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MILESTONE REPORT

Progress on Coupling UEDGE and Monte-Carlo Simulation Codes

M.E. Rensink and T.D. Rognlien

August 28, 1996

Lawrence
Livermore
National
Laboratory

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Introduction

Our objective is to develop an accurate self-consistent model for plasma and neutrals in the edge of tokamak devices such as DIII-D and ITER. The two-dimensional fluid model in the UEDGE code [1-7] has been used successfully for simulating a wide range of experimental plasma conditions. However, when the neutral mean free path exceeds the gradient scale length of the background plasma, the validity of the diffusive and inertial fluid models in UEDGE is questionable. In the long mean free path regime, neutrals can be accurately and efficiently described by a Monte Carlo neutrals model [8]. Coupling of the fluid plasma model in UEDGE with a Monte Carlo neutrals model should improve the accuracy of our edge plasma simulations.

The results described here used the EIRENE Monte Carlo neutrals code [9,10], but since information is passed to and from the UEDGE plasma code via formatted text files, any similar neutrals code such as DEGAS2 [11] or NIMBUS [12] could, in principle, be used.

Coupling Scheme

The Monte Carlo code requires the following input information from UEDGE: the grid and magnetic field orientation; the plasma densities, temperatures and flow velocities; and the ion fluxes incident on various surfaces. The inputs to the UEDGE plasma code from the neutrals model are the source terms for the density, parallel momentum and energy equations of each plasma species in the UEDGE model. One could imagine passing only the atomic neutral density to UEDGE, but this would not accurately model the momentum transfer between plasma and neutrals, which is an essential element in detached divertor plasma operation.

We use a time-dependent simulation method, illustrated schematically in Figure 1, with UEDGE and EIRENE running sequentially in a cycle that is repeated until the plasma has reached a steady state. During each cycle the UEDGE plasma is advanced over a finite time interval, dt, with fixed sources from EIRENE; the EIRENE neutrals are then advanced to steady state with the UEDGE plasma fixed. The capability exists for advancing the neutrals over a finite time interval rather than running them to steady state during each UEDGE/EIRENE cycle, but we did not choose that option in these simulations. The EIRENE code is executed by a call from within the UEDGE code.

Reference Case Input Parameters

For these coupling tests we chose a problem which had been previously used in a comparison of the UEDGE plasma/neutrals model and the coupled B2/EIRENE model. The coupled UEDGE/EIRENE model results enable us to separately identify differences that arise from the plasma model and differences that arise from the the neutrals model. The geometry for the model problem is a rectangular box representing the outer half of the SOL for a single-null divertor configuration, as shown in Figure 2. The poloidal length of the core region is 0.75 meters and the divertor leg length is 0.25 meters. The orthogonal mesh extends radially from 0.01 meters inside the core and private flux regions to 0.04 meters outside the separatrix. There are 64 cells along the poloidal direction, concentrated near the divertor plate where the minimum cell length is 4.4×10^{-4} meters in order to resolve the short mean free path of the recycling neutrals. In the radial direction we use 32 cells, concentrated near the separatrix where the minimum cell width is 6.0×10^{-4} meters. For the UEDGE plasma model we specify fixed density ($7 \times 10^{19}\ \mathrm{m}^{-3}$) and temperatures (150 eV) at the core boundary and zero particle and energy fluxes at all other boundaries except the divertor plate, where a sheath condition applies. The anomalous radial transport coefficients for particle and energy transport are $D_\perp = 0.5\ \mathrm{m}^2\mathrm{sec}^{-1}$ and $\chi_\perp = 0.7\ \mathrm{m}^2\mathrm{sec}^{-1}$. With these input conditions, the power to the outer half of the SOL is 100 kW and the resulting divertor plate temperature is 9 eV near the separatrix strike point, so the plasma is not detached from the plate.

The boundary conditions for the neutrals are determined by specifying the wall and plate materials. The material properties, such as particle and energy reflection coefficients, are contained in a database that can be accessed from the Monte Carlo code. For this test problem, all surfaces are assumed to be molybdenum.

Comparison of UEDGE and EIRENE Neutrals for the Initial Plasma State

The starting point for our time-dependent simulations is a self-consistent steady state from UEDGE using the inertial fluid neutrals model. For our attached plasma case, this should be a good approximation to the final solution one obtains from the more realistic Monte Carlo neutrals model. In Figure 3 we compare the atomic neutral density from the UEDGE and EIRENE models with exactly the same plasma. We expect some differences very close to the divertor plate because the EIRENE model includes hydrogen molecules which originate at the plate and break up within the plasma, while the UEDGE model assumes instantaneous breakup at the plate surface.

Comparison of Steady State Plasma Solutions for Fluid and Monte Carlo Neutral Models

The time evolution of the coupled UEDGE/EIRENE simulation after 1600 iteration cycles is illustrated in Figures 4 and 5. These results were obtained with a UEDGE time step of 5×10^{-6} seconds. In Figure 4 we see that initially the peak plate temperature drops sharply from 9 eV to about 3 eV in less than a millisecond before eventually reaching a steady state value close to 9 eV in a few milliseconds. Similar behaviour is observed for the total hydrogenic radiation as shown in Figure 5. Other global plasma parameters are compared in Table I. Generally, the agreement between the initial (UEDGE fluid neutrals) and final (EIRENE neutrals) solutions is quite good. Plasma profiles on the divertor plate are compared in Figure 6 where we see that the ion density is somewhat narrower with the Monte Carlo neutrals model. Figure 7 shows that the atomic neutral density throughout the divertor region is similar for the two models. There are differences very close to the plate surface which may be attributed to molecules in the EIRENE model. The molecular density, shown in Figure 8, is concentrated near the plate and wall surfaces as expected.

Stability versus Time Step Size

For a numerically explicit coupling scheme, the stability of the coupled system is governed by the size of the time step. Large time steps are desirable for computational efficiency, but lead to numerically unstable behavior. This is illustrated for our model in Figure 9 which shows the short term evolution of the coupled system with three different time steps. With the largest time step, dt=2x10^{-5} sec, the system exhibits undamped oscillatory behavior even in the first few steps. With a moderate time step, dt=1x10^{-5} sec, initial oscillations appear to be damped, but after a few tens of cycles they eventually grow exponentially. Only the smallest time step, dt=5x10^{-6} sec, yields a stable long term solution. This step size is consistent with the experience of the B2/EIRENE modelers for this same problem. For other plasma parameters they find a maximum stable time step as large as dt=1x10^{-4} sec or as small as dt=1x10^{-7} sec; they typically use dt=1x10^{-5} sec. There is no inherent time step limitation associated with the UEDGE plasma model, since it uses a fully implicit solution procedure. Likewise, there is no time step limitation associated with the Monte Carlo neutrals model. The stability requirement arises from the strength of the plasma/neutral coupling and the numerically explicit solution scheme for the coupled system.

