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NSTX-U

Global mixed-material migration modeling of NSTX-U and a parameterized Li-C-O surface model

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57th APS-DPP

Savannah, GA

November 16-20, 2015

PPPL

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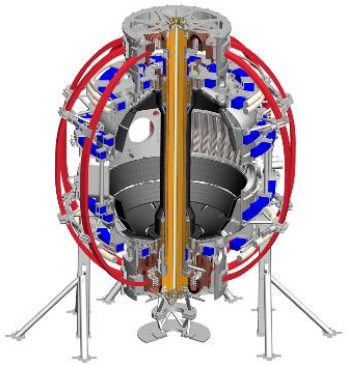


Abstract

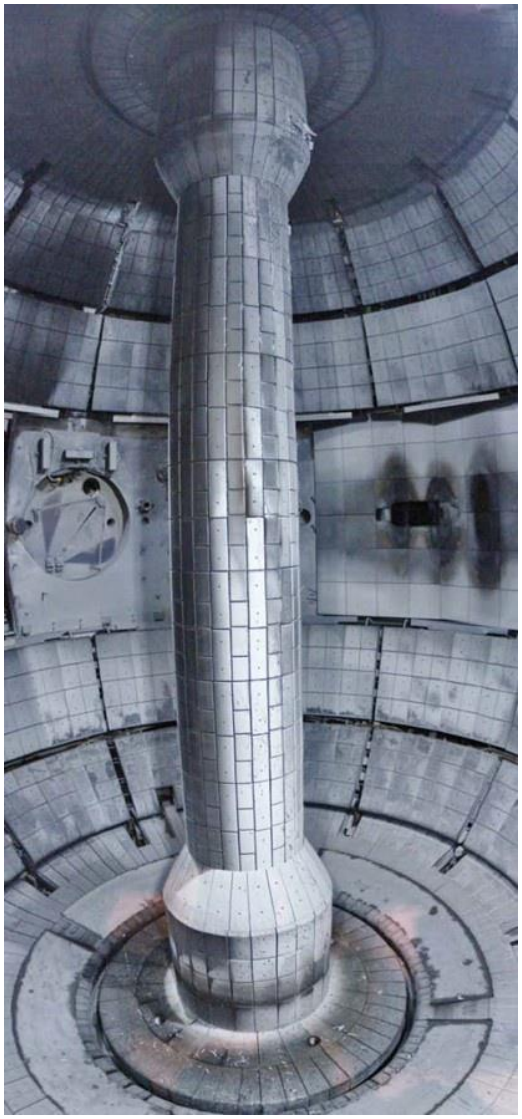
NSTX-U will initially operate with graphite walls, periodically coated with thin lithium films to improve plasma performance. Prior experiments with Li evaporation on NSTX suggest that poloidally inhomogenous mixed-material C/Li/O surfaces will evolve over the course of the campaign due to wall material migration during plasma operation. Understanding the depletion and accumulation of Li in different parts of the machine is a key component of optimizing the Li conditioning process.

To that end, the WallDYN global mixed-material surface evolution model [K. Schmid et al., J. Nucl. Mater. 415, S284-S288 (2011)] has been applied to the NSTX geometry. The WallDYN model couples local erosion and deposition processes with plasma impurity transport in a non-iterative, self-consistent manner that maintains overall material balance.

For this work, a C/Li/O mixed-material erosion model has been generated by parameterizing dynamic sputter and reflection yield calculations from SDTRIM.SP. Li and O migration rates are found to be most sensitive to changes in C surface binding energy and to the presence of high-SBE compounds.

This work is supported by US DOE contract DE-AC02-09CH11466

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



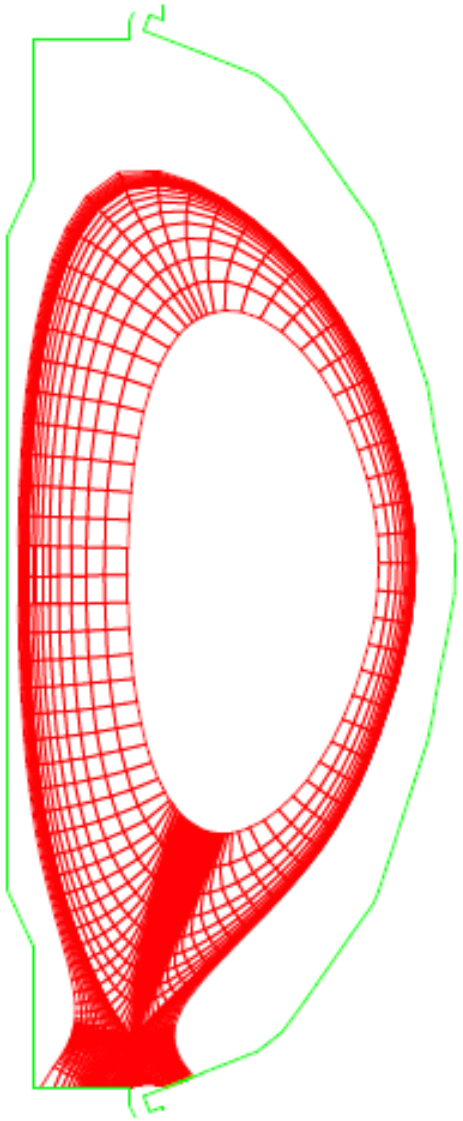
- In mixed material machines, first wall composition evolves in time due to erosion, transport, redeposition, etc.
  - Occurs at different rates for different materials
- Material migration in NSTX-U is complex due to wide range of mixed materials
  - C, Li, O, B, Mo (2016) + compounds/alloys
- NSTX used Li evaporation to improve plasma performance
  - Observed clear evidence of qualitative Li surface changes on time scales of 1-10 shots (migration, passivation, compound formation)
  - Often operated via ad hoc conditioning “recipes” 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)
  - Iterative schemes are computationally intractable

- 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 (~4 hr CPU time)
  - Calculates poloidally-resolved, time-dependent surface concentration and impurity flux evolution
  - Assumes PMI & plasma transport timescales << wall evolution timescale
  - Maintains global material balance

