

Neutral Transport from Wall to Scrape-Off Layer

D. P. Stotler
Princeton Plasma Physics Lab
May 20, 2010

ARIES Town Meeting
“Edge Plasma Physics and Plasma
Material Interactions in the Fusion Power
Plant Regime”

Why Do Neutrals Matter?

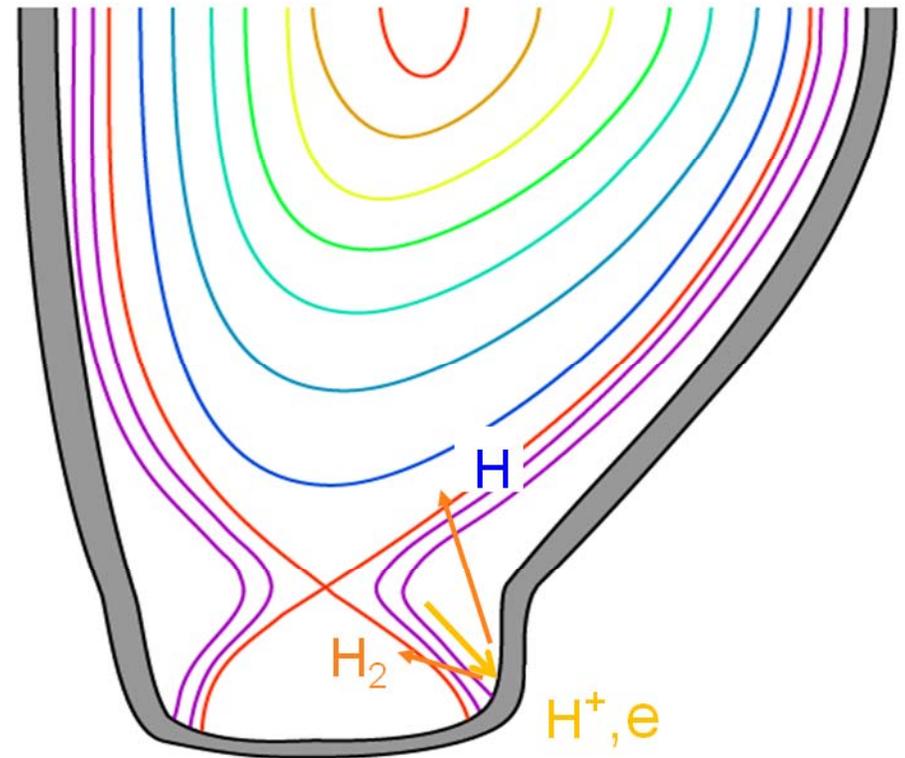
- Wall is sink for plasma, but not mass: recycling
- Sputtered impurities leave wall as neutral atoms & molecules
- Fueling, beam heating, pumping involve neutrals
- Detachment hinges on neutral-plasma interactions
- Play a role in edge transport & turbulence / H-mode (?)
- Increase impurity radiation rate
- Basis for edge & core diagnostics

Outline

- Neutral sources
 - Recycling
 - Sputtering
 - External sources
 - Volume recombination
- Interactions
 - Plasma–material interactions
 - Plasma–neutral reactions
 - Detachment
 - Radiation trapping
- Other stuff

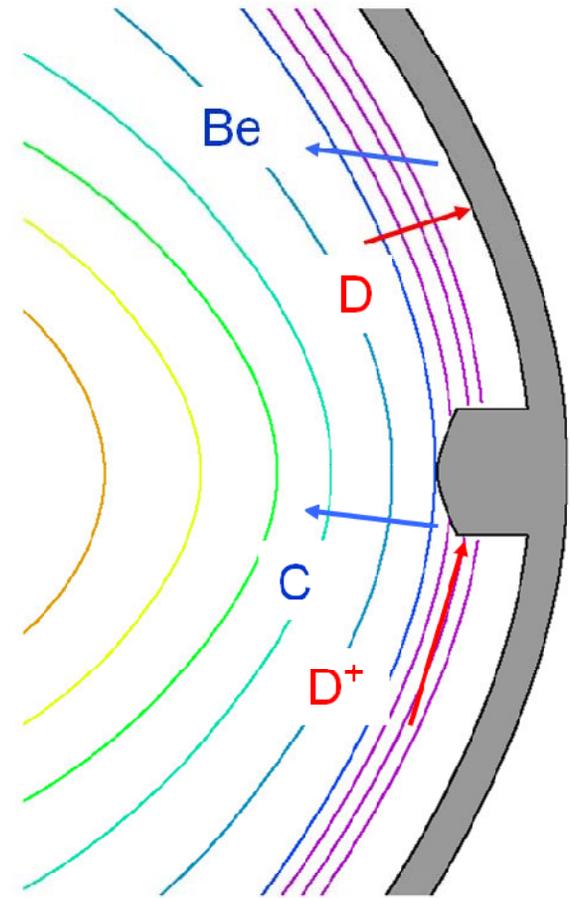
Wall is Sink for Plasma, But Not for Mass: Recycling [Stangeby 2000]

- Flows along open field lines to surfaces,
- Ions accelerated through sheath → PMI:
 - Backscattering → H,
 - Or Absorption,
 - Desorbed as H_2 in steady state.
- H_2 : absorbed & desorbed.
- Kinetic details:
 - Backscattered velocity distribution,
 - Ro-vibrational state of molecules?
- Other issues:
 - Real PMI,
 - Permanent absorption / wall pumping.



