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NSTX-U

Modeling of surface temperature effects on mixed-material migration in NSTX-U

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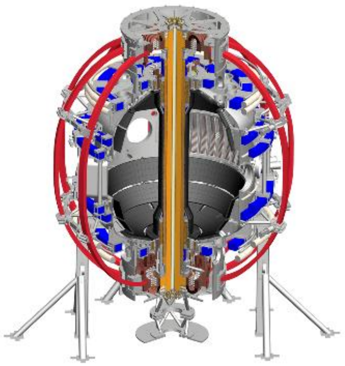
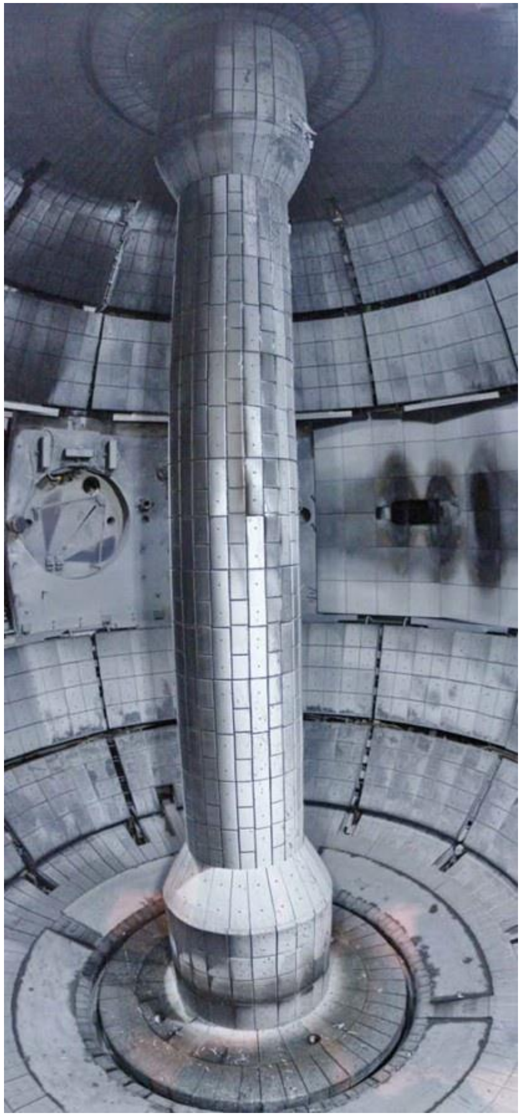


Summary

- Temperature-dependent sputtering of lithium has been added to the WallDYN mixed material migration code
- Thermally-enhanced sputtering leads to small qualitative net change in Li areal density near strike points
  - However, large increase in gross sputtering and redeposition
- Simulations show that a peaked PFC temperature profile (e.g. due to plasma heating) depletes a Li layer faster than an equivalent uniform temperature profile

Material migration is key for understanding wall conditioning and impurity sources in tokamaks

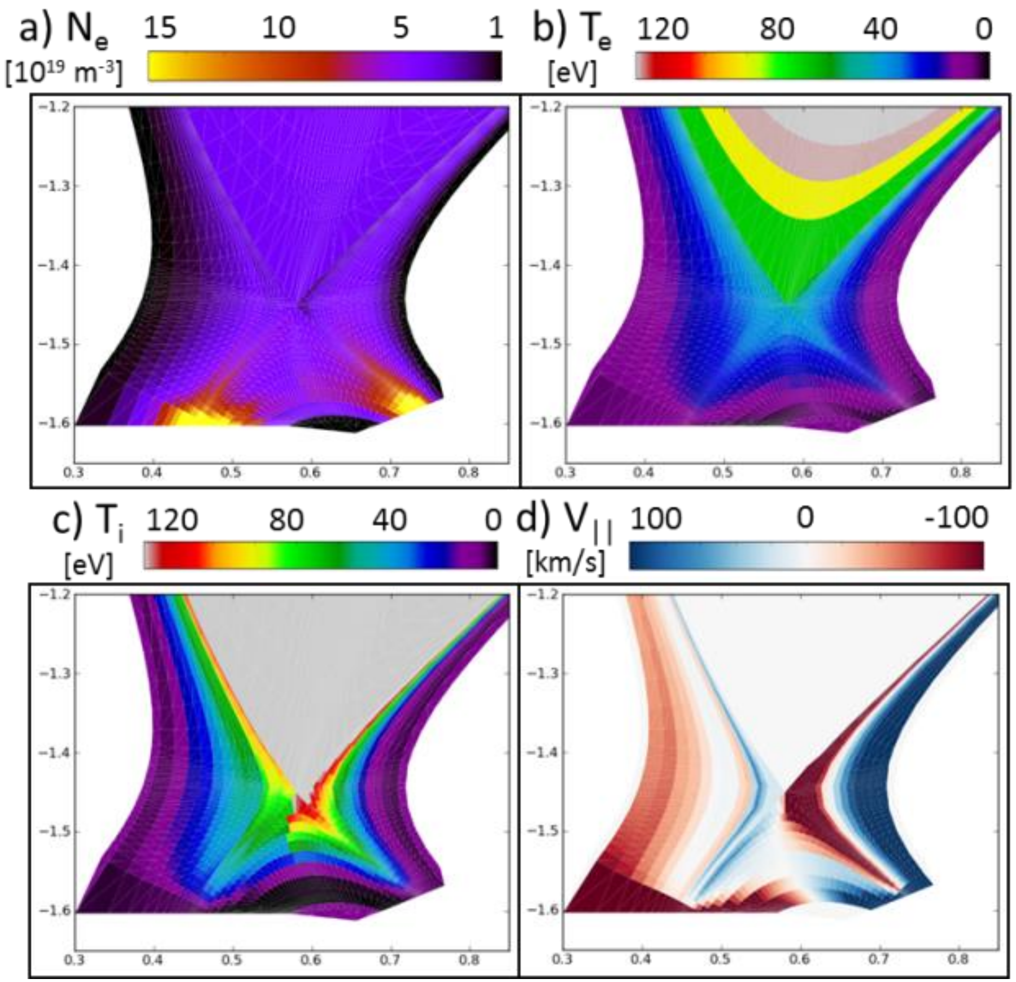


- In mixed material machines, first wall composition evolves in time due to erosion, transport, and redeposition
  - Occurs at different rates for different materials
- Material migration in NSTX-U is complex due to wide range of mixed materials
  - C, Li, O, B, Mo (future) + compounds/alloys
- NSTX used Li evaporation to improve plasma performance
  - Evidence of qualitative Li surface changes on time scales of 1-10 shots (migration, passivation, compound formation)
  - Ad hoc conditioning “recipes” used rather than quantitative understanding

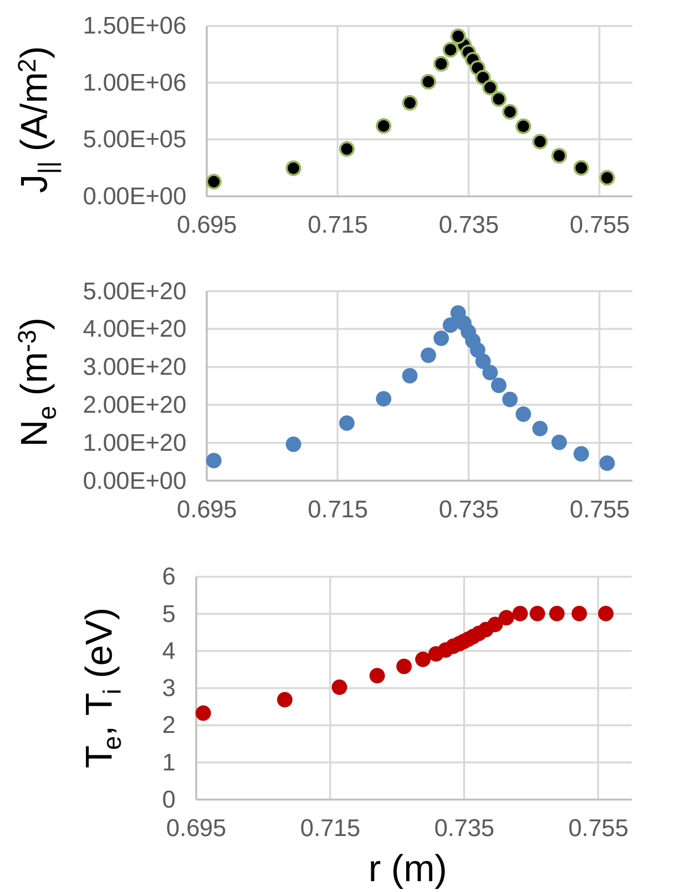
WallDYN calculates material migration in tokamaks in a computationally attractive way

- Interplay between impurity erosion, transport, and deposition means that plasma and wall processes must be treated concurrently
  - Involves wide range of length and time scales (10^{-10}-10^{1} m, 10^{-6}-10^{2} s)
  - Iteration between relevant plasma + surface codes computationally difficult due to scale difference
- Our approach: WallDYN [K. Schmid J. Nucl. Mater. 415 (2011) S284-288]
  - Treats plasma transport and surface processes as rate equations, determined by parameterizing more advanced codes and models
  - Solves differential algebraic system of equations simultaneously rather than iteratively (<1 hr CPU time for 30s plasma exposure on NSTX grid)
  - Calculates poloidally-resolved, time-dependent surface concentration and impurity flux evolution
  - Assumes PMI & plasma transport timescales << wall evolution timescale
  - Assumes single, representative plasma solution for one shot
  - Maintains global material balance

Constant H-mode plasma background: NSTX shot 139396 (0.8 MA, 4 MW NBI heated)