Number of Monte Carlo Flights

The CPU time required for the Monte Carlo calculation is directly proportional to the number of neutral particle flights. The random noise on the spatial profiles of the plasma source terms supplied to UEDGE varies inversely as the square root of the number of neutral particle flights. If the noise level is too high, the UEDGE code will have difficulty solving for the plasma on a given time step. Also, the step-to-step noise level in a given plasma cell may be large. Thus, we choose the number of flights so as to balance these competing requirements. Figure 10 compares the time evolution of the coupled UEDGE/EIRENE system for two such choices, 50K flights and 250K flights. Although the long term evolution is similar, the random step-to-step fluctuations appear to be reduced by using more flights. Spatial contours of the plasma source terms at t=0 are compared in in Figure 11 where we see that a larger number of flights also reduces the spatial noise. It may be possible to obtain steady state solutions with fewer than 50K flights, but we did not run such a test case. With fewer flights one must accept a higher step-to-step noise level in the definition of "steady state". The steady state solution described in this report used 50K flights. We did not attempt to reduce the step-to-step noise with correlated sampling techniques.

Computational Resources

These simulation tests were run on a SPARC 10 workstation with 286 MB of memory. The coupled system was running on just a single processor at any given time. The Monte Carlo portion of the simulation could be speeded up by running flights simultaneously on several processors, but this capability does not yet exist in the EIRENE code.

During each cycle, the UEDGE plasma solver used 60-70 CPU seconds and the EIRENE neutrals solver used 300-500 CPU seconds. Thus, each time step required about 8 CPU minutes and the 1600 steps to the steady state solution used a total of 200 CPU hours. If EIRENE is run in a steady-state mode, the CPU time increases directly with the number of flights as noted in the previous section. The CPU time for UEDGE may increase with the step size or with fewer flights because the plasma solver must work harder to find a solution on each time step. The calculation of the Jacobian for the preconditioner is the most expensive part of the UEDGE solution step; for the cases described here, we calculated the Jacobian about once every 100 time steps.

The memory requirements are set mainly by the UEDGE code; determining factors are the number of cells in the mesh and the choice of pre-conditioner for the Newton solver. For the test cases described here, the size of the UEDGE executable was 80 MB. The size of the EIRENE executable was 45 MB.

Summary

We have obtained a steady state solution with the UEDGE fluid plasma model coupled to the EIRENE Monte Carlo neutrals model. The coupled system approaches steady state on a time scale of several milliseconds. Since the time step size is limited to $dt \leq 5\times10^{-6}$ seconds by stability of the explicit coupling algorithm, the total CPU run time is very long. The Monte Carlo code accounts for approximately 80 % of the total CPU time. We find that the inertial fluid and Monte Carlo neutrals models yield similar results for simulation of an attached plasma.

Conclusions

Clearly, we would prefer to run plasma simulations with the fluid neutrals model for computational efficiency. However, there are several reasons why this may not always be possible: (1) with a structured mesh in UEDGE it is difficult to accurately represent complex divertor and wall configurations, (2) there may be spatial regions where the neutral mean free path is longer than the characteristic scale lengths of the plasma, and (3) it may be difficult to accurately represent molecular effects and some aspects of plasma-wall interactions in a fluid neutrals model . For the simple test problems described in this report, consideration (1) is not an issue. Consideration (2) could be important if we are interested in core fueling by energetic charge-exchange neutrals that originate at the divertor plate, although these neutrals have a negligible effect on the SOL plasma solution. For our test problem the charge-exchange mean free path for hydrogen atoms in the divertor is

$$\lambda_{cx}[\mathrm{m}] = 0.01 \times T^{1/2}[\mathrm{eV}] / n[10^{20}\mathrm{m}^{-3}] = .007\ \mathrm{m}$$

so the fluid treatment should be valid, but λ_{cx}= .20 m is much larger than characteristic SOL scale lengths at the midplane. The neutral-neutral collisonal mean free path in front of the divertor plate is

$$\lambda_{n\text{-}n}[\mathrm{m}] = 0.02 / n[10^{20}\mathrm{m}^{-3}] = .20\ \mathrm{m}$$

so charge exchange dominates the neutral transport processes. At lower densities, the mean free paths become longer and one might expect significant differences between the fluid and Monte Carlo neutrals models. We have not yet tested the fluid model in this regime. For detached plasmas the charge exchange mean free path may increase due to a low ion density in front of the plate. A fluid treatment may still be appropriate if the neutral density increases so that elastic neutral-neutral collisions reduce the total mean free path for neutrals. More simulations are needed to test this hypothesis. In assessing the relative validity of the neutrals models it should be noted that most Monte Carlo simulations do not include neutral-neutral collisions, so the fluid neutrals model may be more realistic in some situations.

Future Work

There are several ways for improving the coupled UEDGE/EIRENE model described here in order to make it a useful tool for divertor simulations. Obviously, a more realistic geometric configuration should be used. Test cases with a detached recombining plasma would more clearly exhibit the differences between the fluid and Monte Carlo neutrals model. The total CPU run time could be reduced by using a larger time step, but this will require a more implicit coupling algorithm. One possibility for doing this is to construct the Jacobian for UEDGE using information from the fluid neutrals model Another possibility is global scaling of the source terms in UEDGE with the total ion flux to the divertor plates; however, previous experience with the B2/EIRENE code indicates that this approach only works in low-recycling situations. It may not be necessary to run the neutrals to steady state on each time step; a substantial reduction in CPU time could be achieved by running the Monte Carlo code in a time-dependent mode.

Acknowledgments

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Table I

Global plasma parameters from steady state solutions with fluid and Monte Carlo neutral models

		fluid neutrals	**Monte Carlo neutrals**
Power to divertor plate		80 kW	104 kW
Ion current to divertor plate		2050 A	2110 A
neutral gas contributions to volume-integrated sources	particles	2000 A	2030 A
	ion parallel momentum	-1.08 N	-0.41 N
	electron thermal energy	-51.3 kW	-50.9 kW
	ion thermal energy	22.6 kW	19.6 kW

Figures

Figure 1 Schematic of UEDGE/EIRENE coupling scheme.

Figure 2 Geometry for UEDGE/EIRENE test problem.

Figure 3 Plasma source terms from UEDGE and EIRENE neutrals models at t=0.

Figure 4 Time evolution of peak plate electron temperature.

Figure 5 Time evolution of total radiated power.

Figure 6 Steady state divertor plate profiles from UEDGE and EIRENE models.

Figure 7 Steady state atomic neutral density in divertor from UEDGE and EIRENE models.

Figure 8 Steady state molecular density in divertor from EIRENE model.

Figure 9 Short term evolution of total radiated power for various time steps.

Figure 10 Short term evolution of peak plate electron temperature for 50K and 250K flights; the solid line denotes data with 250K flights; the 'x' denotes data with 50K flights.

Figure 11 Spatial contours of plasma source terms for 50K and 250K flights at t=0.

