Modeling carbon sputtering and near-surface plasma chemistry*

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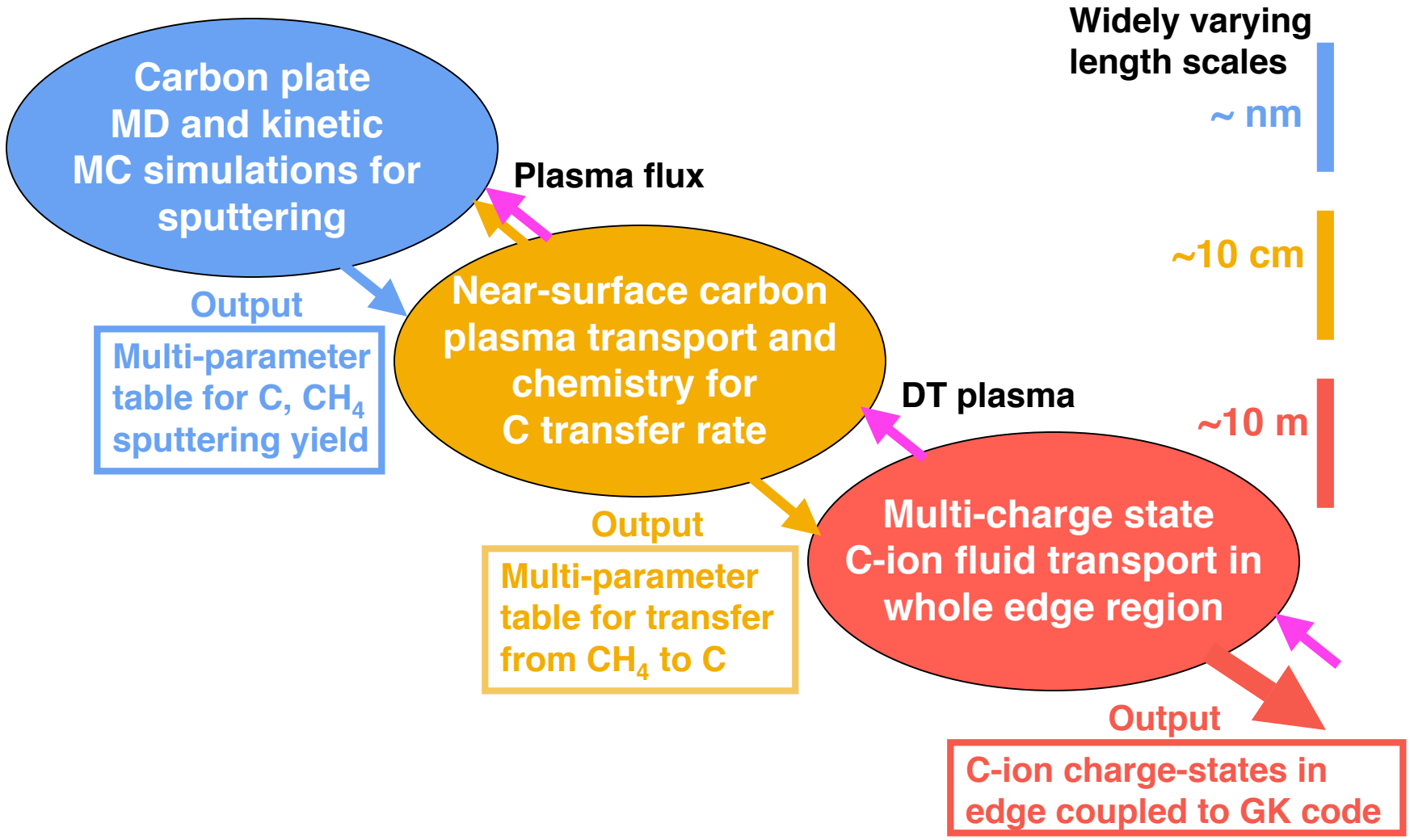
Modeling impurity content in fusion plasmas requires coupling 3 regions

