) until they are ionized by either charge exchange, Eq. (1), or electron impact [4],

Once ionized, the oxygen quickly thermalizes with the protons, rapidly moves along magnetic field lines, and slowly diffuses across them. The oxygen may ionize further,

or it may neutralize by charge exchange and again move rapidly across the magnetic field. Then it might return to the wall, move further into the plasma, or reionize.

To quantify the effect of charge exchange on oxygen loss, a Monte Carlo simulation in slab geometry was performed. The

plasma is characterized by spatially dependent e^- and H^+ temperatures, and e^- and H^0 densities. Trajectories of individual oxygen atoms are followed from the wall to the point in the plasma where they ionize. Plasma-induced O^+ transport is not included in the model, i.e., O ions are confined to magnetic surfaces; only neutral oxygen atoms are allowed cross-field motion. (This approximation will be discussed later.) Ionization and charge exchange rates are calculated at each point along a particle's trajectory and are compared with random numbers in the usual Monte Carlo fashion. This determines a particle's ionization state. The history of a particle is followed until it either: returns to the wall; ionizes to O^{++} ; or moves 10 cm toward the plasma axis. If the first occurs, the oxygen atom is considered to be lost from the plasma. If either of the last two options occur, then that oxygen atom is considered trapped in the plasma. For two different T_e profiles, the percentage of oxygen atoms lost from the plasma because of resonant charge exchange is shown in Figs. 2 and 3. In these computations the spatial distributions of the plasma parameters are given by

$$\begin{aligned} n_e(a-x) &= n_{H^+}(a-x) = 10^{13} (1 + 0.1x) \text{ cm}^{-3} \\ T_e(a-x) &= T_e (1 + 0.1x) \text{ eV} \\ n_{H^0}(a-x) &= n_{H^0}(a) \exp(-x/3) \text{ cm}^{-3} \\ T_H(a-x) &= 5 (1 + 0.1x) \text{ eV}, \end{aligned} \tag{4}$$

where $x(\text{cm})$ is the distance from the edge of the plasma, a is the minor radius of the tokamak, and T_e and n_{H^0} , the electron temperature

and neutral hydrogen density, are indicated on the figures. Two different energies, .02 and 2 eV, were used for the incident oxygen atoms. These are characteristic of oxygen desorbed by thermal processes and H^0 impact, respectively. For all the cases shown here, more than 50% of the O^+ charge exchange neutralizations took place within 5 cm of the wall ($x = 0$). At a 2 eV electron temperature and 10^{12} cm^{-3} electron density the plasma becomes so transparent to the incident O^0 that ~.95% pass beyond the 10 cm limit without ionizing. The results of the simulation are insensitive to the temperature of the background ions over the range $1 < T_i < 10$ eV. As is shown in these figures, by decreasing T_e from 7 eV to 3 eV, a more than 10 fold increase is predicted for the amount of oxygen channeled back onto the wall. Computer runs have also been performed with temperature and density profiles other than equation (4), with the same general result - at $T_e \sim 3$ eV, $n_{H^0} \sim 10^{11} \text{ cm}^{-3}$, and $n_e \sim 10^{13} \text{ cm}^{-3}$ resonant charge exchange between O and H results in $\geq 30\%$ of the incident oxygen atoms being channeled back onto the wall.

To date, there are no direct experimental tests of this model. Measurements of $T_e(a)$, $n_e(a)$, and $n_{H^0}(a)$ have been performed on several tokamaks [5] with characteristic values being $T_e(a) \sim 7$ eV, $n_e(a) \sim 10^{12} \text{ cm}^{-3}$ and $n_{H^0} \sim 5 \times 10^9 \text{ cm}^{-3}$. These conditions should only result in a 1% O loss by O-H charge exchange. This, in fact, is the approximate amount of neutral oxygen inferred by surface analysis techniques [6] to leave the PLT tokamak during the steady state part of the discharge; however this interpretation is not without question, nor has the experiment been repeated on PLT during

high flux H_2 gas pulsing experiments. Such discharges, as are standard for Alcator [7] and high density Pulsator [8] operation, should be characterized by higher $n_{H^0}(a)$ and lower $T_e(a)$; thus O-H charge exchange would be more rapid. In high density Alcator and Pulsator discharges substantially smaller relative amounts of O are present than in their low density discharges. The actual loss of O from the plasma also depends on the sticking probability of O on the wall. Estimates of this from O_2 data give a sticking coefficient near unity [9].

Ion diffusion substantially changes the oxygen transport. Neoclassical transport will cause the O^+ ions to move into the denser and hotter portions of the plasma, thereby increasing the O^{++} formation rate. In tokamak discharges the inward neoclassical ion transport velocity is about 1 cm/ms near the edge [10]. For O-H charge exchange to be competitive with this, the H^0 density at the edge would have to exceed 10^{11} cm^{-3} . At present, no estimate for massive ion transport is possible for the case of H_2 gas puffing experiments, because of the lack of understanding of plasma dynamics during the influx of large amounts of H_2 .

The claim for the importance of chemical processes to oxygen transport is strengthened because many relevant molecular reactions have rates several times faster than reaction (1), and also lead to neutral O formation. Examples are [11]:

PROCESS ($T_i = T_e \sim 3 \text{ eV}$)	RATE ($10^{-9} \text{ cm}^3 \text{ s}^{-1}$)
$\text{O}^+ + \text{H}_2 \rightarrow \text{OH}^+ + \text{H}^0$	2
$\text{OH}^+ + \text{e}^- \rightarrow \text{O}^0 + \text{H}^0$	6
$\text{OH}^+ + \text{H}^0 \rightleftharpoons \text{OH}^0 + \text{H}^+$	1
$\text{O}_2 + \text{e}^- \rightarrow 2\text{O}^0$	20
$\text{H}_3\text{O}^+ + \text{e}^- \rightarrow \text{H}_2\text{O}^0 + \text{H}^0$	6.5

Though these reactions were not explicitly included in our calculations, increasing the (forward) charge exchange rate ($\text{O}^+ + \text{H}^0 \rightarrow \text{O}^0 + \text{H}^+$) by a factor of 5 increased the calculated oxygen loss fraction by a factor of 1.3. Other rapid chemical reactions, not restricted to O^0 formation, which are possible in tokamaks, were also not included in our calculations.

In summary, it is pointed out that numerous low energy chemical processes can occur in the edge or divertor regions of tokamak devices. These processes should be most important during gas puffing, gas blanket, or divertor experiments. Under appropriate conditions, one particular process, O-H charge exchange, can result in the loss of more than 30% of the singly charged oxygen ions from the plasma edge.

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TOP VIEW OF TOKAMAK MIDPLANE

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Fig. 1. Schematic of processes included in the Monte Carlo simulation. Oxygen atoms are desorbed from the wall and enter the cool edge plasma of the tokamak. Ionization by electron impact or charge exchange with H^+ can occur. Subsequently, electron impact ionization to O^{++} or charge exchange neutralization to O^0 occur. The motion of the ions is constrained to magnetic surfaces. Only O^0 is free to move across magnetic surfaces. Some of the neutralized O^0 atoms may return to the wall.

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Fig. 2. Fraction of incident oxygen atoms lost from a 7 eV edge temperature hydrogen plasma because of O-H charge exchange. The fraction depends strongly on the neutral hydrogen density and energy of the incident oxygen atoms. The spatial dependences of the plasma parameters are given in the text.

Fig. 3. Same as Fig. 2, except the edge electron temperature is 3 eV.

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