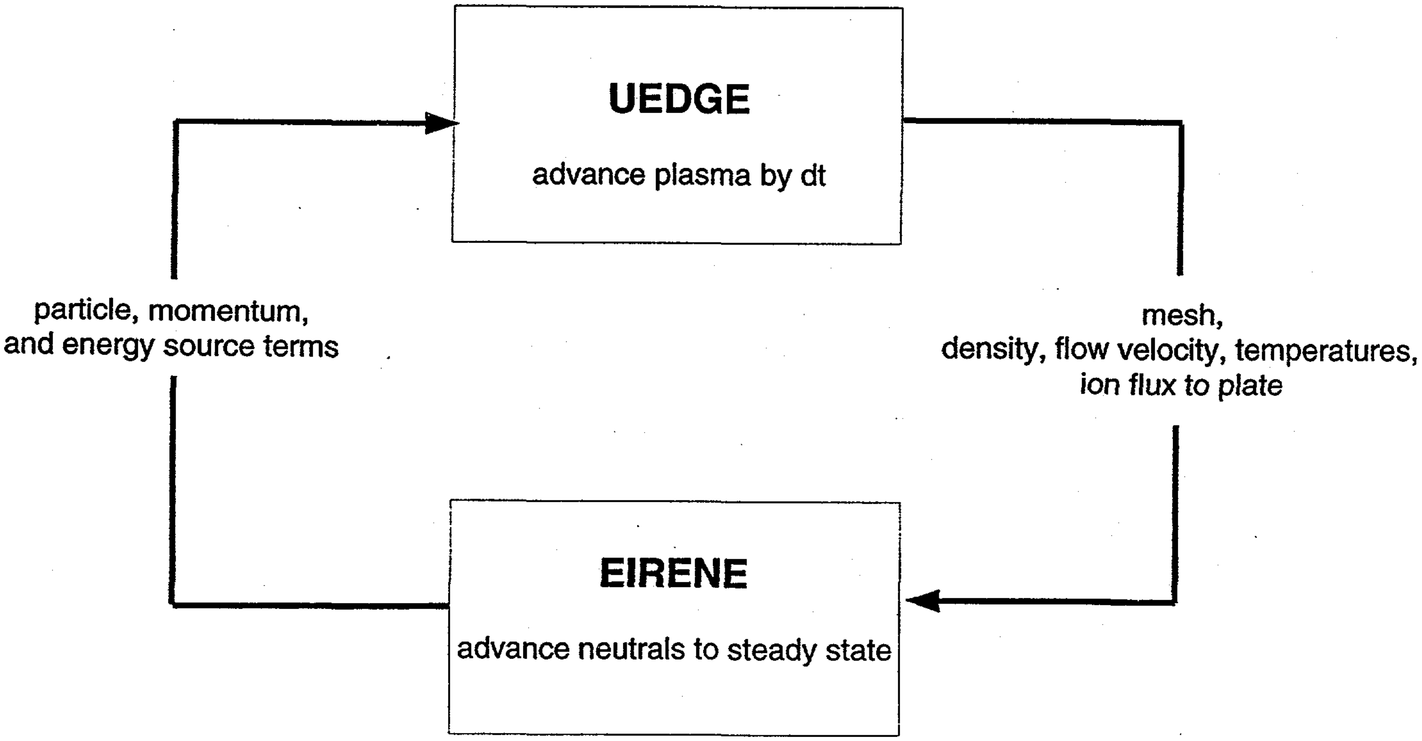

UEDGE
advance plasma by dt
mesh,
density, flow velocity, temperatures,
ion flux to plate
EIRENE
advance neutrals to steady state
particle, momentum,
and energy source terms