Impurities in the edge plasma are important for power balance

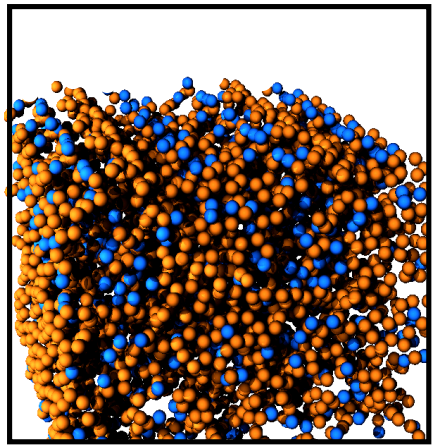


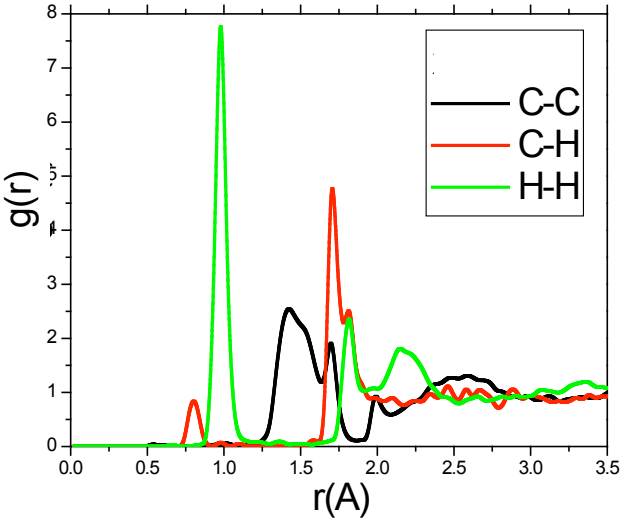
A crucial step for realistic MD simulations is proper construction of the target material

We have succeeded in developing targets corresponding to long-term exposure to reactor plasma as follows:

- start with amorphous graphite formed by pressurized melting and quenching.
- include 25% H (deuterium/tritium) in target to account for plasma exposure.
- anneal C/H target to stabilize structure.
- bombard with tritium/deuterium to include the effect of steady-state exposure.

Resulting carbon MD target showing H (blue)



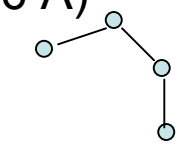


Normalized spatial distribution of lattice ions

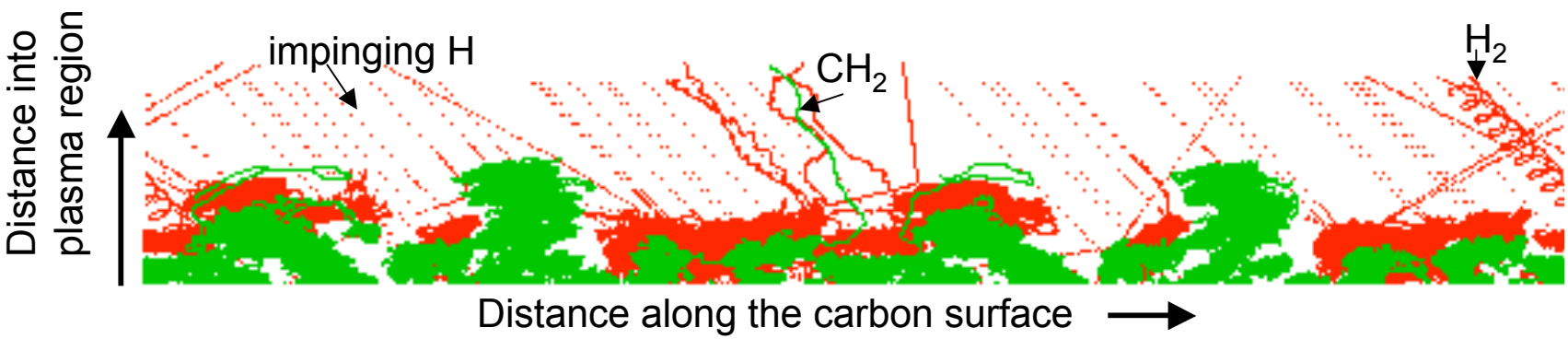
Sputtering MD simulations utilize state-of-the-art AIREBO & Brenner inter-atomic potentials

