Plasma – Material Interactions in a Monte Carlo Neutral Transport Code

What's Not in the Model

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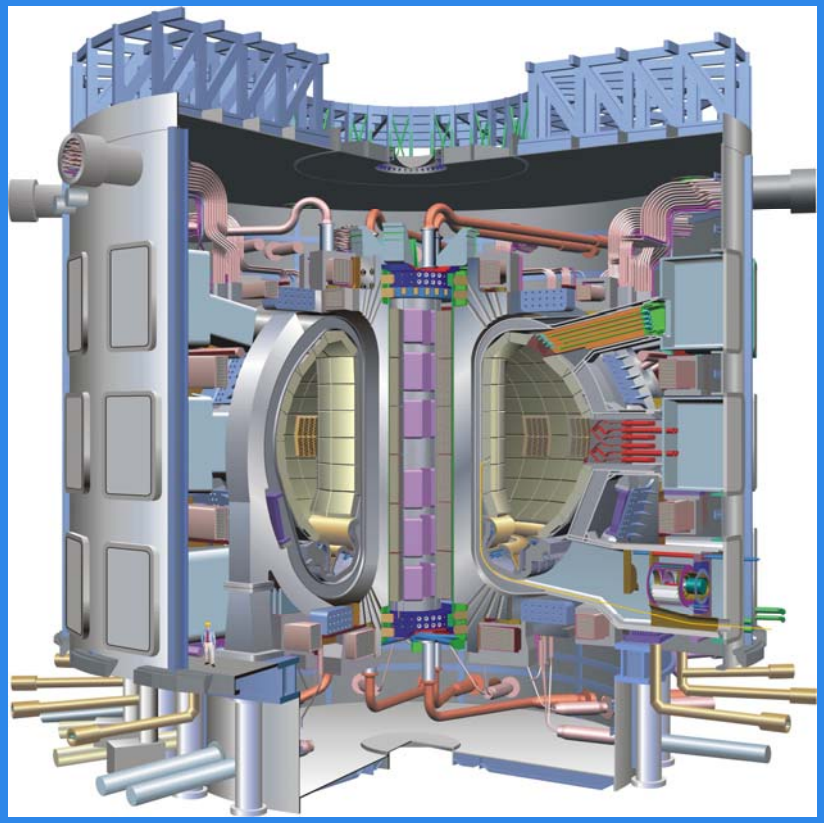
Introduction

- ITER's success crucial to making progress towards practical fusion power [IFRC 2005],
- Several materials related problems could threaten that success,
- Better understanding of plasma-materials interactions in existing experiments will allow us to solve those problems,
  - Most likely via predictive simulation capability based on that understanding.
  - Discuss current state of PMI models in simulations,
  - And prospects for predictive capability.



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Outline

- Boundary of Tokamak Plasmas
- Potential PMI Problems for ITER
- Existing PMI Models
- Areas for Improvement
- Conclusions

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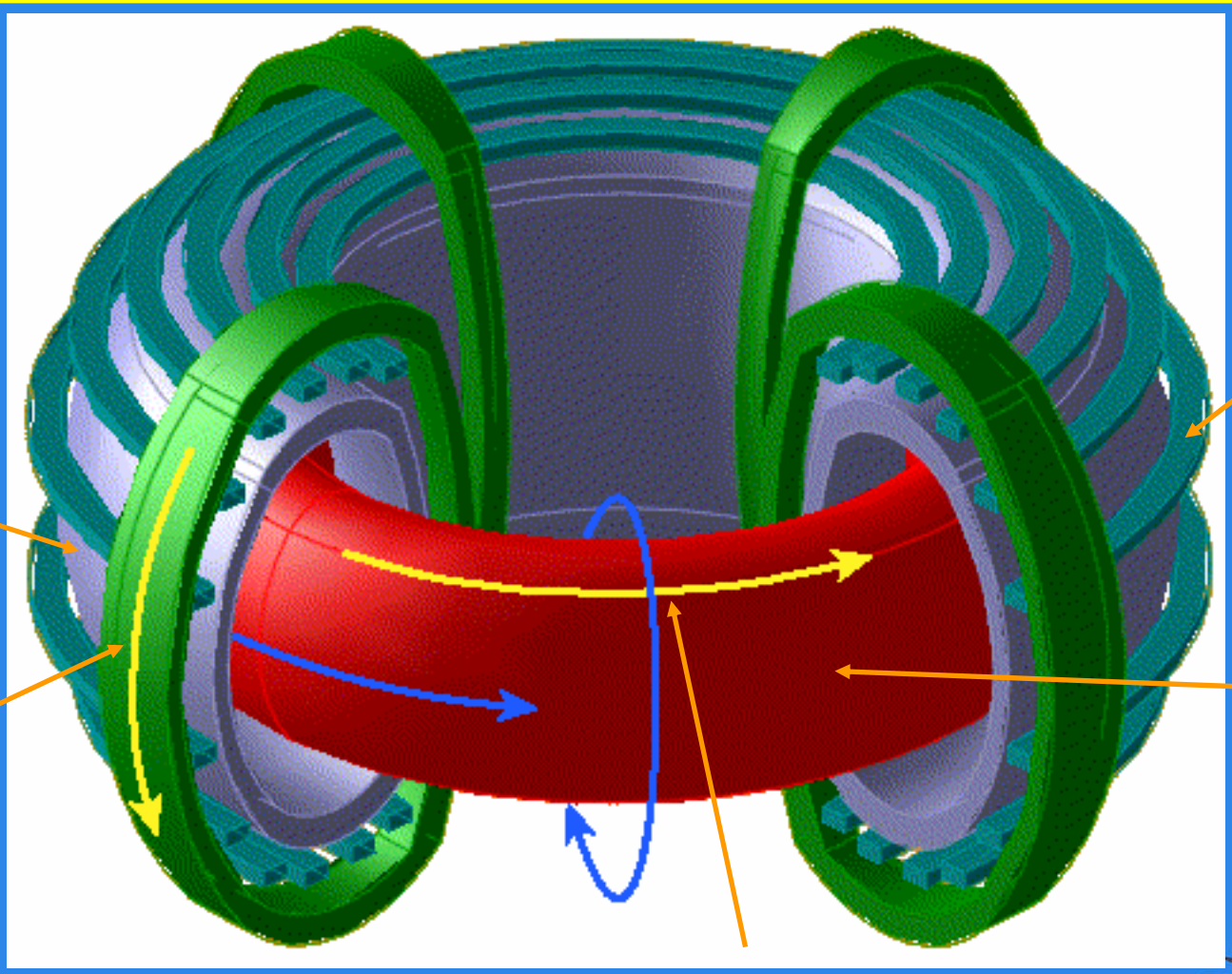
The Most Successful Magnetic Confinement Configuration is the Tokamak