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

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

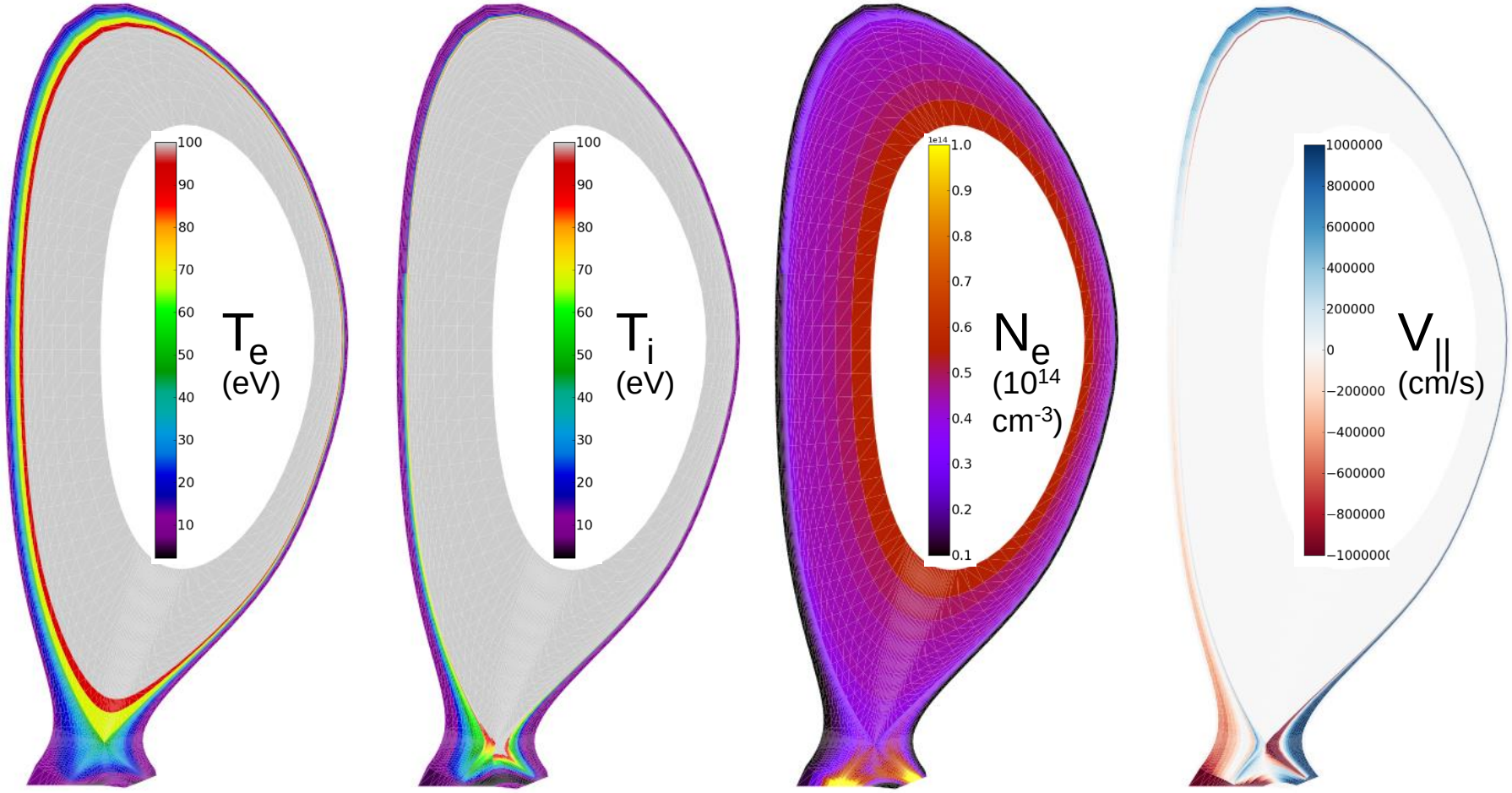
$$\frac{d}{ds}\left(\frac{5}{2}n(s)\cdot v(s)\cdot kT_e(s) - \kappa_{0e}\cdot T_e(s)^{5/2}\frac{dT_e(s)}{ds}\right) = -P_{rad}(s) - P_{helpi}(s) - P_{ei}(s)$$

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

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

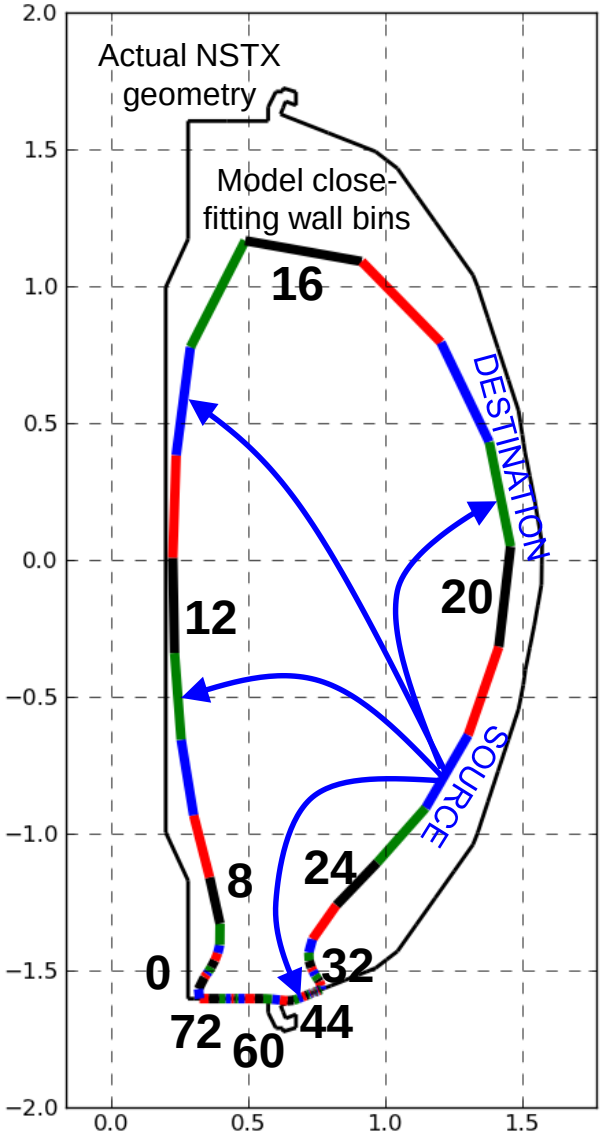
  - Iterate with EIRENE for ionization/power/ momentum sources and sinks
- WallDYN also compatible with SOLPS, etc.