AIREBO (Adaptive Intermolecular Reactive Empirical Bond Order) potential is an extension of REBO that includes:

- Short-range, bonding interactions from Brenner (<3 Å)
- Long-range, non-bonding interactions (<6 Å)
- Torsional interactions (4-body) →



Sputtered-particle trajectories (solid colors) just above the surface

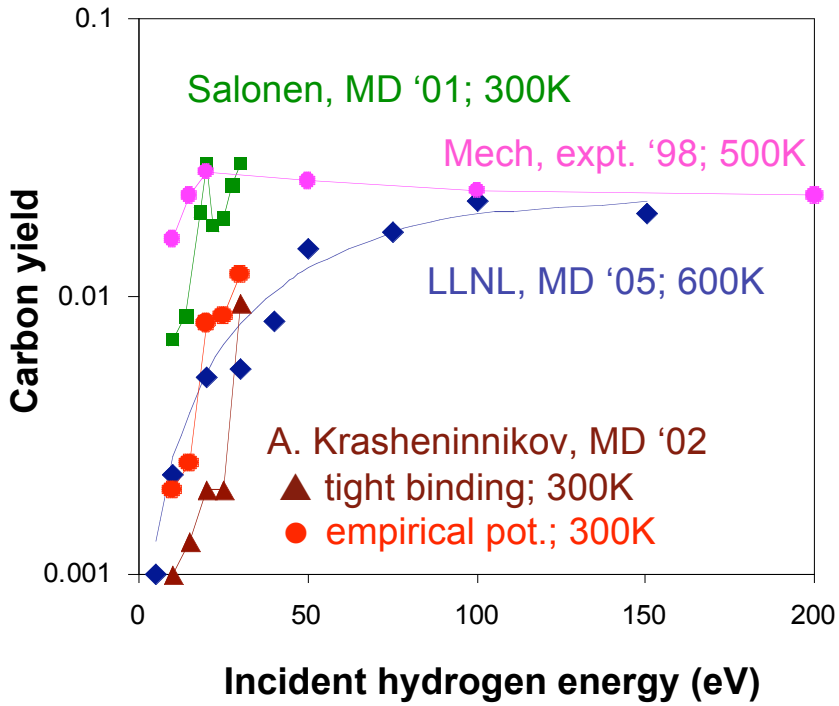


Conditions: T_{surf} = 500K, E_{inc} = 20eV, Θ_{inc} = 30°

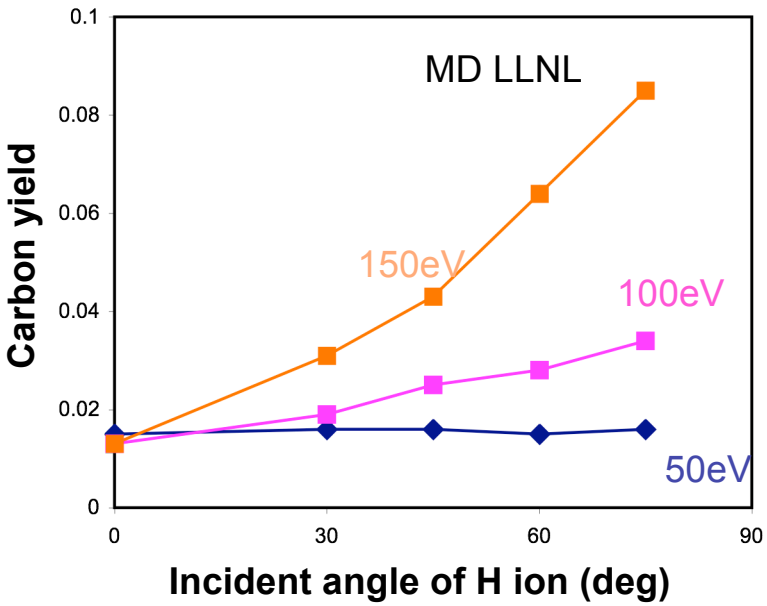