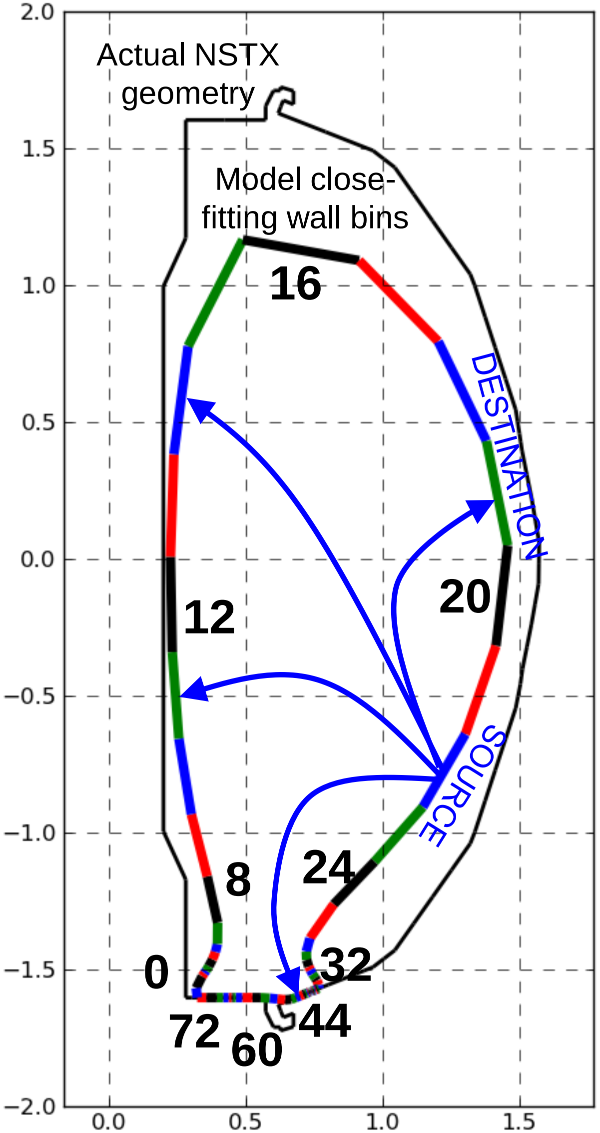


Measured Outer Target Probe Data



– At these plasma parameters, the net force on most impurities is dominated by the friction force (follows $v_{||}$ profile)

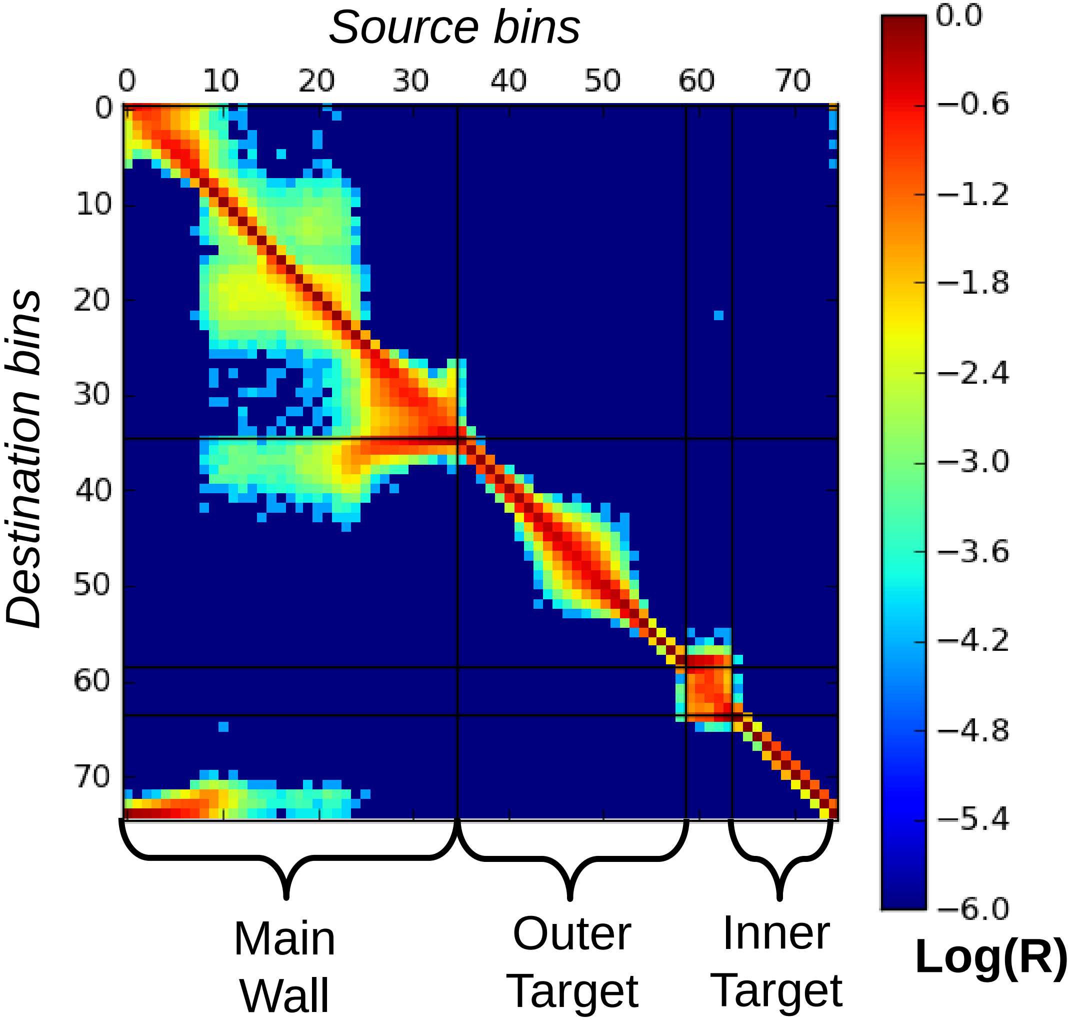
Impurity transport in plasma handled by Monte Carlo impurity code DIVIMP



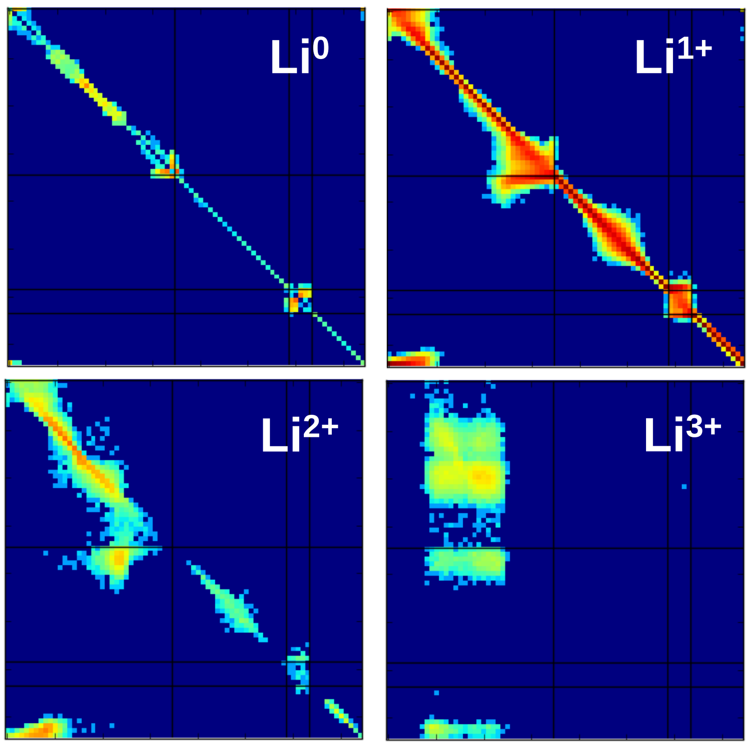
- Wall elements are grouped into 75 bins
  - This work emphasizes resolution @outer target
  - Idealized wall conformal to plasma grid used while extended grid is in development
- 20000 particles are launched from each bin, and the final charge states and deposition locations are recorded
  - Particles are launched as atoms with cosine angular distribution and Thompson energy distribution (to simulate sputtered particles)
- Each DIVIMP run provides a column of the redistribution matrix
  - 225 DIVIMP runs for each plasma solution
- Assumes plasma background does not change with impurity content

Lithium redistribution matrices show that deposition is primarily ionic, local

<u>Charge-integrated Li redistribution matrix</u>



<u>Charge-resolved redistribution matrices</u>



R = probability particle launched from X deposits on Y

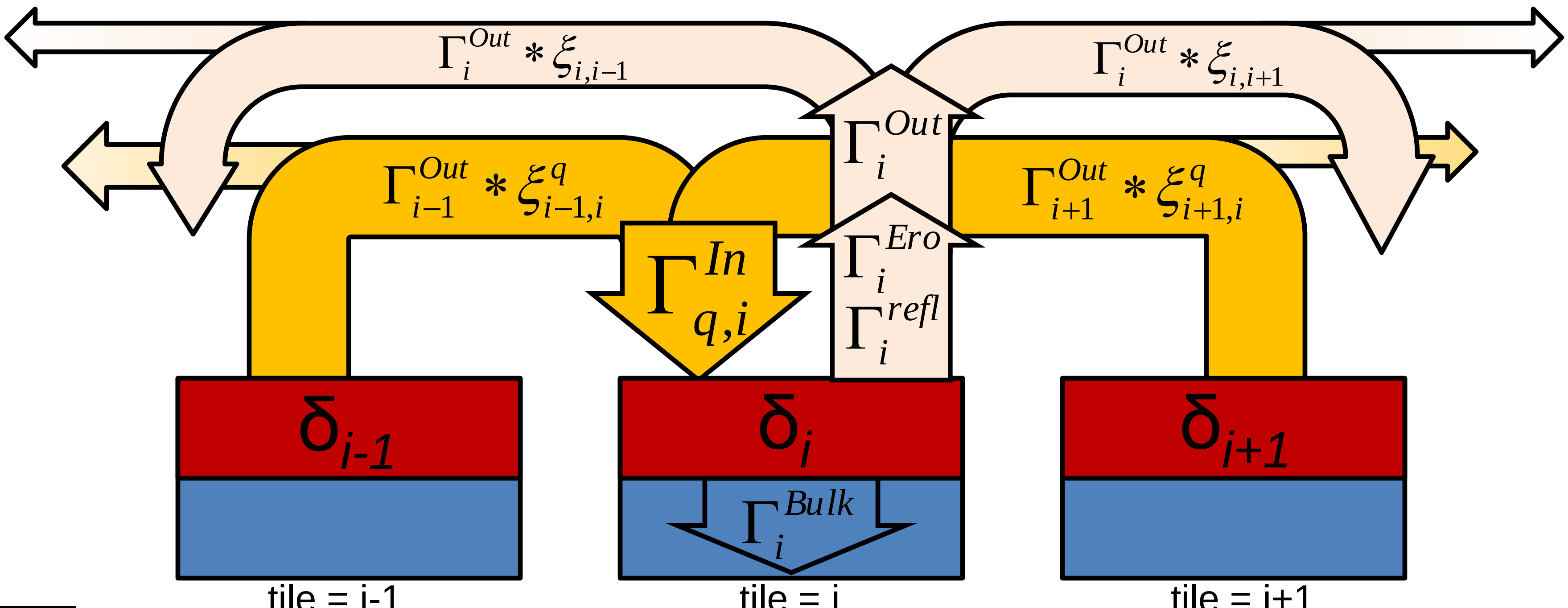
WallDYN couples plasma/surface rates by solving a system of differential-algebraic equations

