

# Monte Carlo impurity studies of carbon dynamics in the DIII-D divertor and scrape-off layer

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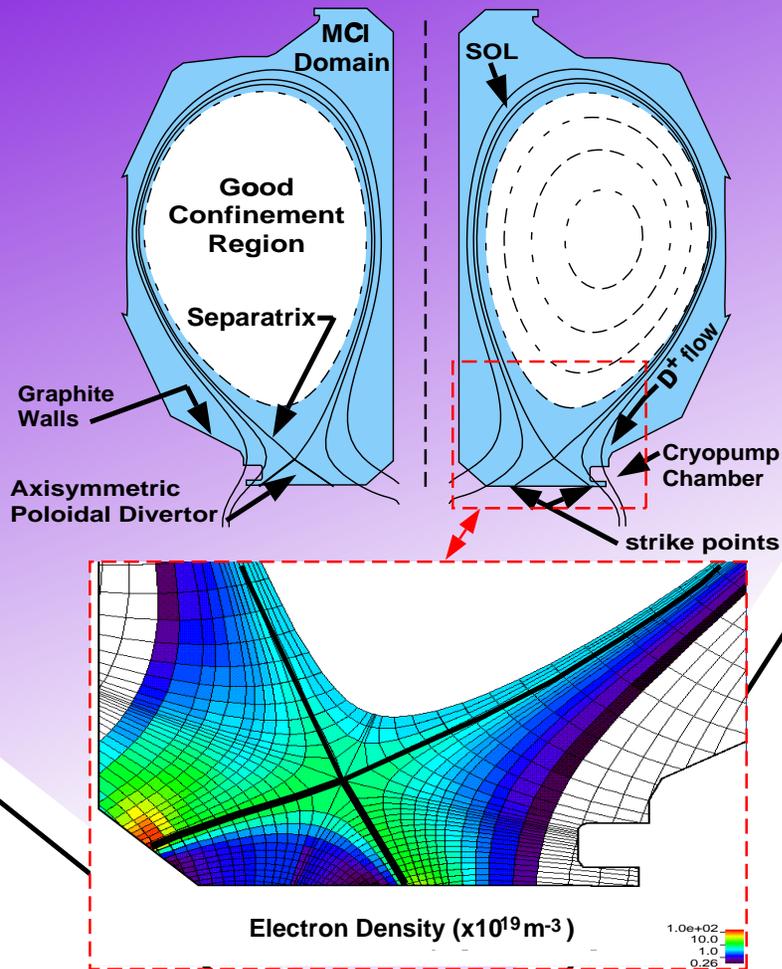
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**Monte Carlo Impurity Studies of Carbon Dynamics  
in the DIII-D Divertor and Scrape-off Layer<sup>1</sup>**

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Ridge National Laboratory — In DIII-D measured sources of carbon  
influx in the divertor have decreased with time and the number of  
boronizations. Over this same period the plasma core carbon content has  
essentially remained constant. In order to better understand these ob-  
servations the Monte Carlo Impurity (MCI) code is being used to study  
carbon sputtering and transport from the DIII-D divertor and wall. A  
comparison with spectroscopic measurements is also being made. Initial  
results show that standard chemical sputtering models yield too much  
carbon radiation in the DIII-D divertor and are unable to reproduce  
the observed carbon source variation. By spatially reducing chemical  
sputtering yields to simulate the effect of boron migration over a series  
of plasma discharges we obtain more realistic levels of carbon radiation  
in the divertor but can not yet explain a constant core carbon content.  
Details of these studies will be presented and preliminary results from  
wall source simulation will be discussed.

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- Prefer Oral Session  
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Special instructions: DIII-D Poster Session 2, immediately following WP West

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# Motivation

## Does chemical sputtering contribute significantly to the core carbon density?

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- In DIII-D there is current very little evidence of chemical sputtering in the divertor region:
  - Strong CD bands were observed in the divertor prior to boronization but have become very weak with addition multiple boron layers over the last few years
  - Over the same period carbon emissions in the divertor have dropped significantly suggesting a reduction in the local carbon source
- While the carbon density in the divertor has fallen, the core carbon content has generally remained constant or increased slightly:
  - Does this imply that the core carbon comes predominantly from wall sources which are unaffected by boron, or
  - Is it possible that chemically sputtered carbon from the divertor does not contribute significantly to the core
- The DIII-D Monte Carlo Impurity (MCI) code is being used to better understand how carbon gets into the core from various locations in the divertor and whether chemical versus physical sputtering sources are more effective in fueling the core
  - Initial results indicate that atomic carbon, due to physical sputtering, has a higher probability of reaching the core than carbon resulting from chemical sputtering with its associated molecular hydrocarbon dissociation/transport

# Monte Carlo Impurity code Overview

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## Background plasma solution

- Supplied by fluid codes such as UEDGE.

## Impurity transport physics

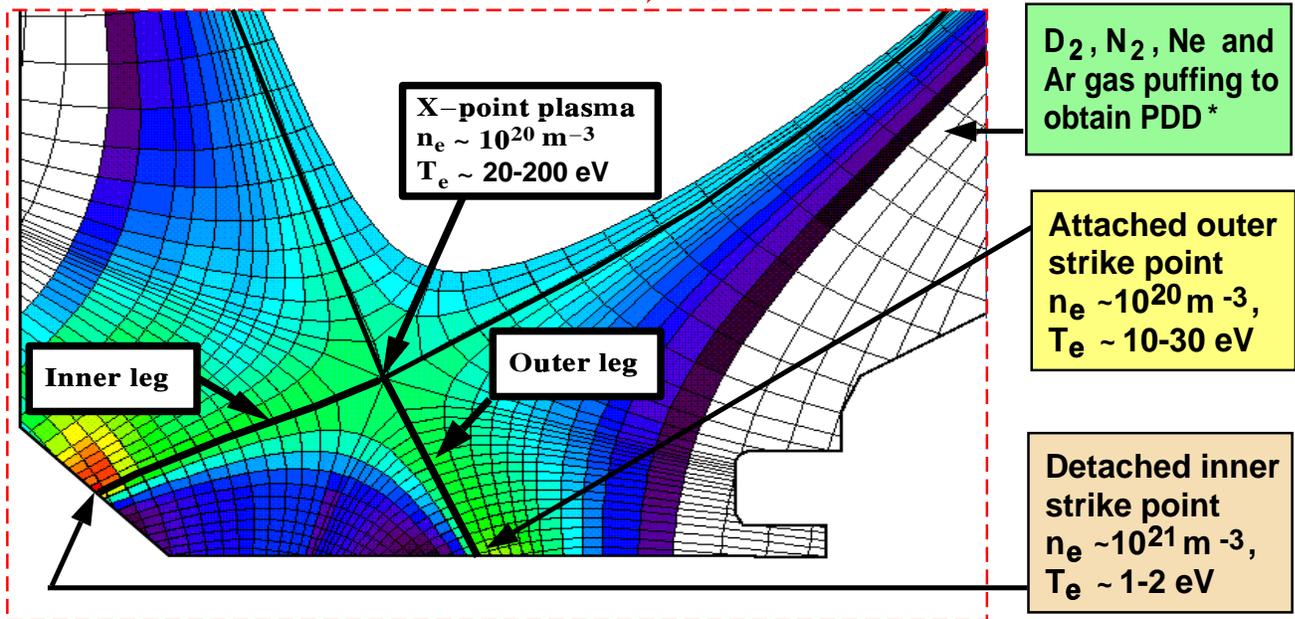
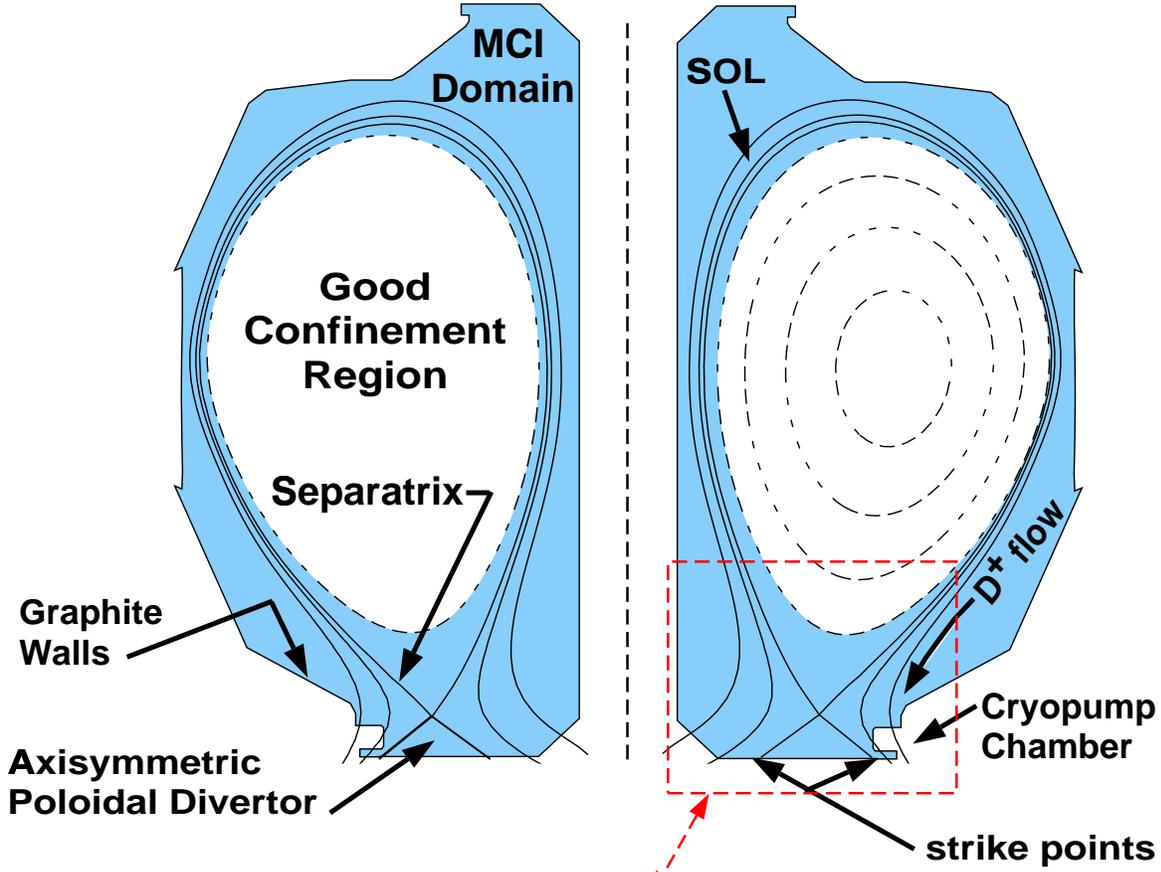
- Forces identical to those used in fluid codes:
  - Classical parallel ion transport that accounts for:
    - collisional diffusion along field lines
    - ion and electron thermal gradients
    - drag due to background ion flows, and
    - parallel electric fields
  - Perpendicular ion transport is anomalous