After 40 D/T impacts: 6H, $2H_2$, CH_2

Our MD simulation results cover a range of impact energies and angles; understanding is developing

Range of results depends partly on different materials/models

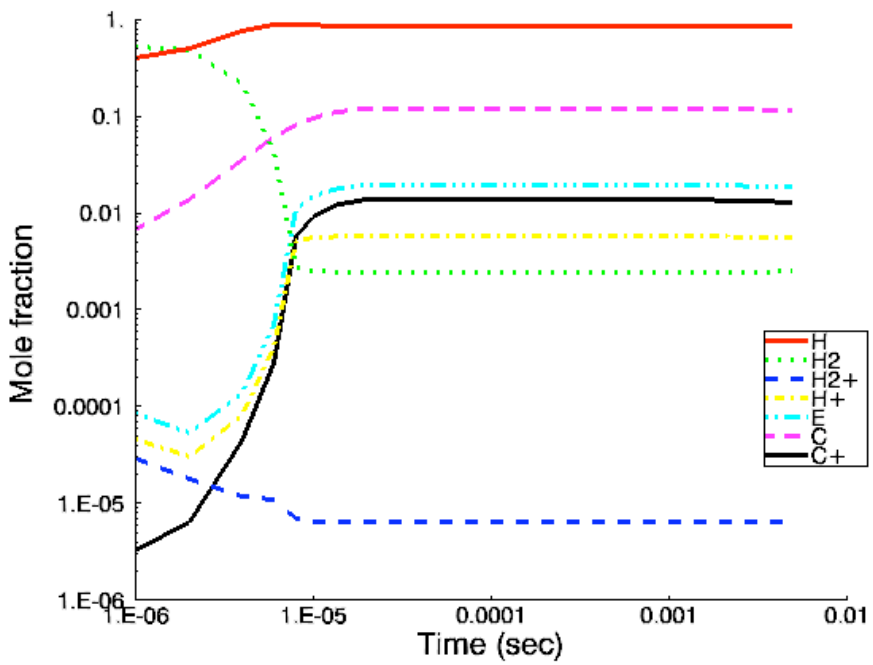


Variations with angle and energy suggest impact of chemical processes



Mech, Haasz et al., J. Nucl. Mat. **255** (1998) 153
Salonen, et al., Phys. Rev. **B63** (2001) 195415
A. Krasheninnikov et al., Comp. Mat. Sci. **25** (2002) 427
LLNL, PFC and LDRD '05