Figure 1

Geometry for Monte Carlo Test Problem

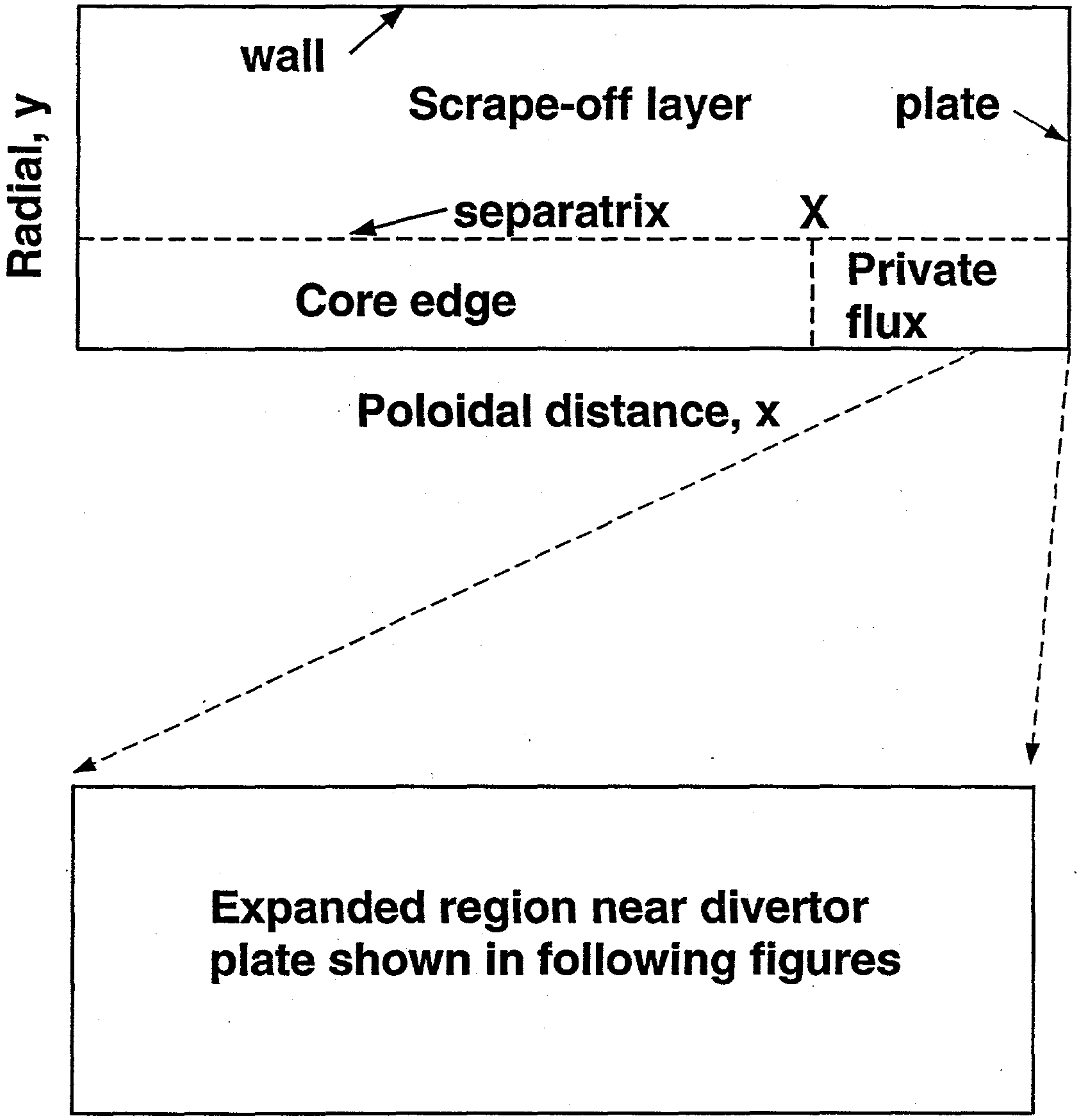
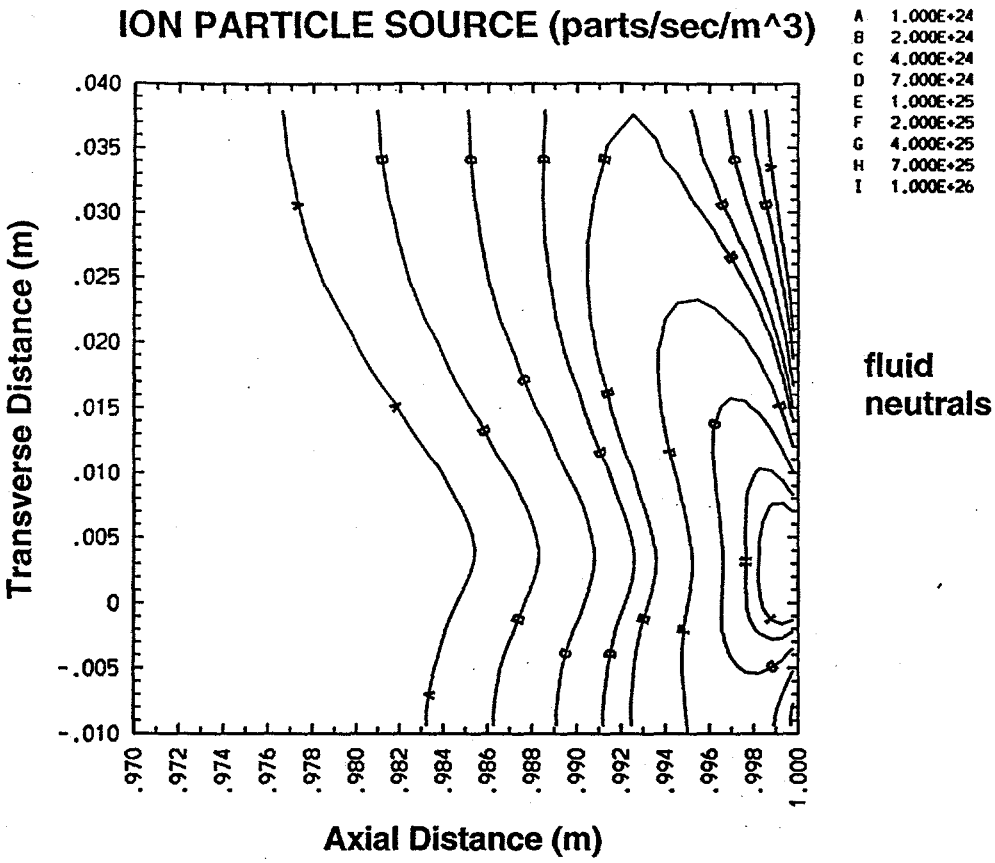
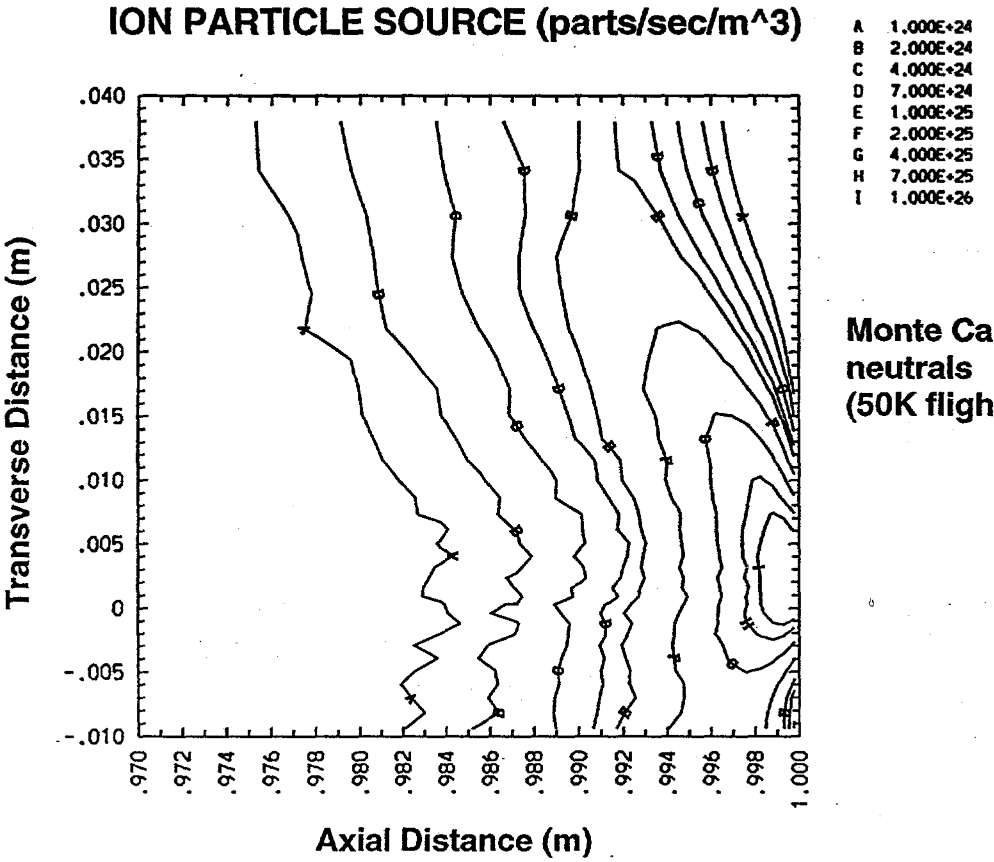


figure 2



fluid neutrals



Monte Carlo neutrals (50K flights)

