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**Particle Reflection and Neutral Transport  
in the Edge of ITER\***

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D. N. Ruzic

University of Illinois  
Urbana, Illinois 61801

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\*The original title of the grant was, "Particle Reflection and Titanium Decay in the Walls of ITER". It was changed by the US ITER team managers to address critical needs of the ITER design.

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## **Abstract**

A 2-D Monte-Carlo simulation of the neutral atom densities in the divertor throat, private flux region, and pump duct of ITER were made using the DEGAS code[1]. Plasma conditions were modelled using the B2 plasma transport code[2]. Wall reflection coefficients including the effect of realistic surface roughness were determined by using the Fractal TRIM code[3]. Results were obtained for both helium and deuterium. Pumping ratios and the effects of geometry are discussed. It is found that the detailed geometry and wall model have a significant effect on the helium pumping ratio and neutral atom density profiles.

[1] D.B. Heifetz et.al. J. Comp. Phys. **46** (1982) 309.

[2] B.J. Braams, NET rep. EUR-FU/XII-80/87/68 (1987).

[3] D.N. Ruzic, H.K. Chiu, J. Nucl. Mater. **162-164** (1989) 904.

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## I. Introduction

This DOE grant supported the principal investigator for two months during the summer of 1989. During this time microscopic surface roughness was discovered to be an important effect on determining the reflection of deuterium, tritium and helium from the wall and divertor surfaces of ITER. These coefficients were calculated and used in the first US simulations of 2-D divertor geometries of the ITER edge design. These simulations, created performed under this contract, show that helium will be pumped more quickly than the D/T gas mixture.

In the steady state of ITER the rate of helium production through thermonuclear fusion will equal the rate at which helium is pumped out of the vessel. If this balance requires an abundance of helium greater than 10% in the core of the ignited ITER plasma, the device may still succeed, but its performance may be marginal. On the other hand, if the helium abundance is only 5%, billions of dollars could be saved by design. The detailed questions of helium pumping is critical to the design and success of ITER.

To calculate the neutral atom density profiles, and thus the removal rates of the atoms, detailed analysis of the geometry and interactions with the walls must be preformed. The work of the principal investigator over the

last year has addressed both of these phenomena. Section II describe the applications of the work done to incorporate microscopic roughness through the use of fractal geometry into a reflection/sputtering model, and section III describes the results from two-dimensional neutral density transport simulations. Even small changes in the geometry or microscopic character of the walls can have large implications to the efficiency of helium removal.

## **II. Particle Reflection**

The TRIM code was modified to include microscopic surface roughness using fractal geometry. that work was carried out by the principal investigator over the last two years and was not supported by this DOE contract. The applications of this code to ITER-related problems was supported by this DOE contract.

These applications were the critical production of reflection and sputtering coefficients for a variety of materials, energies, angles of incidence and incident species. Energy and angular distributions of the reflected and sputtered flux were produced. The requestors and users of this data include:

(1) Dr. Jeffery Brooks, Argonne National Laboratory for use in his redeposition of sputtered material code, REDEP.

(2) Dr. Peter Stangeby, University of Toronto for use in his impurity transport code, LIM.

(3) Dr. Alicia Ehrhardt, Princeton Plasma Physics Laboratory, for use in methane production from tokamak walls simulations.

All three of these researchers are supported by DOE or their national equivalent to work on ITER. Results and journal papers from those studies are still in preparation.

The fractal surface model was also used as a part of this contract to model the surface reactions during neutral atom transport in the divertor region of ITER.

### **III. Neutral Transport in the Divertor Region**

A combination of a charged-particle transport code, B2, and a neutral-atom transport code, DEGAS, were used in this study.

#### **A. Input to Model**

The inputs to the B2 code were: 48MW of input power, H-mode transport coefficients, midplane density at separatrix =  $3.4 \times 10^{19} \text{ m}^{-3}$ . The main result was a sheath temperature of 22.8 eV right on the separatrix and 5.9 eV on the inside and 13.7 eV on the outside of the separatrix. The temperature,

density and flux results from B2 were stretched to fit the realistic geometry as shown in figures 1 and 2.

The surrounding DEGAS zones also need  $T_e$ ,  $T_i$  and  $n_e$  inputs. The inner "private" flux region will sustain a high photo-ionization rate so it was given a  $n_e$  scrape-off length of 5 cm and a rather high minimum density of  $5.11 \text{ cm}^{-3}$ . The  $T_e$  and  $T_i$  scrape-off lengths were 2.5 cm to a minimum  $T_e$  of 2 eV and a minimum  $T_i$  of 4 eV. On the pump duct side the scrape-off distances were more rapid: all three were chosen at 1 cm. There was no minimum to the density, so it quickly became zero. The minimum  $T_e$  was chosen at 1 eV and the minimum  $T_i$  was 4 eV. The 2-D results for  $T_e$ ,  $T_i$ , and  $n_e$  which served as inputs to the DEGAS code are shown in figures 3, 4 and 5.

