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**IMPURITY TRANSPORT CALCULATIONS FOR
A DRIFT-DEPENDENT TOKAMAK SCRAPE-OFF PLASMA***

by

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IMPURITY TRANSPORT CALCULATIONS FOR
A DRIFT-DEPENDENT TOKAMAK SCRAPE-OFF PLASMA

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ABSTRACT

Two dimensional calculations of impurity transport in a high recycling divertor scrape-off region have been made with an updated version of the ZTRANS Monte Carlo computer code. The calculations use plasma parameters for the Doublet 3 divertor, as computed by the Planet Fluid Transport Code. The effects of electric field, particle drift velocities, and thermal forces are included in the calculations. For all impurity species studied, it is found that impurity transport is dominated by frictional forces, over most of the scrape-off region. Light impurities, however, impinge substantially closer to the divertor plate center than do heavy impurities, which tend to impinge at the outer plate boundary.

INTRODUCTION

Compared to hydrogen, impurity transport calculations may involve numerous charge states and more complicated wall interactions and thermal forces. Monte Carlo calculations for trace impurity transport in a fixed background hydrogen plasma can be an efficient means of computing impurity transport. A previous study⁽¹⁾ for the INTOR divertor showed the apparent utility of this approach. Recent analysis of a high-recycling divertor regime has been performed, when drift motion is taken into account. This has been done for the Doublet 3 tokamak using the latest version of the Planet 2-D Plasma Fluid Code.⁽²⁾ In general, the drift motion results in much higher flow velocities than previous computations showed.⁽³⁾ An updated version of the ZTRANS impurity transport code has now been used to study the impurity transport properties of such a regime.

The initial ZTRANS model is described in Ref. (1). Code modifications for this study have included the effect of $\vec{E} \times \vec{B}$ drifts, a revision of the effective collision frequency, and the inclusion of an ion thermal force term that removes the need for a disparate mass approximation. The validity of the ZTRANS model has also been verified by a comparison with a detailed kinetic equation solution code.⁽⁴⁾

The analysis has examined the transport of a variety of light and heavy impurities, all assumed to be present in and diffusing out of the plasma. The present results should be regarded as somewhat preliminary since more work is needed on better matching the Planet data and grid structure to the ZTRANS computational algorithms. General trends, however, related to impurity mass differences and to the near-sonic plasma flow speeds are evident.

The ZTRANS code computes the transport of individual impurity atoms and ions in a fixed background hydrogen plasma. The code essentially solves an approximation of the impurity kinetic equation, valid for time scales of $\tau \gg \tau_c$, where τ_c is the impurity-plasma collision time. The specified plasma parameters are the densities N_e, N_i , temperatures T_e, T_i , plasma parallel flow velocity V_i , and the potential Φ . An orthogonal coordinate system, $(X_{||}, X_R, X_p)$, is used where $X_{||}$ is the coordinate along the (net) magnetic field line, and X_R and X_p are perpendicular to the field. Since in a tokamak the toroidal field is typically much greater than the poloidal field, $X_{||}$ is approximately toroidal, and X_R and X_p can be defined as approximately in the radial and poloidal directions respectively. These terms will be used in this approximate sense (though the code works with the exact geometry). The analysis is two-dimensional since the divertor geometry is toroidally symmetric. The electric field is given by $\vec{E} = -\nabla\Phi$, and may have strong radial and poloidal components.

An impurity ion in a charge state Z is assumed to have thermalizing collisions with the background plasma on a time scale τ_0 . At each collision, the ion acquires a parallel velocity $V_{||} = V_0$ where V_0 is chosen from a normal distribution with mean $\bar{V}_0 = V_i$ (due to frictional forces) and standard deviation $V_{th} = (T_i/M_Z)^{1/2}$ (due to temperature-equilibration), where M_Z is the impurity mass. Between collisions, the ion motion along the field line is subject to acceleration due to the parallel electric field and plasma thermal forces:

$$M_Z \frac{dV_{||}}{dt} = Z|e|E_{||} + \alpha|e|\frac{\partial T_e}{\partial X_{||}} + \beta|e|\frac{\partial T_i}{\partial X_{||}} \quad (1)$$