Figure 3

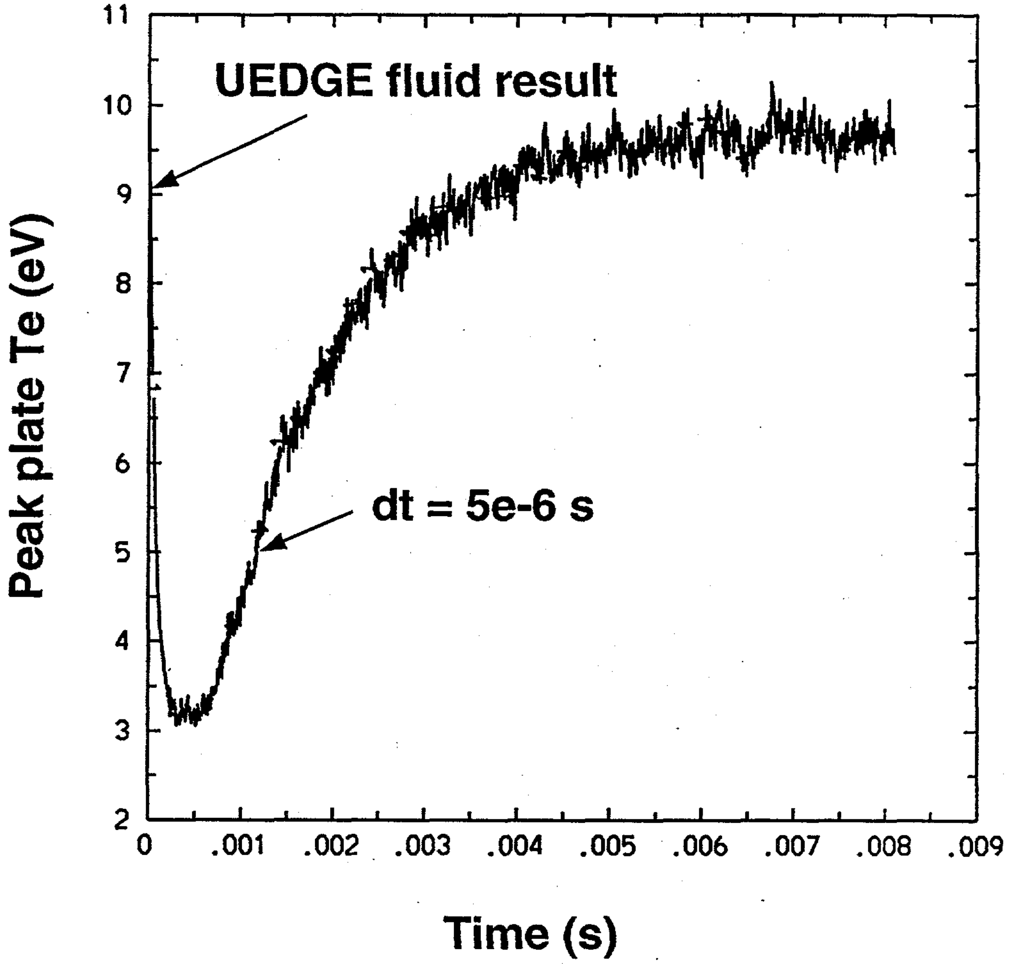

UEDGE fluid result
dt = 5e-6 s
Peak plate Te (eV)
Time (s)
11
10
9
8
7
6
5
4
3
2
0
.001
.002
.003
.004
.005
.006
.007
.008
.009

Figure 4

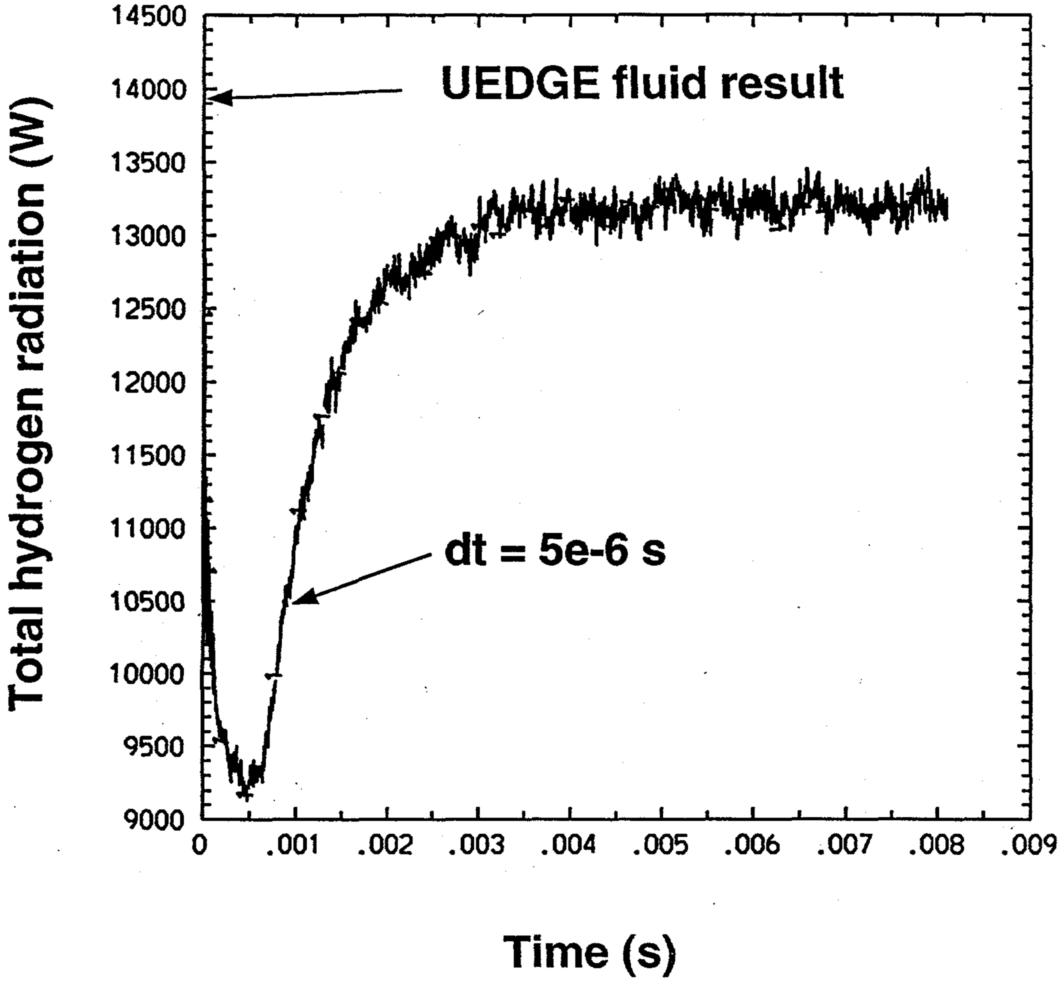
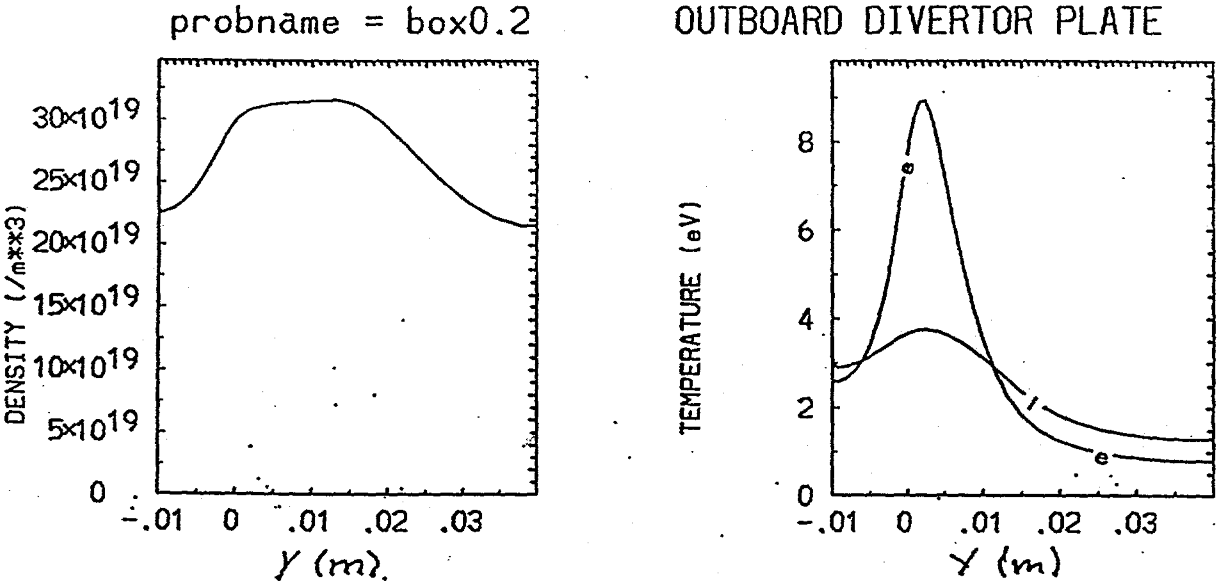

