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#### Abstract

The effect of molecular processes on the transport of neutral gas in tandem mirror halo plasmas is studied using the SPUDNUT neutral transport code. Comparisons to the case where the neutrals are assumed to be incident on the halo plasma as atoms are made. It is found that molecular processes have a strong effect on the transmitted and reflected neutral particle flux. The results are cast in terms of the reflectance and transmissivity coefficients for use in simple point model halo calculations.

#### I. Introduction

Parametric calculations of neutral transport in halo plasmas were done recently by Deng and Emmert. (1) This work used a version of the SPUDNUT (2) transport code which considers only transport of atoms. In reality, however, the neutral gas incident on the plasma is a mixture of molecules at the wall temperature and energetic charge exchange atoms reflected by the wall. H. Howe (3) has extended SPUDNUT to include molecular processes. In this report we reexamine the transport of neutrals in halo plasmas using Howe's version of the SPUDNUT code and compare the results with the atom transport case. We cast the results in terms of the reflectance and transmissivity coefficients, as in Ref. 1, which are useful in simple point model halo calculations.

The plasma model taken is a one-dimensional plasma slab with either parabolic or uniform profiles. The plasma parameters are assumed to be given; we consider here only the neutral transport and do not require that the plasmaneutral system be self-consistent. These results are useful for halo models in which neutral transport is one of several processes involved in the halo. Such models for halo plasmas are under development. (4)

#### II. Molecular and Atomic Processes in the Halo Plasma

The main processes relating to molecular breakup are the following reactions:

dissociative excitation of  $H_2$ ,

$$H_2 + e^- \rightarrow 2 H^0 + e^-$$

ionization of  $H_2$ ,

$$H_2 + e^- \rightarrow H_2^+ + 2 e^-$$

dissociative excitation of  $H_2^+$ ,

$$H_2^+ + e^- \rightarrow H^+ + H^0 + e^-$$

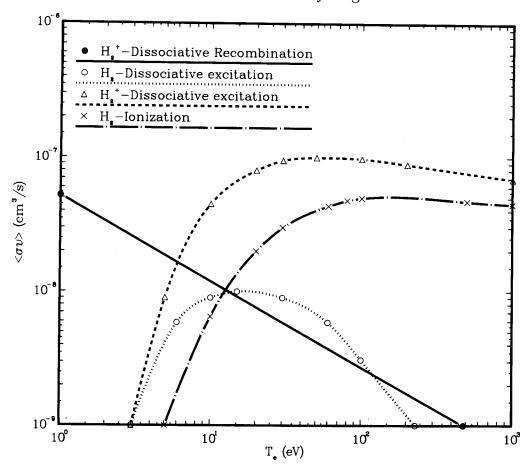
and dissociative recombination of  $H_2^+$ ,

$$H_2^+ + e^- \rightarrow 2 H^0$$
.

We use the symbol H to represent any of the three isotopes of hydrogen. The calculations are actually done for a 50%-50% mixture of deuterium and tritium. The rate coefficients for the above reactions averaged over a Maxwellian electron distribution are given by Jones<sup>(5)</sup> and are shown in Fig. 1.

The molecules incident on the plasma slab are taken to be monoenergetic at the wall temperature and have a cos  $\theta$  angular distribution. According to the reactions above, these molecules either produce  $H^0$  or  $H_2^+$ . Since the  $H_2^+$  molecular ions are trapped by the magnetic field, we need only consider where they are formed and their subsequent breakup into protons and atoms. The protons are also trapped by the magnetic field and constitute part of the ion source term returned by SPUDNUT. The atoms produced from the molecules (often referred to somewhat loosely as Franck-Condon atoms) are assumed to be monoenergetic at energy  $E_0$  (taken here to be 5 eV) and isotropic in direction. Later in this report we show that the results are rather insensitive to the

Fig.1 The Rate Coefficients of Ionization and Dissociation for Molecular Hydrogen



choice for  $\mathbf{E}_0$ . The atoms can subsequently be ionized or undergo charge exchange.