## Carbon source physics

- Sputtering probability calculated on each plasma facing surface using the local background plasma ion flux:
  - Six physical sputtering options.
    - Atomic carbon launched with a Thompson distribution.
  - Chemical sputtering prescribed by the Roth and Garcia-Rosales (RG-R) model [1] or the Roth98 PSI model.
    - Methane dissociation via Ehrhardt and Langer.

[1] J. Roth and C. Garcia-Rosales, Nucl. Fusion 36 (1996) 1647.

# The MCI computational domain extends from the 95% flux surface to the DIII-D walls



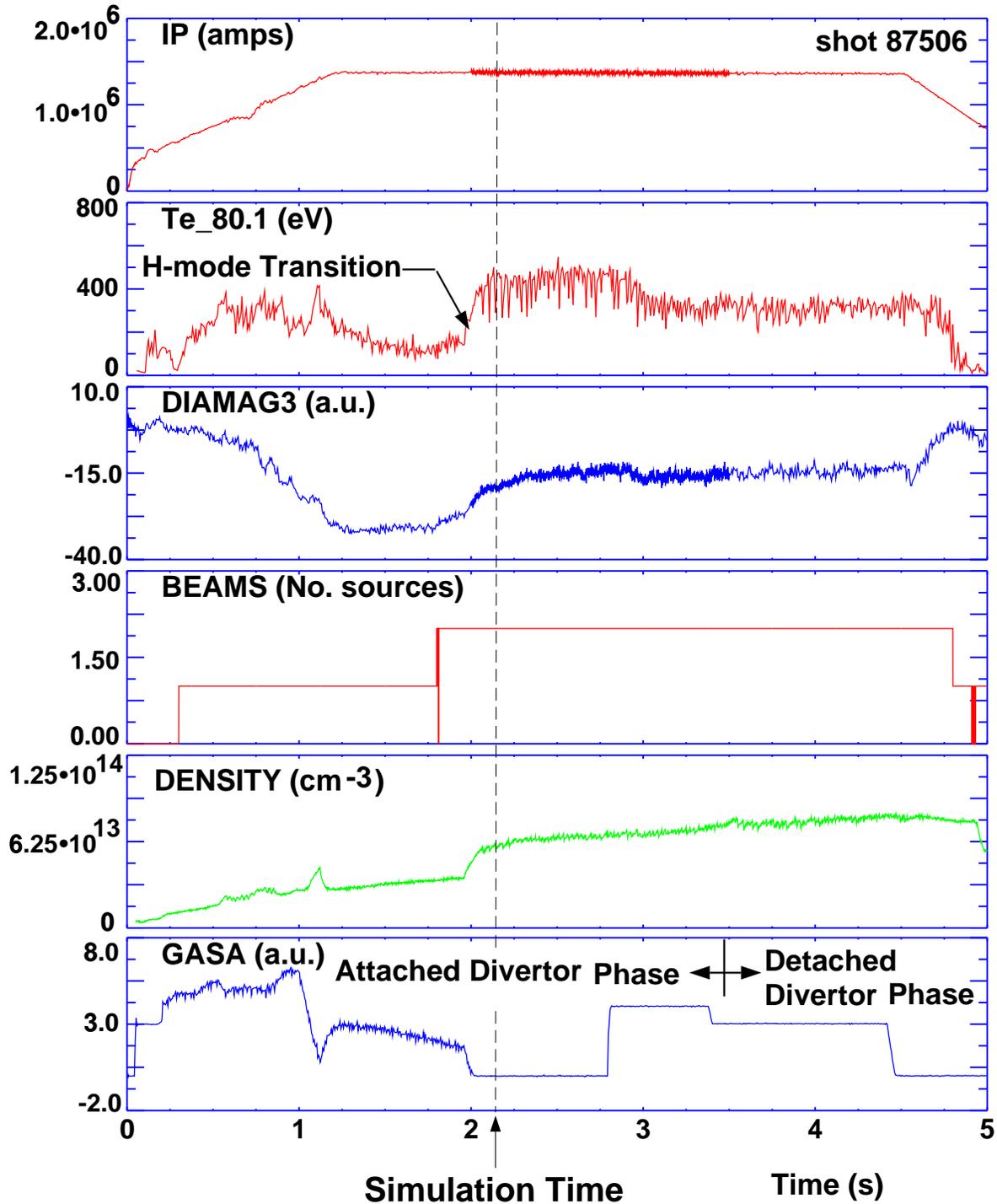
Electron Density ( $\times 10^{19} \text{ m}^{-3}$ )



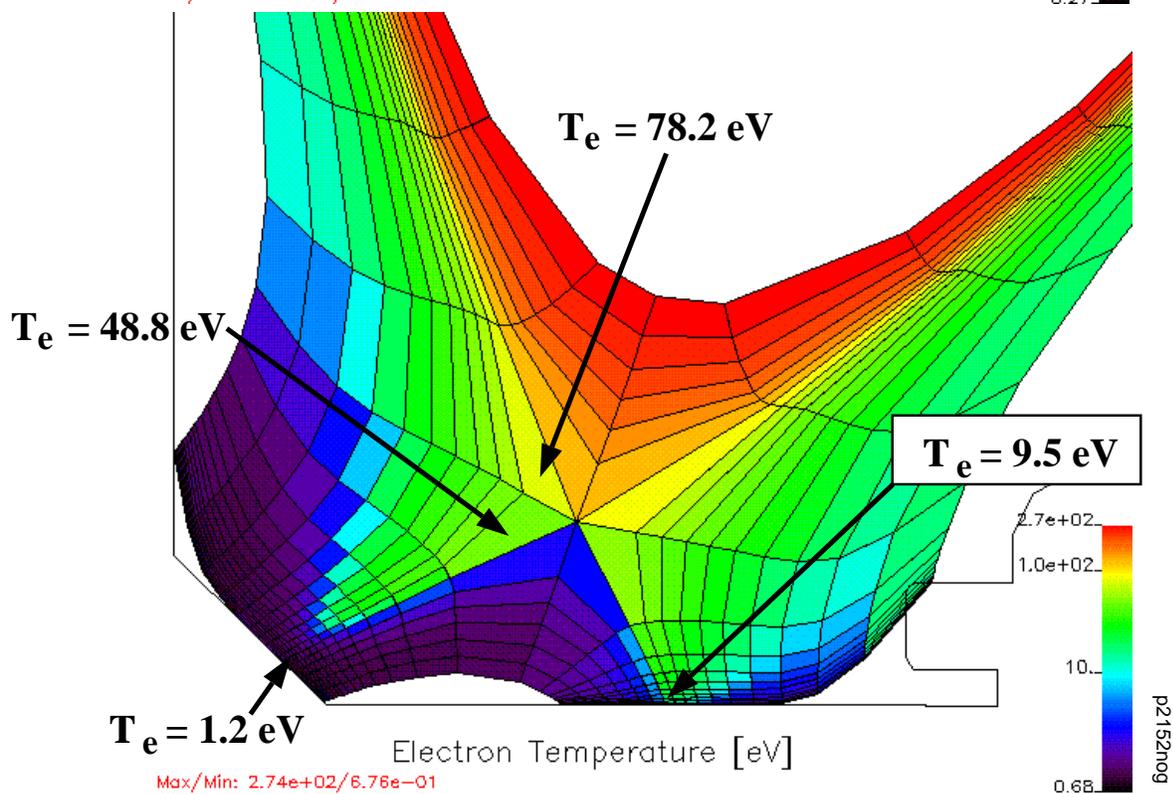
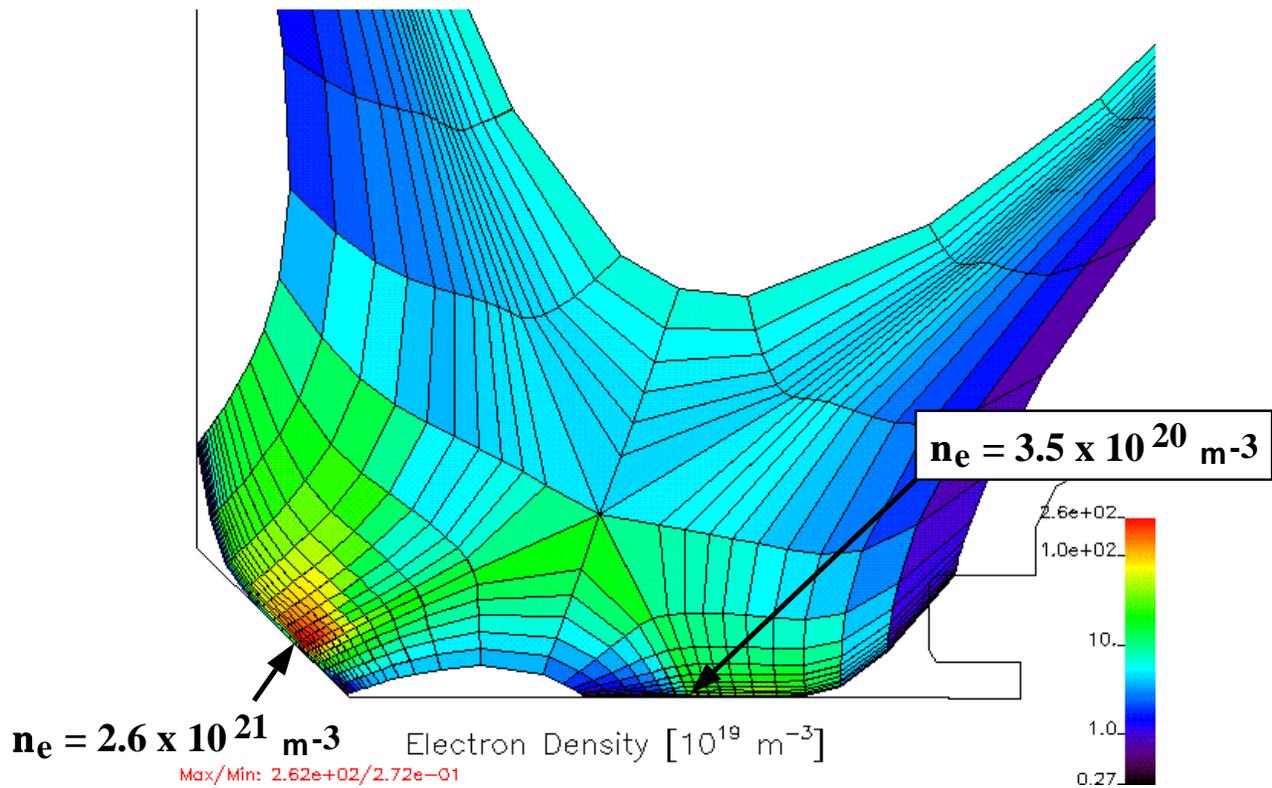
\* PDD => Partially detached divertor