δ_{tile} : Areal density of element on tile

q : Charge state of element

$\xi^{\text{charge state}}_{\text{source,destination}}$: Charge-resolved redist. matrix entry

Subscript for "element" is suppressed on this slide (applies to every term)



$$\frac{d\delta_i}{dt} = \sum_{q=1}^{Nq} \Gamma_{q,i}^{In} - \Gamma_i^{refl} - \Gamma_i^{Ero} + \Gamma_i^{Bulk}$$

$$\Gamma_{q,i}^{In} = \sum_{tile=1}^{NTiles} \left(\Gamma_{tile}^{Ero} + \Gamma_{tile}^{refl}\right) * \xi^q_{tile,i}$$

- Differential-algebraic equation system (~2000 eqs) solved in Mathematica

WallDYN surface model basics

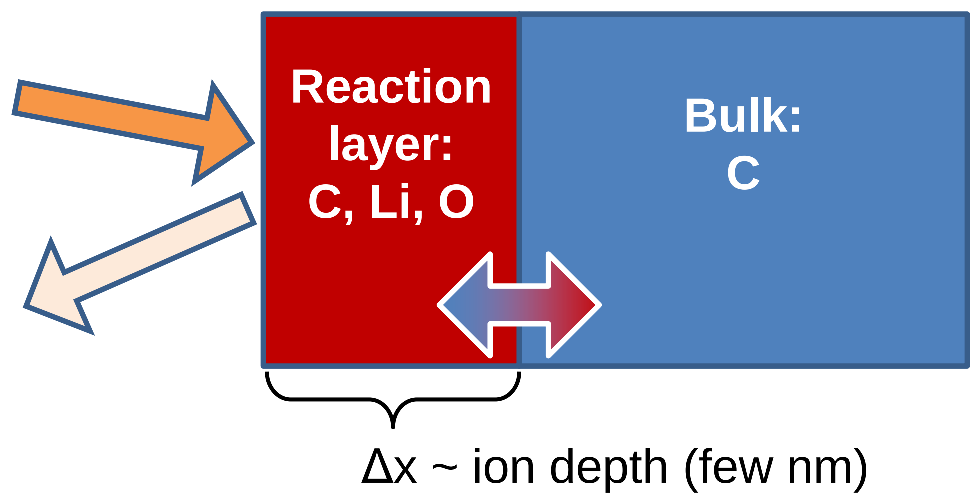
- Homogenous reaction layer on top of homogenous bulk
  - Composition of reaction layer is variable, composition of bulk is fixed
  - All erosion & deposition occurs homogenously in reaction layer
  - Reaction layer width held fixed via bulk exchange
  - Assume that trapped hydrogen does not affect sputtering rates
- Physical sputtering and D-C chemical erosion included
- *New: Thermally-enhanced Li adatom sputtering model*

<u>Incident fluxes:</u>

- Constant D+, D-CX fluxes
- Energy-resolved redeposited impurity fluxes

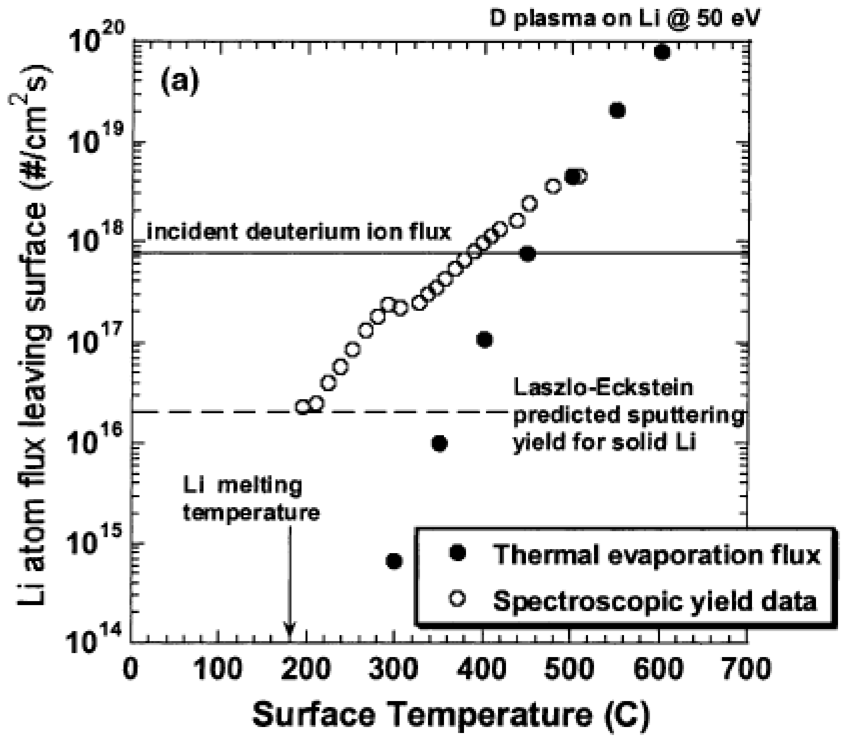
<u>Outgoing fluxes:</u>

- Eroded impurity fluxes
- Reflected impurity fluxes



Test stand Li sputtering studies have shown unexpected thermally-enhanced erosion

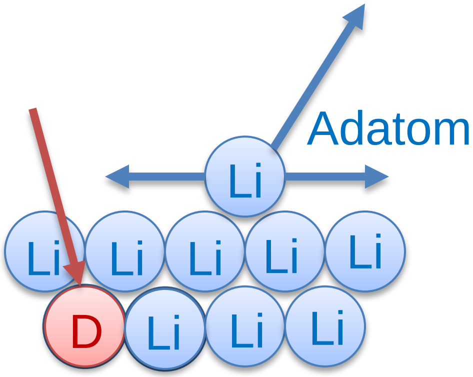
- Enhanced erosion occurs at significantly lower temperatures than evaporation onset
  - Important at temperature ranges used in liquid Li divertor schemes
  - Dependent on incident species
  - Independent of incident flux/energy in most datasets
    - Reason for outlying datasets not fully understood
- Not accounted for in previous WallDYN simulations
- Be also shows thermally-enhanced erosion at T>1000K

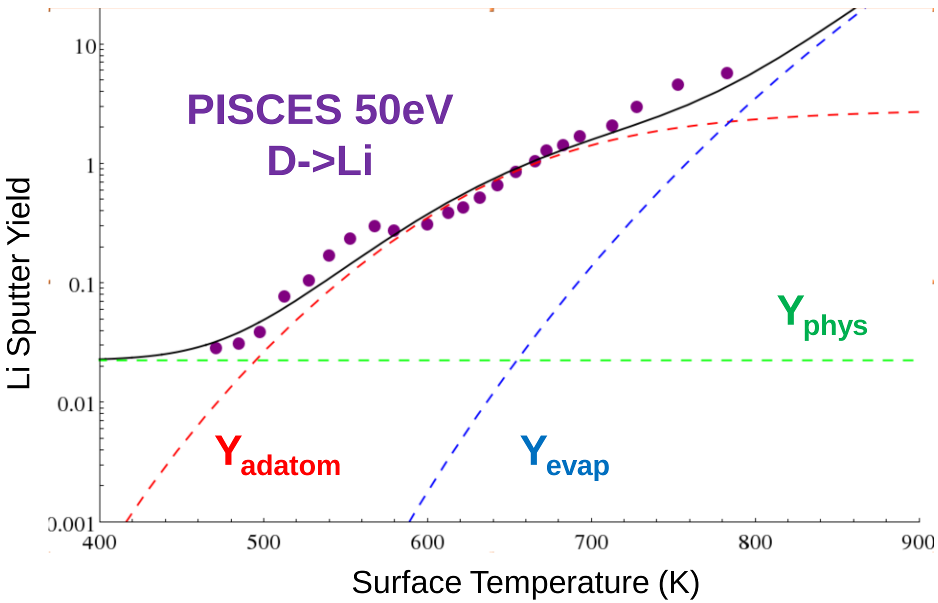


From Doerner JNM 2001

Adatom sputtering model adequately describes observed Li erosion enhancement

- What is an adatom?
  - Atom in excited state that does not have sufficient energy to sputter following sputtering cascade
  - Either diffuses across surface to recombination site, or evaporates/sublimates
  - Yield depends on ratio of adatom surface binding energy to surface diffusion activation energy