Stabilizing and shaping magnetic fields are generated by currents in other coils

vacuum vessel

plasma

Current driven through coils distributed around torus creates primary magnetic field

An external transformer induces a current in plasma around torus that creates a smaller magnetic field

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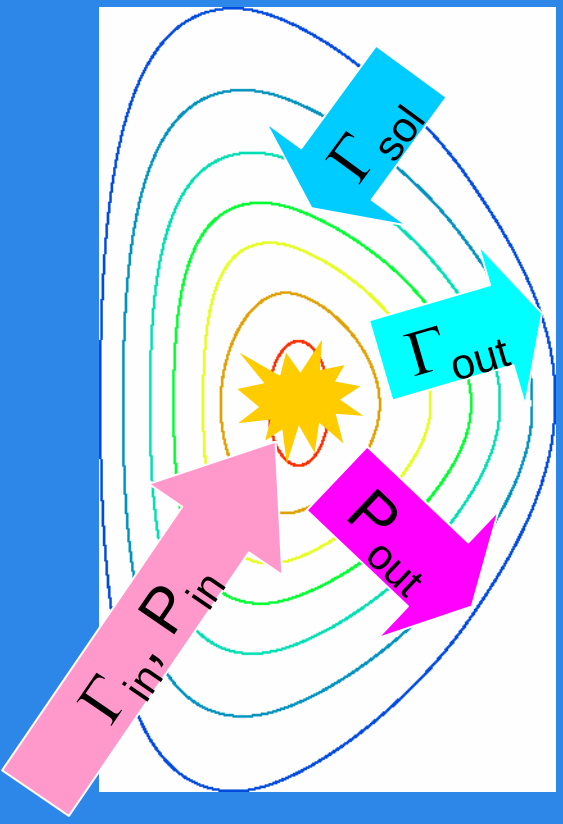
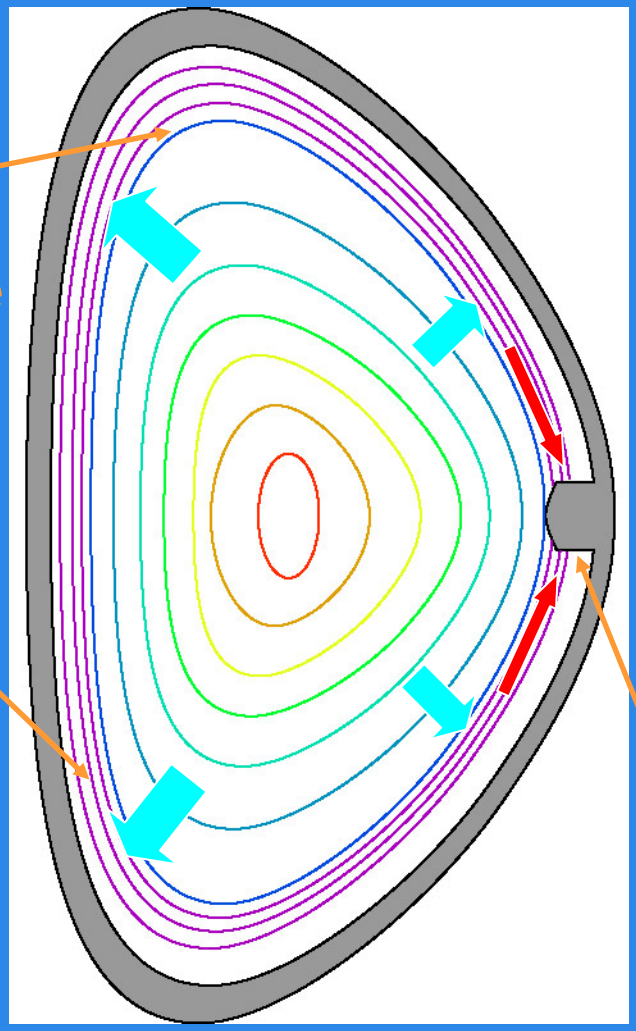
In Steady State, Have Power & Particle Flows To Material Boundaries