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



– 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

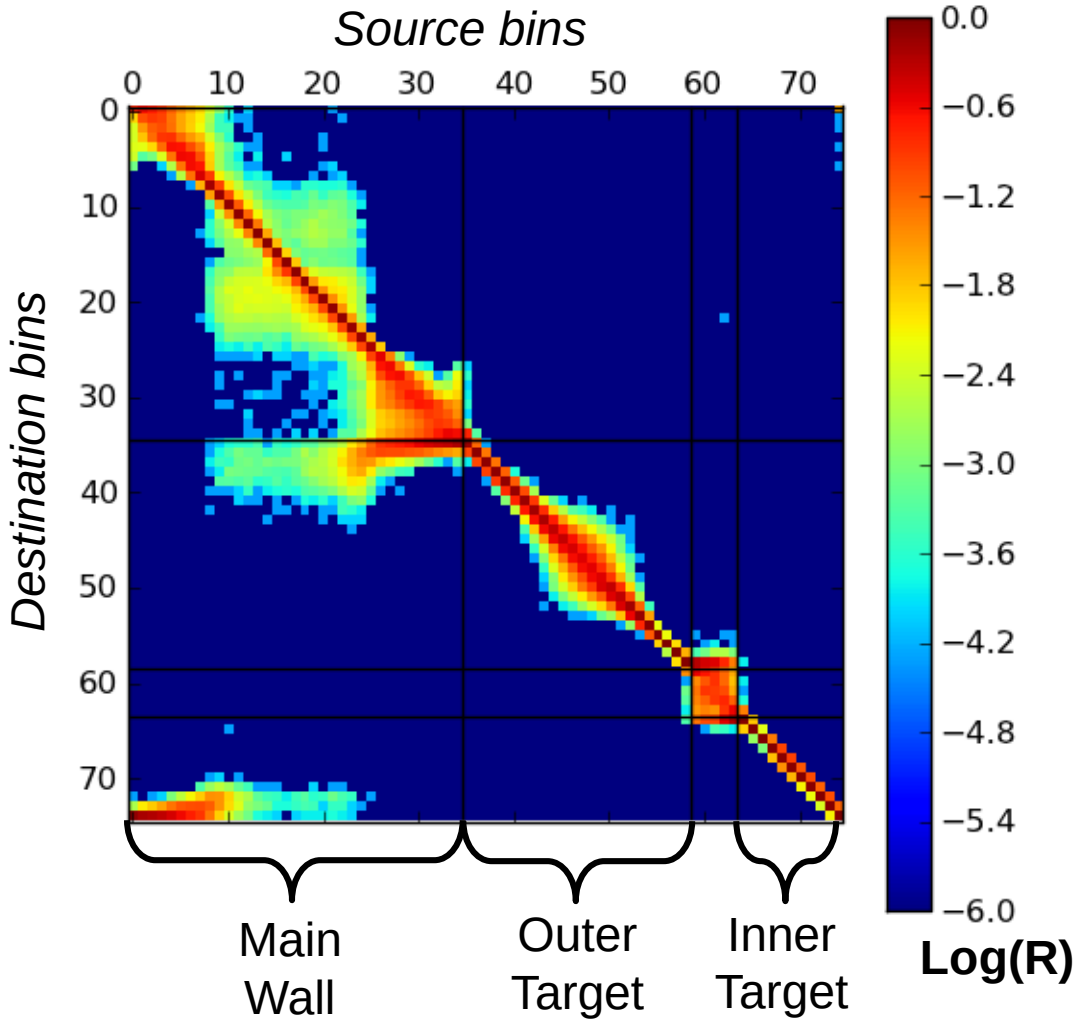


- Wall elements are grouped into 75 bins
  - This work emphasizes resolution @outer target
- 20000 particles are launched from each bin, and the final charge states and deposition locations are recorded
  - Particles are launched as atoms with cosine angular distribution and Thompson energy distribution (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

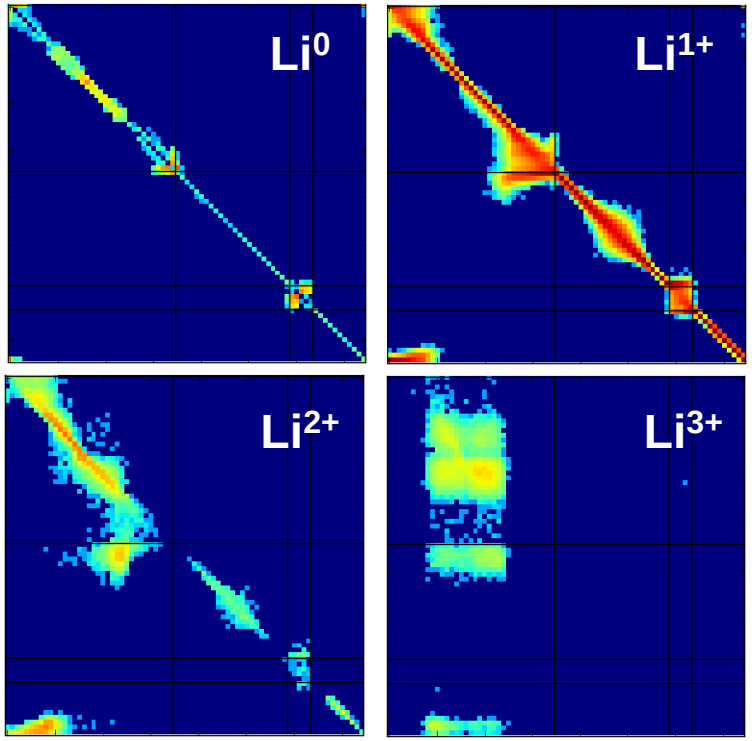
Why use an idealized close-fitting wall instead of the actual NSTX wall coordinates?
→ See *Future Work – Model Improvements*