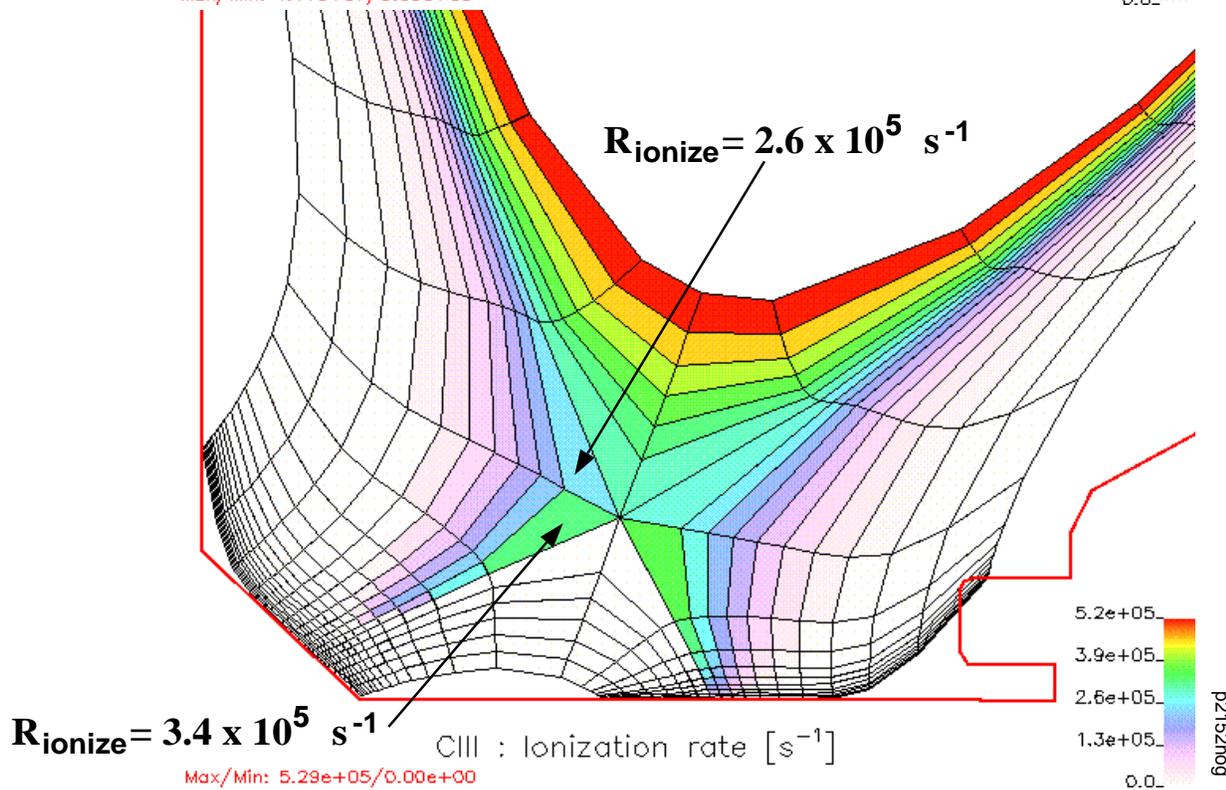
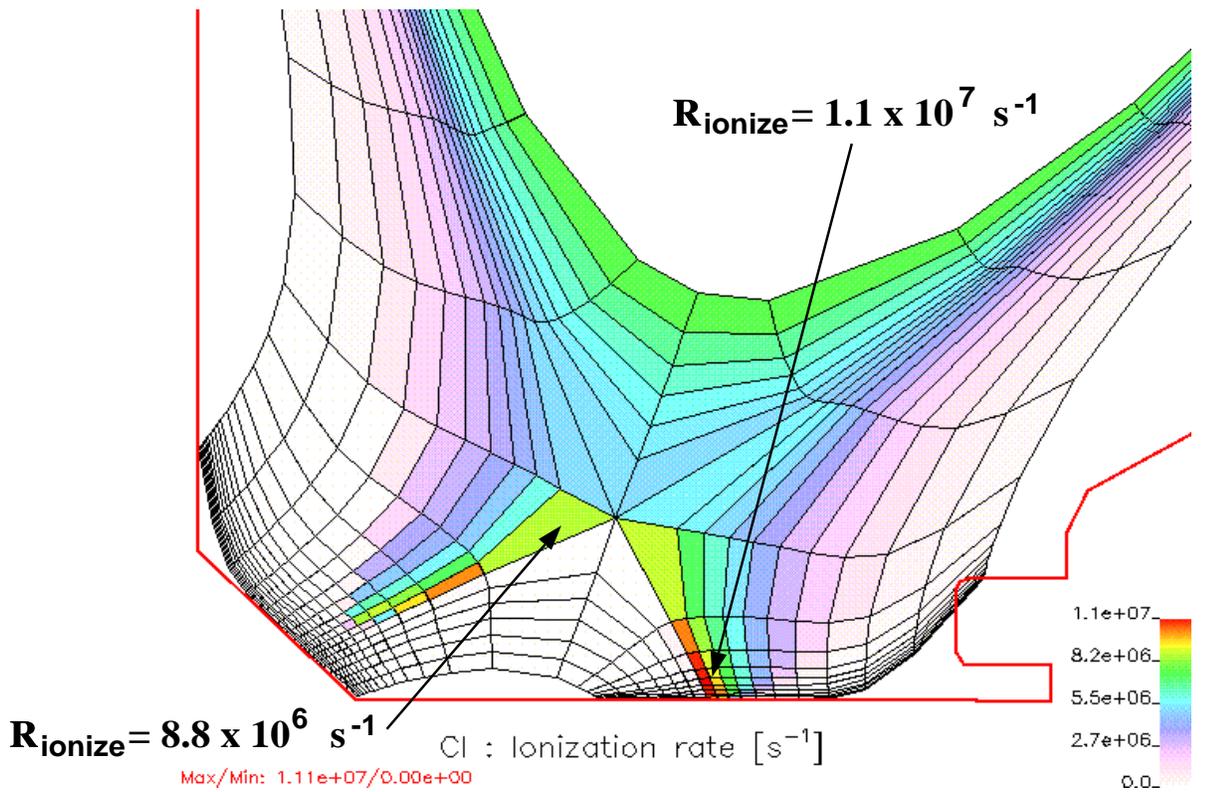
# Simulations done with attached outer strike points provide good physics benchmarks