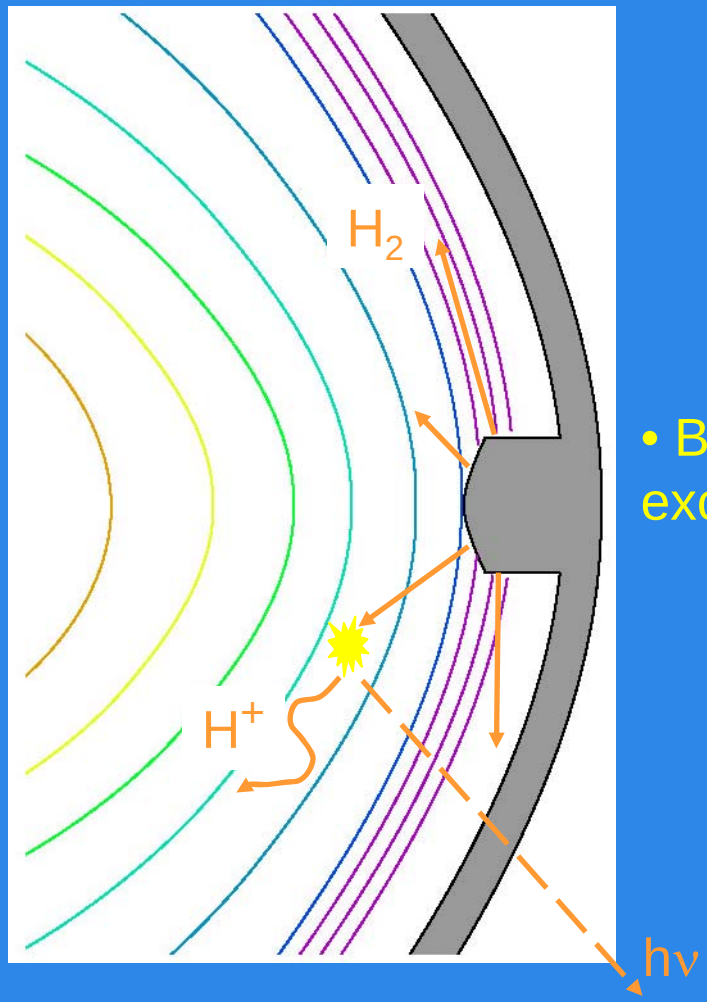
- In a reactor, 80% of fusion power leaves as neutrons,
  - Captured in blanket.
- Other 20% flows out of plasma & strikes material boundaries.
- Particle flows replace fuel ions & remove He ash.
- In non-DT experiment, $P_{out} = P_{in}$,
- Particle flows determined by competition between sources (core & edge) and diffusion.
- General reference: [Stangeby 2000]

Simplest Plasma-Material Interaction Configuration Is the Limiter



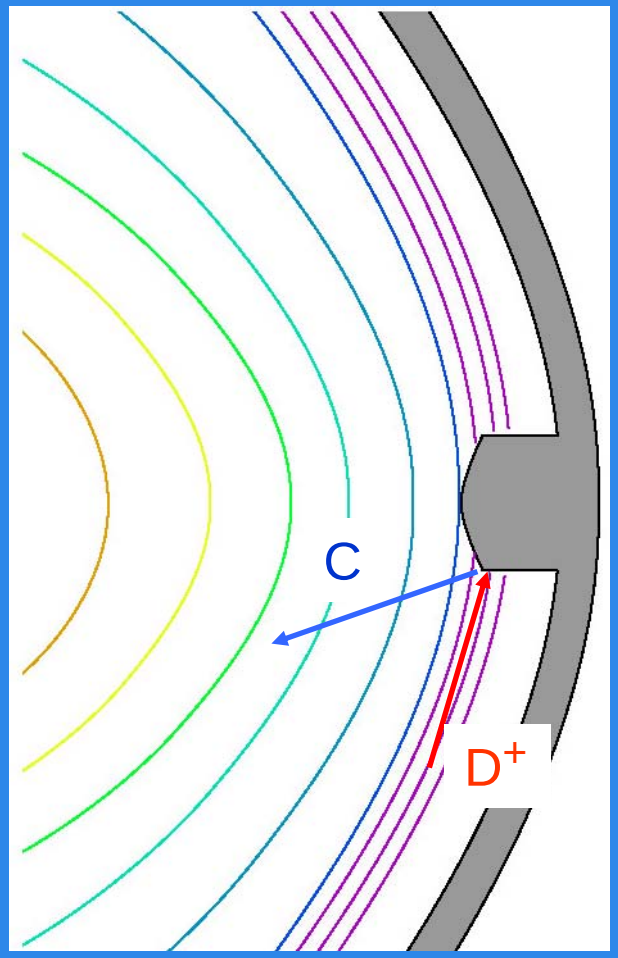
- Limiter location defines last-closed flux surface,
  - Intercepts open field lines / flux surfaces ⇒ scrape-off layer (SOL).