Lithium redistribution matrices show that deposition is primarily ionic, local

Charge-integrated Li redistribution matrix



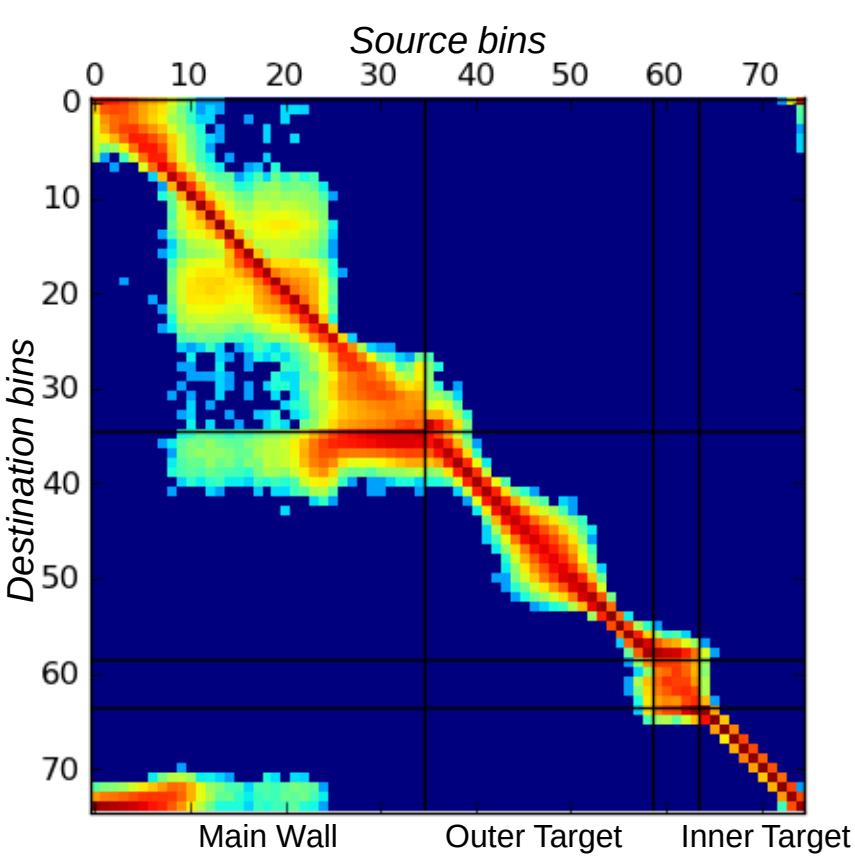
Charge-resolved redistribution matrices



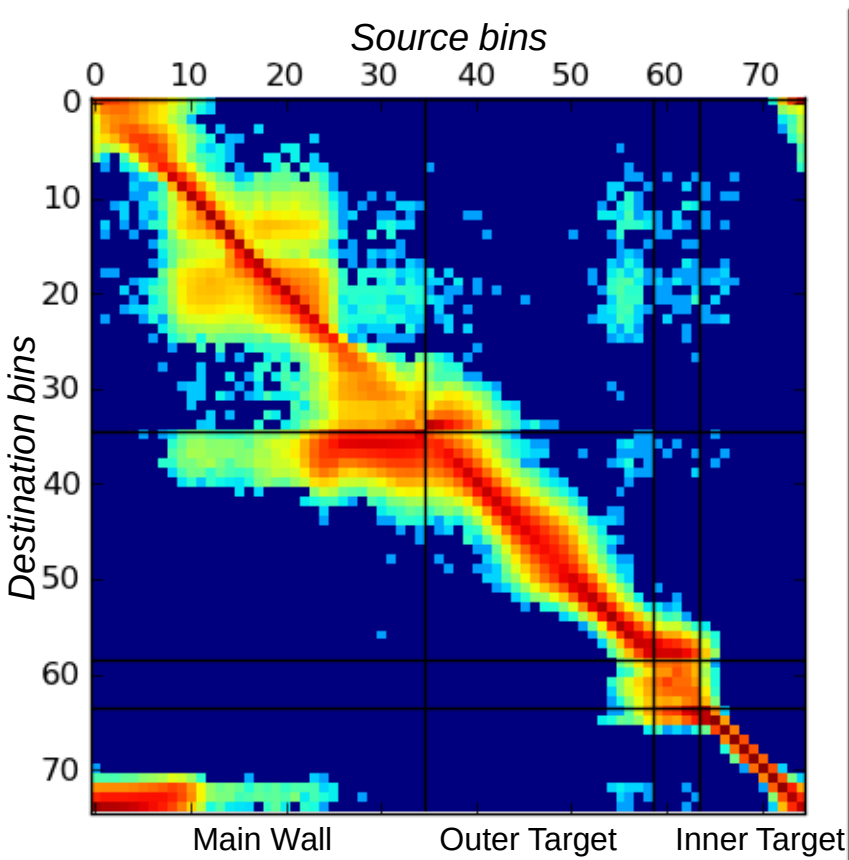
R = probability particle launched from X deposits on Y

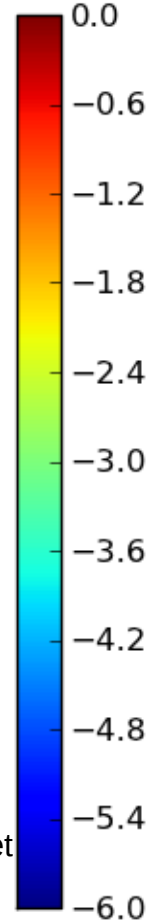
Carbon, Oxygen redistribution matrices are qualitatively similar to Lithium

Charge-integrated C redistribution



Charge-integrated O redistribution





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

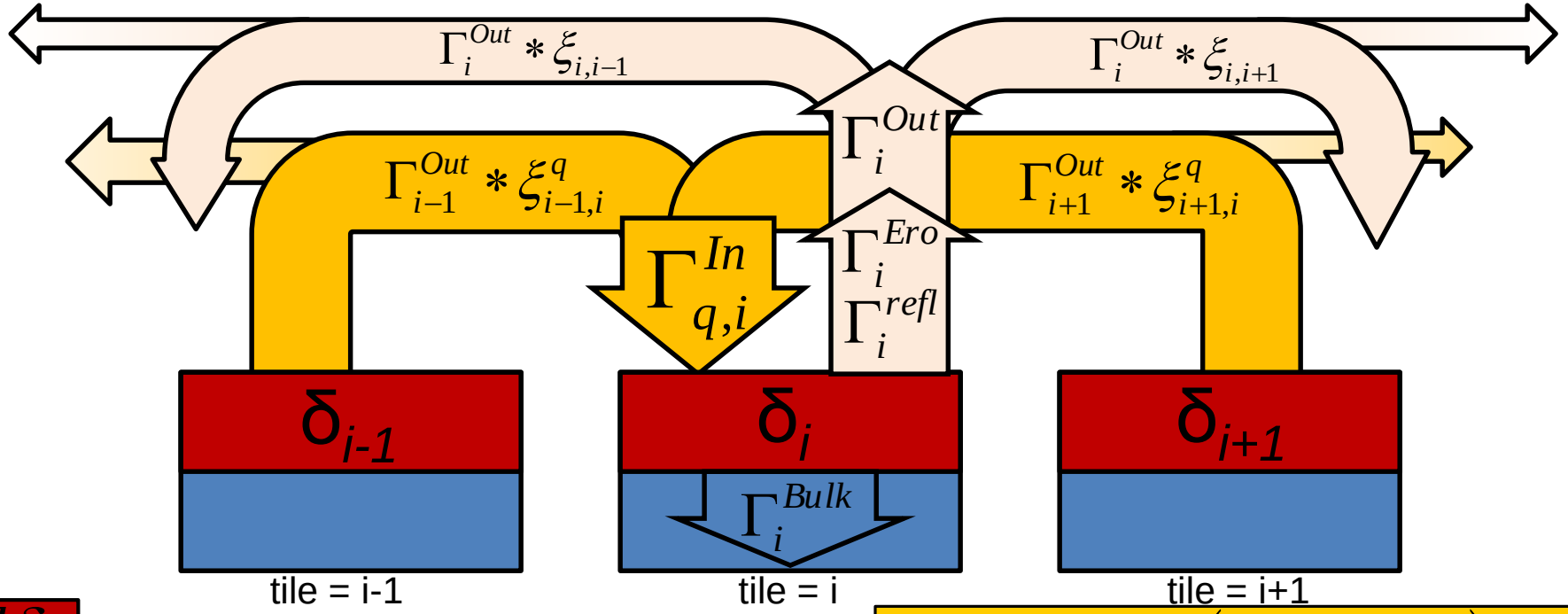
WallDYN couples plasma/surface rates by solving a system of differential-algebraic equations