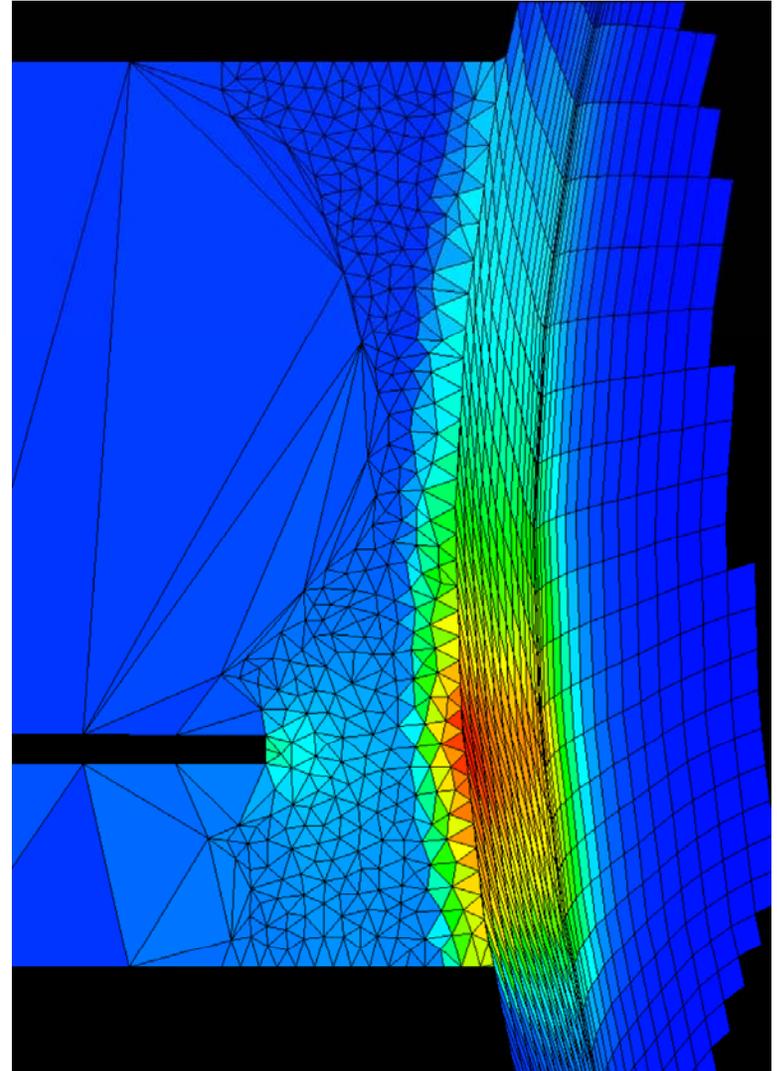
Sputtered Impurities Leave Wall as Neutral Atoms & Molecules

- \Rightarrow cross magnetic field lines.
- Particles knock off substrate atoms \Rightarrow physical sputtering.
- E.g., ions going through sheath when $T_e > 100$ eV.
- Or atoms CX'ing with hot ions,
 - Main chamber erosion & deposition issue for ITER [Kotov 2009].
- Chemical sputtering
 - Usually refers to hydrocarbons formed on graphite.



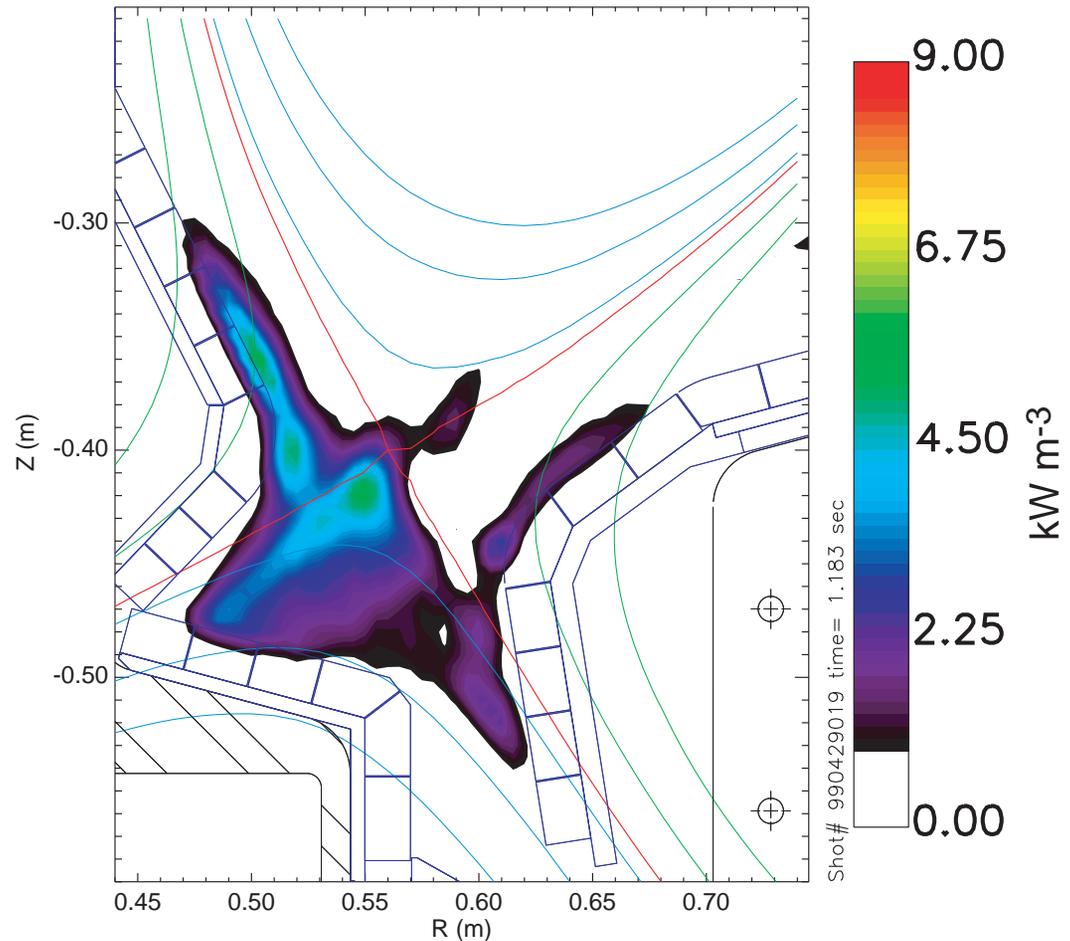
Fueling, Beam Heating, Pumping Based on Neutrals