Limiter Acts as a Sink for Plasma Particles and Power



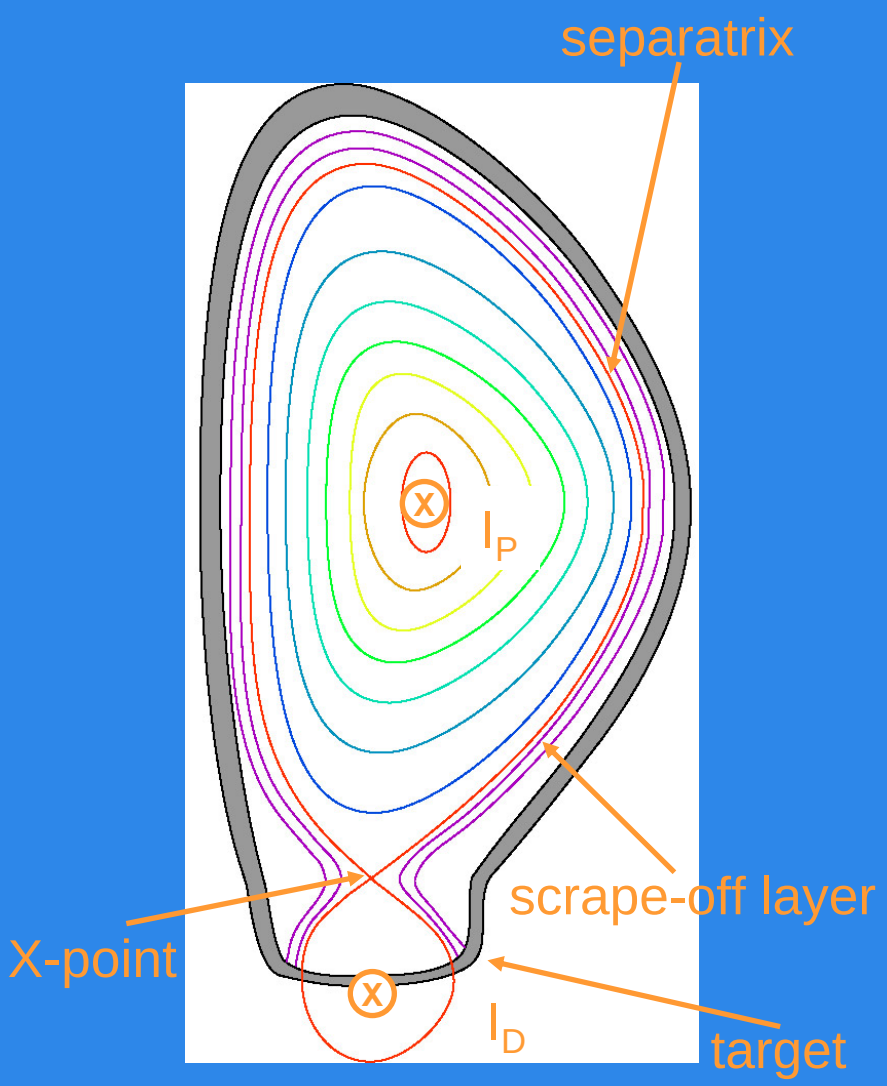
- Not for mass, however:
  - Electrons & ions recombine at surface,
  - In steady-state, resulting neutral atoms & molecules recycle back into plasma.
  - Neutrals travel freely across field lines,
  - & be ionized near or far from limiter
  - $\Rightarrow$ plasma can refuel itself.
- Before being ionized, H atoms can be excited by electron impact,
  - Radiatively decay & emit photons,
  - $\Rightarrow$ Markers of ionization.
  - E.g., n = 3 $\rightarrow$ 2 transition (Balmer-alpha or H_α) at ~6560 Å dominates visible emissions & is often used for diagnostics.

High T_e Near a Material Can Lead to Impurity Sputtering



- Particles striking a material at high enough energy can knock off substrate atoms ⇒ physical sputtering.
- Becomes a significant particle source for E ~ few 100 eV – 1 keV,
  - ⇒ Is a concern for T_e > 100 eV.
- Can lead to self-sputtering,
  - Efficient due to similar projectile & substrate mass,
  - And due to Z > 1.
- Sputtered impurities can harm core,
  - Efficient radiators ⇒ P_{rad},
  - Dilute hydrogen fuel.