The flux to the plate was scaled such that the total current of particles striking the sheath in the B2 code was the same as the total  $D^+$  current hitting the plate in the DEGAS code. The flux profile is shown in figure 6.

## **B. Recycling**

The B2 code operates on the following principle with respect to recycling: the net current from the plasma into the edge equals the loss of particles at the plate. In this run a recycling coefficient of 0.999 was used as an input.



That means for every 1000 particles that strike the plate 1 particle was lost. Therefore only 1 particle (net) enters from the plasma. By comparison, Sugihara shows a recycling coefficient of 0.988.

The DEGAS code is given a current on the plate and calculates the current that exits through the pump duct. This ratio depends on the geometry and the input plasma parameters. In this case for every 1000 D<sup>+</sup> ions that struck the plate  $69 \pm 10$  went down the duct: a recycling coefficient of  $0.931 \pm 0.010$ . Geometry is partly to blame for this discrepancy. The present simulation has a pump throat of 160 cm and assumes that pumps cover 100% of the toroidal extent. More realistic assumptions are a 120 cm throat and 20% coverage leading approximately to a linear reduction of 15 per cent which in-turn gives a recycling coefficient of 0.989.

In order to verify whether the present plasma parameters were consistent with the 0.933 recycling, a DEGAS run was made with "recycling" turned "on". This means that once a test-flight is ionized, that ion follows a flux surface, crashes into a surface, neutralizes and is born once again. The computational time increases dramatically. The only loss mechanism for a test flight is to find the pump! In this case (run 5) only 100 flights were run. For the 100 particles that exited, 431 struck the plate! The recycling was only  $0.77 \pm 0.033$ . It should not have been that easy for a re-ionized/re-neutralized atom to avoid yet

another re-ionization. The electron temperature in the divertor should be higher.

This recycling run does show, however, that a tilted plate does propel neutrals to the outside edge. flights in DEGAS clearly shows the out-board walking phenomenon that is expected to occur.

The absolute magnitudes of the recycling fluxes require some care. These simulations are two-dimensional but ITER is a 3-D future object. Currents that are quoted are really numbers of particles per second per unit length. That length is a depth into the plane in a toroidal direction. The input from B2 is  $1.5e23$  #/s/m. In DEGAS the input flux to the plate is  $1.5e21$  #/s/cm. the number exiting through the pump is  $(4.48 \pm 0.70)e19$  D0/s/cm at an average energy of 6.38 eV and  $(2.94 \pm 0.43)e19$  D2/s/cm at an average energy of 0.068 eV. This gives a total of  $(1.04 \pm 0.16)e20$  D/s/cm.

### C. Helium

Doubly ionized Helium was added to the DEGAS simulation. Since no B2 runs with He were available a simple assumption of 10 per cent helium was used. That is, the density and flux of He++ was taken to be .10 times the D+ density and flux. The temperature was identical. In this simulation no background He+ or D2+ was considered, though those can be added to DEGAS.

Helium has a higher wall reflection coefficient at low energy than Deuterium. Since energetic He travels farther and straighter than D2 a higher rate of He is expected at the duct. The input current on the plate was  $1.5e20$  He<sup>++</sup>/s/cm. The current down the duct was  $3.34 \pm 21e19$  He/s/cm. This gives a Helium recycling of  $0.777 \pm 0.014$ . For an input ratio of 10 D per 1 He on the plate, approximately 3.1 D per 1 He exit the simulation. This is good news. If the He flux is peaked more toward the outboard edge, as some suspect, the ratio could be even more favorable. Sugihara shows an enhancement as well. His recycling for He is  $1.000 - 0.015$  while his D/T recycling is  $1.000 - 0.008$  according to the "Global Particle Balance" figure. This gives a factor of 1.8 enhancement compared to our 3.23 factor.

This ratio of D to He flux is quite dependent on the reflection coefficients used in the simulation. This run uses Fractal TRIM data for number, energy and angular reflection characteristics.

#### **D. Densities**

DEGAS calculates neutral densities by scoring where the neutral atoms are when they make collisions. Usually there are enough collisions to create an adequate representation of the neutral density. In regions of no plasma however,

one must introduce "fictitious" collisions to track where the neutral atoms are. These collisions do nothing to alter the physics of the simulation. The particles' energy, and direction are not changed. It is merely an accounting device.

The density of neutral D is shown in figures 7 and 8. the density of neutral D2 molecules is shown in figures 9 and 10. The density of neutral He is shown in figures 11 and 12. Note the sharp drop in these parameters where the plasma is hot.

An examination of the private flux region shows a considerable relative helium abundance. Unfortunately the magnitude of the density is not large enough to pump.