Charge exchange atoms or Franck-Condon atoms incident on the wall can be reflected as energetic atoms. For incident energies above 10 eV, we use the reflection coefficients of Oen and Robinson,  $^{(6)}$  while for energy less than 10 eV, the reflection coefficient is reduced in accordance with the calculations of Baskes.  $^{(7)}$ 

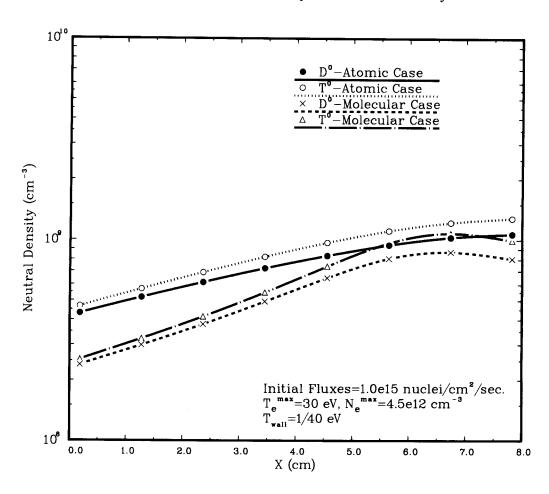
For comparison with the earlier work, we also present calculations where only atoms are incident on the plasma halo. In this case the atoms have an energy of 5 eV and a cos  $\theta$  angular distribution. To compare with the incident molecule case, the incident flux in both cases is the number of nuclei incident per unit area per unit time.

In the calculations presented in the next section, the plasma halo has either uniform or parabolic density and temperature profiles of the form  $(f_{max} - f_{min})(1 - (x/h)^2) + f_{min}$ . The main plasma-halo plasma interface is at x = 0 and the wall is at x = h. We take h = 8 cm for this work. When parabolic profiles are used, the boundary density is 5% of the maximum density in the halo and the boundary temperature is 3 eV. The plasma species is 50% D and 50% T. The neutral transport calculations are done only over the range x = 0 to 8 cm. Any neutrals penetrating the halo and entering the main plasma are assumed to be absorbed there and do not reenter the halo.

#### III. Results and Comparisons

Figure 2 shows the neutral atom density profiles in the halo plasma for parabolic plasma density and temperature profiles; the halo plasma parameters used are indicated on the figure. Results for both an atomic and a molecular incident flux are given. For the same initial flux, the neutral density is

Fig.2 Neutral Atom Density Profiles In Steady State



lower in the molecular case. This is because breakup of  $H_2^+$  produces  $H^+$  as well as  $H^0$ . In addition, the  $H^0$  produced is isotropic and therefore has an equal probability of heading back to the wall as penetrating deeper into the plasma. The maximum in the neutral atom density is located a couple of centimeters from the wall. This indicates that most of the incident molecules are broken up within this distance; this peak shifts inward as the wall temperature is increased.

In order to discuss the calculations, it is useful to consider the fractional yield of  ${\rm H}^0$  and  ${\rm H}^+$  from the breakup of  ${\rm H}_2$ . This is shown in Fig. 3 as a function of the electron temperature. We see that, at low  ${\rm T}_{\rm e}$  (< 10 eV), the yield is mostly atoms, while at high  ${\rm T}_{\rm e}$  the yield is equal fractions of ions and atoms.

Figure 4 shows the reflectance versus the integrated line density in the halo for parabolic halo profiles. The reflectance is defined as the total atomic flux incident on the wall divided by the initial flux of atoms or molecules (not including the reflected flux from the wall) incident on the plasma halo. The reflectance is higher in the molecular case because the Franck-Condon atoms are born near the wall and half of them are directed back towards the wall. The reflectance increases as the line density increases because of the greater probability of reflecting back the inward-going atoms by charge exchange. When the integrated line density is low, most of the atoms incident on the wall are at the energy  $\rm E_{0}$ , while the spectrum shifts toward the plasma temperature as the line density increases because charge exchange atoms are more dominant then. Figure 5 shows the transmissivity (flux penetrating the halo divided by the initial flux) for the same conditions. The transmissivity

Fig.3 Fraction of  $D^{\rm 0}$  and  $D^{\rm +}$  from Molecular Dissociation as a Function of  $T_{\rm e}$ 

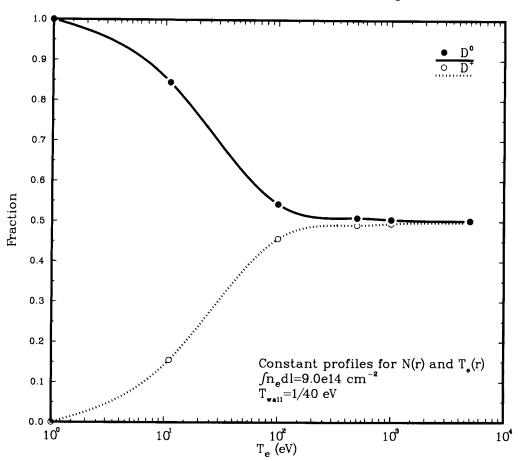


Fig.4 Reflectance versus Integrated Line Density for Different Initial Fluxes (Atomic and Molecular)