Tokamak Divertor Configuration Moves the Plasma Material Interaction Away From Core



- Divertor created by adding coil I_D with current in same direction as I_P.
- In between, get B_{pol}=0.
  - This is the X-point.
  - Corresponding surface is separatrix; becomes the LCFS.
  - Separates SOL from core plasma.
- SOL field lines strike material surface at the divertor targets.
- Divertors concentrate particles & power.
  - Facilitates pumping,
  - But complicates power handling!

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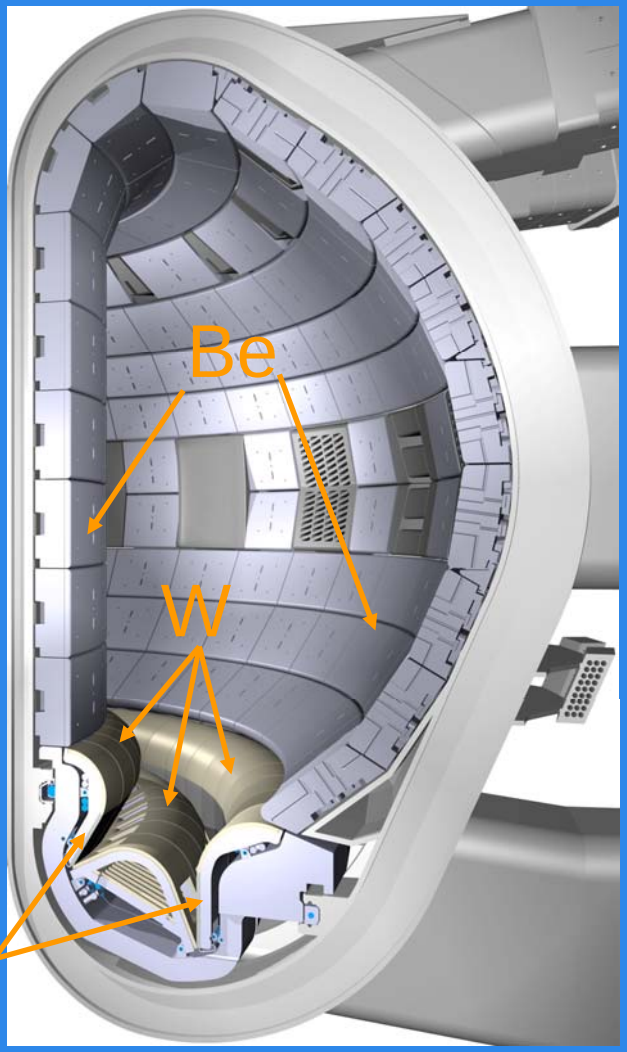
ITER Will Use a Mix of Plasma Facing Materials