- Gas Puff:
 - Easy to install & control,
 - Flexible timing, composition, rate,
 - Easy to simulate!
 - Big drawback: poor penetration,
- Higher density methods more efficient:
 - Pellet,
 - Supersonic gas injection,
 - Molecular clusters.
 - Better not just due to speed,
 - On HFS, aided by ∇B drift [Lang 1997].
 - Difficult to model because of impact on plasma parameters & equilibrium.
- Neutral beam injection:
 - Reliable heating with extensive database.
 - Deep core fueling in present day devices.
 - Can be modeled.
 - Basis for several diagnostics.



Volume Recombination of Hydrogen Can Be Dominant Neutral Source

- If T_e low enough, say, < 1 eV.
- Detect by D_γ / D_α ,
- Ratios & rates come from atomic physics model.
- Recombination included in edge simulation codes,
 - Sensitivity to T_e complicates interpretation of experimental data [Lisgo 2005].
- Observed in detached plasmas.



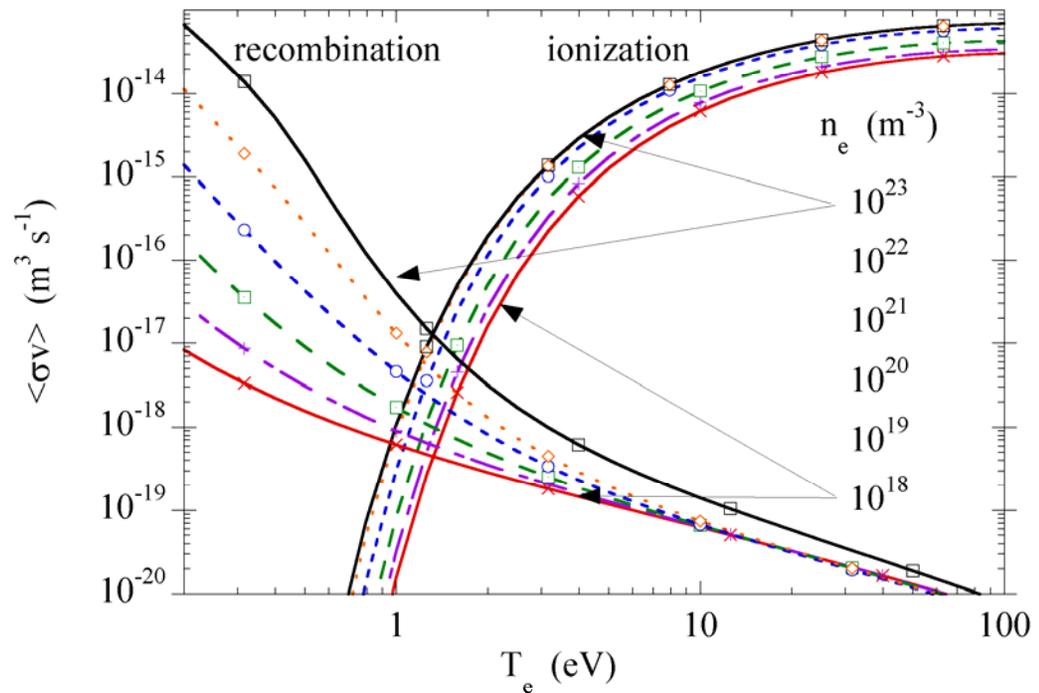
[Boswell 2001]

Outline

- Neutral sources
 - Recycling
 - Sputtering
 - External sources
 - Volume recombination
- Interactions
 - Plasma–material interactions
 - Plasma–neutral reactions
 - Detachment
 - Radiation trapping
- Other stuff

Electron Impact Ionization of Hydrogen is a Multi-Step Process

- Collisions excite, de-excite, & ionize,
- Atoms can decay radiatively.
- Timescales comparable \Rightarrow treat all.
- Ionization of H($n=0$) is one of thousands [Loch 2009].
- Excited states equilibrate faster than ground state changes,
 - \Rightarrow collisional radiative model.
 - Yields effective rates of ionization and recombination for ground state.
 - Functions of n_e & T_e .
- & line emission (D_α), total radiation, electron cooling rates.
- Assumes plasma optically thin.
- Similar data for He [Loch 2009], Li [Loch 2006]...

