Plasma – Surface Interactions in a Monte Carlo Neutral Transport Code

What’s Not in the Model

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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.
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 / H₂ fraction,
  - & on neutral kinetic distribution, e.g., energy & rotational / vibrational excitation of H₂.
  - PSI model impacts all of these.
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 ↔ reflection [Eckstein 1991],
  - In general described by \( P(E_{\text{in}}, \theta_{\text{in}}; v, \alpha, \phi) \).
  - Codes like TRIM have been used to generate such data,
    - Stored in “Bateman” format.
  - But, much simpler models also used,
    - E.g., \( R_n(E_{\text{in}})f(\theta_{\text{in}}) \), \( R_E(E_{\text{in}})f(\theta_{\text{in}}) \) 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 \( (T_{\text{wall}}) \),
  - Cosine or Maxwell flux angular distribution.
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.
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 $T_{\text{wall}}$ to be evaluated consistently.
What Else Are We Missing?

1. Low $E_{\text{in}}$ Limit of Reflection
2. Recycling Kinetics
3. Sheath Physics
4. Changes in Material State
5. Liquid Surfaces
6. Synergistic Effects
7. Diagnostics & Experimental Data
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 $E_{in} \lesssim 3$ $E_{sbe}$.
- 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.
- Which is it???

- [Vietzke 2002] describes three H₂ desorption processes,
  1. Thermal: cosine at $T_{\text{wall}}$
  2. Prompt desorption following recombination of adsorbed H: cosine at 4 $T_{\text{wall}}$, some vibrational excitation,
  3. Recombination of incoming & adsorbed H: incoming energy goes into H₂ translational, vibrational, rotational energy.

- [Brezinsek 2002] demonstrated $T_{\text{wall}}$ dependence of H / H₂ fraction in recycled flux,
  - Also: evidence for vibrationally excited H₂ coming from surface.

- What about charge state distribution?
  - Not all neutral [Ehrenberg 1996], [Meyer]!
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].
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.
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!
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 H₂ vibrational & rotational distribution [Vietzke 2002].

- But, have plenty of work to do before fully investigating these effects!
7. Sophisticated Codes Require Sophisticated Experiments & Measurements

- See discussion in [Federici 2001],
- 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\textsubscript{2} fraction, T\textsubscript{rot}, T\textsubscript{vib}. 
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.