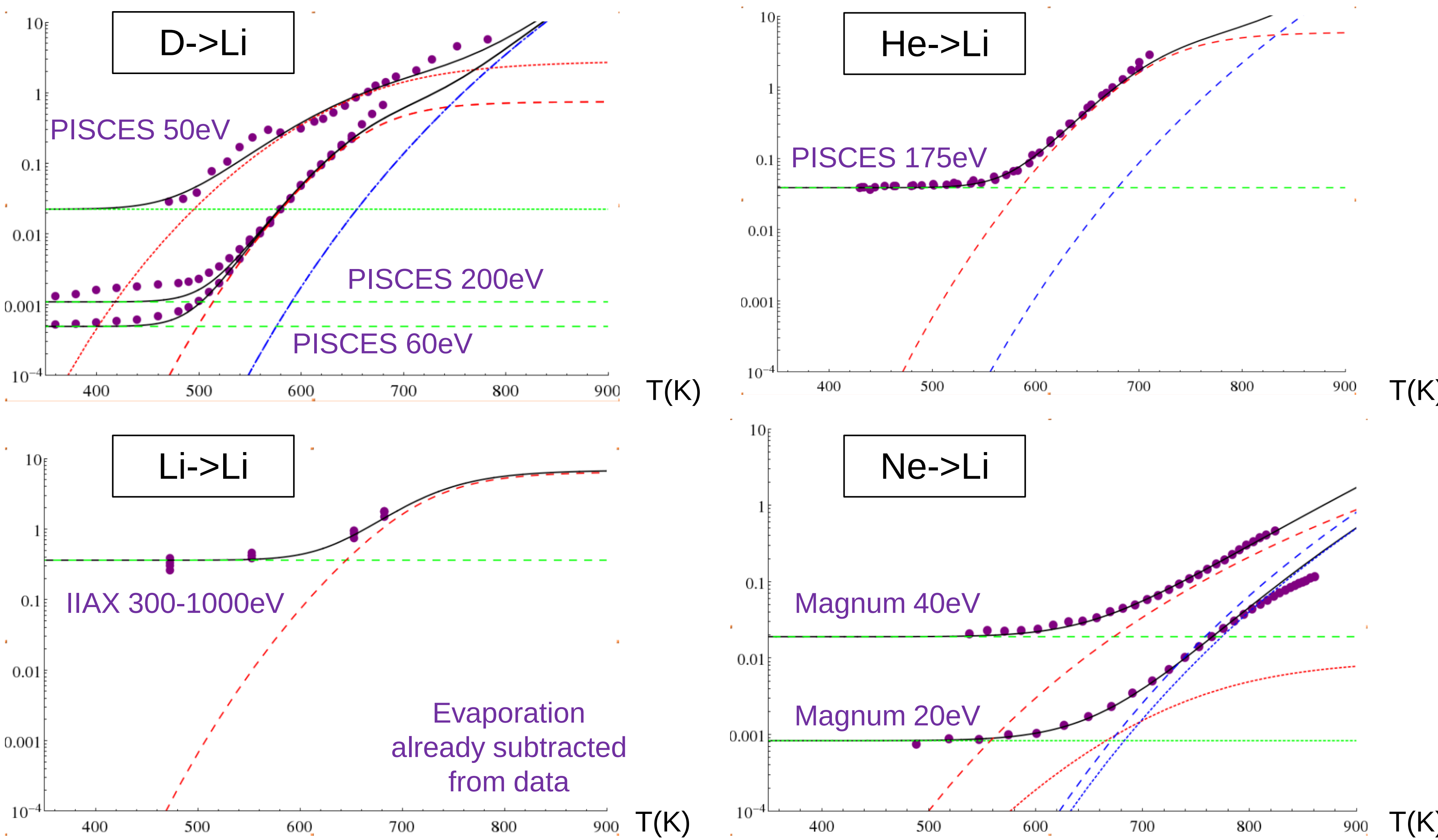
- Adatom sputtering model:

$$\Gamma_{Ero}(E,T) = Y_{phys}(E)\Gamma_{in} + Y_{adatom}(T)\Gamma_{in} + \Gamma_{evap}(T)$$

$$Y_{adatom} = \frac{Y_{ad}}{1 + A * \exp(E_{eff}/kT)}$$

3 fit parameters: Y_{ad}, A, E_{eff}

Fits made to existing temperature-dependent Li sputtering datasets and added to WallDYN

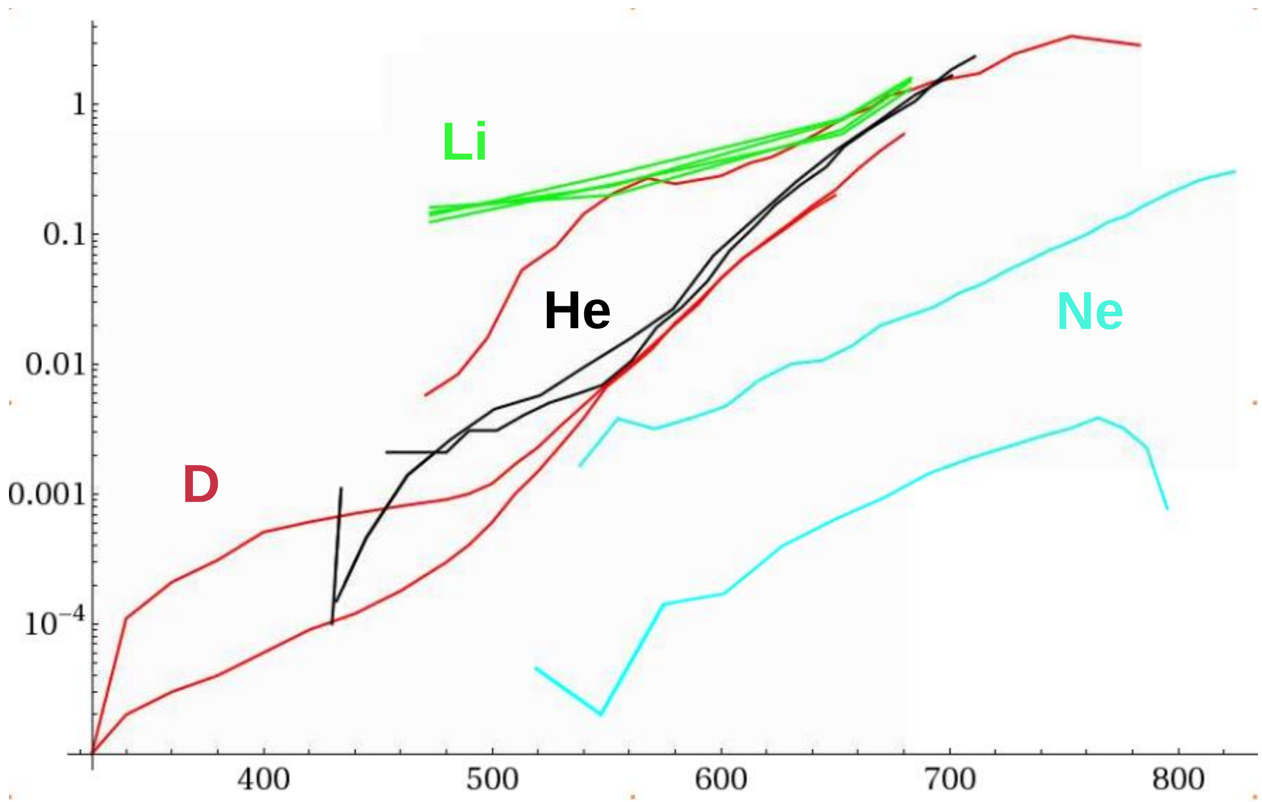


Thermally-enhanced Li sputtering term shows no trends with incident mass

- No datasets exist for $Y_{C\text{->}Li}$, $Y_{O\text{->}Li}$ vs temperature
- Given lack of data or trends, assume $Y_{adatom,C/O} = 0$ in these simulations
  - Gross surface behavior is dominated by $Y_{D\text{-}Li}$, so effect expected to be small

Adatom yield for X -> Li

$$Y_{adatom} = Y_{tot} - Y_{phys} - Y_{evap}$$



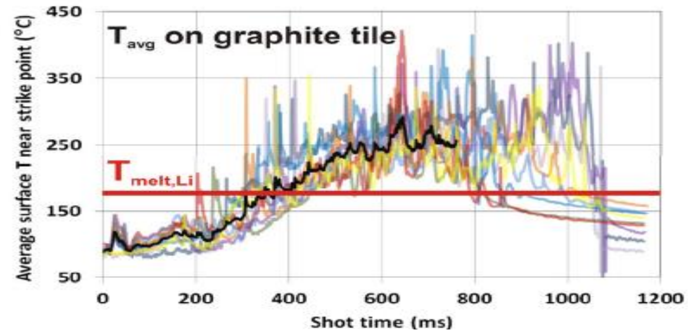
Exercise WallDYN model with 2 temperature profiles, representing likely reactor scenarios

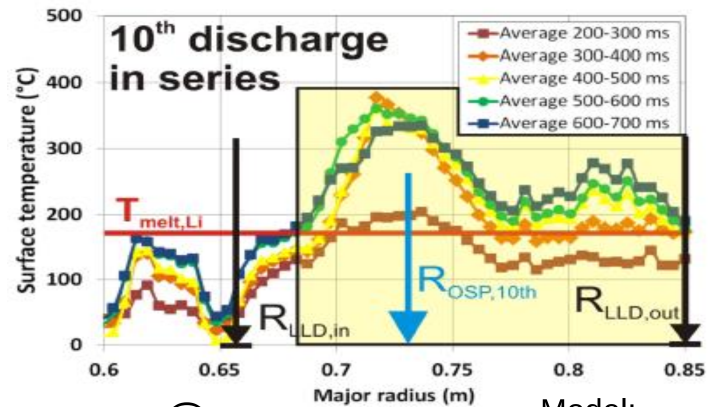
- Scenario 1: uniform wall temperature
  - Conceptually similar to actively heated PFCs
  - Ad hoc model 300K, 400K, 500K, 600K
    - T>>600K not properly modeled in WallDYN due to how extreme Li evap. fluxes can change near-surface plasma

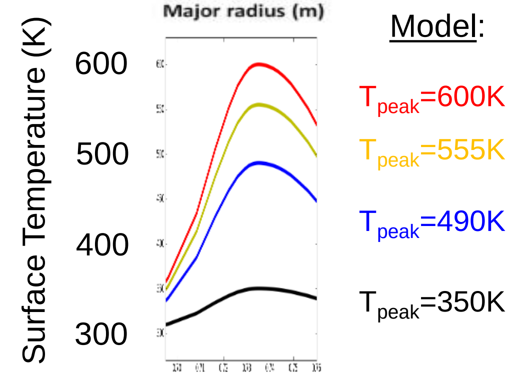
- Scenario 2: wall temp. peaked at strike point
  - Conceptually similar to PFCs naturally heated by plasma during a single discharge
  - Peak T, profile width set

    by 2010 IR data
    - T_{peak}=350K, 490K, 555K, 600K
    - T=300K outside divertor grid