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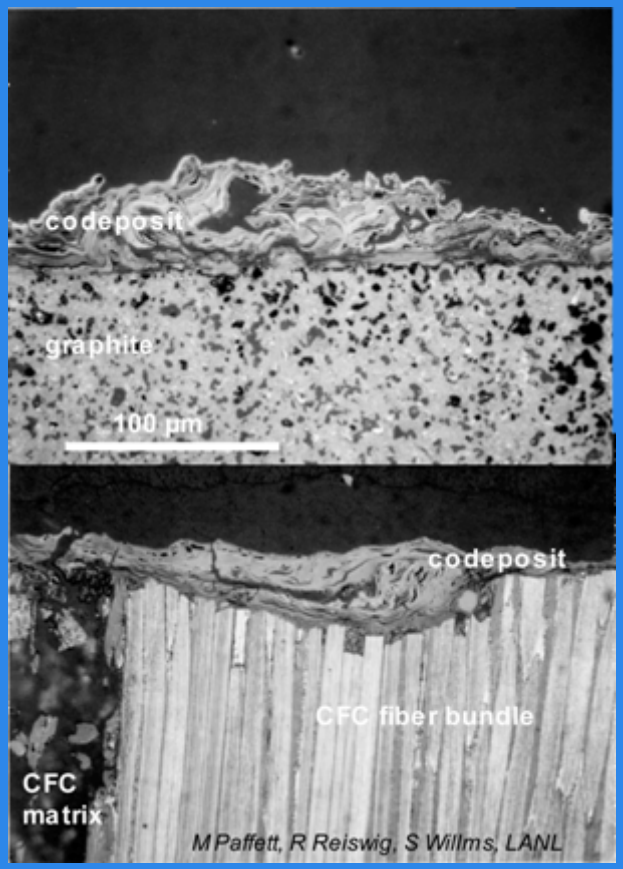
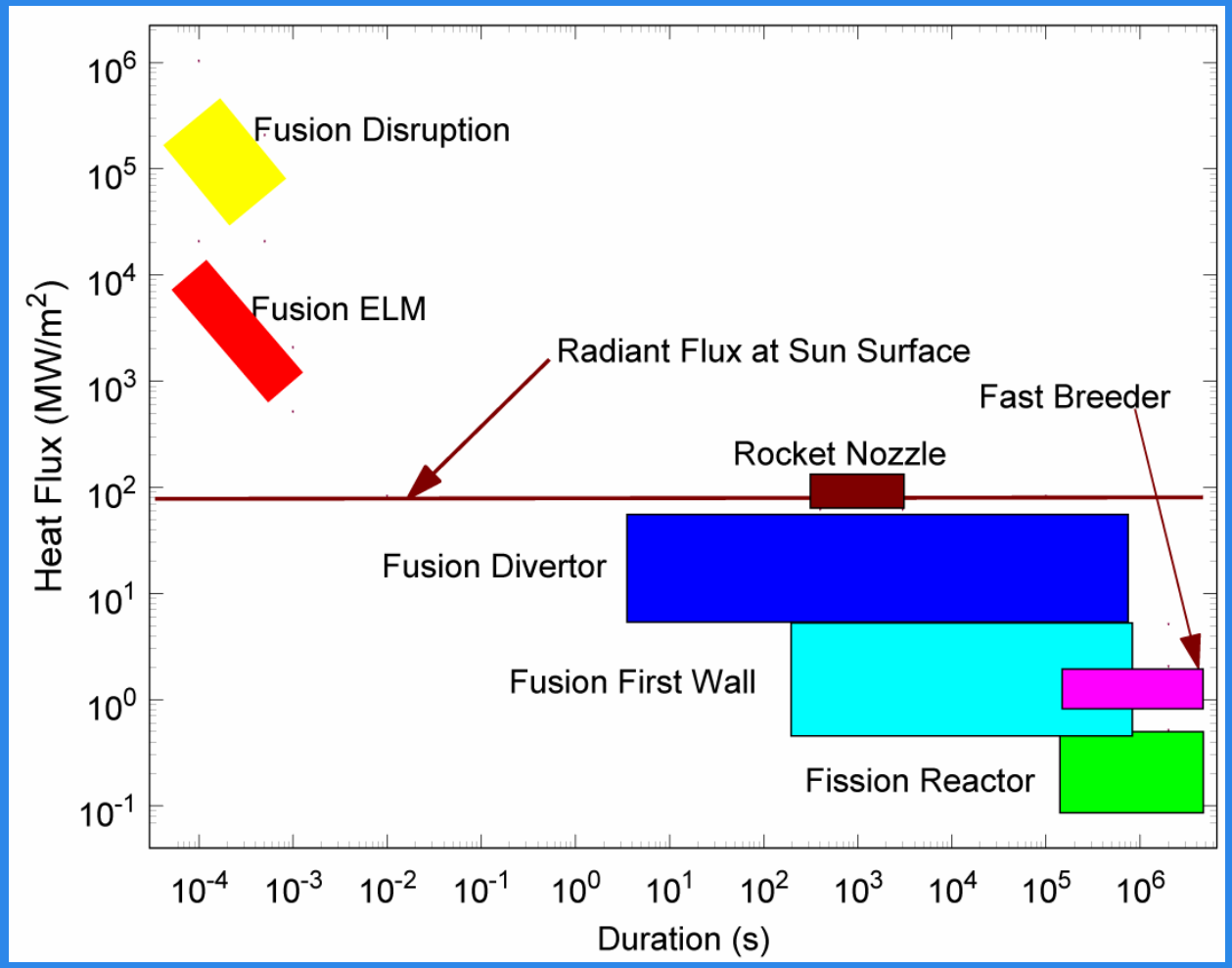
- Main chamber: Be.
- Divertor surfaces mostly W,
  - Except for target strike points, C.
- Existing tokamak database dominated by all carbon machines,
  - More aggressive research with ITER relevant materials under way.
- Divertor plasma parameters:
  - $n_e = 10^{20} – 10^{21}$ m^{-3},
  - $T_e = 0.1 – 100$ eV,
  - $n_D = 10^{19} – 10^{20}$ m^{-3},
  - $P_{D2} = 0.1 – 10$ Pa (plenum).

Will Need to Understand Hydrocarbon Behavior

- Safety concerns limit amount of in-vessel tritium in ITER [Federici 2001],
  - Trapped in redeposited hydrocarbons,
  - Extrapolation of existing data ⇒ serious problem.
- Mechanisms of hydrocarbon creation, transport, & deposition not completely understood.
- Starting point: data for dissociation & ionization of hydrocarbons improving,
  - CH_y, C_2H_y, C_3H_y [Janev 2002, Janev 2004],
  - See also HYDKIN reaction analysis tool: http://www.eirene.de/eigen/index.html
- Tritium removal techniques also being pursued.