An examination of the flux to the exit plane does show a significant phenomenon. The flux to the upper half of the exit is 50% higher than the flux to the lower half. If the duct need be made smaller, the bottom should be cut away.

#### **E. Future Work**

B2 runs with Helium need to be made and used for input in DEGAS. Likewise, the neutral densities calculated from DEGAS should be fed back into the B2 simulations. A variety of geometries should be used, particularly the ones in S.A. Cohen's memo file number ITER-IL-Ph-13-9-U-, dated July 5, 1989.

If this contract is renewed as anticipated, a full three-dimensional geometry will be simulated.

**F. Figures**

The figures are shown on the following pages.

Figure 1

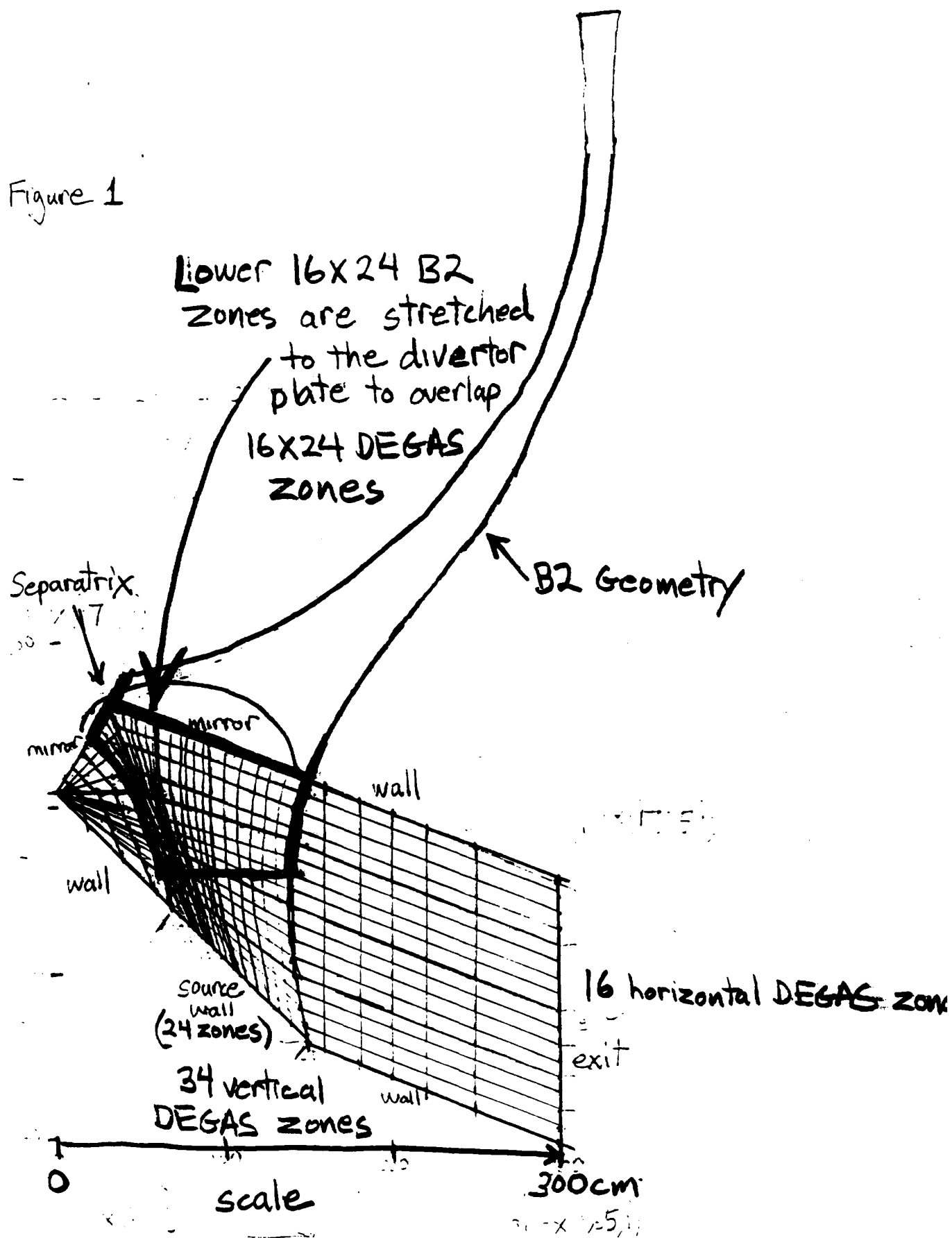


Figure 2

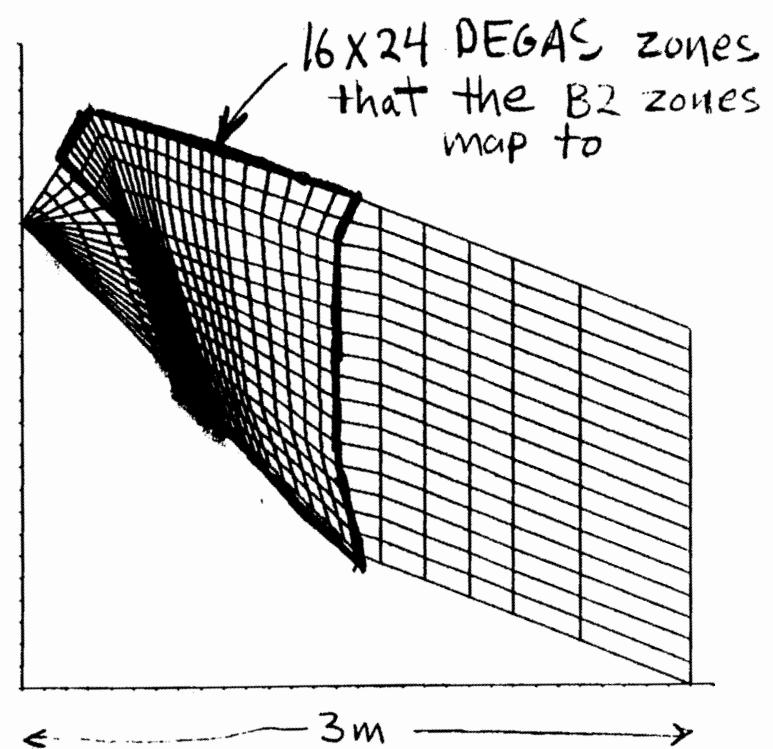


Figure 3

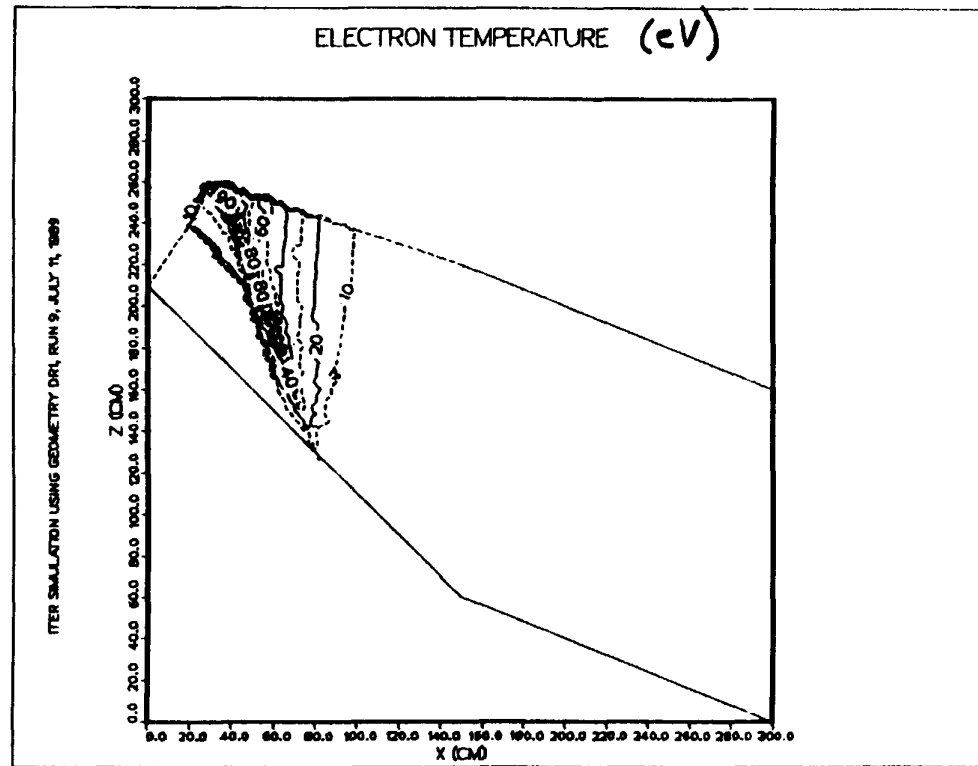