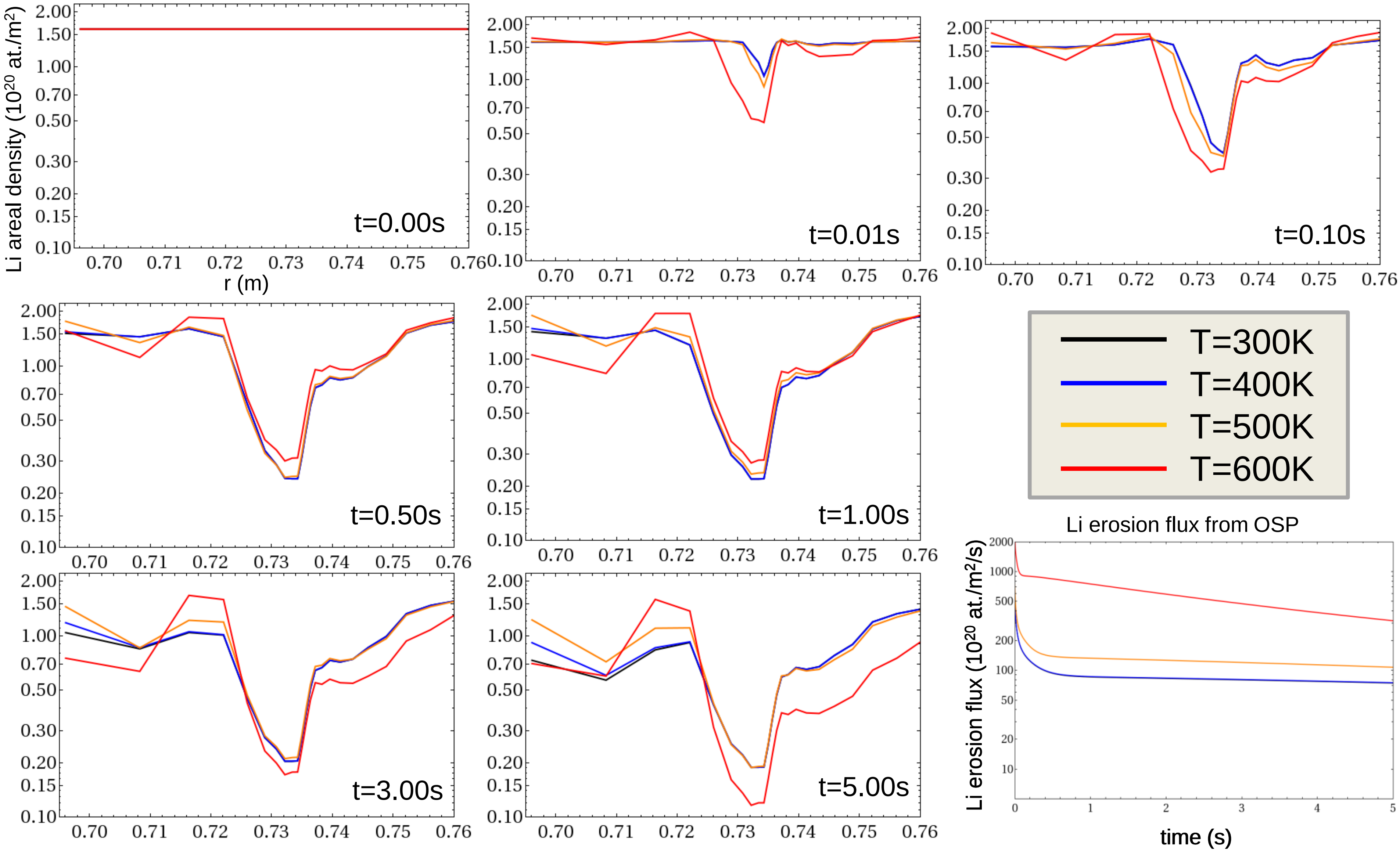
From McLean JNM 2013





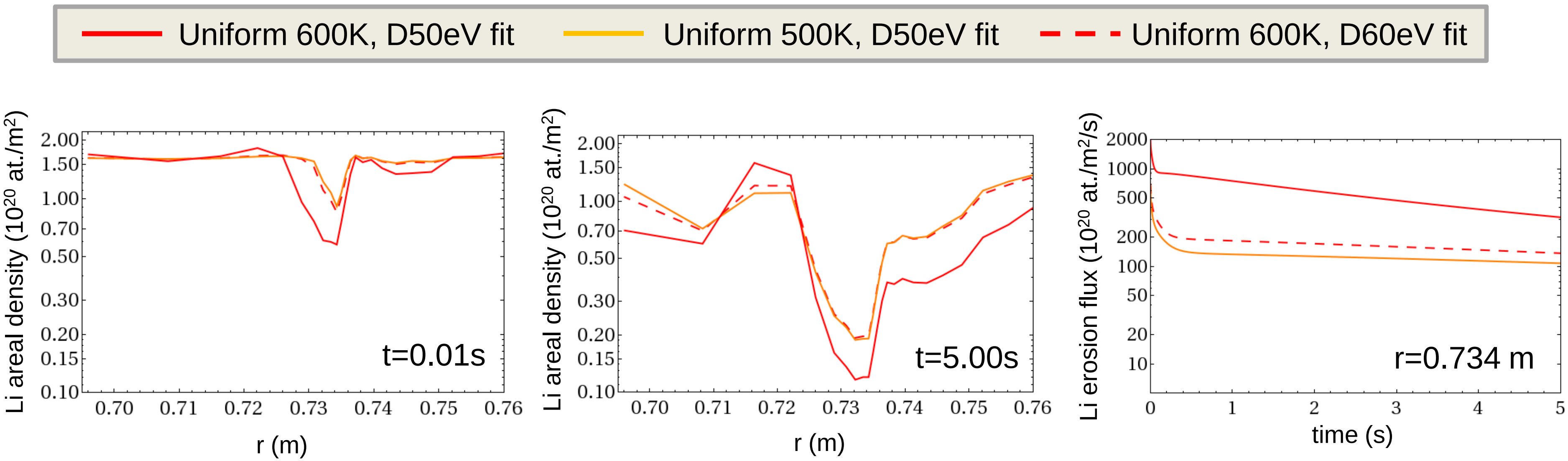


WallDYN results: uniform wall temperatures



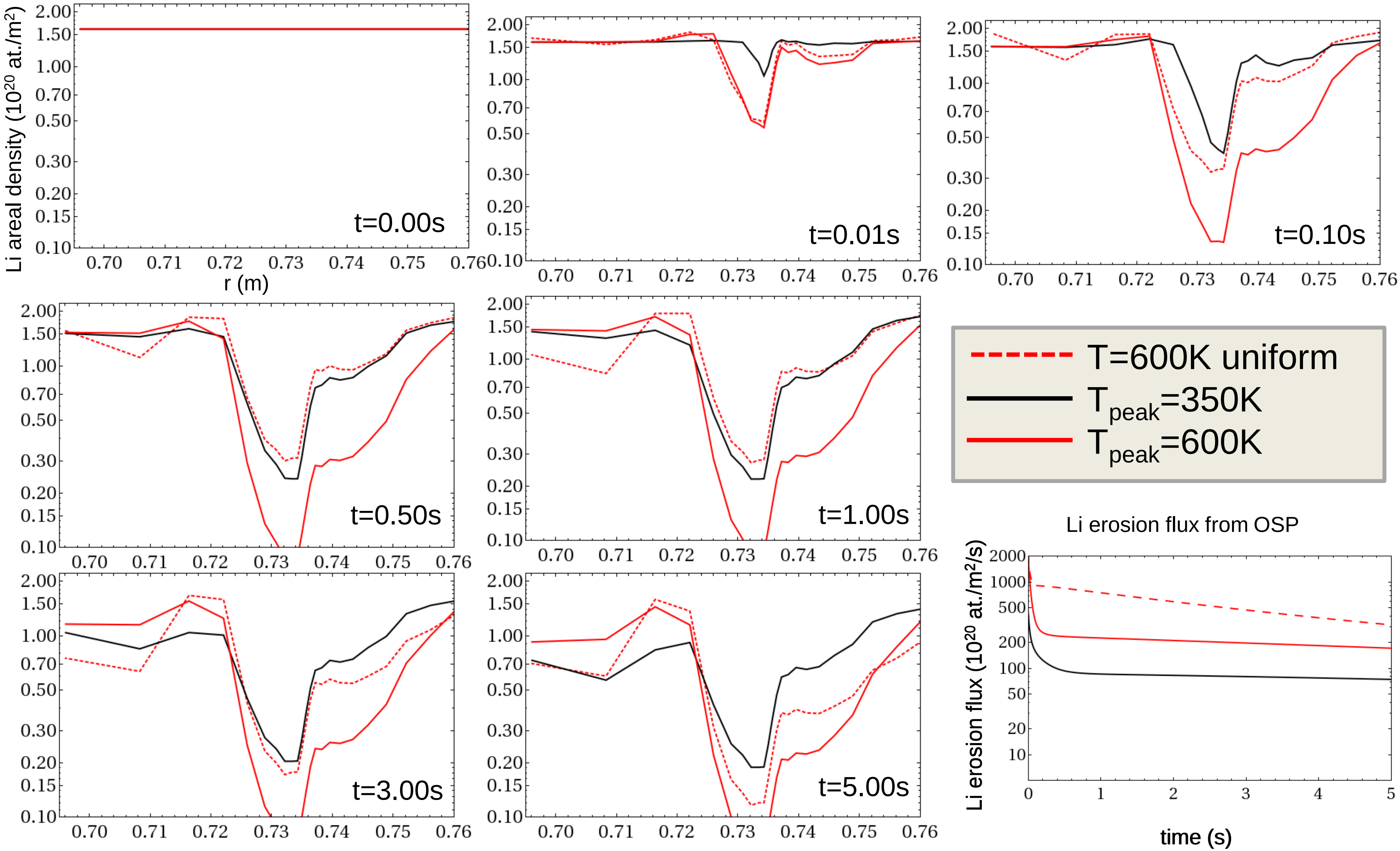
Using different D->Li data can lead to significant changes, but effect can be captured via T_{eff}