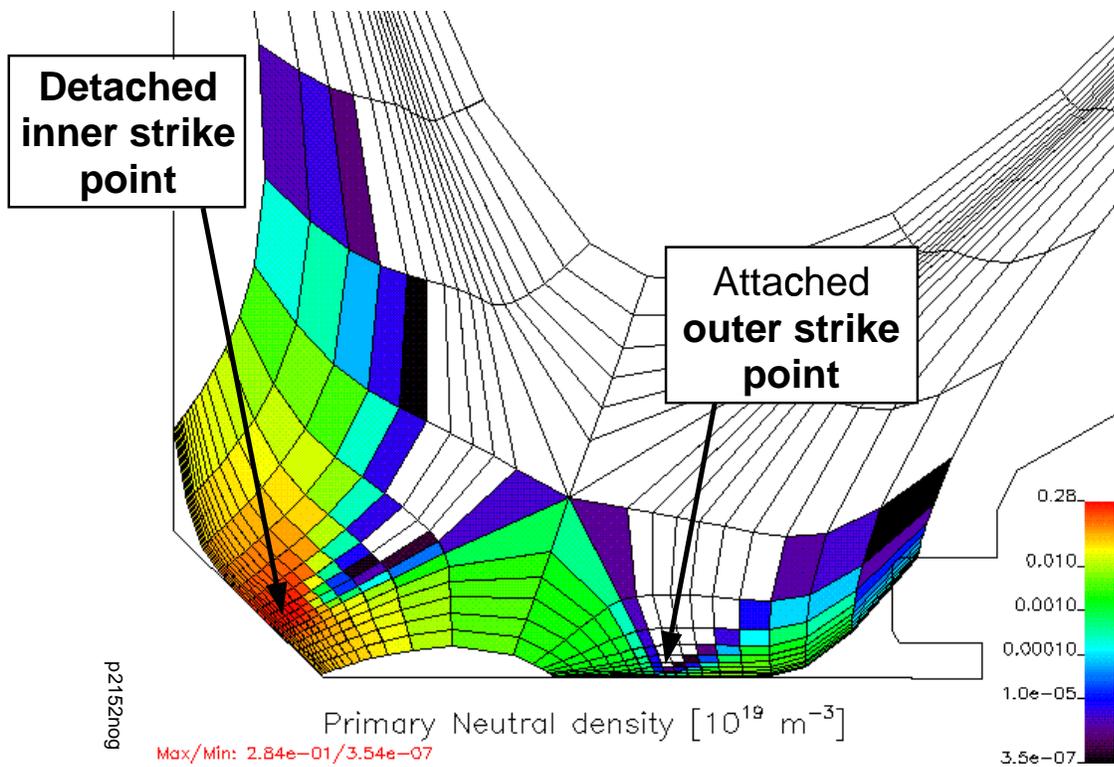
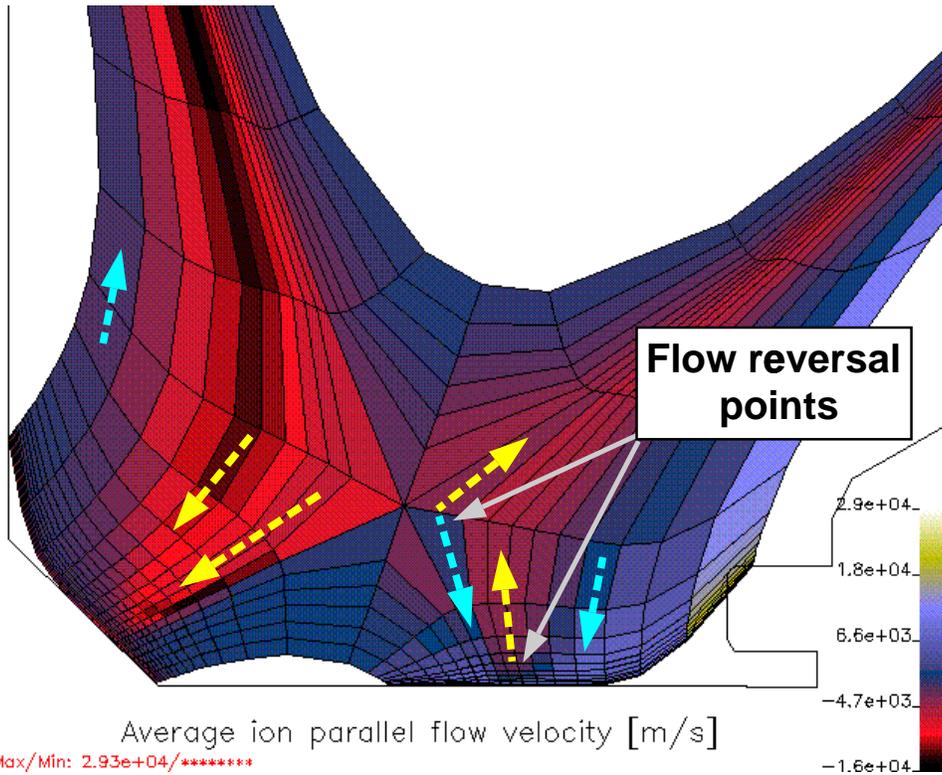
# Fluid codes are used to calculate the MCI background plasma



# Cell specific atomic data is processed using the fluid background plasma



# UEDGE solution has large flow reversal region at outer strike point with a detached inner leg

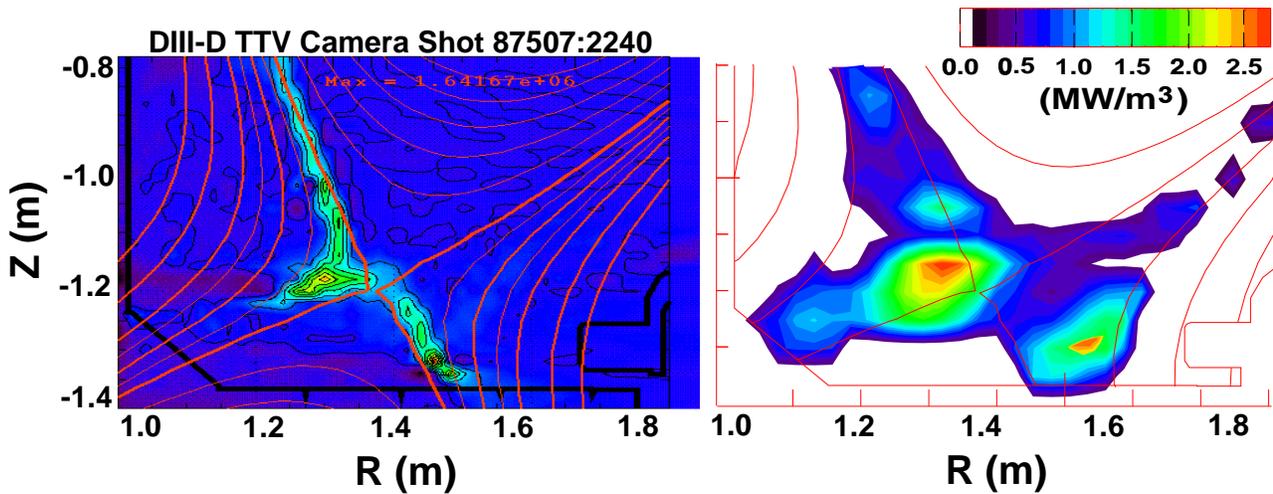


# MCI's sputtering and transport models are benchmarked against measured emissions

## Measured 2D spatial emissions

TTV carbon line radiation

Bolometric total radiated power



CIII ( $\lambda = 465$  nm) emission

Shot 87507,  $t = 2240$  ms

- Qualitatively and quantitatively compared to MCI's simulated 2D line radiation and total radiated power.

## Spatially integrated total radiated power

- Quantitatively compared to MCI's total radiated power integrated over the divertor and SOL region.

# MCI simulation results are particularly sensitive to the carbon sputtering physics

Goal -> Benchmark sputtering models

$$Y_{\text{TOT}} = Y_{\text{PHY}} + Y_{\text{CHEM}}$$

- The total carbon sputtering yield ( $Y_{\text{TOT}}$ ) may depend on both physical and chemical sputtering processes.