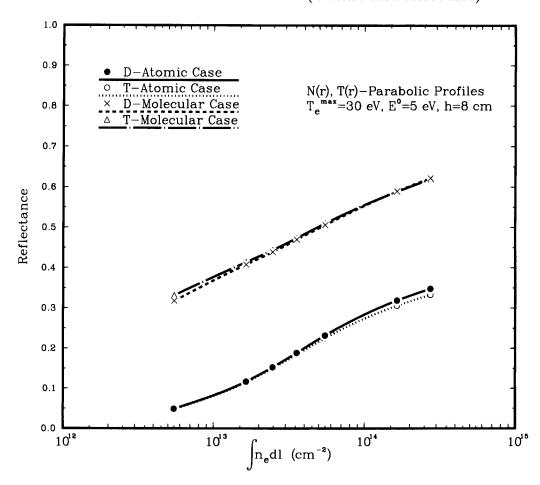
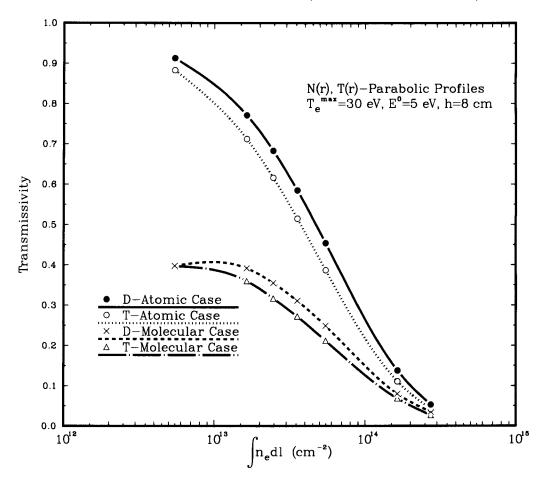


Fig.5 Transmissivity versus Integrated Line Density for Different Initial Fluxes (Atomic and Molecular)



is lower for the molecular case because molecular breakup produces a reduced inward-going flux of atoms compared with the incident atomic flux case.

Figures 6 and 7 show the corresponding results when the plasma halo has a uniform density and temperature. The biggest change is in the reflectance for the incident molecule case. This is due to the temperature dependence of the fractional yield. At high density the molecules don't penetrate as far, and thus break up in a colder plasma where the fractional yield favors Franck-Condon neutral production. This effect is missing in a uniform temperature plasma.

Figures 8-11 show the reflectance and transmissivity versus electron temperature for uniform profiles; Figs. 8 and 9 are for a low line density and Figs. 10 and 11 are for a higher line density. The transmissivity is a minimum at about 80-100 eV, which is where the ionization rate for both molecular and atomic hydrogen is a maximum. This suggests that the minimum in the transmissivity is due to the increased attenuation caused by ionization. The reflectance for the molecular case is composed of two components, the cold neutrals produced by molecular breakup, and the hot neutrals produced by charge exchange with the plasma. These components are shown separately in Figs. 8 and 10. Over most of the range, the cold component dominates in the flux of atoms incident on the wall. Of course, the hot component is more important in determining the sputtering of the wall.

The average energy of the reflected and transmitted neutral atoms is shown in Fig. 12 versus the line density. The transmitted atoms in the atomic and molecular cases have much the same energy. The average energy of the reflected neutrals is much different in the two cases. The atomic case has a much higher energy because all the neutrals are reflected by charge exchange

Fig.6 Reflectance versus Integrated Line Density for Different Initial Fluxes (Atomic and Molecular)