- Significant differences exist in PISCES D->Li datasets
  - 50eV dataset chosen as "standard" because it matches Y_{phys} from TRIM
- Effect of different D fits on WallDYN results:



- "Effective" T is 100K lower when using alternate D->Li dataset
- Recent work (Abrams NF 2016) has shown that D implantation also reduces thermal enhancement of Li sputtering
  - Further work is required to self-consistently incorporate this into WallDYN

WallDYN results: wall temperature peaked at strike point



Discussion

- For T<450K, temp-dependent Li sputtering can be ignored
- At higher T, Li migration patterns are qualitatively similar but quantitatively different
  - 10x higher Li erosion flux at high T (but higher redeposition flux too…)
- Individual transport steps are very small (~1cm near SP), and this has consequences for Li coverage
  - Rapid SP erosion leads to Li buildup immediately outside SP, which subsequently redeposits back at the SP once SP is aqeduately depleted
  - Thermally-enhanced erosion can change the timescales of transient erosion and redeposition, as well as increase gross lithium erosion
- A temperature profile peaked at the SP will deplete a Li coating faster than an equivalent uniform temperature profile
  - SP erosion is just as fast, but backfill from outside OSP is reduced
- Uncertainties in D->Li datasets do have an effect on model, but this analysis should provide an upper bound on thermal effect

Next steps for material migration modeling in NSTX-U

- Validation of Li WallDYN model for NSTX-U postponed to resumption of operations due to coil failure

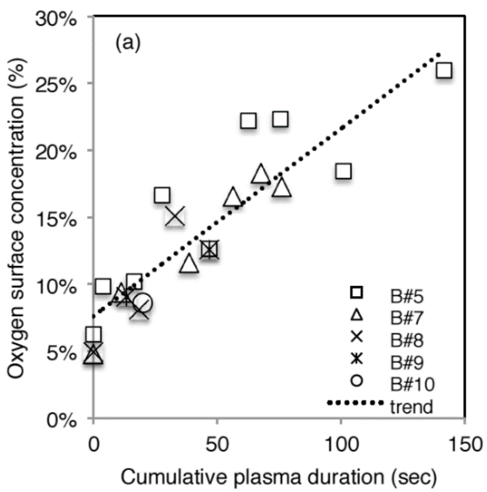
- Boronization (via dTMB) used in 2016 campaign, and WallDYN will be matched to available data
  - Key similarities between Li and B migration
    - Similar plasma transport patterns
    - Similar physical sputtering rates
  - Key differences between Li and B migration
    - Different chemical properties (especially D retention)
    - No temperature-dependent sputtering for B

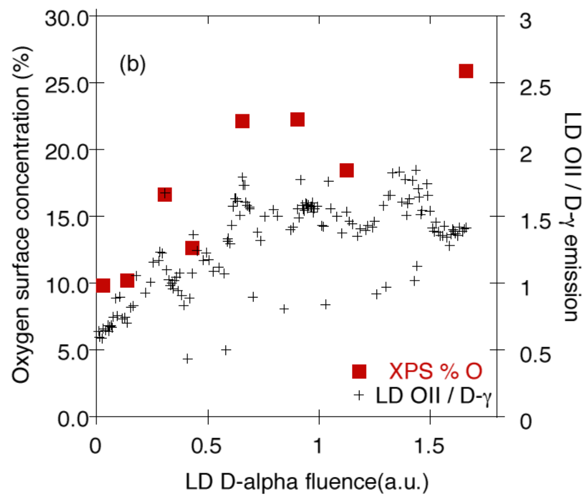
- This will be the first application of WallDYN to a fully low-Z machine, and to a spherical torus!

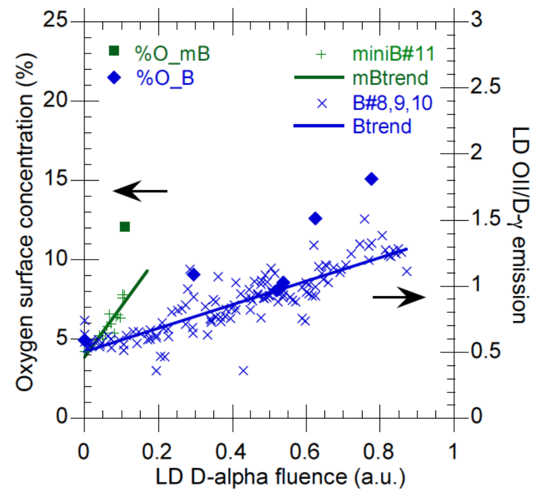
MAPP and spectroscopic data show clear evolution of divertor PFCs following boronization

- Suppression of O immediately following boronization, followed by a steady increase in O after plasma exposure
  - Consistent with thin-film B erosion
  - Rate of O increase depends most strongly on type of boronization (full bottle vs. ¼ bottle "mini")
- Comparatively little dependence on specific plasma configs.
  - Suggests campaign-integrated modeling approach may be successful

From Skinner PSI 2016

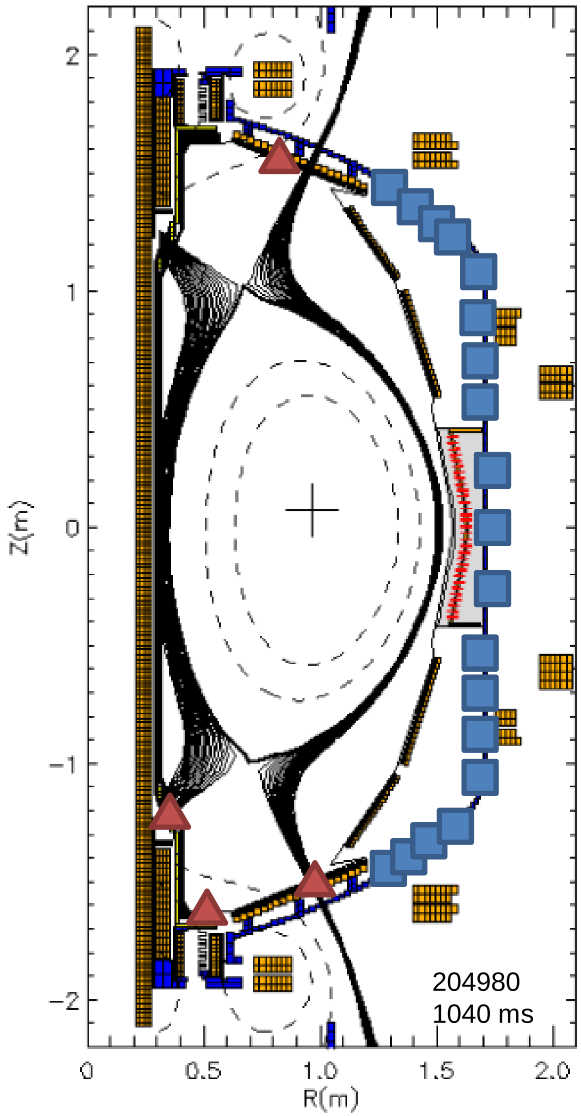






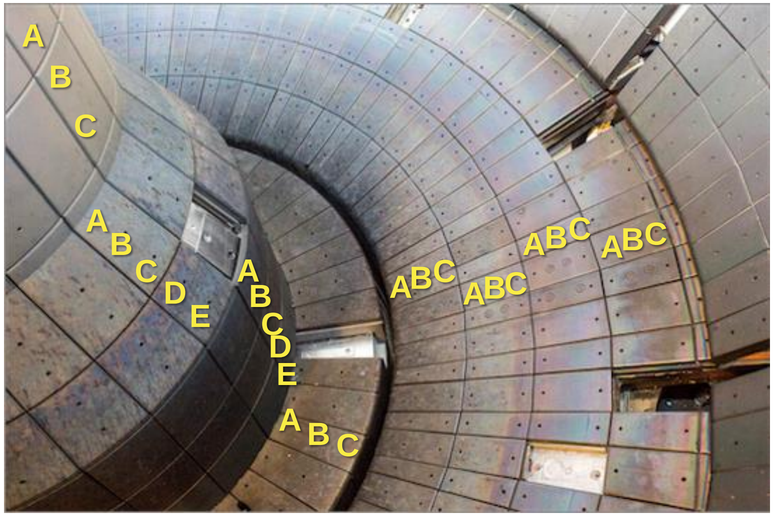
See also Tue AM Skinner GO6.8, Bedoya GO6.9

Post-mortem analysis is beginning on tiles and coupons exposed to 2016 NSTX-U campaign