Six physical sputtering models are used in MCI

Smith78

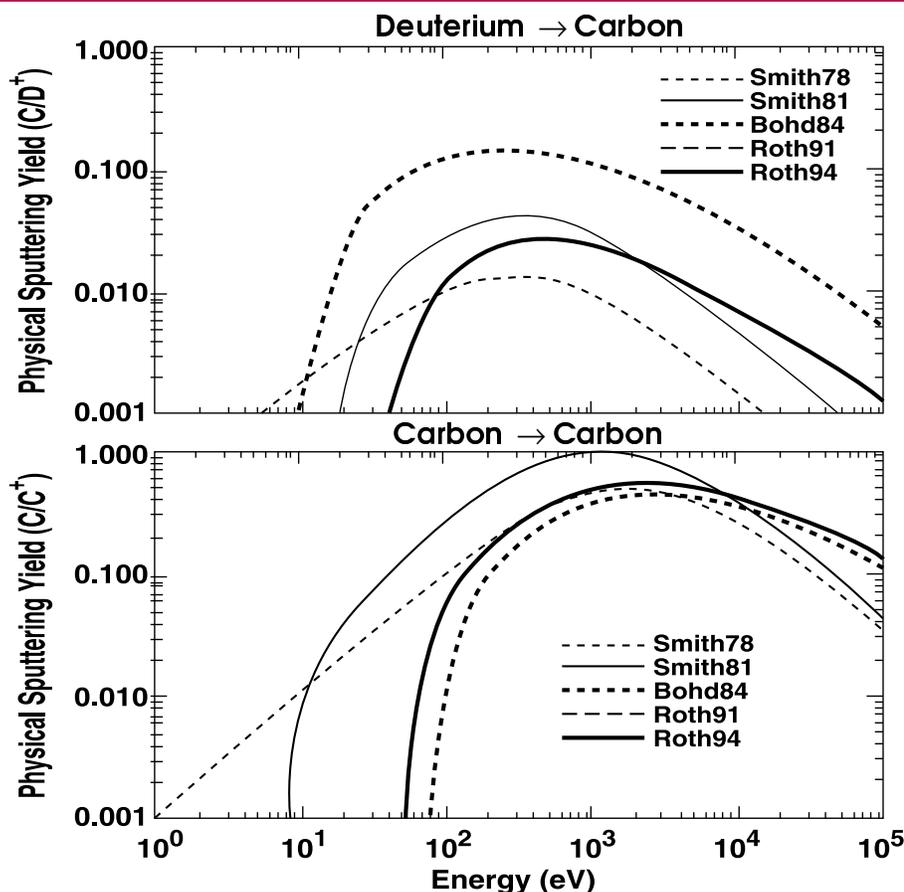
Smith81

Bohd84

Roth91

Roth94

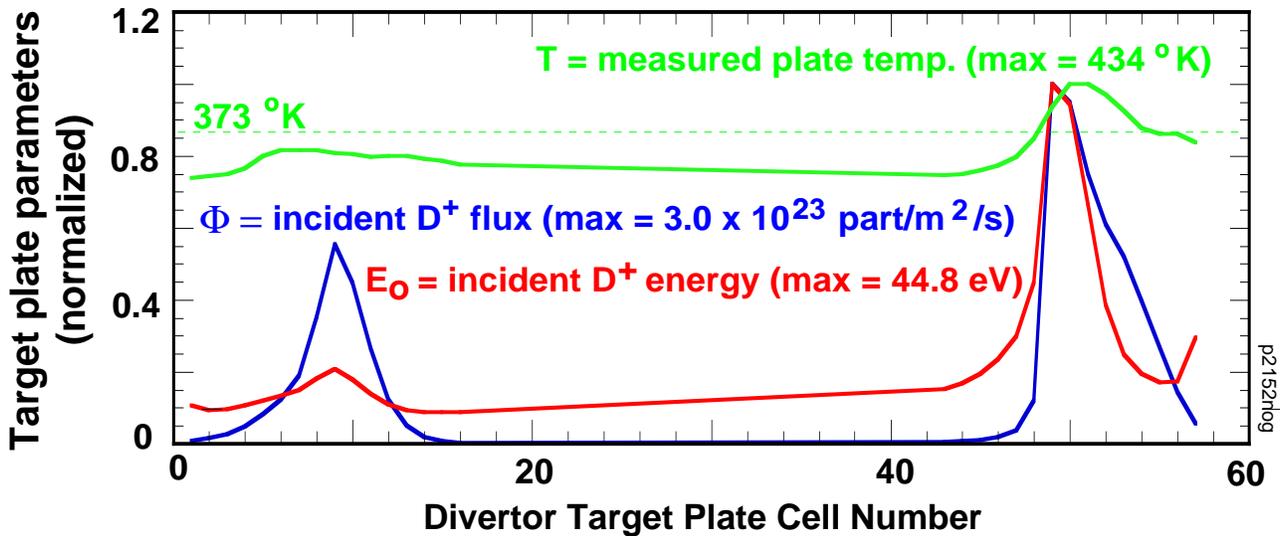
Y=Const.



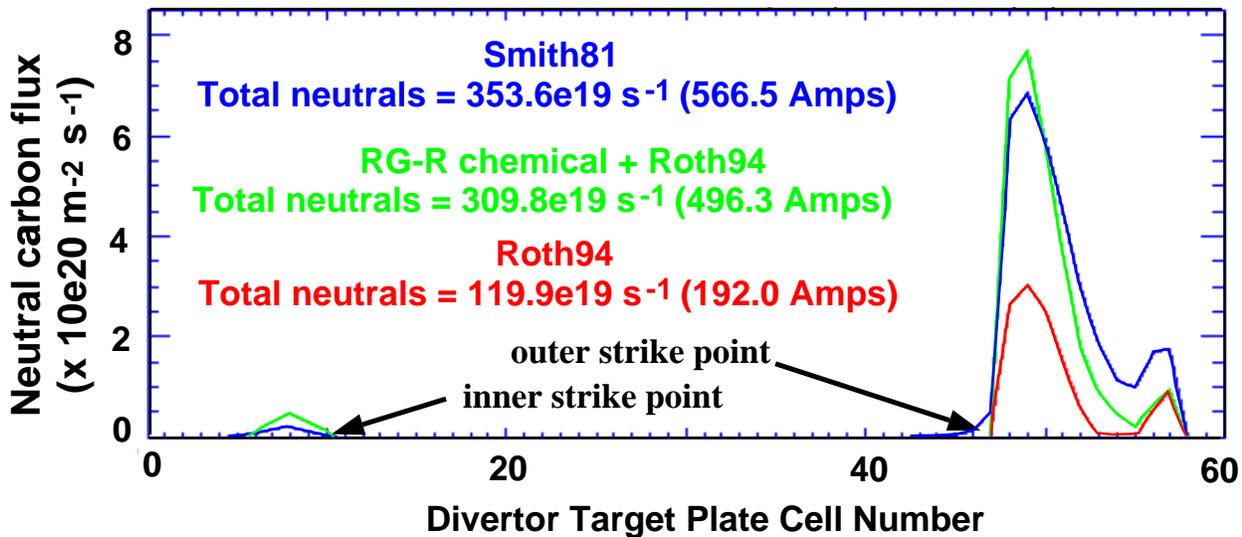
- Some models predict a two order of magnitude increase as the incident particle energy goes from 10 -> 100 eV.

# Excluding neutral flux contributions RG-R chemical sputtering produces about the same CI flux as the Smith81 model

Divertor target plate parameters used to calculate physical and chemical sputtering yields



Comparison between the RG-R chemical sputtering model, driven by a D<sup>+</sup> flux only, and two physical sputtering models



# Divertor + SOL carbon inventory and radiated power increase with RG-R sources as compared to constant physical sputtering

Shot 87506, t = 2240 ms

measured divertor + SOL radiation:  $P_{carbon}^{div+SOL} = 1718 \text{ kW}$

Species	Inventory (x 10 <sup>17</sup> )	Fraction (%)	
CI	0.355	14.00	Total carbon influx = 31.5 A  Ave. carbon lifetime = 1.29 ms  Calculated $P_{carbon}^{div+SOL} = 258 \text{ kW}$
CII	0.362	14.27	
CIII	0.097	3.84	
CIV	0.086	3.38	
CV	0.709	27.99	
CVI	0.315	12.42	
CVII	0.610	24.10	
Total C	2.533		
CI	2.474	8.99	Total carbon influx = 2150.0 A  Ave. carbon lifetime = 0.21 ms  Estimated $P_{carbon}^{div+SOL} = 4110 \text{ kW}$
CII	2.829	10.28	
CIII	1.428	5.19	
CIV	1.150	4.18	
CV	8.535	31.03	
CVI	3.717	13.51	
CVII	7.378	26.82	
Total C	27.510		

p2177nog

- Changes in the radial profile of the carbon source distribution affect the charge state balance but do not have a significant impact on the 2D spatial distribution of the carbon radiation.

# Uncertainties are found in the carbon source physics when measured target plasma parameters are used in MCI

Shot 87506, t = 2240 ms  
 measured divertor + SOL radiation:  $P_{carbon}^{div+SOL} = 1718$  kW

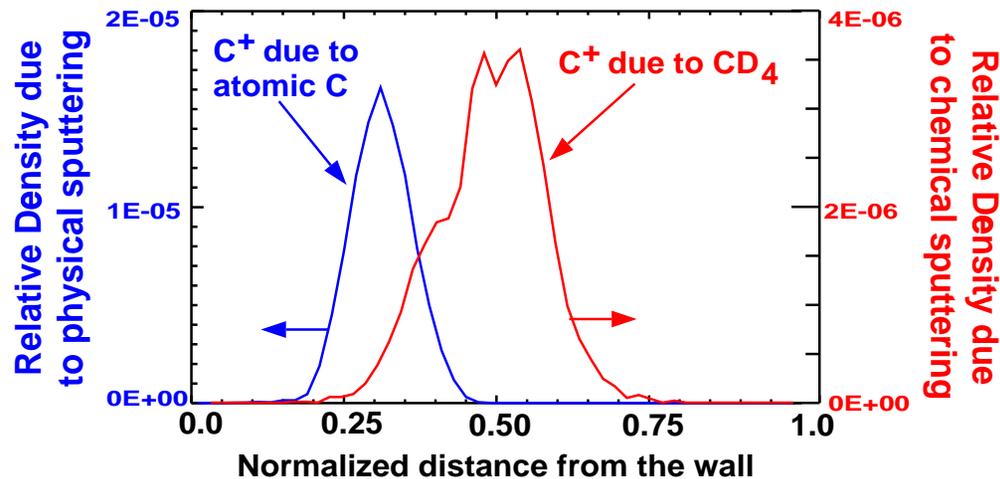
MCI simulation results using  
 measured target plate plasma

Phys. sputtering source model	Chem. sput.	Inventory (x 10 <sup>17</sup> )	Rad. P. (kW)	C Source (A)	
Roth94	RG-R	15.270	1690	496.3	1.6% ↓
Smith78	RG-R	27.880	2862	533.5	
Smith81	RG-R	30.470	3467	1078.4	
Bohdansky84	RG-R	125.700	14190	4292.1	
Roth91	RG-R	16.630	1721	478.4	0.2% ↑
Y = 10 <sup>-3</sup>	RG-R	16.000	1573	225.1	8.4% ↓
Roth94	none	2.633	384	192.0	
Smith78	none	9.822	1096	229.1	
Smith81	none	10.690	1344	566.5	21.8% ↓
Bohdansky84	none	87.510	9961	2637.9	
Roth91	none	2.353	346	180.8	
Y = 10 <sup>-3</sup>	none	2.768	272	31.6	

p2177nog

- The Roth91 physical sputtering model driving the RG-R chemical sputtering source gives the best match between the measured total power and the simulated total power.