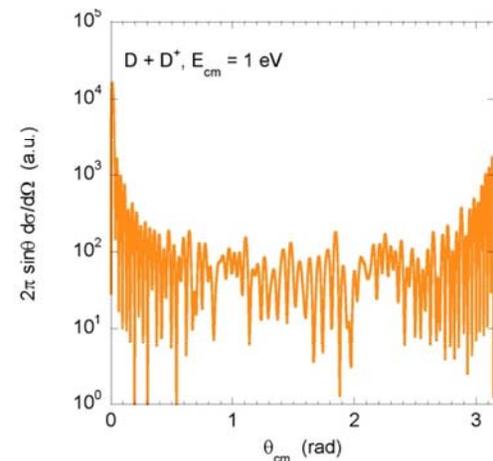
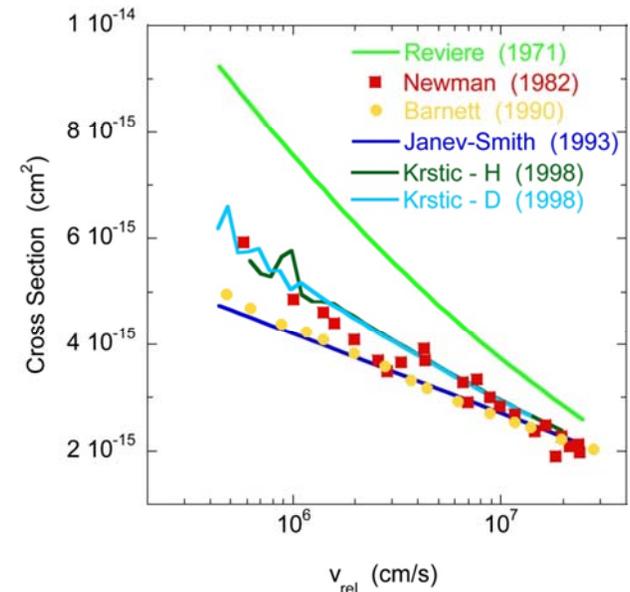


[Post 1995]

$$\frac{Dn_0}{Dt} = -n_0 n_e S_{\text{eff}} + n_i n_e R_{\text{eff}}$$

Charge Exchange & Elastic Scattering Exchange Momentum & Energy Between Ions & Neutrals

- $\text{H} + \text{H}^+ \rightarrow \text{H}^+ + \text{H}$,
 - Pure CX: 180° scattering in center of mass,
 - Below ~ 1 eV, momentum transfer from elastic scattering also important.
 - Fully quantal calculations of $d\sigma/d\Omega$ describe as single reaction [Krstic 1998].
- $\text{H}_2 + \text{H}^+ \rightarrow \text{H}_2 + \text{H}^+$,
 - Elastic scattering transfers energy to $\text{H}_2 \Rightarrow$ longer mfp [Krstic 1998].
- Neutral-neutral: $\text{H} + \text{H}$, $\text{H} + \text{H}_2$, ...
 - Nonlinear \Rightarrow iterative BGK [Kotov 2006],
 - Significant impact on ITER neutral pressure & pumping [Kukushkin 2005].

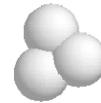


H₂, H₂⁺: How Big Does the Zoo Need to Be?

- Lower T_e ⇒ H₂ longer lifetime ⇒ additional processes,
 - Vibrational excitation & de-excitation,
 - ⇒ ion conversion: H₂(v) + H⁺ → H₂⁺ + H,
 - More species: H₃⁺, H⁻.
- Predicted “Molecule Assisted Recombination” [Krasheninnikov 1997],
 - AUG modeling [Fantz 2001], showed instead “Molecule Assisted Dissociation”!
- “Collisional radiative” rates for H₂, H₂⁺: [Sawada 1995], [Greenland 2001], [Pigarov 2002], [Kotov 2006],
 - Treating H₂(v) as “excited state”.
- In ITER simulations, H₂ CR model increases PFR pressure & neutral power flux to targets. [Kukushkin 2005].
- In general, should include H₂(v) [Reiter 2007],
 - But, has not had significant impact on macroscopic divertor parameters.



$$\frac{dn_{H_2}}{dt} = -(D_{H_2} + S_{H_2} + I_{H_2}) n_e n_{H_2}$$



$$\frac{dn_{H_2^+}}{dt} = S_{H_2} n_e n_{H_2} - (R_{H_2^+} + D_{H_2^+} + S_{H_2^+}) n_e n_{H_2^+}$$

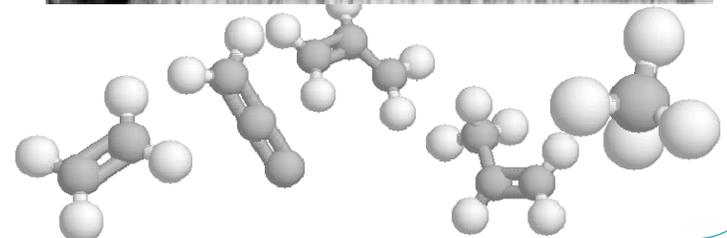
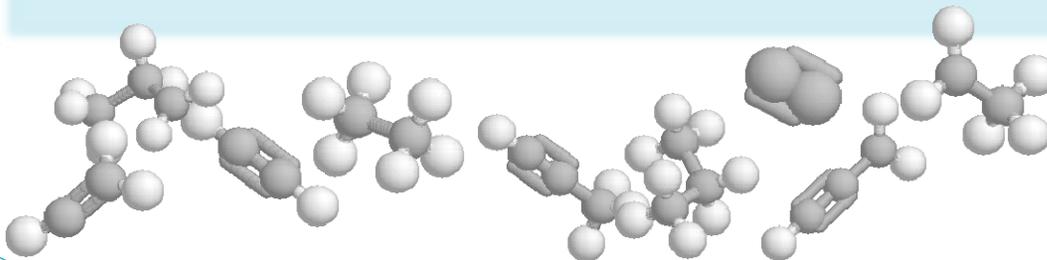
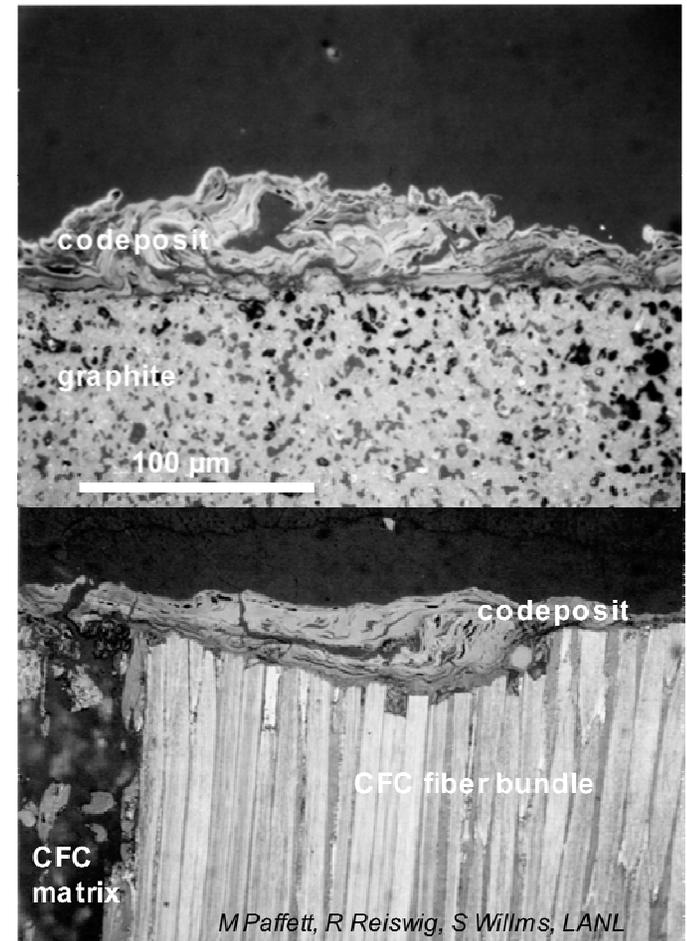