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)



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

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

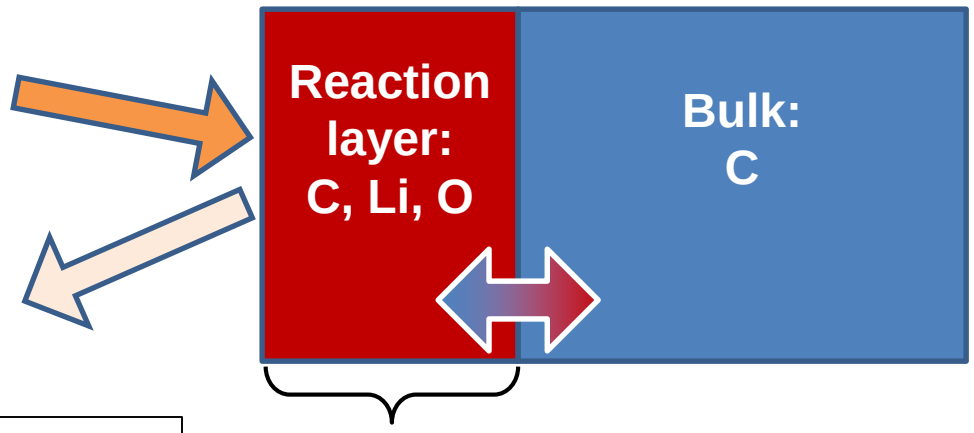
- Differential-algebraic equation system (~2000 eqs) solved in Mathematica

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

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

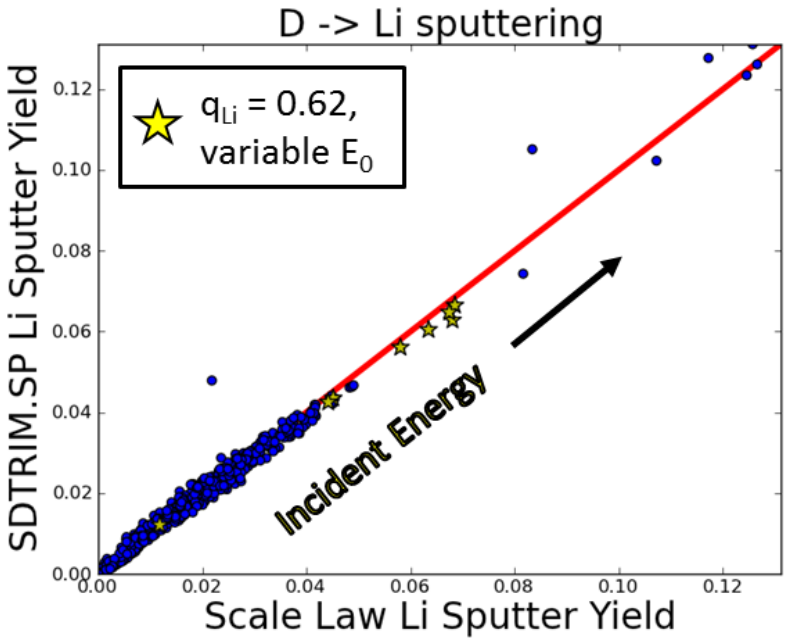
Outgoing fluxes:
- Eroded impurity fluxes
- Reflected impurity fluxes