# RG-R and Roth98 chemical sputtering result in too much radiation when neutral flux contributions are included



CD<sub>4</sub> molecules from chemical sputtering result in deeper carbon penetration, increased carbon inventories and more radiated power

## Experimental results

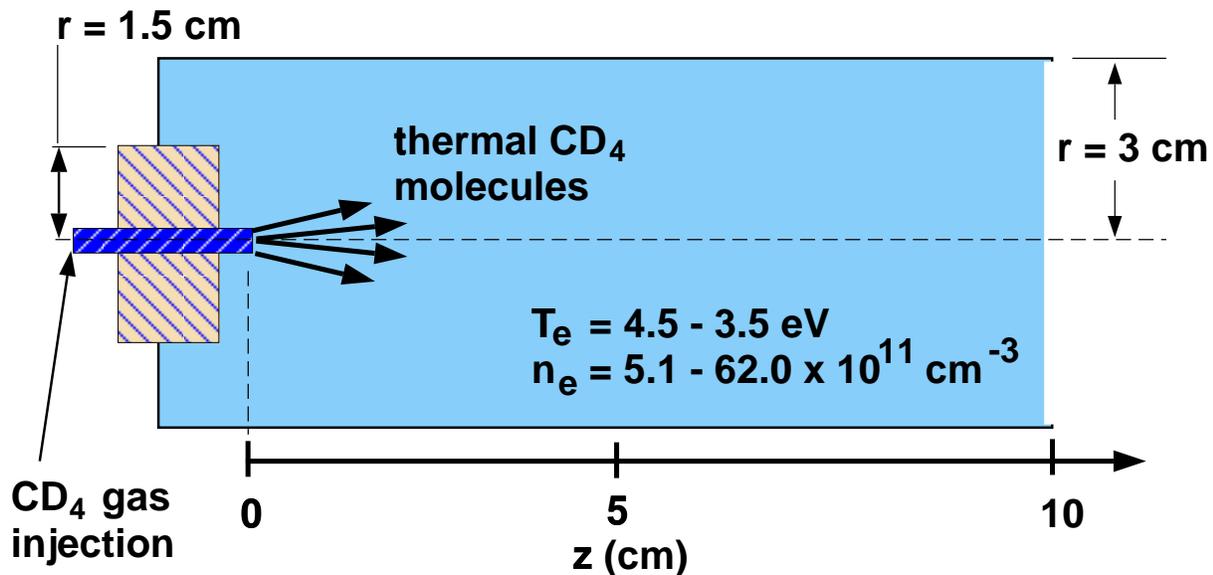
Shot 87506, t = 2240 ms: measured divertor + SOL radiation:  $P_{carbon}^{div+SOL} = 1718$  kW

## MCI results

	Phys. sput. model	Chem. sput.	Inventory (x 10 <sup>17</sup> )	C Source (A) from D+ only	Rad. P. (kW)	Est. Rad. P. w. neut. (kW)	$\frac{\Delta P}{P}$
	Roth94	Roth98	33.45	798.6	3398	4587	↑ 167%
	Roth94	RG-R	15.27	496.3	1690	2113	↑ 23%
	Roth94	none	2.63	192.0	384	442	↓ 74%
p2177nog	Smith81	none	10.69	566.5	1344	1545	↓ 10%

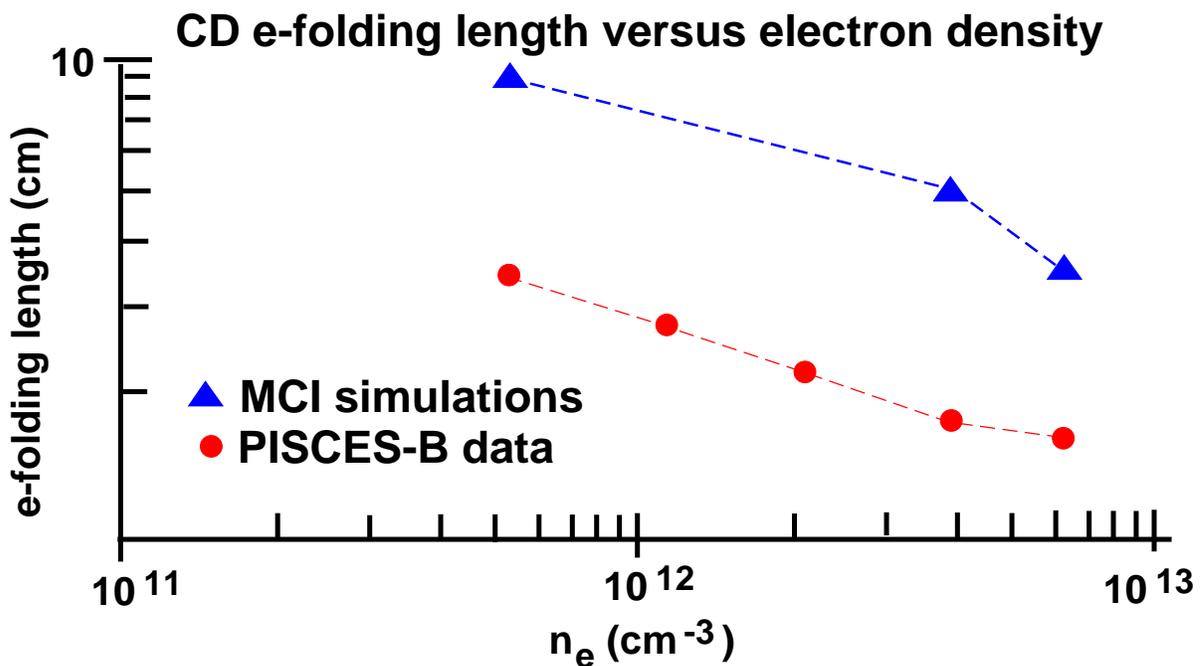
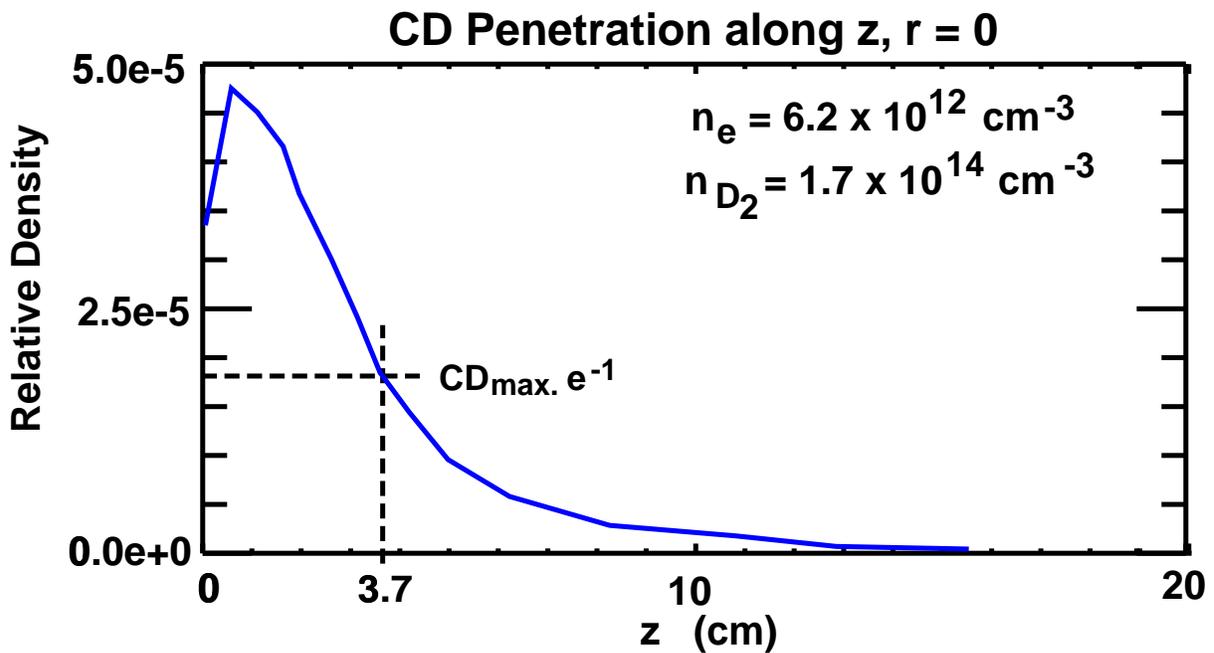
# MCI's Molecular dissociation and transport models are validated with PISCES data