Initial reaction-diffusion model being used to rank importance of species



Ion-neutral reactions

$H2 + H^+ \Rightarrow H + H2^+$

$H + H2^+ \Rightarrow H2 + H^+$

Electron impact ionization

$e^- + H2 \Rightarrow H2^+ + 2e^-$

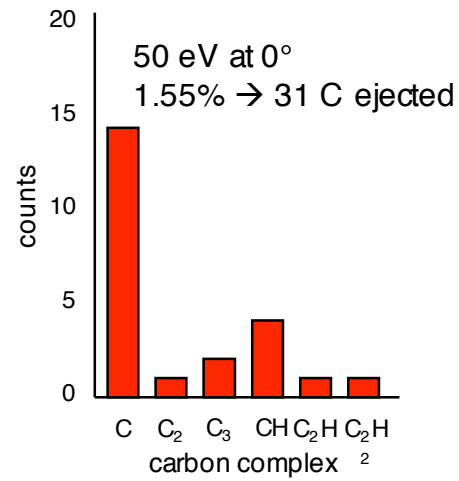
$e^- + H \Rightarrow H^+ + 2e^-$

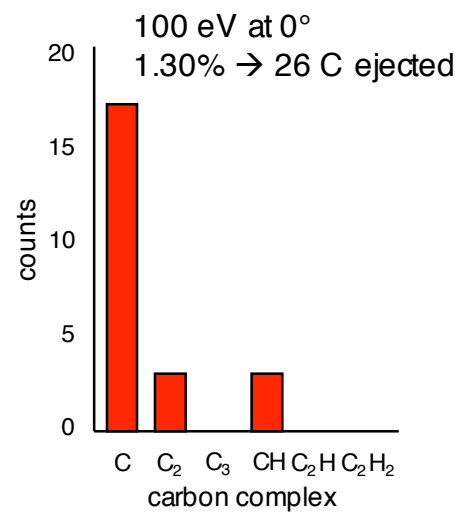
$e^- + H2 \Rightarrow 2H + e^-$

$e^- + C \Rightarrow C^+ + 2e^-$

Next step:
Include sputtered hydrocarbon.