Figure 4

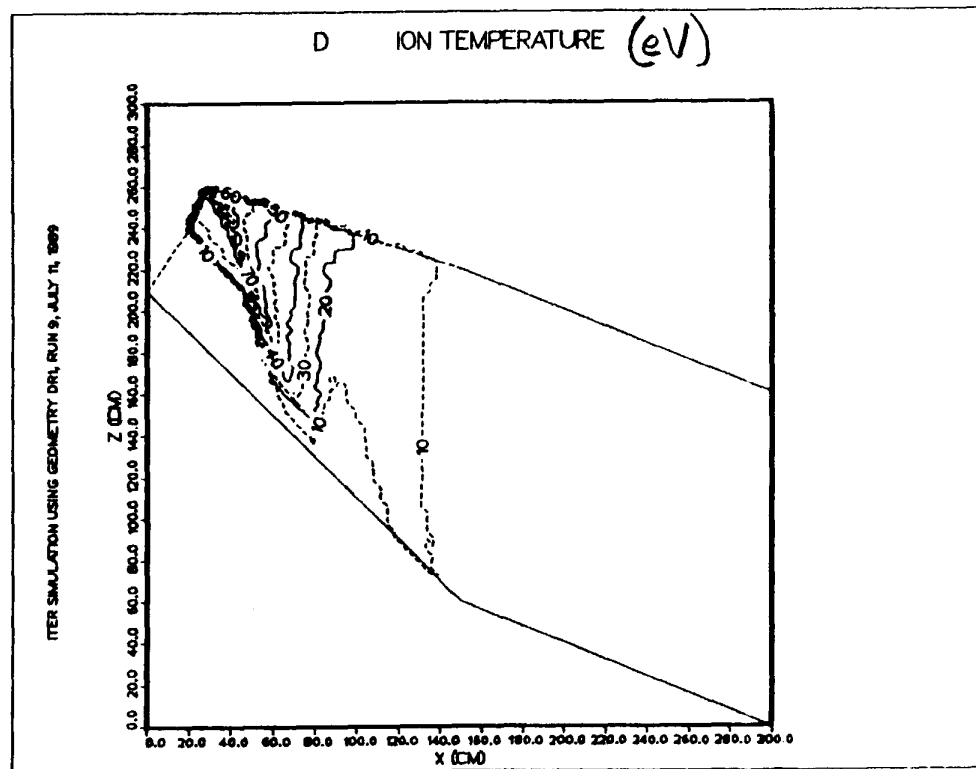


Figure 5

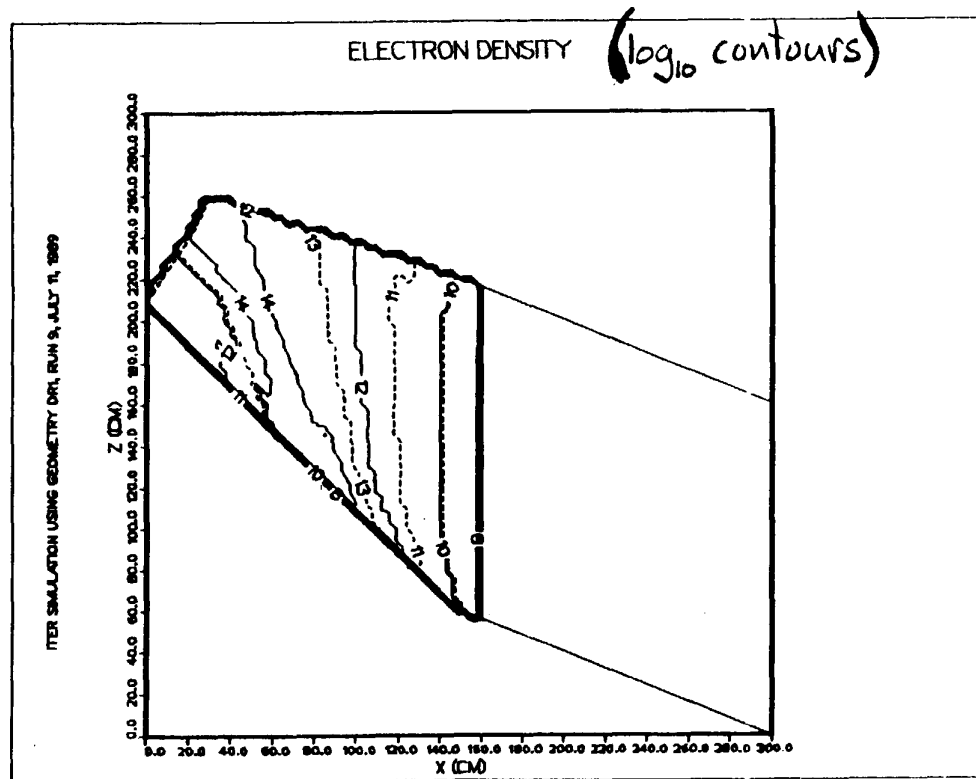


Figure 6

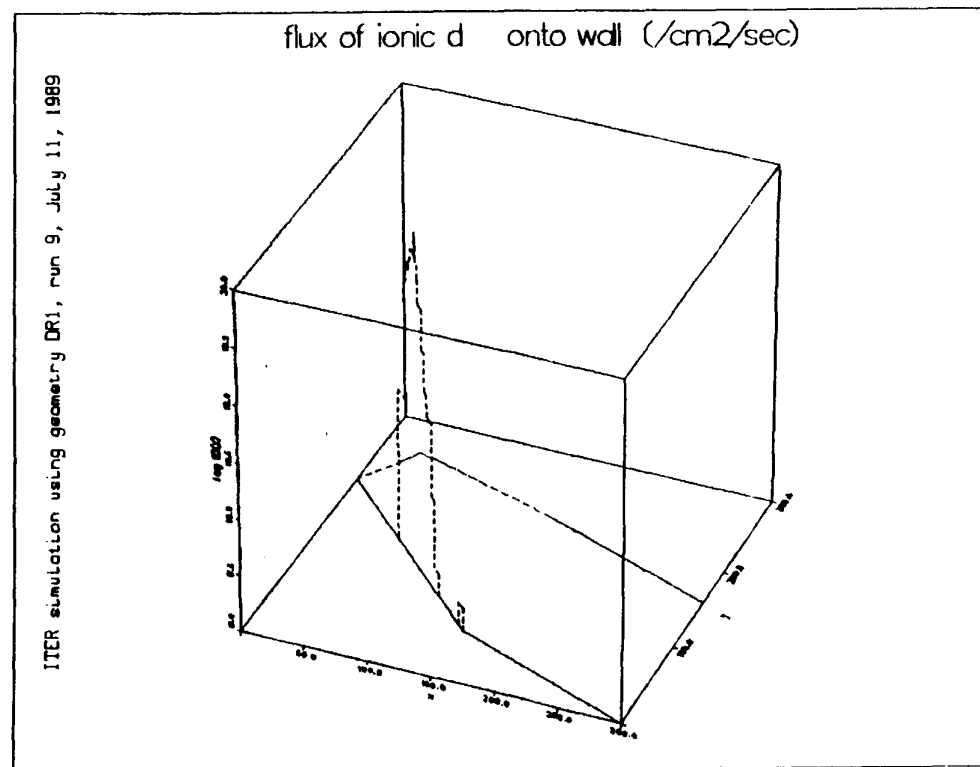


Figure 7

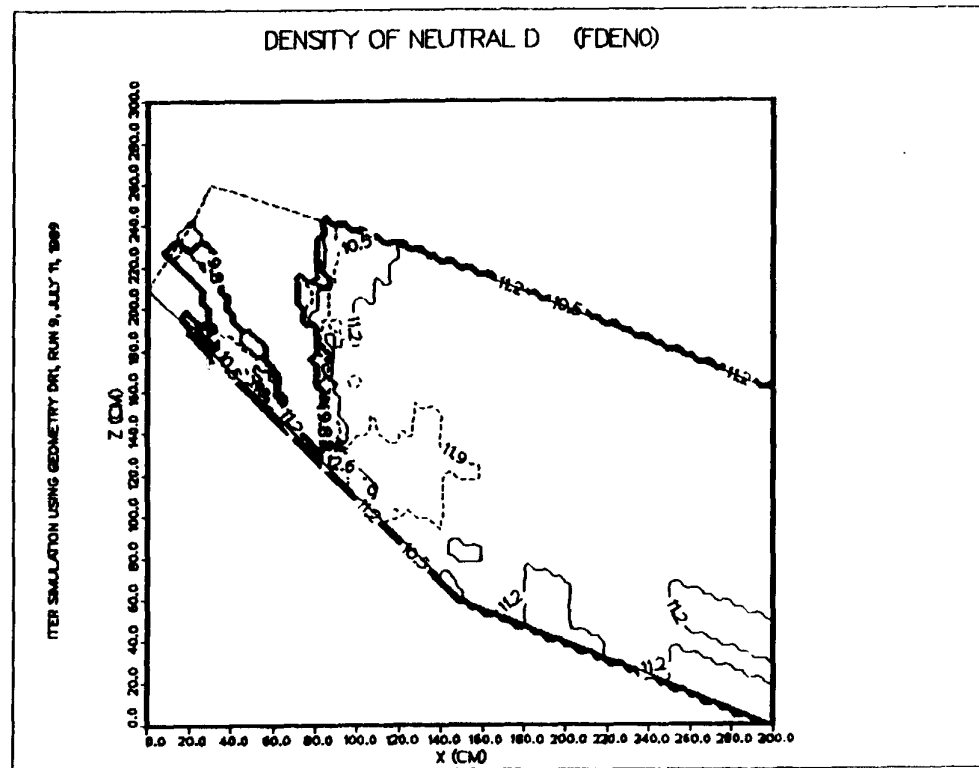


Figure 8