ITER Divertor Target Heat Fluxes In Context [Herrmann 2003, Kukushkin 2005]



[M. A. Ulrickson, Sandia National Labs]

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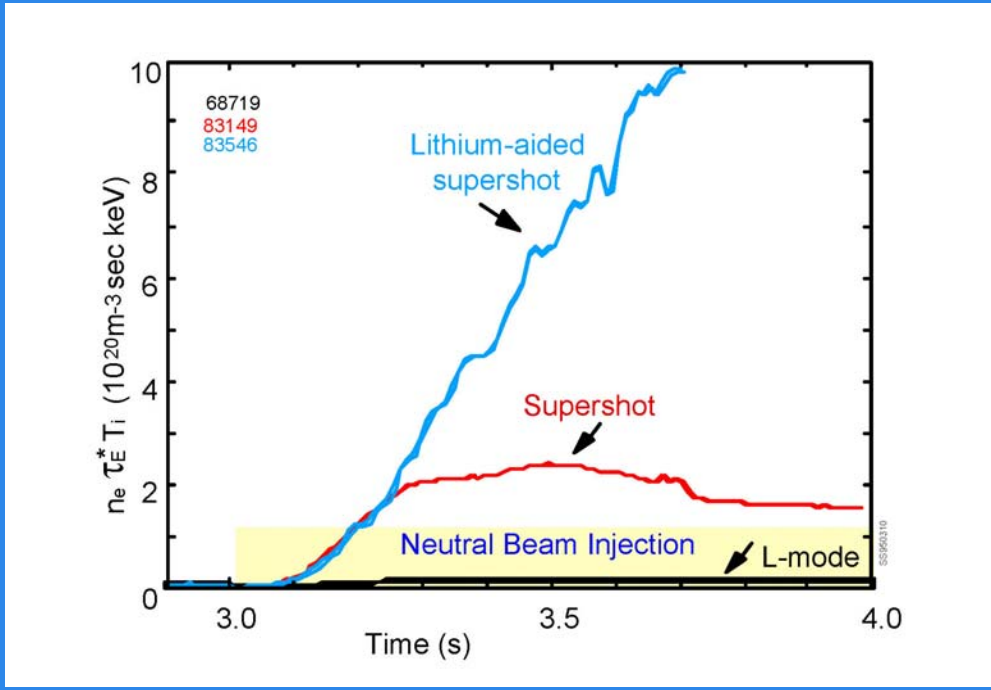
Experimentally Most Important Impact of PMI Missing from Existing Simulation Codes

- Have wide agreement that core plasma performance sensitive to "wall conditions" ↔ recycling.
- Best discharges obtained with "conditioned walls",
  - E.g., via discharge cleaning, B or Li coatings,
- TFTR Li, pellets & DOLLOP, is an extreme example.
- But, existing simulations do not differentiate between these 3 conditions.



[Mansfield 2001]

Incomplete PMI Model Hinders Other Physics Work

- **Particle balance analysis more complicated than power balance,**
  - Instead of a "check" on analysis, particle balance used to infer wall sources & sinks!
  - In a code, power balance more complicated.
- **Diagnostic interpretation uses emission rates to infer particle fluxes,**
  - But, the relation between them depends on H / H_2 fraction,
  - & on neutral kinetic distribution, e.g., energy & rotational / vibrational excitation of H_2.
  - PSI model impacts all of these.

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Model Currently Used in DEGAS 2 is Relatively Simple

- DEGAS 2 work has focused on H-related physics,
  - See: http://w3.pppl.gov/degas2
  - Leave discussion of sputtering, erosion, redeposition & other impurity processes to others.
- Backscattering $\leftrightarrow$ reflection [Eckstein 1991],
  - In general described by $P(E_{in},\theta_{in};v,\alpha,\phi)$.
  - Codes like TRIM have been used to generate such data,
    - Stored in "Bateman" format.
  - But, much simpler models also used,
    - E.g., $R_n(E_{in})f(\theta_{in})$, $R_E(E_{in})f(\theta_{in})$ in DEGAS's refl.dat; used with outgoing cosine distribution.
- Absorption
  - Specified as a fraction of incident flux,
  - "Recycling coefficient" can vary in space.
- Desorption
  - In steady state, everything else!
  - Thermal energy distribution (T_{wall}),
  - Cosine or Maxwell flux angular distribution.

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Can We Do Better Now?

- A predictive modeling capability will require more detail,
  - Particularly to simulate ITER,
    - Longer pulse, higher heat & particle fluxes.
- But, don't think we want an MD model of every atom in vacuum vessel!
  - Can we summarize material state with a modest number of added parameters?
  - Probably need some sort of reduced model based on that set since high dimension tables difficult to generate, store, & search.

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There Have Already Been Attempts to Do Just This! Integrated Models

1. [Hillis 2001] used coupled EIRENE – WDIFFUSE to analyze JET D → H exchange experiments.
2. [Mioduszewski 2001] examined space & time dependent recycling by combining model for D trapping with DEGAS-computed fluxes.
3. [Warrier 2004] combined empirical formulas for several PSI processes into single suite of subroutines & added 1-D heat diffusion equation to allow T_{wall} to be evaluated consistently.

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What Else Are We Missing?

1. Low E_{in} Limit of Reflection
2. Recycling Kinetics
3. Sheath Physics
4. Changes in Material State
5. Liquid Surfaces
6. Synergistic Effects
7. Diagnostics & Experimental Data

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1. What is Low E_{in} Limit of Reflection?