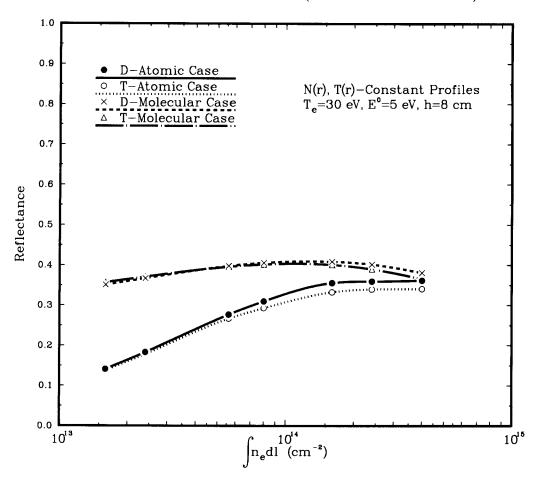


Fig.7 Transmissivity versus Integrated Line Density for Different Initial Fluxes (Atomic and Molecular)

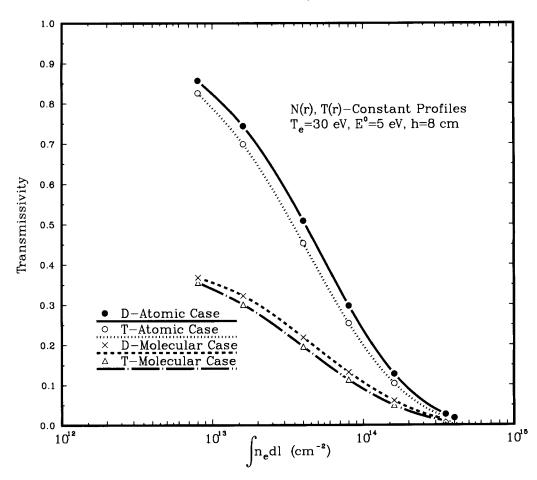


Fig.8 Comparison of Reflectance for Atomic and Molecular Initial Fluxes

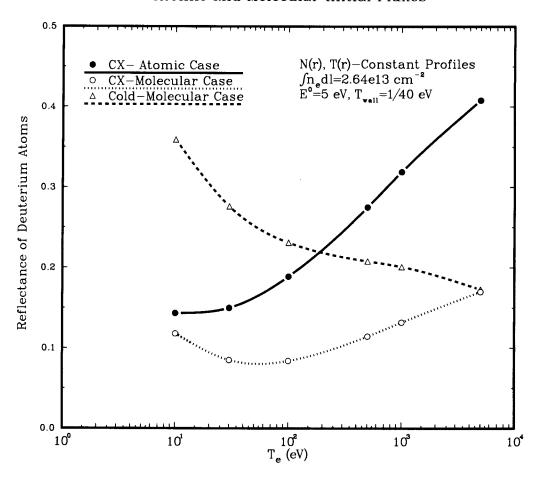
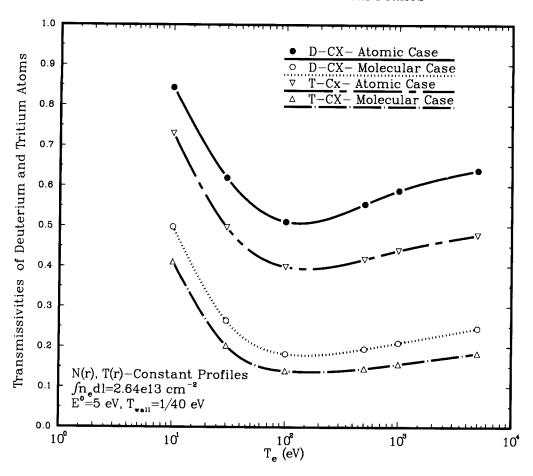
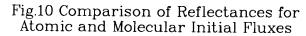