where $|e|$ is the electron charge and α, β are the respective coefficients for the electron and ion thermal forces. The former coefficient is taken from the Braginski⁽⁵⁾ result for ion-electron collisions; $\alpha = 0.71 Z^2$. Following the Braginski, Fokker-Plank methods, Terry⁽⁶⁾ has recently derived the ion thermal force term for an arbitrary mass and arbitrary energy impurity ion. By integrating Terry's expression over a maxwellian distribution of impurity ion energies, to represent the average force over a period $\tau = \tau_0$, we have obtained the following value for β :

$$\beta = 3Z^2 (1 + \gamma) \left[.7795 - \frac{1.2292}{(1 + \gamma)^{1.5}} + \frac{.2329\gamma}{(1 + \gamma)^{2.5}} + \frac{.3904\gamma^2}{(1 + \gamma)^{3.5}} \right] \quad (2)$$

where $\gamma = M_i/M_Z$.

The variation in the ion thermal force, with impurity mass is shown in Table 1 for $M_i = 2.5$ AMU (DT). Included is the force for a deuterium-tritium "test particle".

As shown, for a negative temperature gradient, helium would tend to be attracted to the divertor plate by the ion thermal force. The force is repulsive for heavier impurities. Both ion and electron thermal forces are strongly dependent on charge state.

Table 1. Ion-impurity thermal force coefficient.

Species	γ	B/Z^2
DT	1	-2.38
He	.63	-1.10
Be	.28	.281
Fe	.045	1.34
W	.014	1.49
--	0	1.56

The collision time used in the code is $\tau_0 = 2\tau_c$, $\tau_c = \frac{1}{\nu}$, where

$$\nu = \frac{4 (2\pi)^{1/2} N_i e^4 \log \Lambda}{3 (4\pi \epsilon_0)^2 T_i^{3/2}} \left\{ \frac{M_i}{M_Z (M_Z + M_i)} \right\}^{1/2} Z^2$$

is the Braginski collision frequency.

Between thermalizing collisions, the ions move in the radial direction due to diffusion and drift and in the poloidal direction due to drift, as expressed by:

$$\Delta X_R = V_R \Delta t + \Delta X_D \quad (3)$$

$$\Delta X_P = V_P \Delta t \quad (4)$$

where $V_R = E_p/B$ is the radial drift velocity, $V_P = E_R/B$ is the poloidal drift velocity, Δt is the time step, and ΔX_D is the diffusion term. The latter is chosen from a normal distribution with zero mean and a standard deviation of $\sqrt{D\Delta t}$. The Bohm diffusion coefficient, $D = T_e/16B$, was used in the simulation.

The charge state of an impurity is determined from the local rate coefficients for electron impact ionization and recombination by a Monte Carlo method described in Ref. (1). Rate coefficients from the atomic physics code of Hulse⁽⁷⁾ and other sources⁽⁸⁾ are used. Particle-boundary interactions are computed as described generally in Ref. (1). For the present calculations, helium is backscattered from the first wall and divertor plate while other impurities are assumed to stick. Ions near the divertor plate are assumed to be accelerated through a sheath potential of $3T_e$.

DOUBLET 3 SCRAPE-OFF PLASMA

The grid system used for the Planet calculations of the D-3 divertor configuration is shown in Fig. 1. The magnetic field strength is $B = 1.5T$. The inclusion of drift velocities is found to result in near sound speed flows over much

of the scrape-off. Parallel flow velocities, however, are still negative (pointing away from the divertor plate) over much of the region including the separatrix field line above the x-point. Hydrogen fluid motion, which depends on the parallel flow, and diamagnetic and $\bar{E} \times \bar{B}$ drift motion, is generally such that hydrogen flows towards the divertor plate. Impurity flow, as will be shown, is in general highly mass dependent.