- Linear devices such as PISCES-B at UCSD are ideal for validating the detailed physics modules used in MCI



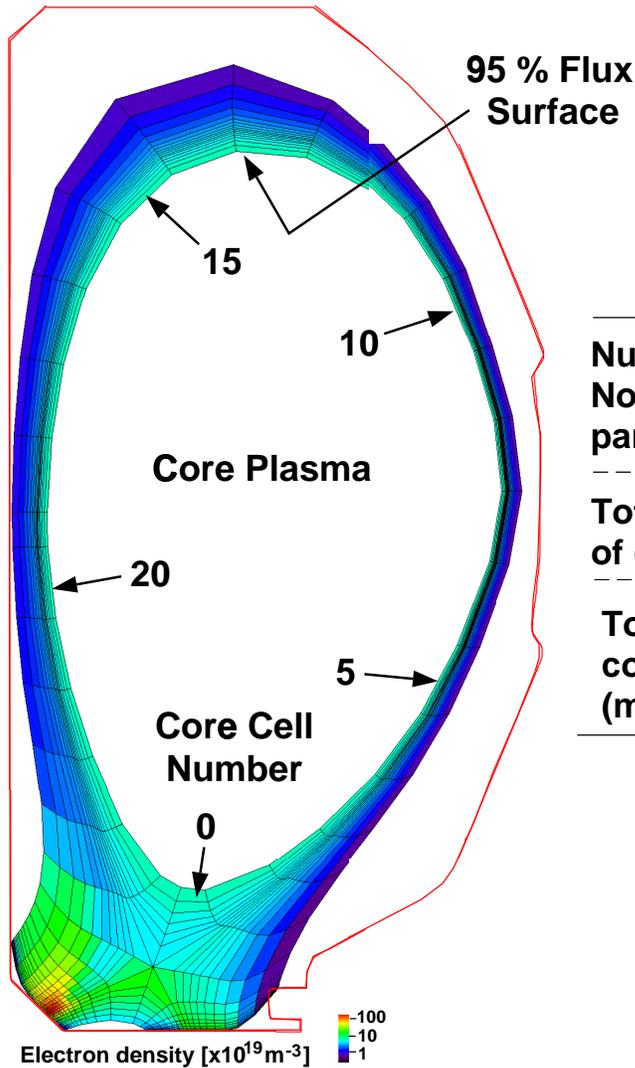
- Ehrhardt and Langer [PPPL-2477, Sept. 1987] methane dissociation, with MCI transport physics, is being validated using data from PISCES-B where the:
  - parallel ion and electron thermal gradient forces are relatively weak compared to tokamak divertors
  - neutral deuterium densities are large compared to the plasma density ( $1-1.75 \times 10^{14} \text{ cm}^{-3}$ )
  - $E_{||} = 1.75-2.25 \text{ V/m}$  and  $D^+$  flow ( $v = 10.1-11.4 \text{ km/s}$ ) are directed toward the methane source
  - $D_{||} \gg D_{\perp}$ , radial transport is dominated by neutral collisions and molecular gyroradius effects

# MCI's Molecular dissociation and transport models are being validated with PISCES data



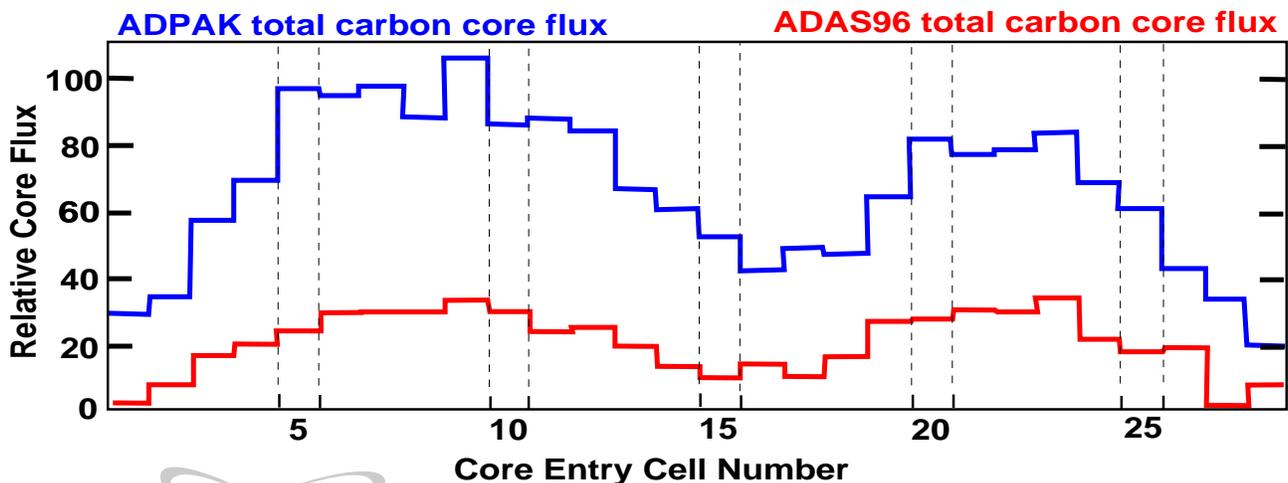
- A 3D neutral collision and a velocity diffusion model are being implemented in MCI which should significantly reduce the CD penetration depth

# The average core carbon density is a factor of 7 lower with ADAS96 versus ADPAK data



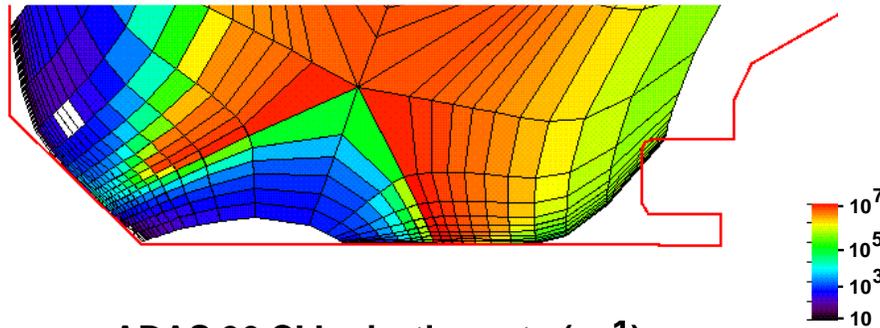
	ADPAK	ADAS96
Number of Non-recycling particles	443,292	1,563,528
Total Number of core entries	3,670	1,200
Total carbon core density ( $\text{m}^{-3}$ )	9.87e17	1.36e17

Integrated carbon sputtering current =  $3.3\text{e}21 \text{ s}^{-1}$  (566.5A)

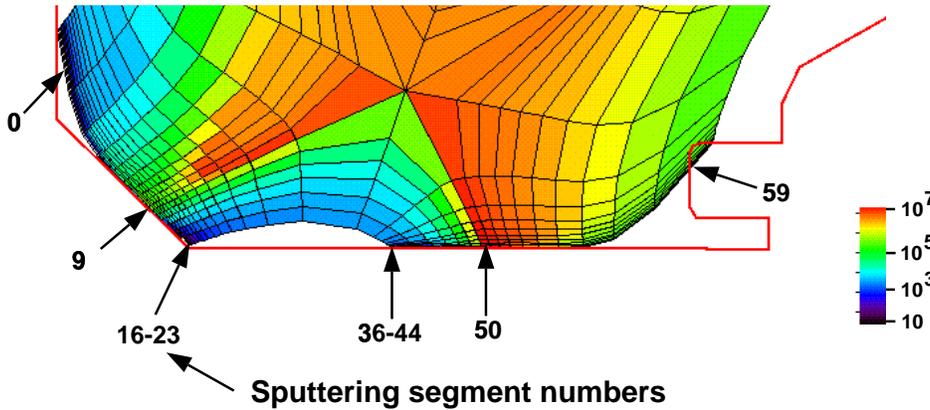


# Most of the core carbon due to divertor sources originates from low sputtering yield regions

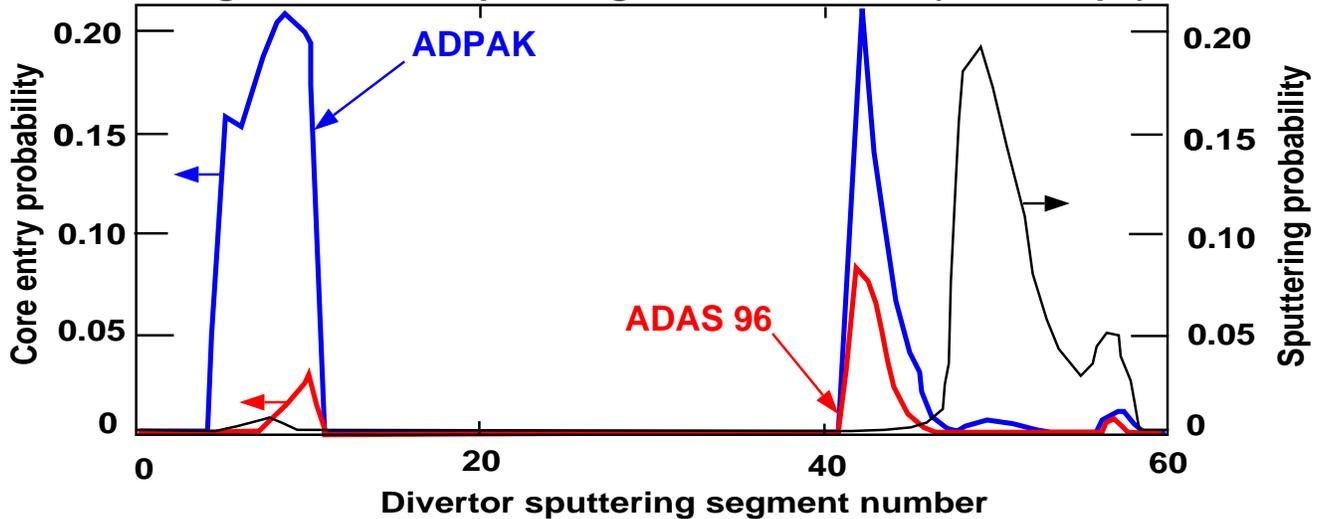
ADPAK CI Ionization rate ( $s^{-1}$ )