Sputtered hydrocarbons predicted by MD are now being added to find net C yield



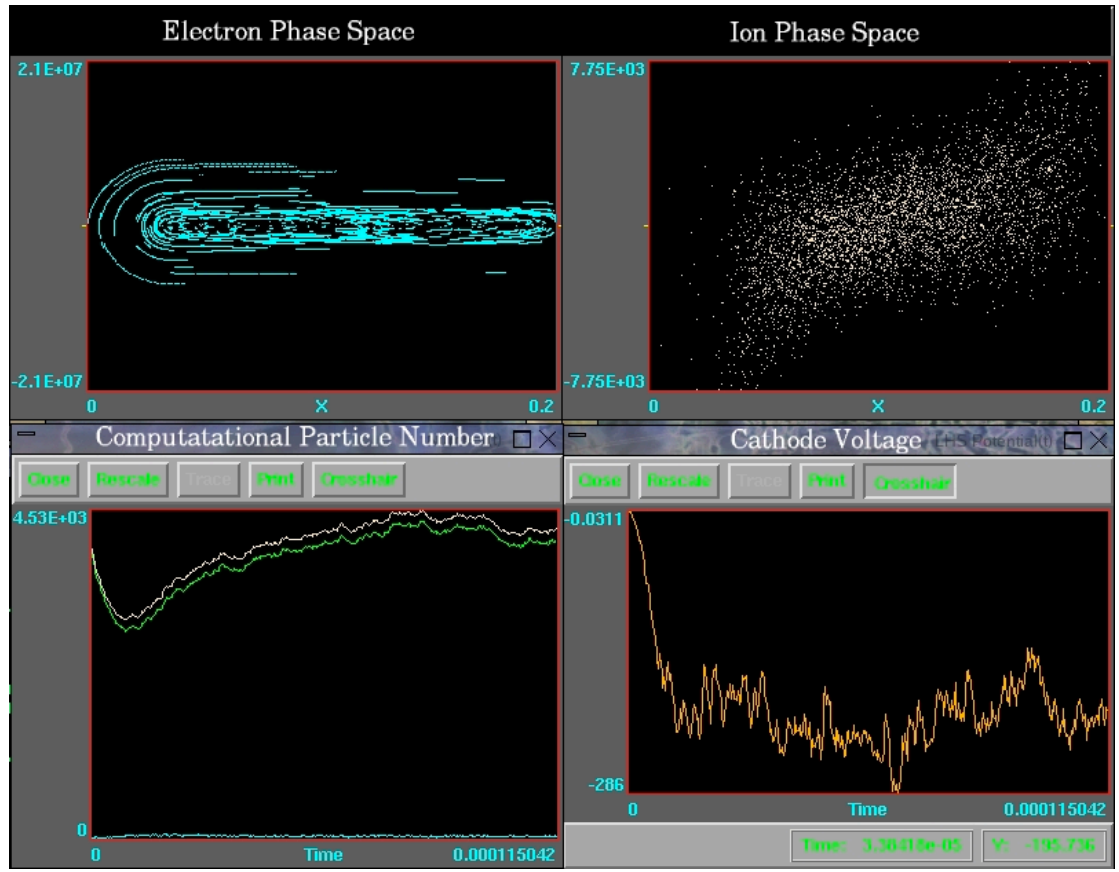


XOOPIC can use full particle electrons, but we need more efficient Boltzmann electron model

- PIC ions, Boltzmann-PIC hybrid electrons
- Electrons above specified threshold treated as particles – retains kinetic effects, Monte Carlo collision model
- Electron bulk modeled as inertialess Maxwell-Boltzmann distribution:

$$n(\mathbf{x}) = n_0 \exp\left(-q\phi(\mathbf{x})/T\right)$$

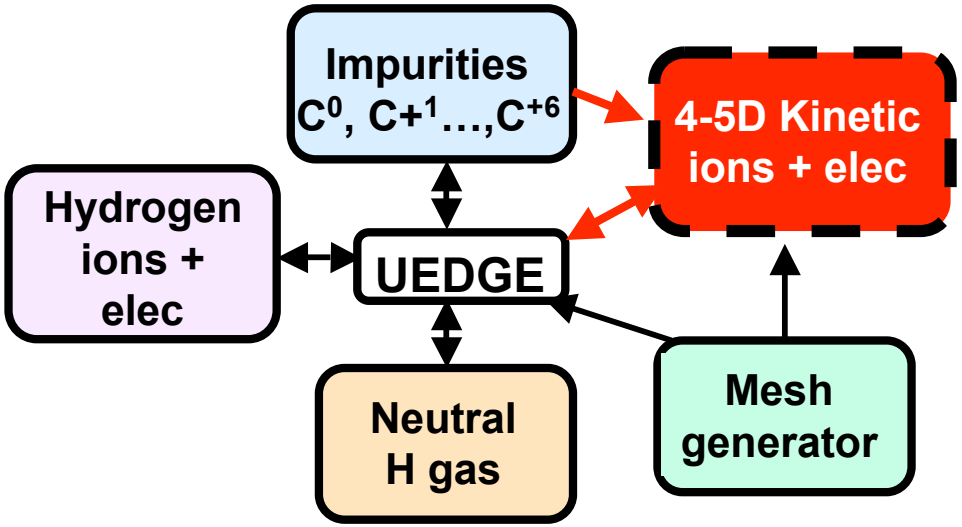
- Can choose arbitrary Boltzmann electron distribution function, f(E), e.g. with cutoff tails.
- Boltzmann species collisions based on f(E)