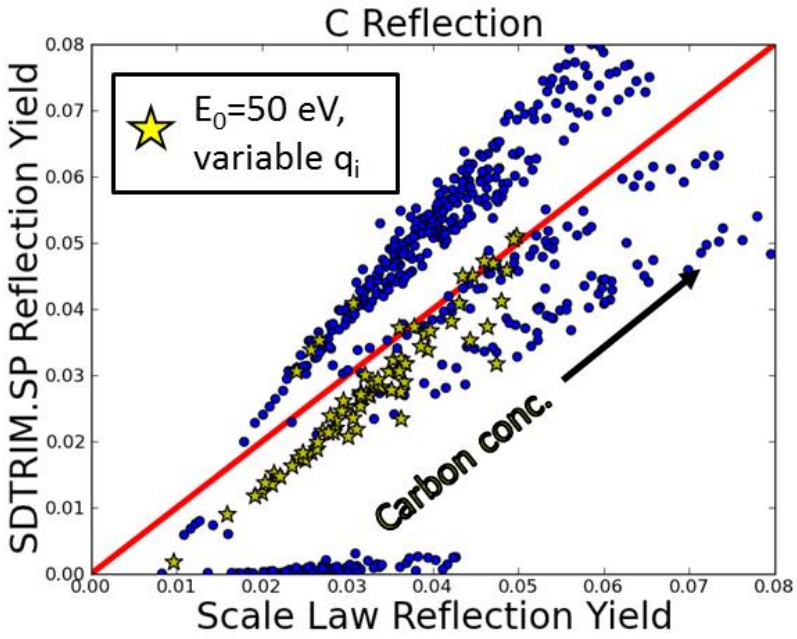


Reaction layer width same as MAPP XPS range
→ See *Future Work – Experiments*

Analytic 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

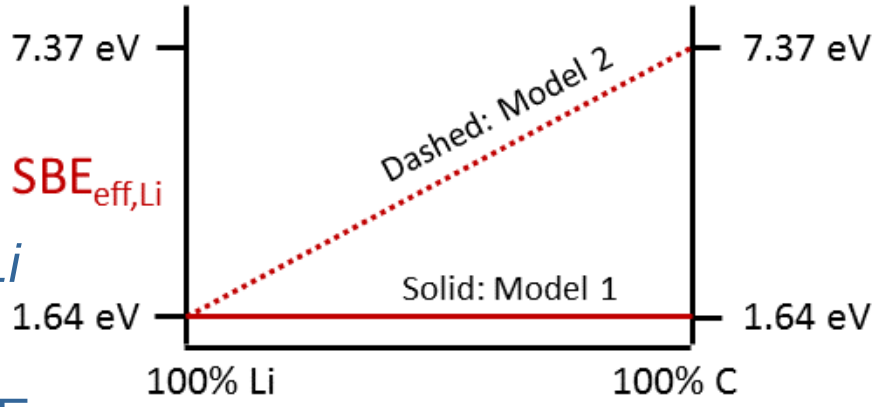
Surface binding energy (SBE) is the key input parameter for sputtering in SDTRIM.SP

- Element i is sputtered if perpendicular recoil energy > $SBE_{eff,i}$
- Ansatz: $SBE_{eff,i} = \Sigma_j q_j * SBE_{ij}$ q_j = concentration of element j

SBE_{ij}(eV)	i = Li	i = C	i = O
j = Li	1.64	SBE_{C-Li}	SBE_{O-Li}
j = C	SBE_{Li-C}	7.37	SBE_{O-C}
j = O	SBE_{Li-O}	SBE_{C-O}	2.58

- Diagonal components: sublimation energy (well known)
- Off-diagonal components: ?

- Ex: $SBE_{eff,Li}$ with q_O=0
  - Model 1: $SBE_{Li-C} = SBE_{Li}$
    => $SBE_{eff,Li} = SBE_{Li}$
  Intuitively: Li-C bonds behave like Li-Li
  - Model 2: $SBE_{Li-C} = SBE_C$
    => $SBE_{eff,Li} = q_{Li}*SBE_{Li} + q_C*SBE_C$
  Intuitively: Li-C bonds behave like C-C



Sensitivity scan conducted to test importance of mixed-material SBEs on overall surface evolution

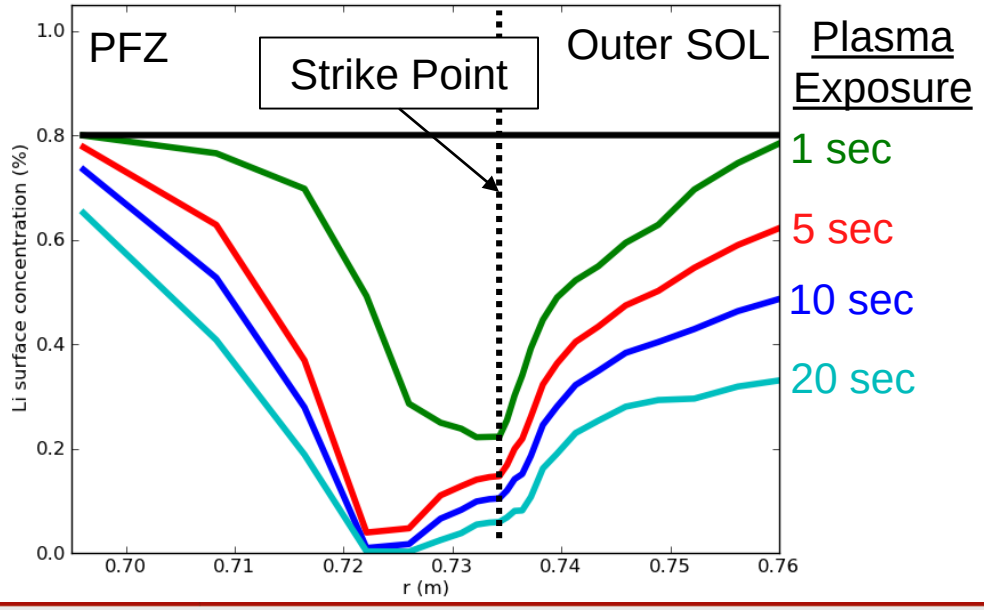
SBE_{ij}(eV)	i = Li	i = C	i = O
j = Li	1.64	(1)	(3)
j = C	(1)	7.37	(2)
j = O	(3)	(2)	2.58

Mixed SBE models tested:		
(1)	**(2)**	**(3)**
1.64	2.58	1.64
1.64	2.58	2.58
1.64	7.37	1.64
1.64	7.37	2.58
7.37	2.58	1.64
7.37	2.58	2.58
7.37	7.37	1.64
7.37	7.37	2.58