ADAS 96 CI Ionization rate ( $s^{-1}$ )

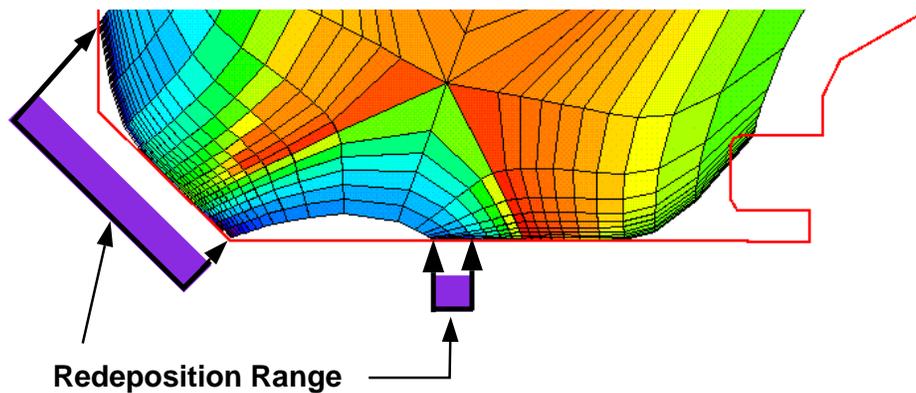


Integrated neutral sputtering rate =  $3.34e21$   $s^{-1}$  (566.5 Amps)



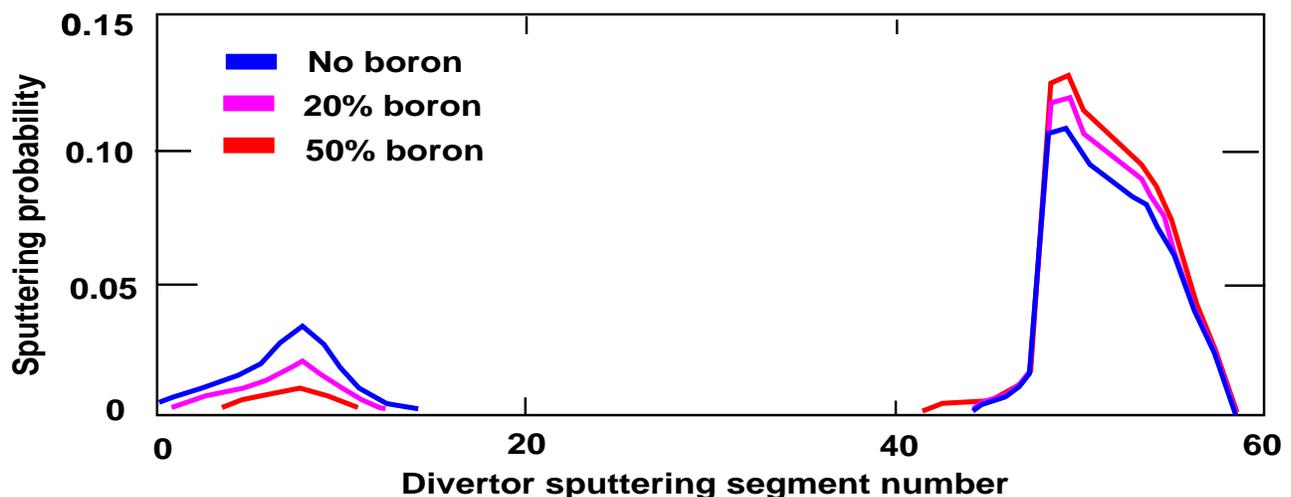
# Boron reduces the chemical sputtering source originating from the divertor targets without affecting physical sputtering

- A non-uniform boron layer is simulated in MCI in order to model the effect of erosion near the outer strike point and redeposition near the inner strike point.



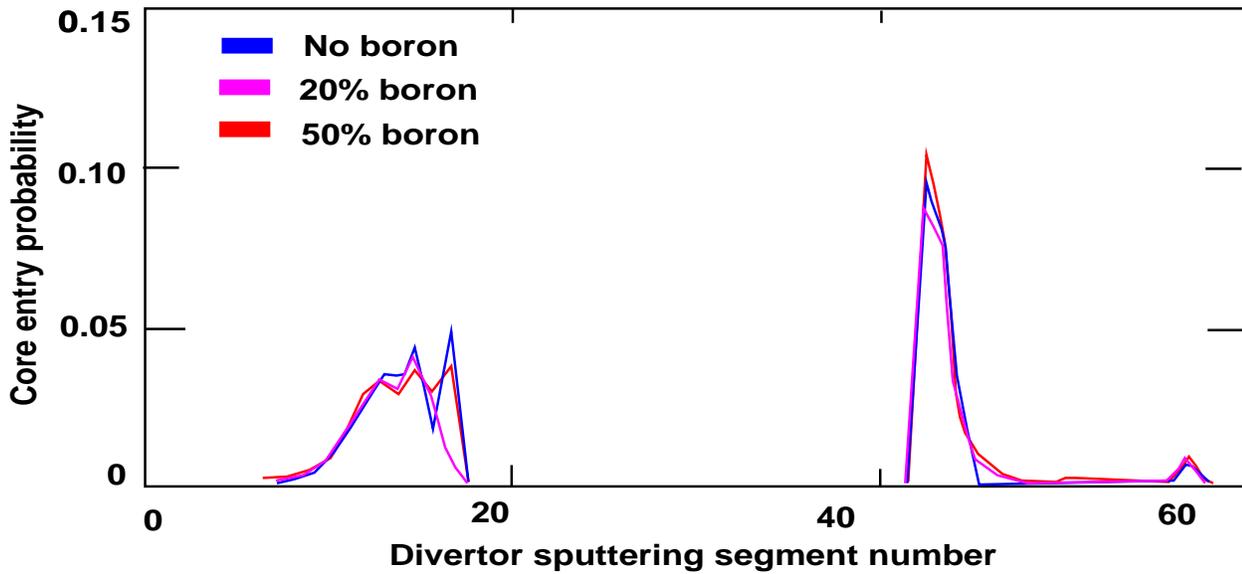
- Three mixtures of boron and carbon: no boron, 20% boron, and 50% boron, are compared in the MCI simulations. The mixed layer is only applied to the redeposition range shown above.

Sputtering probability from each divertor target segment with various boron mixtures



# Boron reduces the chemical sputtering source rate and increases the core carbon density

Probability of entering the core from each divertor target segment with various boron mixtures



Percent boron	Total C flux (A)	Total number of core C particles	Total number of div. + SOL C particle (E19)	Total div. + SOL power (kW) E19
0	14937.6	899	1.74	5518
20	13461.3	885	0.96	3920
50	12757.5	1025	0.51	2966

- Increasing the boron fraction reduces the carbon density and radiated power the divertor and SOL while increasing penetration probability near segment #44 and the core C.
- These results are consistent with the DIII-D measurements and highlight the point that energetic atomic carbon, from physical sputtering, has a higher probability of entering the core than thermal molecules from chemical sputtering.

# Results and conclusions

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- **MCI simulations with mixed boron and carbon divertor targets show that molecular carbon from chemical erosion is less likely to reach the core plasma than atomic carbon from physical sputtering.**
  - **Increasing the boron/carbon fraction on the target plate surfaces reduces the carbon density and total radiated power in the divertor and SOL while increasing the carbon density in the core plasma.**
  - **These results agree with DIII-D measurements but only represent carbon contributions from the divertor. MCI is being also used to assess the relative importance of wall sources for determining the core carbon density**
  - **Accurate atomic data and carefully validated molecular dissociation models, using PISCES data, are particularly important for understanding why molecular carbon is less effective in reaching the core than atomic carbon**
- **Since atomic carbon leaves the target plates with more energy than molecular carbon it can penetrate deeper into the plasma in regions where the CI to CII ionization rates are small compared to the molecular dissociation rates. Most of the divertor carbon reaching the core originates from regions where sputtering rates are small but atomic neutral carbon mean free path lengths are long.**



MCI WWW page  
[lithos.gat.com/mci](http://lithos.gat.com/mci)