$$\frac{dn_H}{dt} = (2D_{H_2} + I_{H_2^+}) n_e n_{H_2} + (2R_{H_2^+} + D_{H_2^+}) n_e n_{H_2^+} - I_H n_e n_H + R_H n_e n_{H^+}$$

$$\frac{dn_{H^+}}{dt} = I_{H_2} n_e n_{H_2} + (D_{H_2^+} + 2S_{H_2^+}) n_e n_{H_2^+} + I_H n_e n_H - R_H n_e n_{H^+} \quad \text{[Kotov 2006]}$$

Another Reason to Get Rid of Carbon

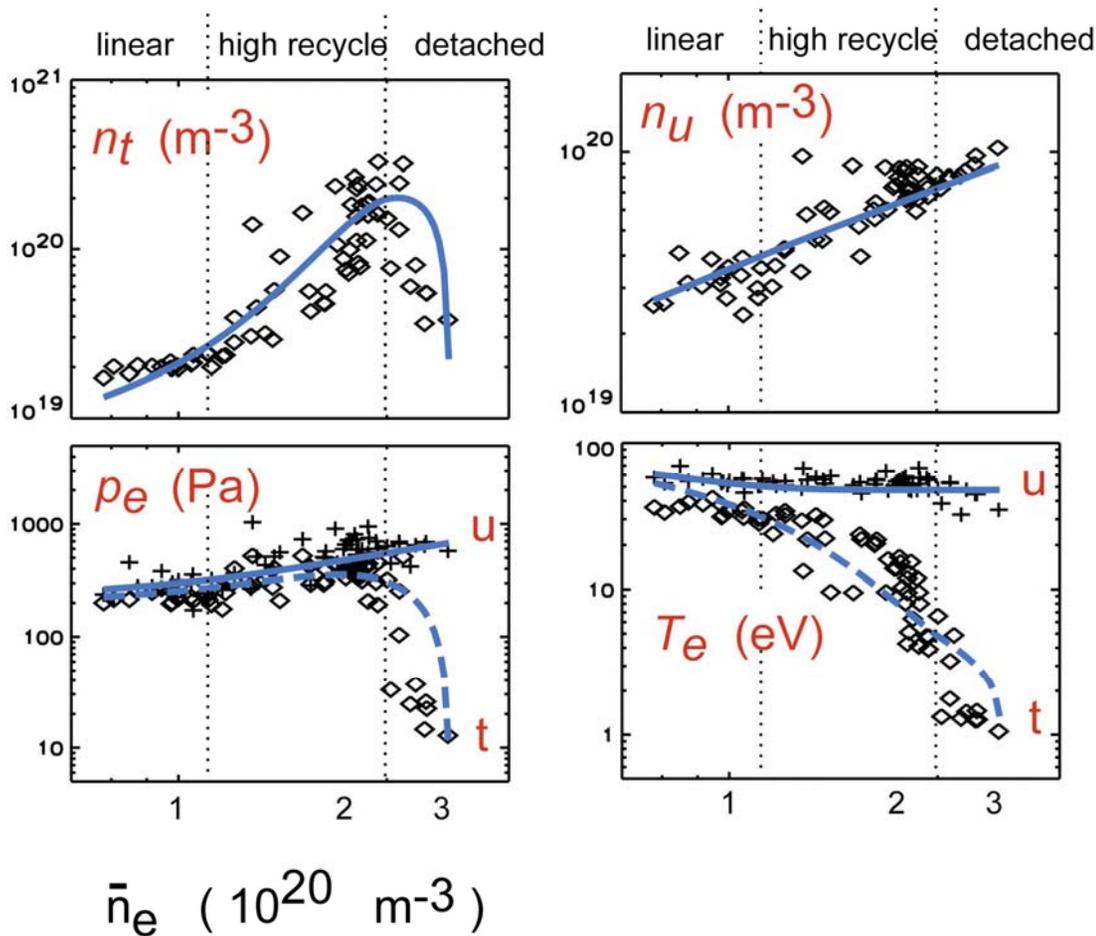
- Would like to avoid carbon because of T inventory [Federici 2001].
- If we really understood hydrocarbon creation, transport, & deposition...
- Starting point: data for dissociation & ionization of hydrocarbons,
 - CH_y , C_2H_y , C_3H_y [Janev 2002], [Janev 2004],
 - HYDKIN reaction analysis tool:
<http://www.hydkin.de>
- Resulting systems very complicated!
 - 700 processes for C_3H_y !
 - Many more fragmentation channels.
- Different pathways dominate at low (1 - 2 eV) & high T_e (> 10 eV) [Reiter 2009] \Rightarrow simpler models may be possible.