For simplicity, we analyzed impurity transport for the outer (large major radius) half of the scrape-off region only, from the top of Fig. 1 to the outer divertor plate (i.e., for $x \geq 50$ cm). Results for the inner region should be similar. The first wall is taken as the outer flux line in Fig. 1. For the ZTRANS calculations, impurity ions were launched uniformly on the separatrix field line from near the top to a point just above the x-point. A total of about 11,000 particles per simulation were used. The initial ion charge state used was the local coronal equilibrium value. For helium, a particle history terminates if it re-enters the plasma (either as a neutral or ion). Other species terminate upon re-entering the plasma or impinging on the wall or divertor plate.

RESULTS

The ZTRANS simulations are summarized in Table 2. The impurity ion density in the scrape-off zone is shown in Fig. 2 for helium and Fig. 3 for iron. The density profiles for oxygen and tungsten are similar to the results for iron. In these figures D_{PERP} is the coordinate perpendicular to the separatrix field line.

The helium and iron density profiles are fairly similar above the x-point region, but substantially different below the x-point. Iron tends to flow along the outer scrape-off field lines where the plasma fluid velocity, V_i , always points towards the divertor plate. The iron density is low near the divertor plate center. Helium, in contrast, exhibits substantially higher density near the plate center ($D_{\text{PERP}} = 0$, $y < 10$ cm). Figure 4 compares the particle flux to the divertor plate for He, Fe, and W. Results for DT test particles (not shown) are similar to helium but are more centrally peaked.

Some of the differences between He and heavier ion transport are due to the effects of neutral He transport which tends to spread out the helium ion flux, due to multiple ionizations and divertor plate impingements. Other differences are due to the smaller mass, which affects the collision frequency and the impurity thermal velocity.

The thermal and parallel electric field forces constitute only a second order effect ($\lesssim 10\%$) over most of the scrape-off region. A measure of the relative effects of collisional friction and thermal and E_{\parallel} forces, is the quantity

$$K = \left| \frac{V_i}{\frac{1}{2} a \tau_0} \right| \text{ where the acceleration } a = \frac{dV_{\parallel}}{dt} \text{ is given in Equation (1). It was found}$$

that $K \approx 10 - 100$ over the scrape-off zone, except near the divertor plate, for the impurities studied.