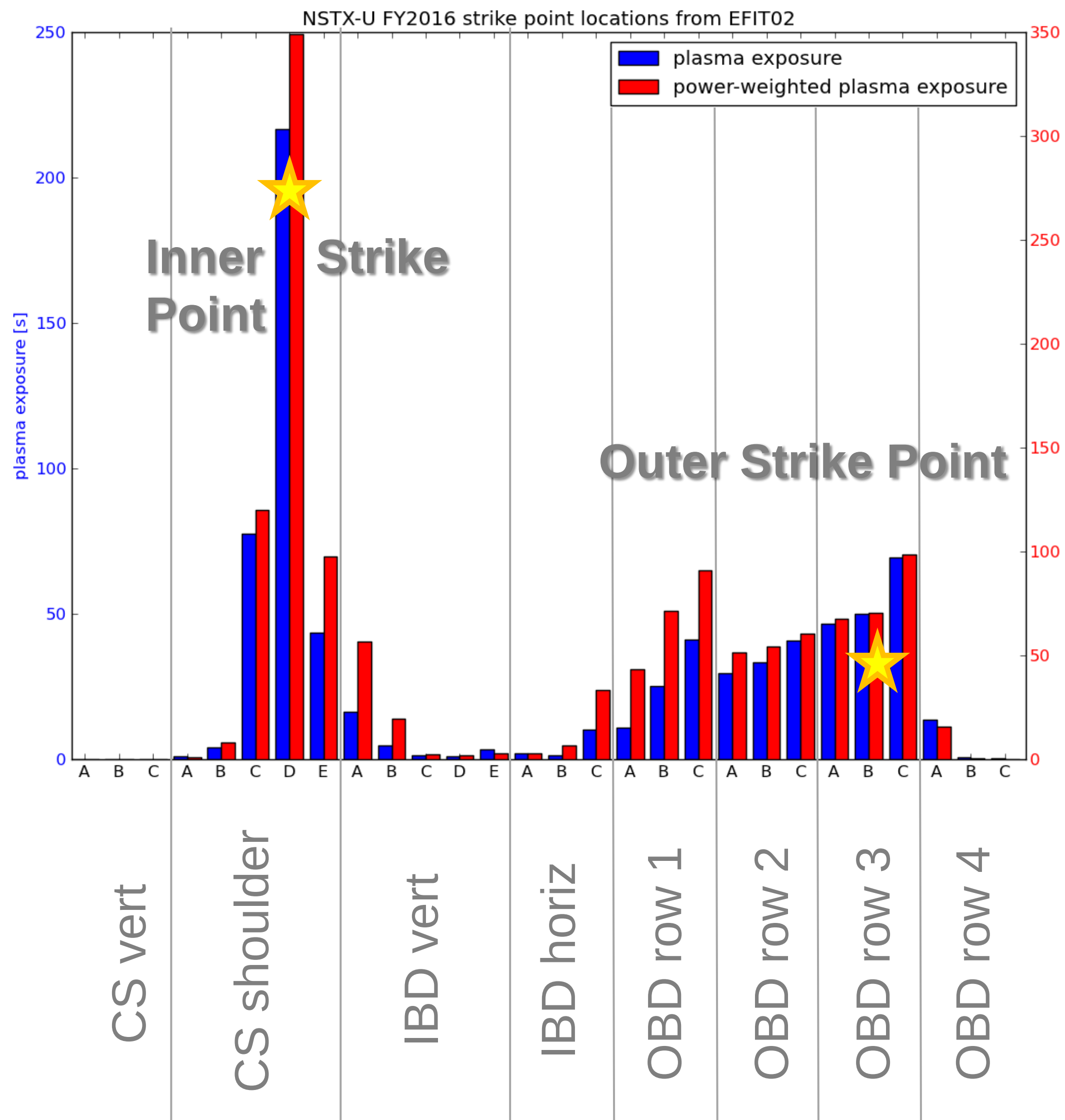


- Tile cores taken from graphite PFCs in 4 poloidal locations (▲)
  - Lower centerstack shoulder (ISP)
  - Lower horizontal inner divertor (PFZ)
  - Lower row 3 outer divertor (OSP)
  - Damaged upper outer divertor
  - HR-XPS, depth profiles, imaging, SIMS
- 23 1” Si coupons welded to vacuum vessel wall (■)
  - Poloidal & toroidal array
  - Line of sight to plasma via gaps between passive plates
  - NRA, RBS
- Analysis is PPPL/Princeton/UIUC collaboration

Most common 2016 NSTX-U discharge parameters identified for representative modeling



- Most common shape was double-null L-mode fiducial (★ on histograms)
  - ISP/OSP on cored tiles
  - Good candidate for campaign-integrated WallDYN modeling
  - Will also need to evaluate effect of OSP sweep



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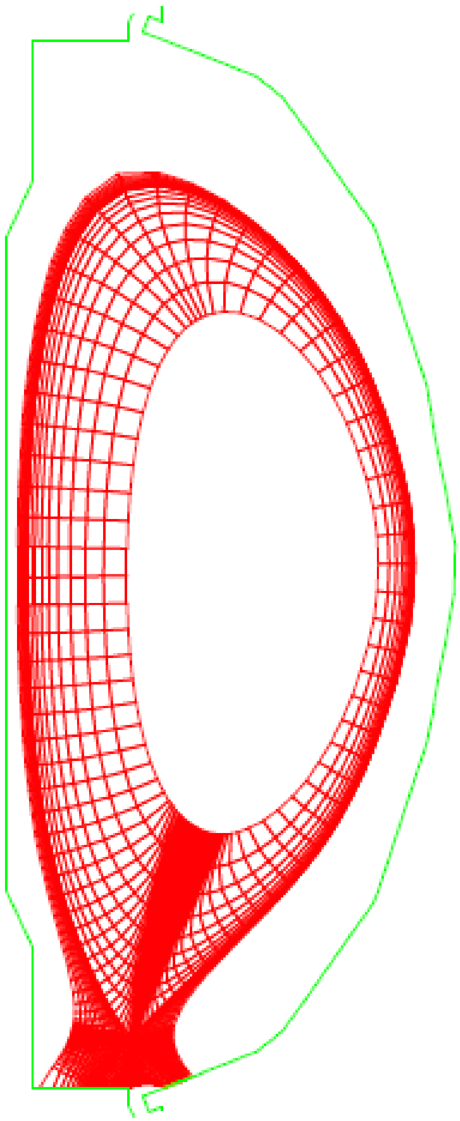
Plasma backgrounds generated by OEDGE suite (OSM + EIRENE + DIVIMP)



- Onion Skin Model (OEDGE SOL opt 22):
  - Target Langmuir probe data give boundary conditions for T_e, T_i, N_e
  - Solve fluid conservation equations in successive grid cells along field-aligned flux tubes

$$\frac{d}{ds}\left(n(s)\cdot v(s)\right)=S_{ioniz}(s)-S_{recom}(s)$$

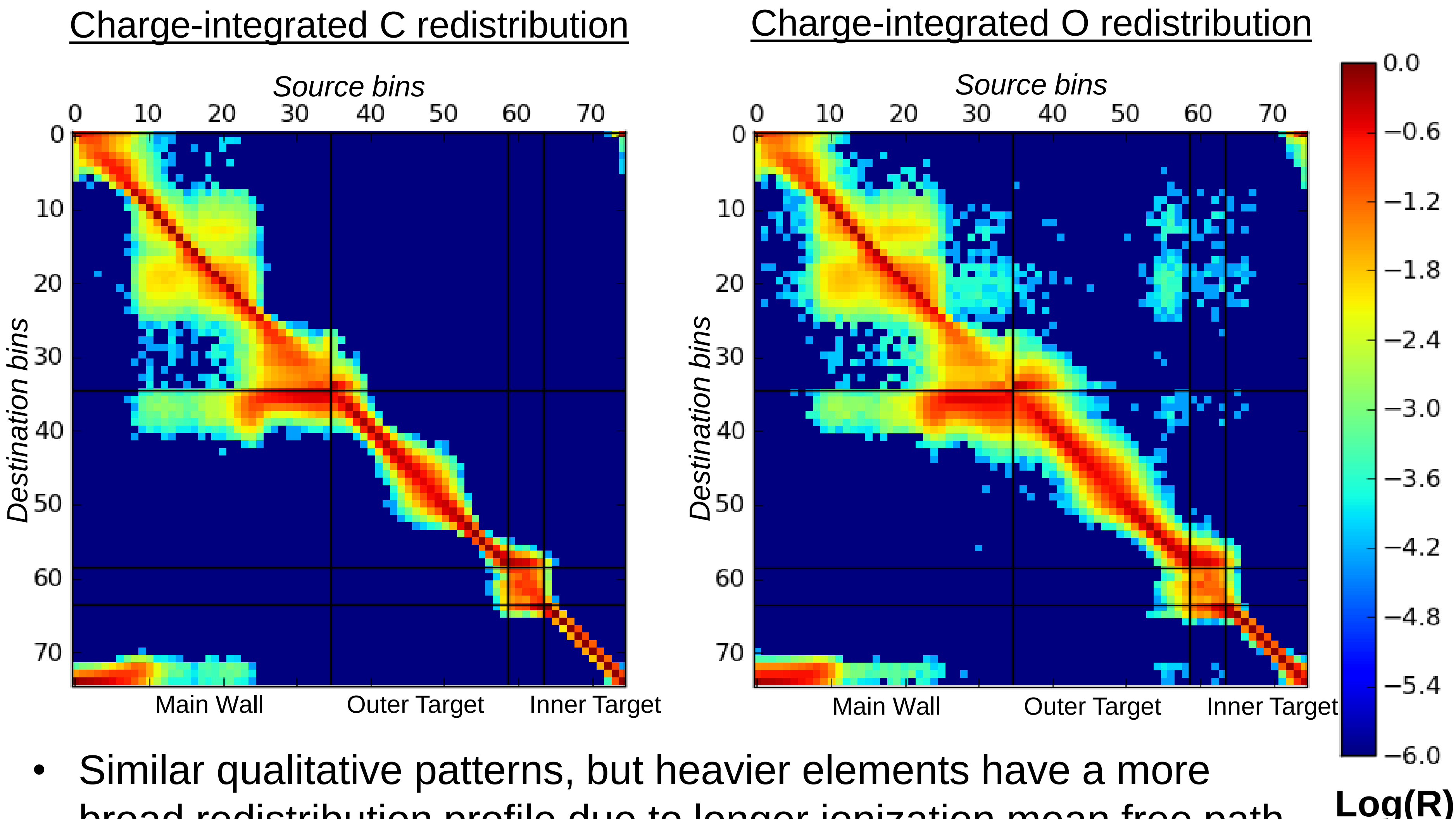
$$\frac{d}{ds}\left(\frac{5}{2}n(s)\cdot v(s)\cdot kT_e(s)-\kappa_{0e}\cdot T_e(s)^{5/2}\frac{dT_e(s)}{ds}\right)=-P_{rad}(s)-P_{helpi}(s)-P_{ei}(s)$$

$$\frac{d}{ds}\left(\frac{5}{2}n(s)\cdot v(s)\cdot kT_i(s)+\frac{1}{2}m\cdot n(s)\cdot v(s)^3-\kappa_{0i}\cdot T_i(s)^{5/2}\frac{dT_i(s)}{ds}\right)=-P_{cx}(s)+P_{ei}(s)$$

$$\frac{d}{ds}\left(n(s)\cdot\left(kT_e(s)+kT_i(s)\right)+n(s)\cdot m\cdot v(s)^3\right)=S_{mom}(s)$$

  - Iterate with EIRENE for hydrogenic ionization/power/momentum sources and sinks
- WallDYN also compatible with SOLPS, etc.