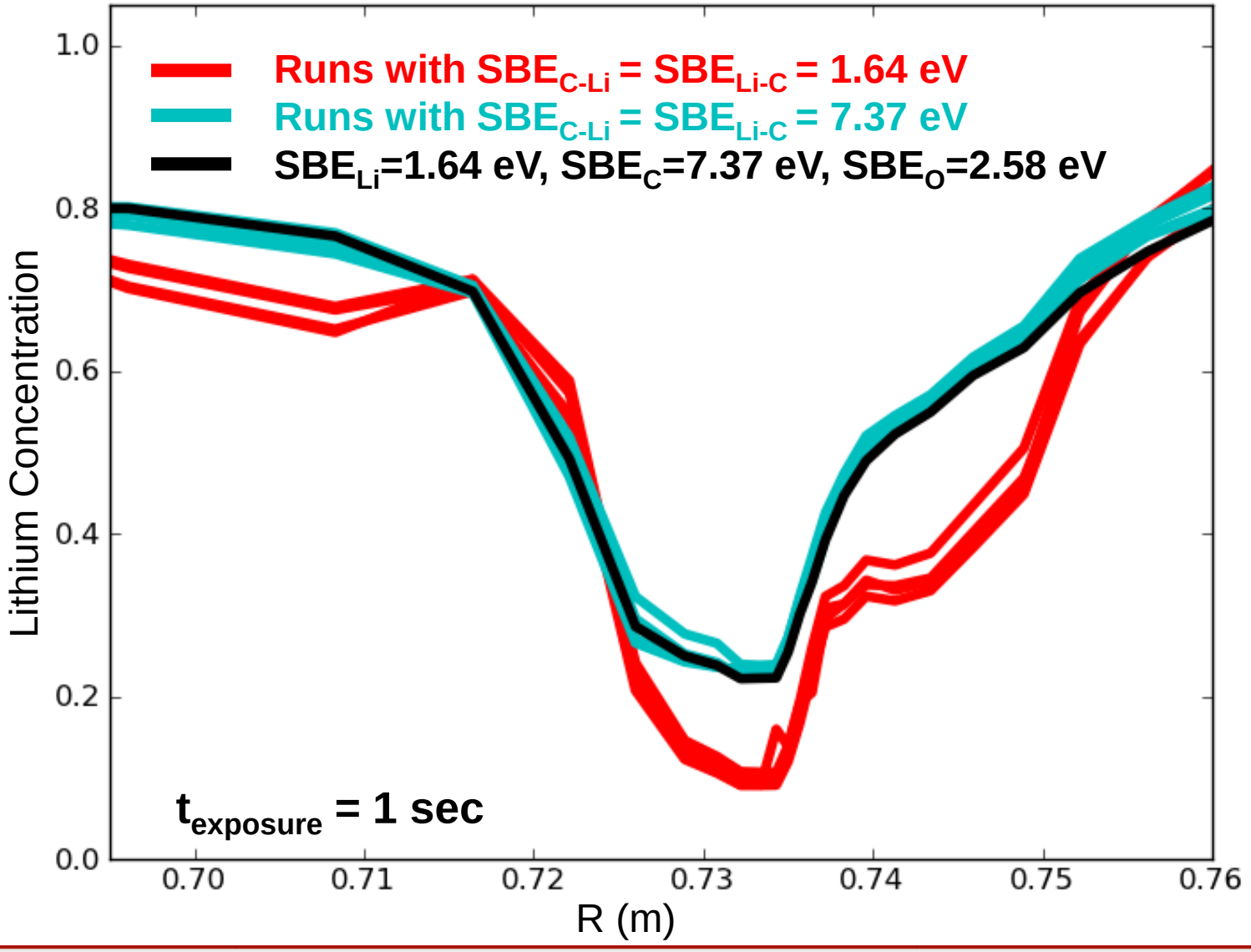
Constant SBE models tested:

- SBE_{Li}=1.64, SBE_{C}=7.37, SBE_{O}=2.58
- SBE_{Li}=6.64, SBE_{C}=12.37, SBE_{O}=7.58

- Assumption: mixed-material SBEs affect each element the same (e.g. $SBE_{Li-C}=SBE_{C-Li}$)
- Figure of merit: Li, O conc. evolution at outer target surface
  - Initial atomic concentration: 80% Li, 10% C, 10% O

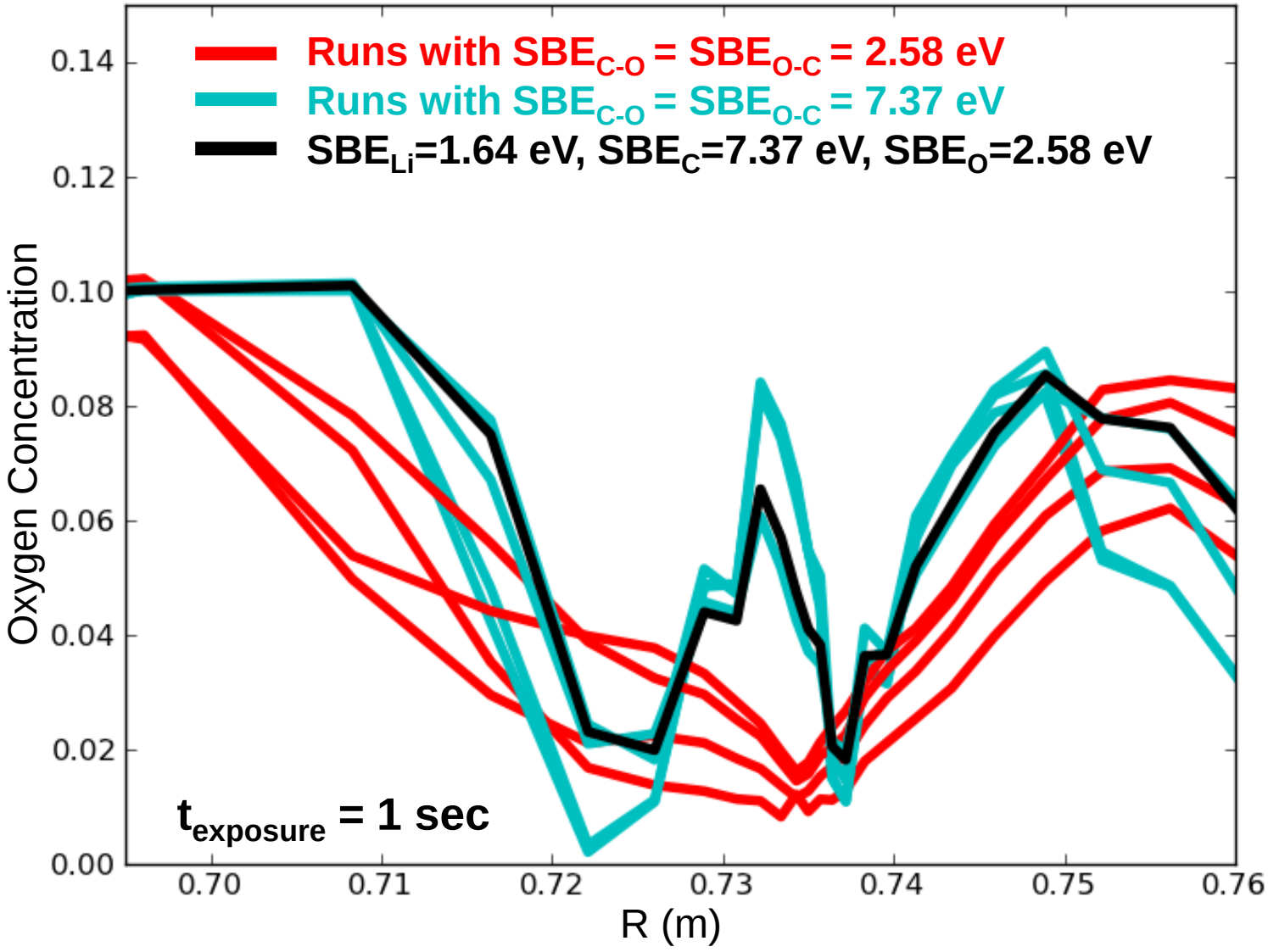


Scan shows that Li concentration results are strongly correlated with C-Li binding interaction