14500
14000
13500
13000
12500
12000
11500
11000
10500
10000
9500
9000
0
.001
.002
.003
.004
.005
.006
.007
.008
.009
UEDGE fluid result
dt = 5e-6 s
Total hydrogen radiation (W)
Time (s)

Figure 5

Plate Profiles of Density and Te Show Some Differences in Two Models

UEDGE Fluid Neutrals Model



EIRENE Monte Carlo Neutrals Model

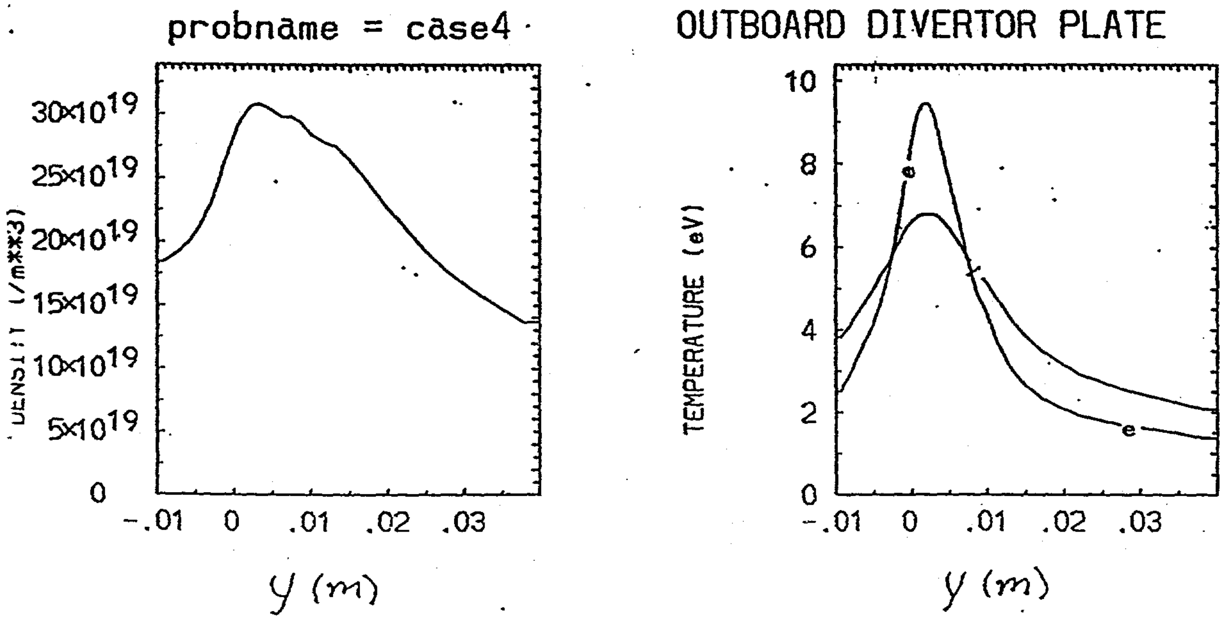
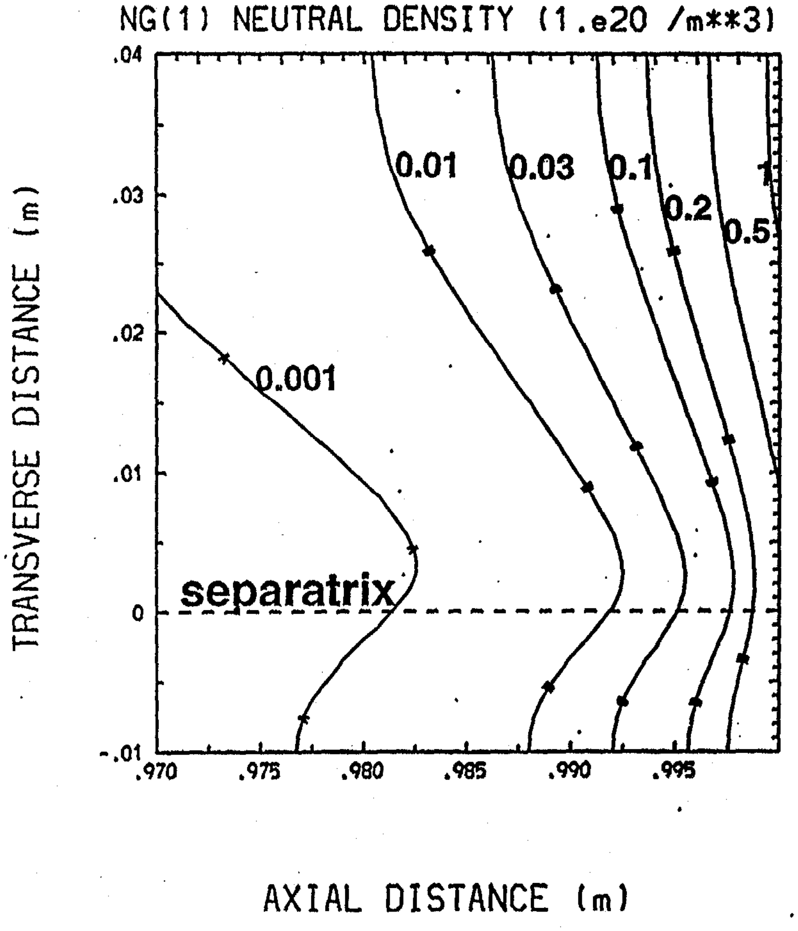