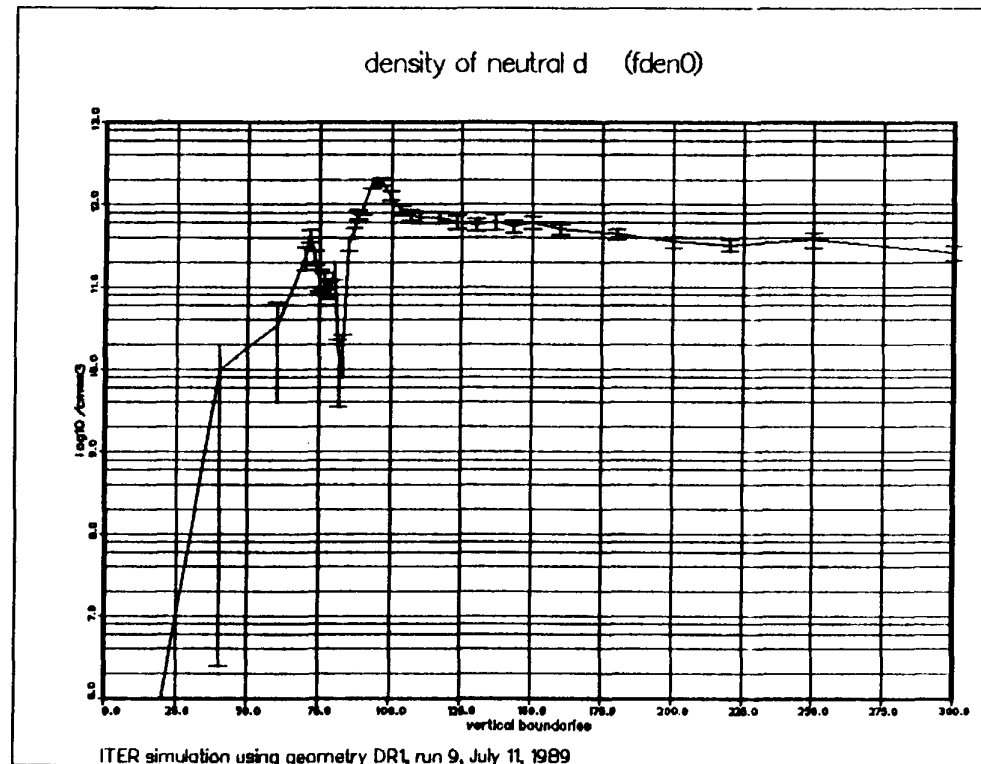


Figure 9

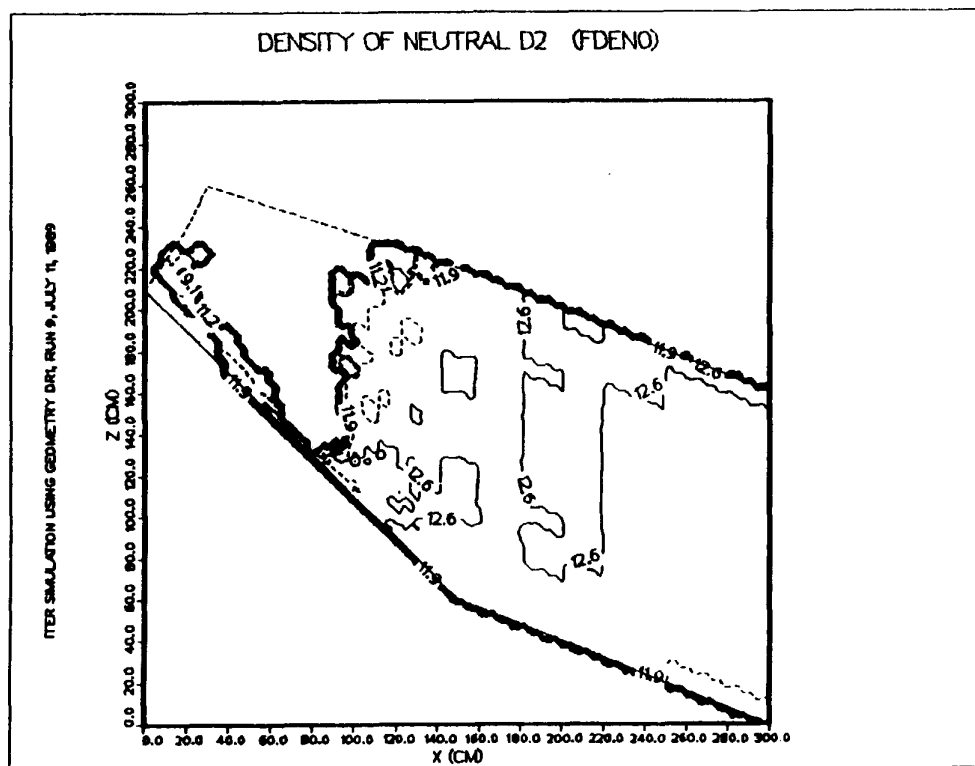


Figure 10

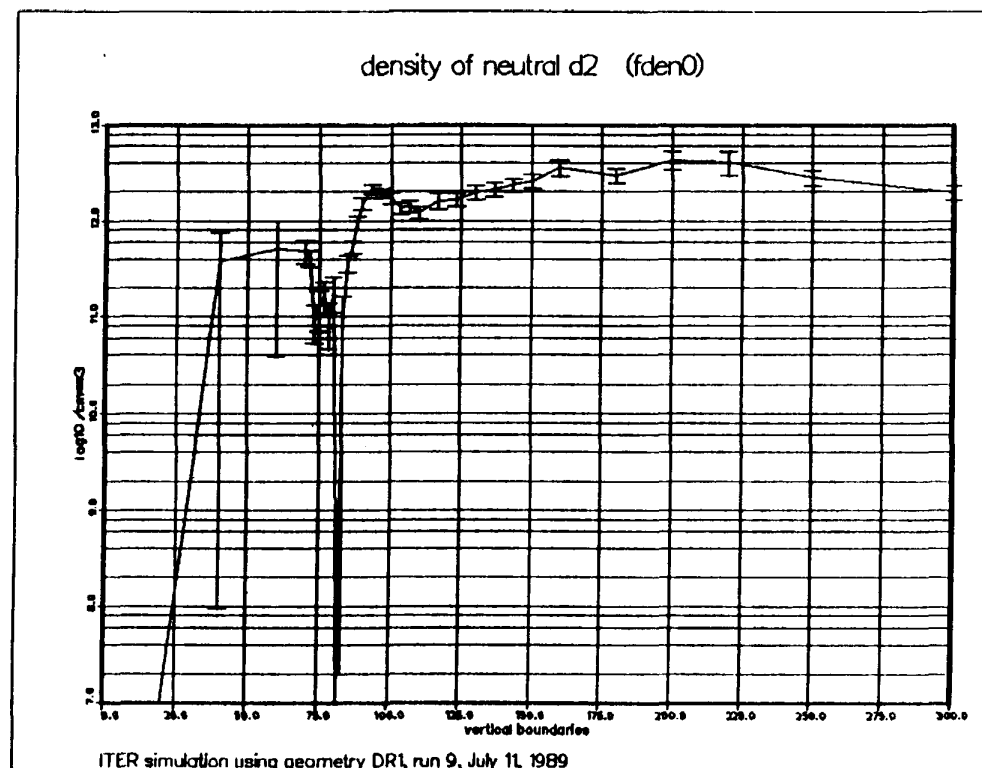


Figure 11

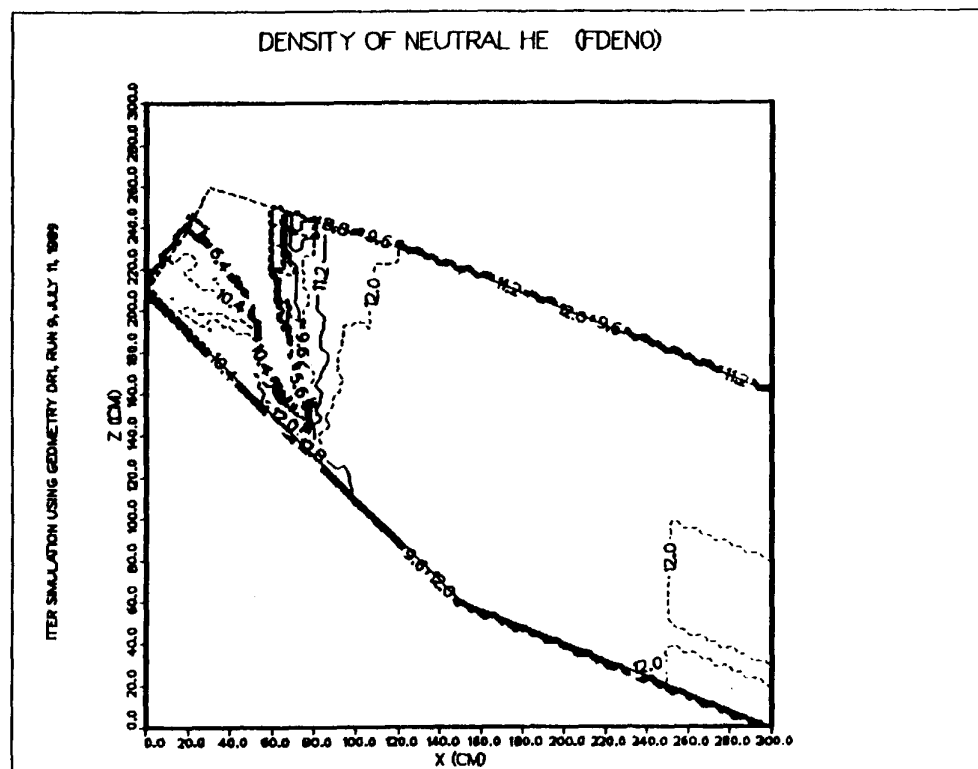




Figure 12

