Plasma – Surface Interactions in a Monte Carlo Neutral Transport Code

What's Not in the Model

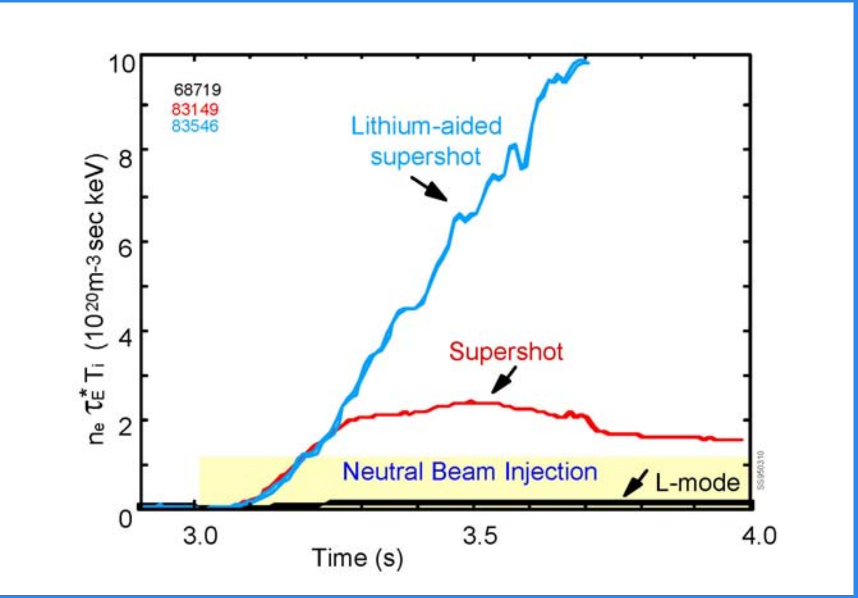
D. P. Stotler
Princeton Plasma Physics Lab

Outline

- Motivation
- Background
- Some Existing Integrated Models
- What Are We Missing?
- Conclusions

What Do We Need to Develop a Predictive Simulation Capability?

- That's a long list!
- But, PSI models have not received as much attention as other areas.
- Yet, 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.

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Incomplete PSI 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,
  - Sputtering, erosion, redeposition & other impurity processes well covered by others here.
- 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 $\rightarrow$ 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.

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, $R_n \to 1$ at low E_{in},
  - Rather, R_n should decrease for $E_{in} \lessapprox 3\ E_{sbe}$.
- But, [Vietzke 2002] argues that incident energy unlikely to be completely absorbed by phonons & that R_n should $\to$ 1 below 1 eV,
  - Shows supporting experimental data.
- Which is it???

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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]!

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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.

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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.

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 $\Rightarrow$ 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 2004] $\Rightarrow$ importance of verification & validation.
- Dedicated laboratory facilities, e.g.,
  - PISCES-B [Doerner 2003],
  - MIRF [Meyer 2005],
  - U. Wisconsin [Whyte].
- 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.