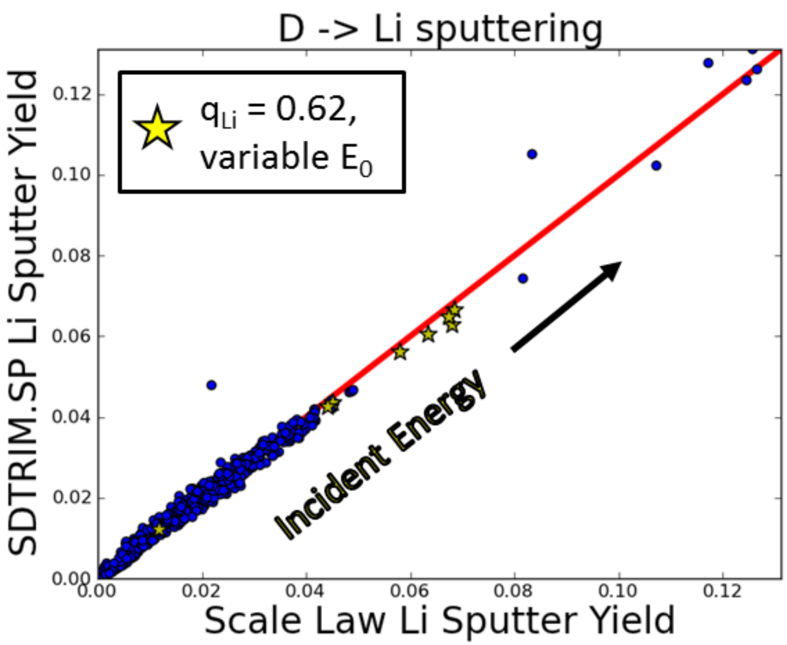
Carbon, Oxygen redistribution matrices are qualitatively similar to Lithium

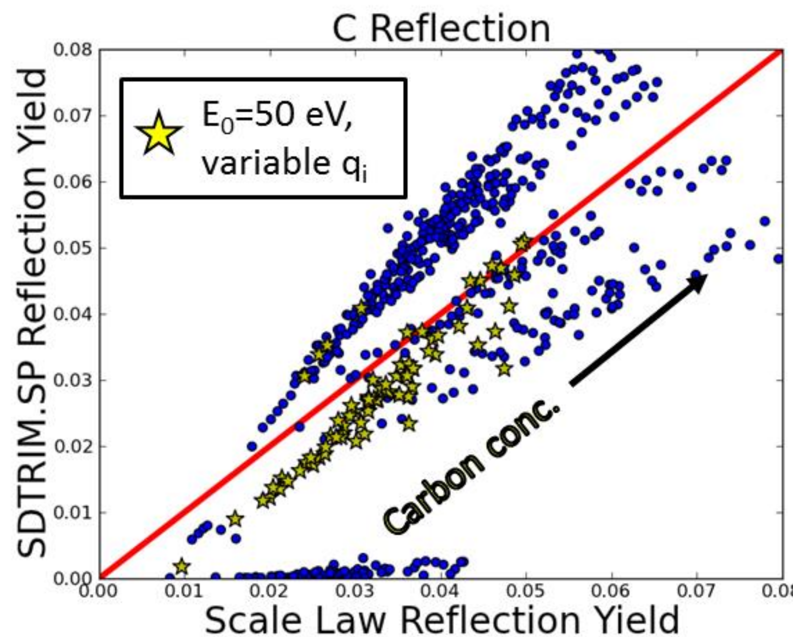


- Similar qualitative patterns, but heavier elements have a more broad redistribution profile due to longer ionization mean free path

Analytic physical erosion rates generated by fitting scale laws to SDTRIM.SP results

- SDTRIM.SP varied over projectile/energy/surface composition (1600+ runs)





$$Y_{sput}^{FIT} = Q * s_n(E_0/E_{TF}) * (1-(E_{th}/E_0)^{2/3}) * (1-E_{th}/E_0)^2 * (1 + \Sigma_i\, q_i * a_i)$$

Bohdansky formula — Composition dependence

q_i = concentration of element i

Fit parameters: Q, E_{th}, a_C, a_{Li}, a_O

$$Y_{refl}^{FIT} = \rho_{refl} * E_0^{\alpha} * (1 + \Sigma_i\, q_i * b_i)$$

Composition dependence

q_i = concentration of element i

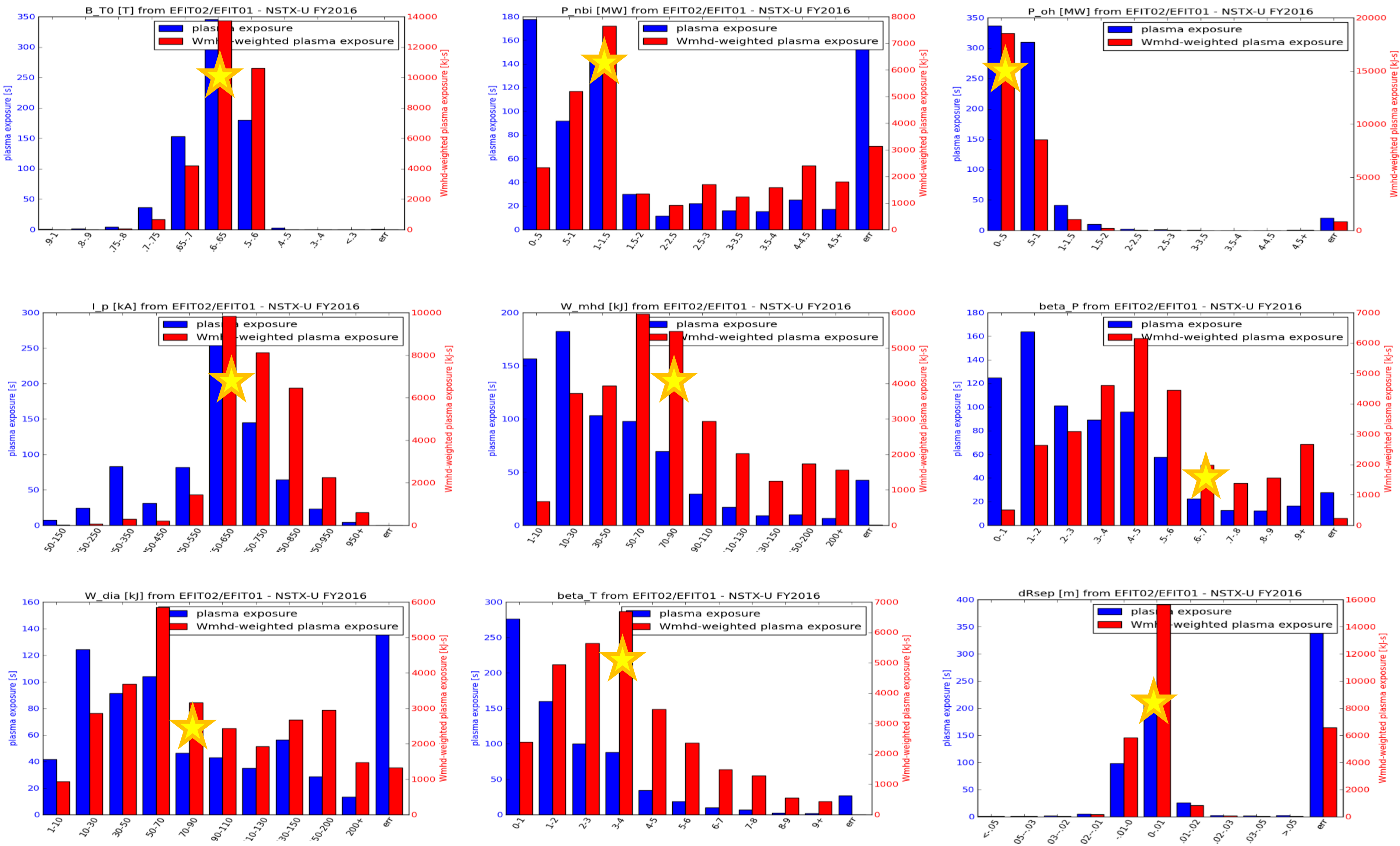
Fit parameters: ρ_{refl}, α, b_C, b_{Li}, b_O

Adatom fit parameters

$$\Gamma_{adatom} \big/ \Gamma_{in} = Y_{ad} \big/ 1 + A * \exp(E_{eff} / kT_{Surf})$$

Incident Species	Reference	Y_{ad}	A	E_{eff}
D 50eV	Doerner JNM 2001	2.9	9.6e-6	0.70
D 60eV	Doerner JNM 2003	0.749	2.3e-9	1.17
D 200eV	Doerner JNM 2003	0.749	2.3e-9	1.17
D 20eV	Abrams NF 2016	Unable to fit w/o D implantation		
He 175eV Hi flux	Doerner JNM 2003	5.97	3.3e-9	1.24
He 175eV Lo flux	Doerner JNM 2003	5.97	3.3e-9	1.24
Ne 20eV	Abrams NF 2016	0.01	8.2e-6	0.81
Ne 40eV	Abrams NF 2016	4.2e6	57	0.88
Li 300eV	Allain PRB 2007	6.5	5.0e-9	1.22
Li 500eV	Allain PRB 2007	6.5	5.0e-9	1.22
Li 700eV	Allain PRB 2007	6.5	5.0e-9	1.22
Li 1000eV	Allain PRB 2007	6.5	5.0e-9	1.22

Other discharge parameters throughout 2016 campaign also well represented by L-mode fiducial



Other discharge parameters throughout 2016 campaign also well represented by L-mode fiducial