M Paffett, R Reiswig, S Willms, LANL

Partial Detachment Allows ITER to Radiate 60 – 70% of Divertor Power

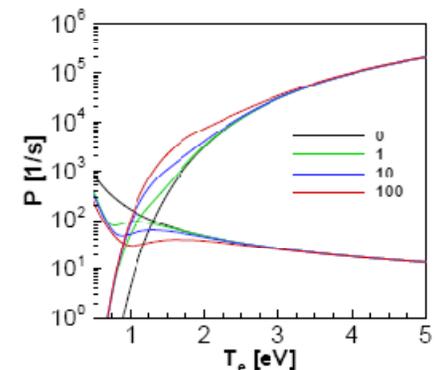
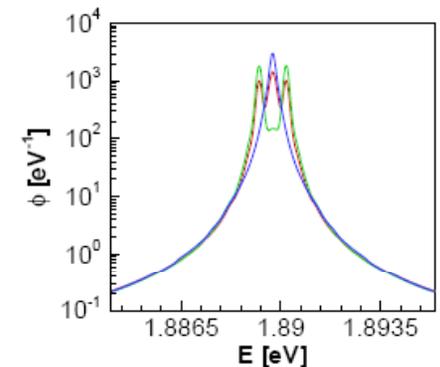
- Via photons & neutrals [Pitts 2009].
- $j_{\text{sat}} \downarrow$, but $D_{\alpha} \uparrow$ with increasing $\langle n_e \rangle$ [Stangeby 2000],
 - & $T_e < 1 - 2$ eV or pressure drop along field line.
- Complicated interplay of many processes \Rightarrow different types of detachment.
 - Ion-neutral friction to removes momentum & power,
 - Recombination may be present, but not controlling,
 - Radiation trapping.
- Simulation of observed detachment behavior difficult [Wischmeier 2009].



[Pitcher 1997]

Lyman- α MFP \ll Local Dimensions for ITER Divertor

- For Ly- α ~ 0.2 cm / $n_D(10^{20} \text{ m}^{-3})$ [Post 1995],
 - \Rightarrow Photons reabsorbed by atoms \Rightarrow “trapped”.
- Couples plasma \leftrightarrow neutrals \leftrightarrow radiation,
 - & line shape effects important.
- EIRENE models photons in same way as atoms & molecules,
 - Add photo-excitation to H CR model [Reiter 2002],
 - Include Zeeman splitting, and, for Ly- α , fine structure Zeeman-Stark profiles [Reiter 2007].
 - 2x increase in ITER n_e , lower T_e [Reiter 2007].
 - $\sim 100\%$ of Ly- α trapped & 60–90% inner divertor ionization due to “radiative stimulated ionization”.
- Alternative: add plasma transport model to NLTE code CRETIN [Adams 2004],
 - Used to benchmark modified CR rates [Scott 2004] $\Rightarrow S_{\text{eff}}(n_e, T_e, L)$, $R_{\text{eff}}(n_e, T_e, L)$ & use in existing plasma & neutral transport codes.
 - Approximate treatment may suffice for high opacity [Scott 2004], [Kotov 2006].

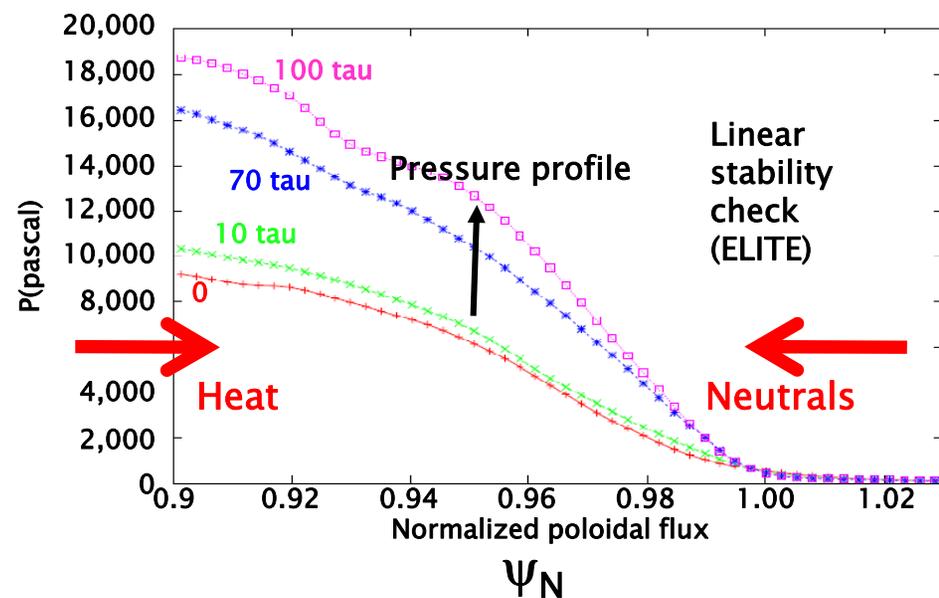


[Adams 2003]

How Important are Neutrals for Edge Turbulence & Transport?