Figure 6

Atomic Densities Are Similar Away from Plate

UEDGE Fluid Neutral Density



EIRENE Atomic Density

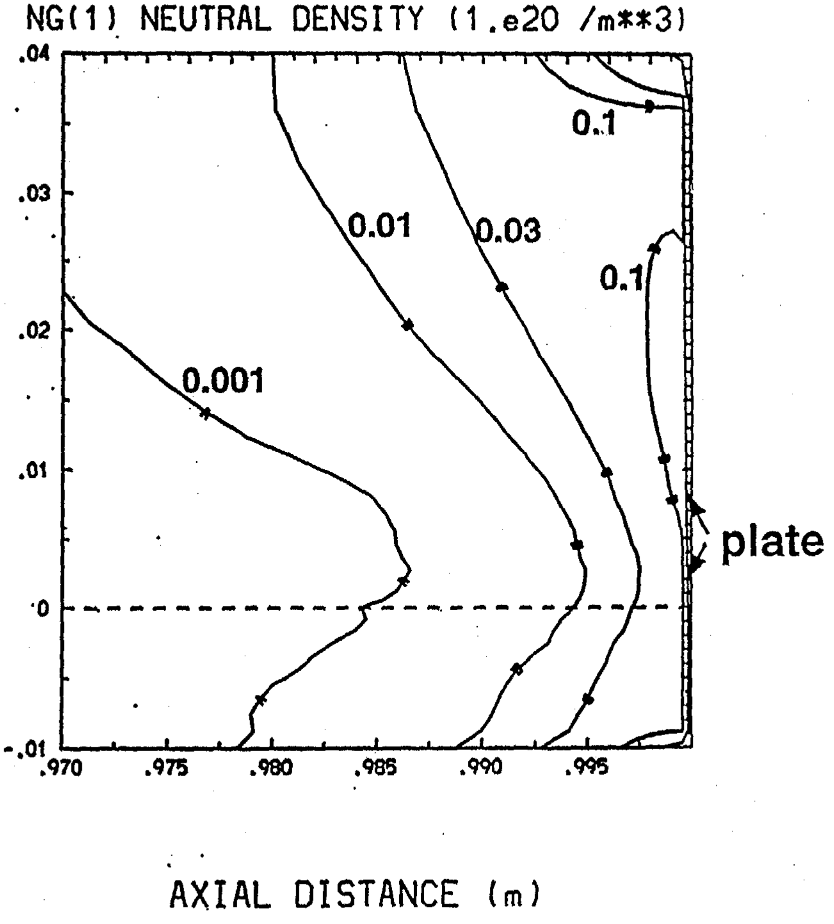


Figure 7

Final EIRENE Molecular Gas Density

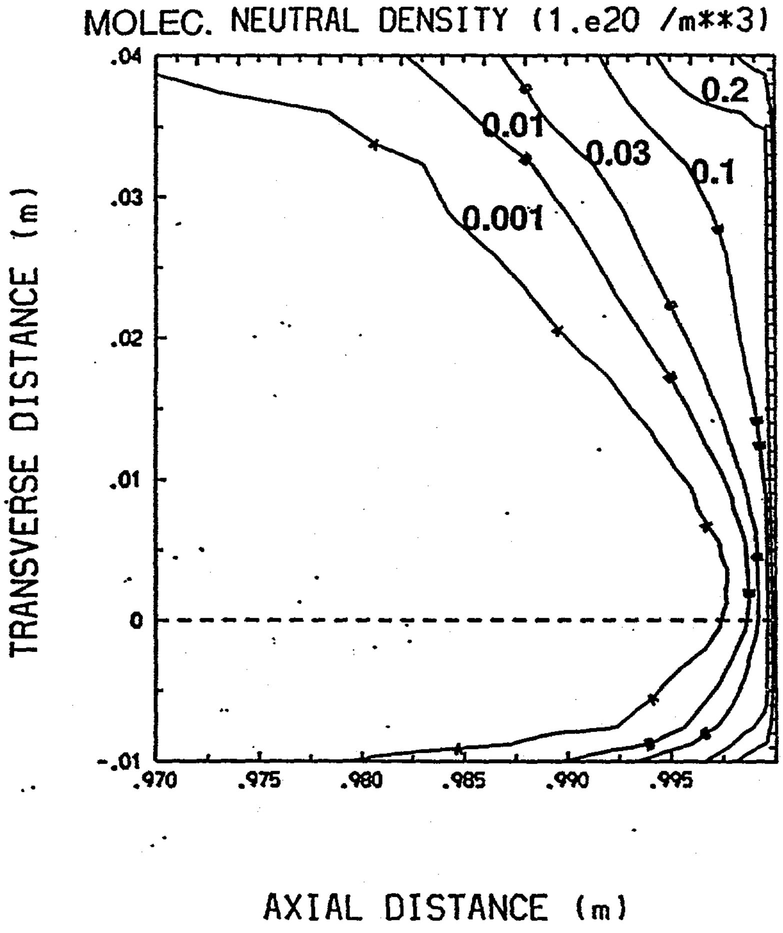


Figure 8

UEDGE/EIRENE Coupling Requires Small Timestep for Stability

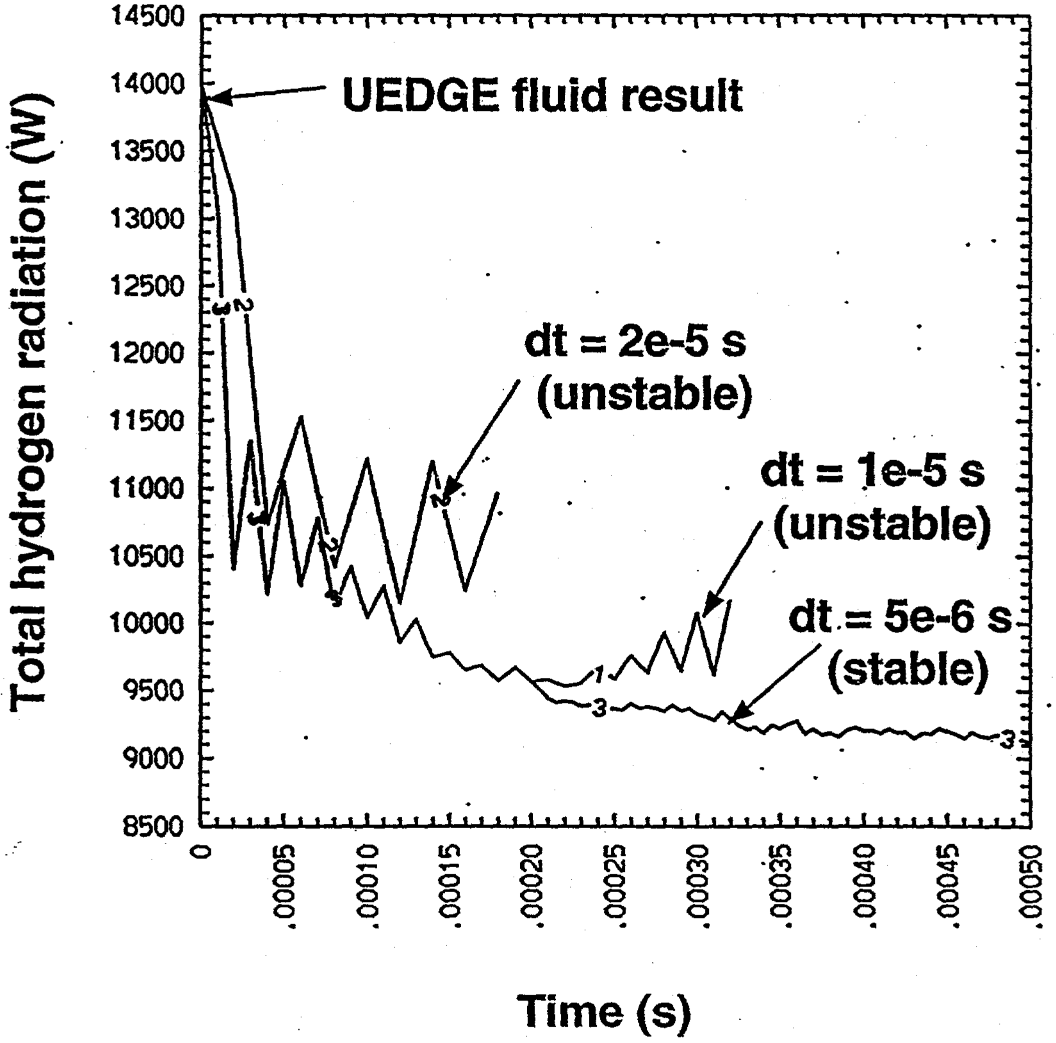