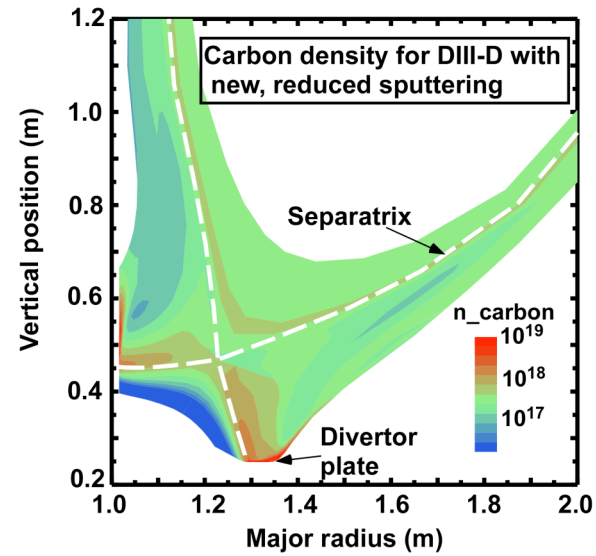


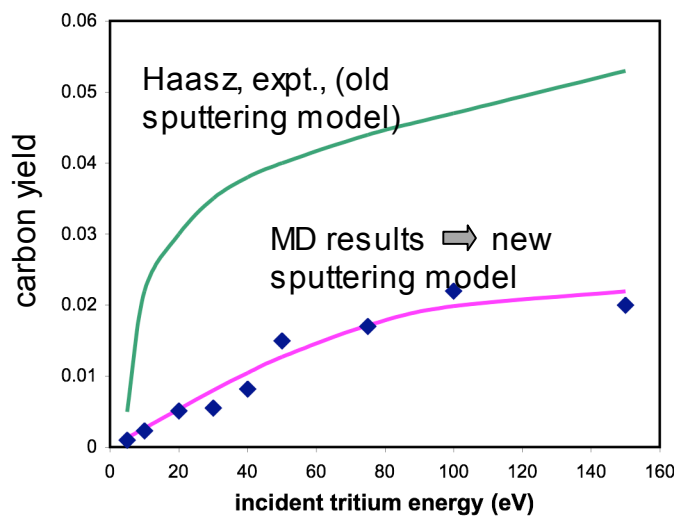
Current-driven 1D DC discharge runs up to 100 times faster than full PIC electron model.

Based on Cartwright et al., *Phys. Plasmas* **7**, 3252 (2000).

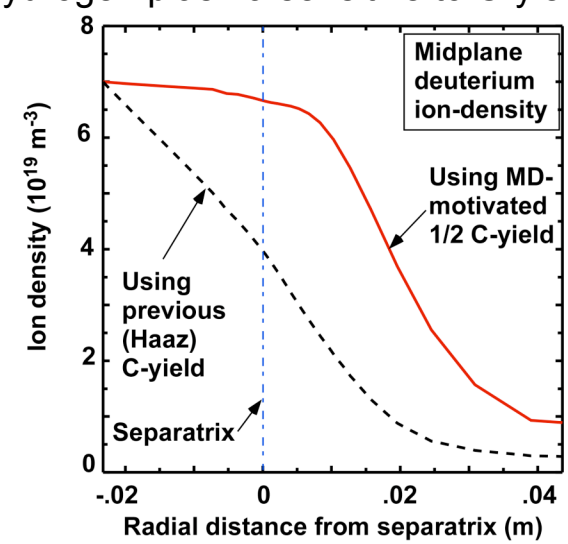
Full edge profile of carbon ions (charges Z= 1-6) from fluid UEDGE provides impurities