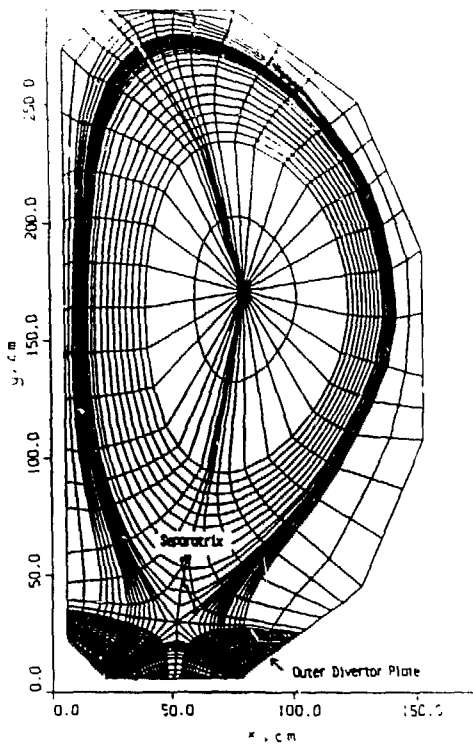


FIG. 1 DIVERTOR SCRAPE-OFF GEOMETRY

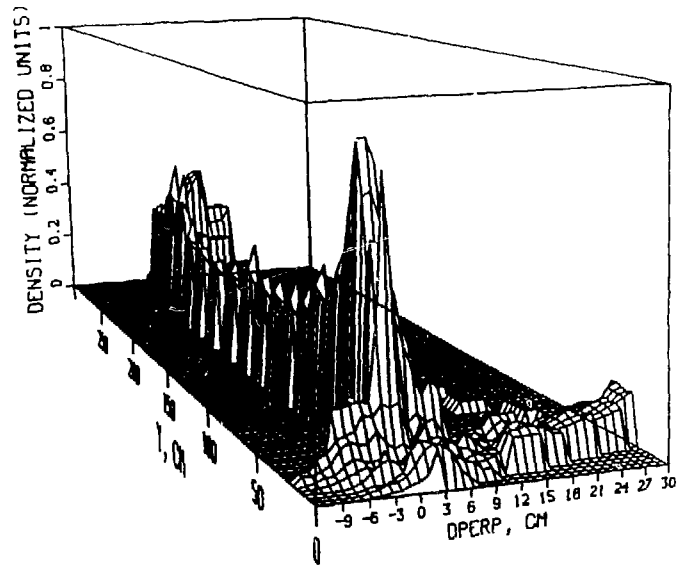


FIG. 2 HELIUM DENSITY IN THE OUTER SCRAPE-OFF REGION.

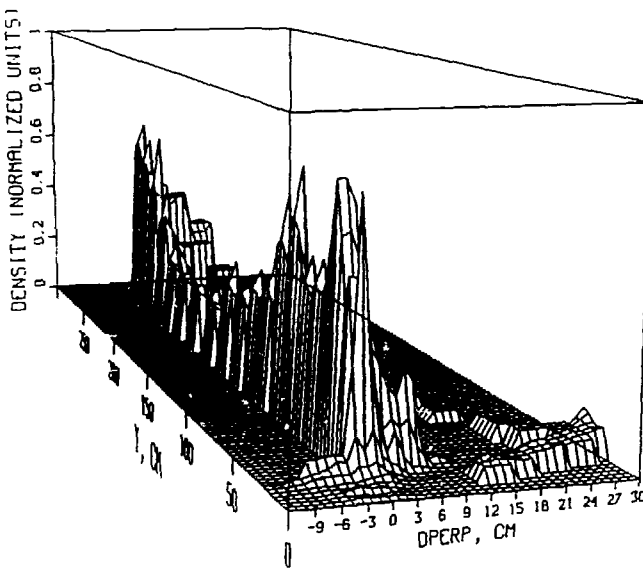


FIG. 3 IRON DENSITY IN THE OUTER SCRAPE-OFF REGION.

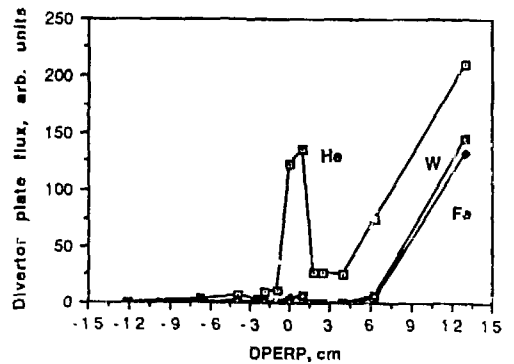


FIG. 4 ION FLUX TO THE DIVERTOR PLATE.

As shown in Table 2, only a small fraction of the helium diffusing from the plasma impinges on the divertor plate. This is similar to results for INTOR.⁽¹⁾ The implications of this phenomenon on helium pumping for future power reactors is a key issue and needs further assessment.

Table 2. ZTRANS Results Summary

Species Launched	Fraction Hitting Divertor Plate	Fraction Hitting Wall	Predominant Charge State	
			Above x-Point	Below x-Point
D-T ^d	.023	.002	1	1
He	.015 ^b .058 ^c	.001 ^b .01 ^c	2	2
O	.014	.001	8	7
Fe	.013	.002	11	8
W	.014	.002	12	8

^aTreated as test particles.

^bBefore recycling.

^cIncluding recycling.

DISCUSSION

Monte Carlo impurity transport calculations were made for a high recycling divertor regime, characterized by generally high plasma fluid speeds. Light impurities, being more mobile, tend to flow along the separatrix and impinge near the divertor center while heavy impurities tend to flow only near the outer boundary where the plasma parallel flow is always towards the divertor plate. Only 1-2% of all impurities diffusing from the plasma reach the divertor plate. The thermal and parallel electric field forces were found to be important only close to the divertor plate, for this regime. As in past calculations, it was found that charge states, near the divertor plate, for medium and high Z impurities, are higher than the local coronal equilibrium value. This is due to the long recombination time compared to the particle transit time from the higher temperature edge plasma region to the plate.

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