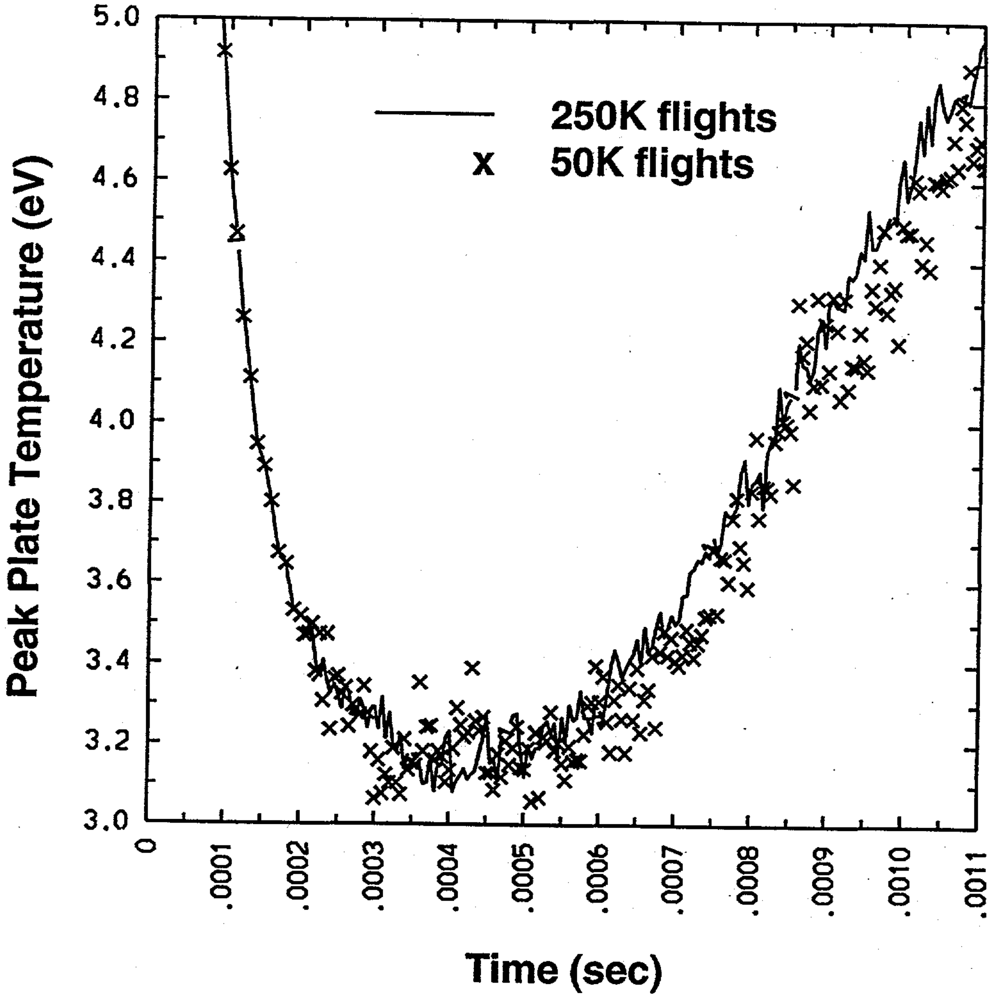
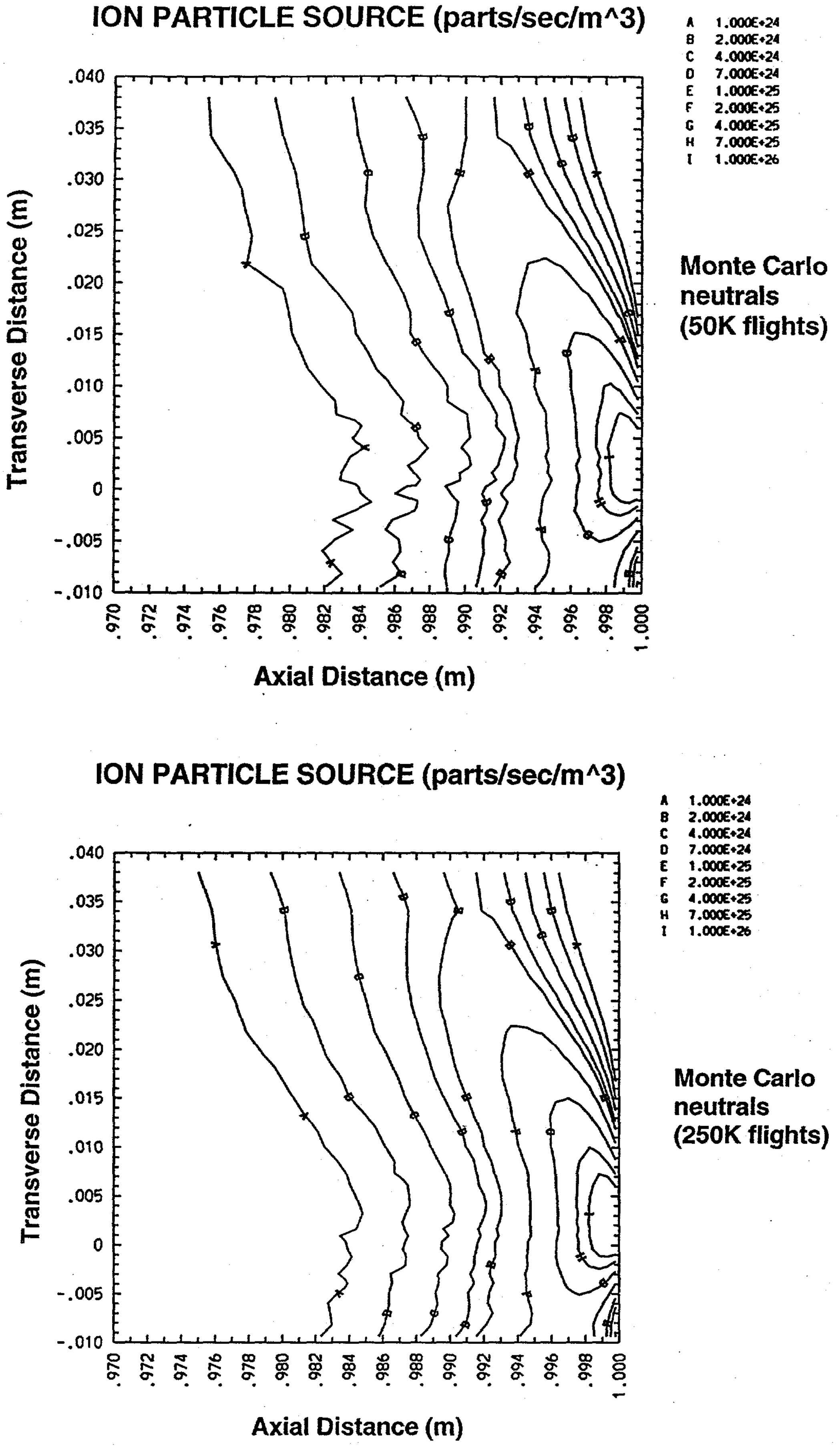


Figure 9



250K flights
x 50K flights
Peak Plate Temperature (eV)
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
0
.0001
.0002
.0003
.0004
.0005
.0006
.0007
.0008
.0009
.0010
.0011
Time (sec)

Figure 10



Monte Carlo neutrals (50K flights)

Monte Carlo neutrals (250K flights)

Figure 11