- [Eckstein 1991] points out that some BCA simulations yield, incorrectly, $R_n \rightarrow 1$ at low E_{in},
  - Rather, R_n should decrease for $E_{in} < 3\ E_{sbe}$.
- But, [Vietzke 2002] argues that incident energy unlikely to be completely absorbed by phonons & that R_n should $\rightarrow 1$ below 1 eV,
  - Shows supporting experimental data.
- The two situations likely associated with different amounts of absorbed H.
- Also: recent MD simulations of low E reflection of H on W [Henriksson 2006].

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2. More Detailed Models Do Exist for Recycling Kinetics

- [Vietzke 2002] describes three H_2 desorption processes,
  1. Thermal: cosine at T_{wall},
  2. Prompt desorption following recombination of adsorbed H: cosine at 4 T_{wall}, some vibrational excitation,
  3. Recombination of incoming & adsorbed H: incoming energy goes into H_2 translational, vibrational, rotational energy.
- [Brezinsek 2002] demonstrated T_{wall} dependence of H / H_2 fraction in recycled flux,
  - Also: evidence for vibrationally excited H_2 coming from surface.
- What about charge state distribution?
  - Not all neutral [Ehrenberg 1996, Meyer 2006]!

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3. Sheath Physics Determines Ion Impact Energy & Angle

- DEGAS 2 model is relatively simple,
- Canonical references: [Stangeby 1986, Chodura 1986].
- More detailed models exist,
  - Particle Trajectories [Cohen 1998],
  - Sheath structure in highly inclined field [Chodura 1986], [Riemann 1994].
- Secondary electron effects?
  - Straightforward to include [Stangeby 1986],
  - Determined by material properties,
    - More detailed discussion: [Schou 1996].

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4. What Phenomena Impact the Material State?

- Wall conditioning: "bake-out" or "discharge cleaning" ⇒ reduced H concentration,
  - E.g., [Causey 2002, Hillis 2001, Ehrenberg 1996]
- Coatings intended to absorb H & lower impurity influx,
  - Most common now: B, Be, and Li,
  - E.g., [Causey 2002]
- Changes in surface structure ("roughness") or phase due to erosion, redeposition, irradiation,
  - E.g., [Federici 2001]
  - Even more complicated in presence of > 1 PFC material, as in ITER.
    - Coster beginning to address this [Coster 2006].

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Some Examples: Changes in Absorption

- [Ohya 2001, Golubeva 2003], (probably many others) examined impact of C & W layers on reflection & trapping,
  - [Ohya 2001] also considered dynamic effects.
- Modifications of trapping character by energetic He ion irradiation, e.g. [Nagata 2003],
- [Atsumi 2003] considered impact of neutron irradiation on H retention & diffusion in C,
  - Experimental data & proposed model.

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5. Do Liquid Surfaces Need to Be Modeled Differently?

- **Variety of configurations:**
  - Thin films or coatings,
  - Thick (> 1000 Å) surfaces (e.g., CDX-U),
  - Flowing liquid.
- **[Bastasz 2001] covers some relevant issues:**
  - Slightly different E_{sbe} has small impact on sputtering,
  - But, near surface density stratification could have significant effect,
  - Evaporation must be considered,
  - Trapping, diffusion of H, He are of great interest,
    - See also [Causey 2002].
  - **Conclude from this that a liquid surface model will be qualitatively different!**

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6. Are There Synergistic Effects?

- Some processes are known to depend strongly on surface temperature,
  - E.g., evaporation, chemical sputtering,
  - Need to model temperature evolution ⇒ self-consistent solution with incident heat flux,
  - If system actively cooled, need to model it!
  - Even further complicated by presence of flakes or other local modifications of thermal conductivity.
- Dependency on particle flux?
  - E.g., chemical sputtering.
- Impact on kinetic details?
  - E.g., incoming fluxes might alter outgoing H_2 vibrational & rotational distribution [Vietzke 2002].
- But, have plenty of work to do before fully investigating these effects!

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7. Sophisticated Codes Require Sophisticated Experiments & Measurements

- See discussion in [Federici 2001],
  - Related: Post's "Prediction Challenge" [Post 2005] ⇒ importance of verification & validation.
- Dedicated laboratory facilities, e.g.,
  - PISCES-B [Doerner 2003],
  - MIRF (ORNL) [Meyer 2006],
  - U. Wisconsin [Wright 2007].
- Incident flux measurements in tokamaks,
  - Hydrocarbon deposition, e.g., [Skinner 2005].
- Also, more detailed spectroscopy,
  - E.g., [Brezinsek 2002] measured H / H_2 fraction, T_{rot}, T_{vib}.

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Conclusions

- Plenty of room for improvement!
- Some of the above can be included straightforwardly:
  - Better sheath model,
  - More detailed recycling kinetics.
- Plan on handling spatially & temporally varying material state,
- Hard part is determining a set of parameters that adequately characterizes that state & a reduced model based on it.

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