- Investigated by Center for Plasma Edge Simulation
 - SciDAC Proto-FSP, C. S. Chang - PI.
- Developing simulations of edge pedestal buildup & ELM crash via:
 - XGC0 - kinetic neoclassical guiding center particle code [Chang 2004],
 - DEGAS 2 - kinetic Monte Carlo neutral transport code,
 - ELITE- Linear MHD code,
 - M3D - Extended MHD code.
- Roles in problem:
 - XGC0 - Plasma transport, self-consistent E_r ,
 - DEGAS 2 - Ionization source feeding pedestal buildup,
 - ELITE- detect ELM instability,
 - M3D - simulate nonlinear ELM crash.
- Other impacts of neutrals being investigated,
 - E.g., modifications to ion distribution function.

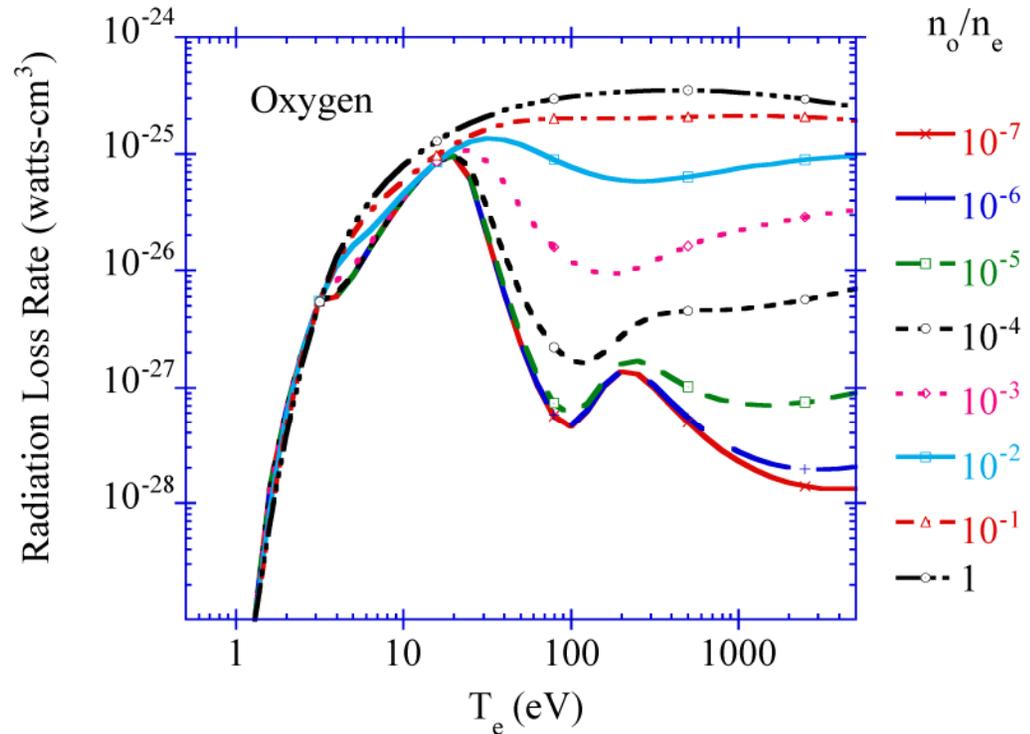
Pedestal buildup in XGC0



[Park 2007]

Pumping, Impurity Radiation & Diagnostics

- Helium pumping [Kukushkin 2009]
 - Code results given high credibility,
 - Used to evaluate divertor design.
- Impurity CX with H,
 - Reduces average charge state \Rightarrow increased radiation.
- Neutral based diagnostics
 - CX recombination spectroscopy,
 - Gas puff imaging, etc.
 - Beam emission spectroscopy,
 - Motional Stark Effect.



[Post 1995]

Conclusions

- Do we understand neutral transport?
 - Why else would we develop detailed 3-D, kinetic, neutral transport models?
- But, we don't have a complete picture:
 - Simulations depend on uncertain plasma parameters,
 - Incomplete atomic physics data,
 - And rudimentary PMI.
- We've got a lot of work to get to a predictive model:
 - Fusion Simulation Program,
 - Expanding PMI research effort.

References

- [Adams 2004] M. L. Adams and H. A. Scott, “Effect of Hydrogen Line Radiation on the Divertor Target Plate Incident Heat Flux”, *Contrib. Plasma Phys.* 44, 262 (2004).
- [Boswell 2001] C. Boswell et al., “Observations of Cold, High Density Plasma in the Private Flux Region of the Alcator C-Mod Divertor”, *J. Nucl. Mater.* 290–293, 556 (2001).
- [Chang 2004] C. S. Chang, S. Ku, and H. Weitzner, “Numerical Study of Neoclassical Plasma Pedestal in a Tokamak Geometry”, *Phys. Plasmas* 11, 2649 (2004).
- [Fantz 2001] U. Fantz et al., “Hydrogen Molecules in the Divertor of ASDEX Upgrade”, *J. Nucl. Mater.* 290–293, 367 (2001).
- [Federici 2001] G. Federici et al., “Plasma–Material Interactions in Current Tokamaks and their Implications for Next Step Fusion Reactors”, *Nucl. Fusion* 41, 1967 (2001).
- [Greenland 2001] P. T. Greenland, “Collisional–Radiative Models with Molecules”, *Proc. R. Soc. Lond. A* 457, 1821 (2001).
- [Janev 2002] R. K. Janev and D. Reiter, “Collision Processes of CH_y and CH_y^+ Hydrocarbons with Plasma Electrons and Protons”, *Phys. Plasmas* 9, 4071 (2002).
- [Janev 2004] R. K. Janev and D. Reiter, “Collision Processes of $\text{C}_{2,3}\text{H}_y$ and $\text{C}_{2,3}\text{H}_y^+$ Hydrocarbons with Plasma Electrons and Protons”, *Phys. Plasmas* 11, 780 (2004).
- [Kotov 2006] V. Kotov, “Numerical Study of the ITER Divertor Plasma with the B2–EIRENE Code Package”, Ph. D. Dissertation, Ruhr–Universität Bochum (2006).