Fig.9 Comparison of Transmissivities for Atomic and Molecular Initial Fluxes





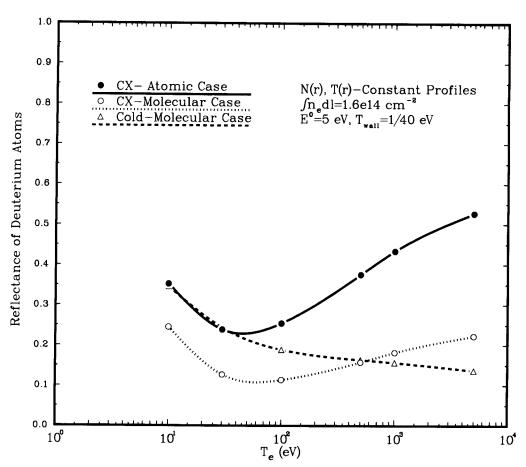


Fig.11 Comparison of Transmissivities for Atomic and Molecular Initial Fluxes

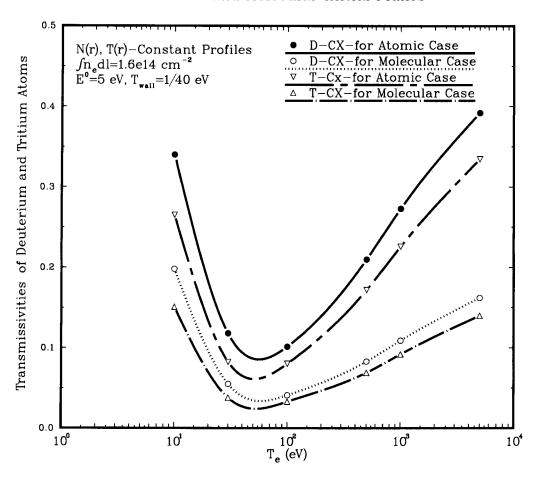
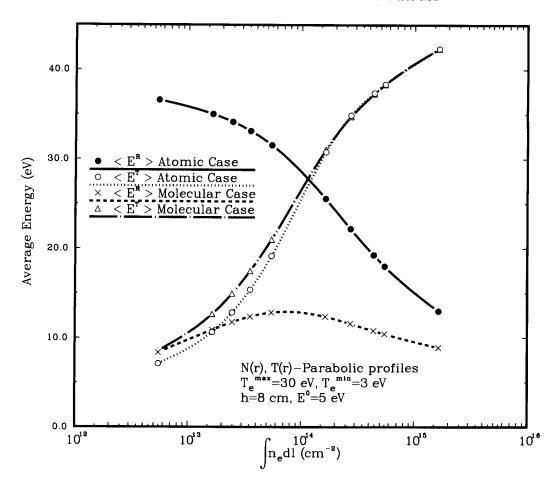


Fig.12 Average Energy of Reflected and Transmitted Neutrals



and therefore leave the plasma with an energy determined by the ion temperature roughly one mean free path into the plasma. The molecular case shows a much lower average energy because the backward-going Franck-Condon atoms produced by molecular breakup also contribute to the reflected flux and reduce the mean energy of the outgoing neutral atoms.

Finally, we consider the sensitivity of the results to the choice for the energy  ${\rm E_0}$  at which the neutral atoms are created. Figure 13 shows the variation of the reflectance and transmissivity with  ${\rm E_0}$  for parabolic density and temperature profiles; the incident flux is molecular for these calculations. The reflectance and transmissivity are rather insensitive to the choice for  ${\rm E_0}$ . Calculations done with a different (higher) ion temperature show a similar result. Consequently, we conclude that the choice for  ${\rm E_0}$  is not critical. Of course, at very low ion temperature (< 5 eV) the results should be more sensitive to  ${\rm E_0}$ , but this is not an interesting parameter range for halo plasmas, since the halo would not be able to shield the core plasma from incident neutral gas and impurities.

#### IV. Summary

We have utilized the SPUDNUT code to study the transport of neutral particles in tandem mirror halo plasmas. The particles incident on the halo can be either neutral atoms or molecules. Using a series of comparison calculations, we have found that these two cases can give quite different results for the reflected and transmitted neutral atom flux and for the mean energy of the atoms incident on the wall. We conclude that it is necessary to include the molecular processes to get an accurate calculation of neutral atom transport.

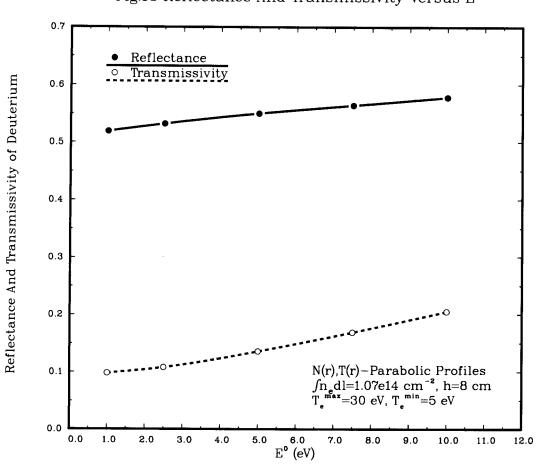


Fig.13 Reflectance And Transmissivity Versus  $\boldsymbol{E^0}$ 

#### Acknowledgement

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