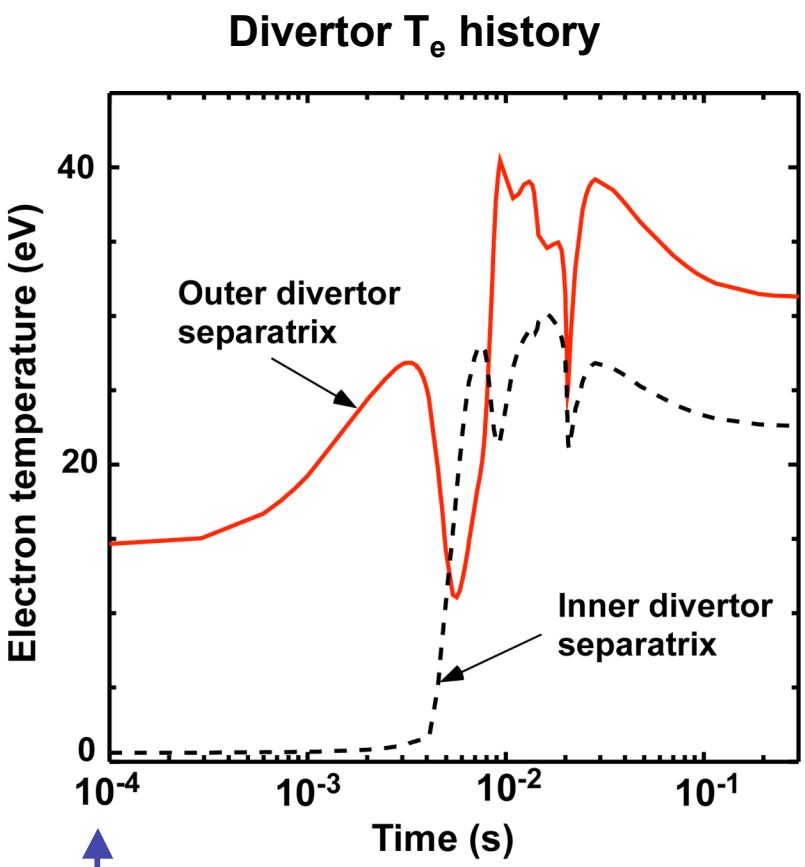


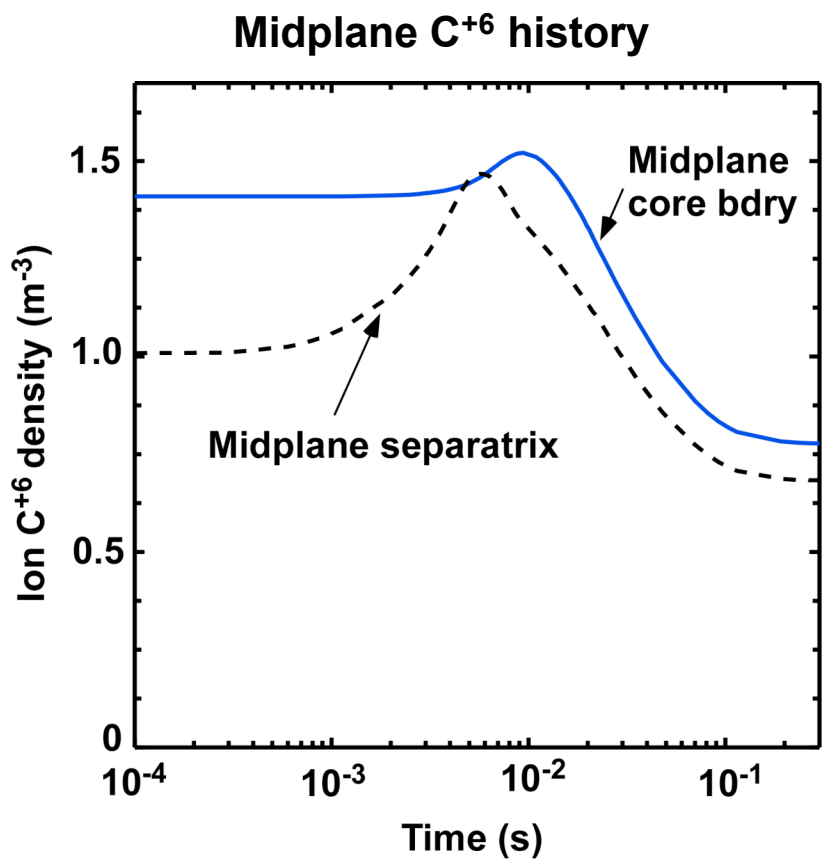


Hydrogen plasma sensitive to C-yield



Reduced carbon sputtering induces change from "detached" inner divertor to "attached"





Change from 100% to 50% of Haaz '97 sputtering model

Summary

- Developed realistic chemically-evolved (surface roughness) C/H targets using annealing and deposition
- State-of-the-art carbon interaction models were applied to producing new multi-variable chemical/physical sputtering
- Implemented and began testing chemical-rate methodology (ChemKin) to identify dominant hydrocarbon species
- Initial demonstration of edge plasma sensitivity to carbon content
- Implemented fast Boltzmann electron model for developed near-surface dynamics via XOOPIC plasma/neutral code