References (cont.)

- [Kotov 2009] V. Kotov, D. Reiter, A. S. Kukushkin, and H. D. Pacher, *Phys. Scr.* T138, 014020 (2009).
- [Krasheninnikov 1997] S. I. Krasheninnikov, “Plasma–Neutral Gas Interaction in a Tokamak Divertor”, *J. Nucl. Mater.* 241–243, 283 (1997).
- [Krstic 1998] P. S. Krstic and D. R. Schultz, “Elastic and Related Transport Cross Sections for Collisions Among Isotopomers of $H^+ + H$, $H^+ + H_2$, $H^+ + He$, $H + H$, and $H + H_2$ ”, *At. Plasma–Mater. Data Fus.* 8, 1 (1998).
- [Kukushkin 2005] A. S. Kukushkin et al., “Effect of Neutral Transport on ITER Divertor Performance”, *Nucl. Fusion* 45, 608 (2005).
- [Kukushkin 2009] A. S. Kukushkin et al., “Analysis of the Optimized Divertor in ITER”, *Nucl. Fusion* 49, 075008 (2009).
- [Lang 1997] P. T. Lang et al., “High–Efficiency Plasma Refuelling by Pellet Injection from the Magnetic High–Field Side into ASDEX Upgrade”, *Phys. Rev. Lett.* 79, 1487 (1997).
- [Lisgo 2005] S. Lisgo et al., “OSM–EIRENE Modeling of Neutral Pressures in the Alcator C–Mod Divertor”, *J. Nucl. Mater.* 337–339, 139 (2005).
- [Loch 2006] S. D. Loch et al., “Generalized Collisional–Radiative Model for Light Elements. A: Data for the Li Isonuclear Sequence”, *At. Data and Nucl. Data Tables* 92, 813 (2006).
- [Loch 2009] S. D. Loch, C. P. Balance, M. S. Pindzola, and D. P. Stotler, “The Role of Excited State Ionization Data on H and He Generalized Collisional–Radiative Coefficients”, *Plasma Phys. Control. Fusion* 51, 105006 (2009).
- [Park 2007] G.Y. Park, J. Cummings, C.S. Chang, N. Podhorszki, S. Klasky, et al., “Coupled Simulation of Kinetic Pedestal Growth and MHD ELM Crash”, *J. Phys. Conf. Series* 78, 012087 (2007).

References (cont.)

- [Pigarov 2002] A. Yu. Pigarov, “Collisional Radiative Kinetics of Molecular Assisted Recombination in Edge Plasmas”, *Physica Scripta* T96, 16 (2002).
- [Pitcher 1997] C. S. Pitcher et al., “SOL Power and Pressure Balance in Alcator C-Mod”, Proc. Of 24th EPS Conference, 1997, Berchtesgaden, Germany, vol. 21A, part II, p. 581.
- [Pitts 2009] R. A. Pitts et al., “Status and Physics Basis of the ITER Divertor”, *Phys. Scr.* T138, 014001 (2009).
- [Post 1995] D. E. Post, “A Review of Recent Developments in Atomic Processes for Divertors and Edge Plasmas”, *J. Nucl. Mater.* 220–222, 143 (1995).
- [Reiter 2002] D. Reiter et al., “Towards Radiation Transport Modelling in Divertors with the EIRENE code”, *Plasma Phys. Control. Fusion* 44, 1723 (2002).
- [Reiter 2007] D. Reiter et al., “Detailed atomic, molecular and radiation kinetics in current 2D and 3D edge plasma fluid codes”, *J. Nucl. Mater.* 363–365, 649 (2007).
- [Reiter 2009] D. Reiter, B. Koppers, and R. K. Janev, “Hydrocarbons in Edge Plasmas: a Sensitivity Analysis”, *Phys. Scr.* T138, 014014 (2009).
- [Sawada 1995] K. Sawada and T. Fujimoto, “Effective Ionization and Dissociation Rate Coefficients of Molecular Hydrogen in Plasma”, *J. Appl. Phys.* 78, 2913 (1995).
- [Scott 2004] H. A. Scott and M. L. Adams, “Incorporating Line Radiation Effects into Edge Plasma Codes”, *Contrib. Plasma Phys.* 44, 51 (2004).
- [Stangeby 2000] Peter C. Stangeby, *The Plasma Boundary of Magnetic Fusion Devices* (Institute of Physics Publishing, Philadelphia, 2000).
- [Wischmeier 2009] M. Wischmeier et al., “Current Understanding of Divertor Detachment: Experiments and Modelling”, *J. Nucl. Mater.* 390–391, 250 (2009).

Interpretation of Light Emission

- Neutral transport calculations readily yield volumetric light emission (e.g., D α) amenable to calculation of synthetic diagnostics and comparison with experimental data.
- However, emission rates may be sensitive to T_e ,
 - And n_e , T_e may vary locally over short times due to intermittent turbulent transport,
 - Because emission nonlinear function of T_e , time average emission \neq emission at average T_e .
- Interpretation further complicated by light reflections,
 - Occasionally problematic in past,
 - Much more so with full metal machines and shiny Li coatings,
 - For Li, using Ly- α lines instead.