- Dominant variable is SBE_{C-Li} for all exposure times
- SBE_{Li-O} appears as subdominant variable after long exposure times
- Note that constant SBE model (black) tracks with SBE_{C-Li}=7.37 eV (cyan)

Scan also shows correlation of O concentration results with C-O binding interaction



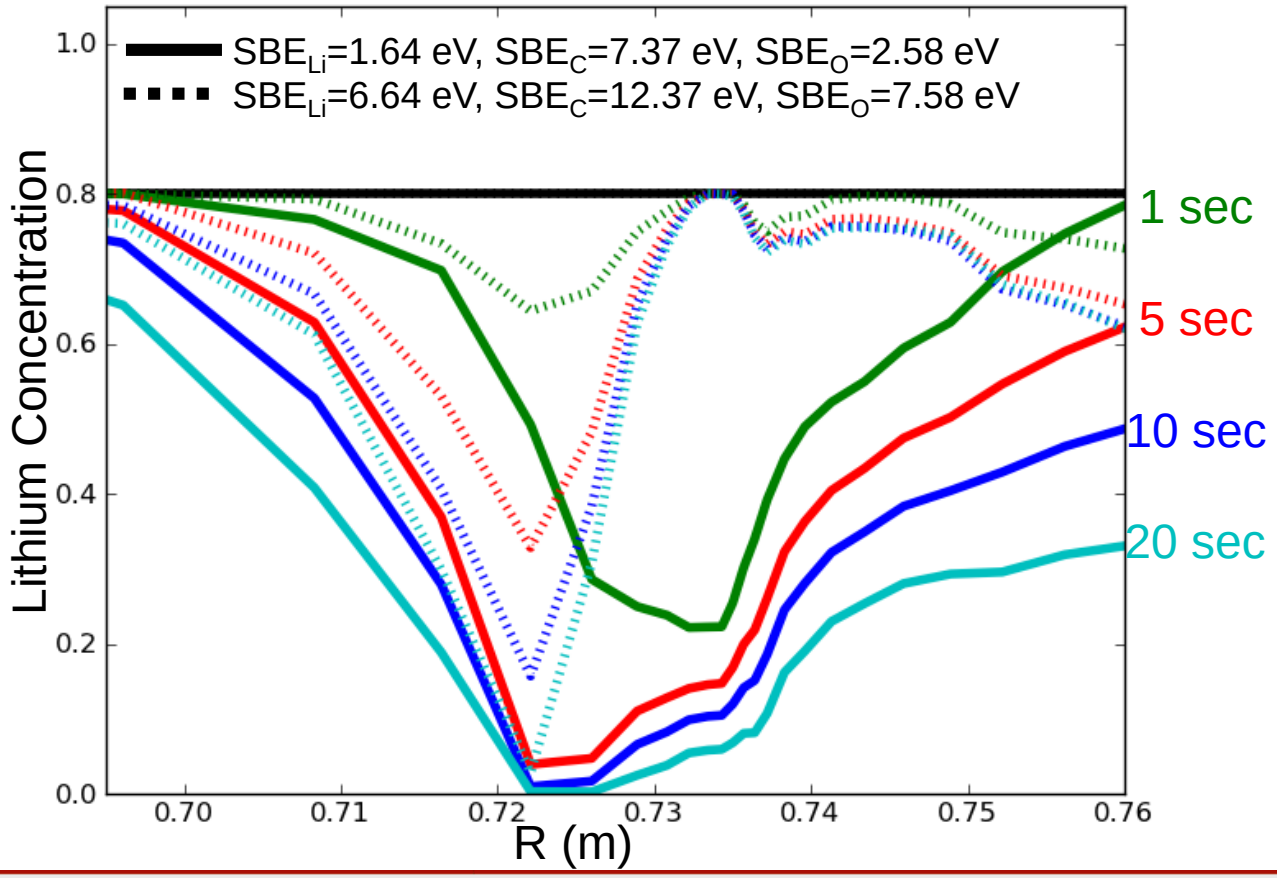
- Dominant variable is SBE_{C-O} for all exposure times
- Note low O concentration compared to Li, C
- Note that constant SBE model (black) tracks with SBE_{C-O}=7.37 eV (cyan)

Discussion

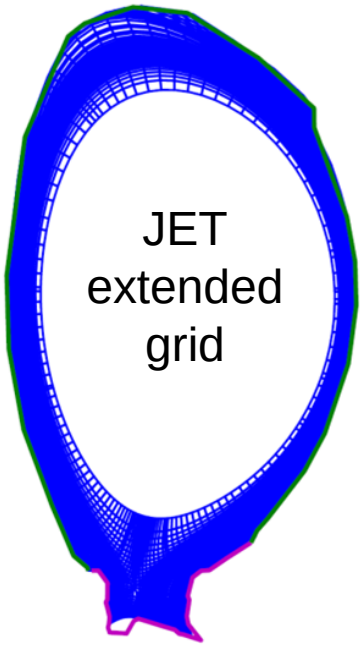
- Changes in carbon sputtering ($SBE_{C,eff}$) are what govern lithium & oxygen migration results in WallDYN!
  - If $SBE_{Li,eff}$ was the dominant parameter, you would expect the constant SBE model (black) to track with SBE_{C-Li}=1.64 eV (red), since both use a constant $SBE_{Li,eff}$=1.64 eV
  - This is not the case! Constant SBE model (black) tracks with SBE_{C-Li}=7.37 eV (cyan) because both use a constant $SBE_{C,eff}$=7.37 eV
  - Same behavior occurs with SBE_{C-O}
- Occurs due to the mixing of a high SBE bulk (SBE_C=7.37 eV) with low SBE surface materials (SBE_{Li}=1.64 eV, SBE_O=2.58 eV)
  - Li-O binding effects are subdominant due to low O concentration, and small difference between SBE_{Li} and SBE_O
  - A similar dynamic will likely occur when using high-Z bulk materials (SBE_{Mo}=6.81 eV, SBE_W=8.79 eV)

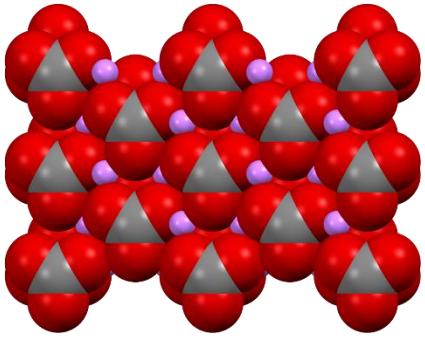
Quick exploration: What effect does adding a compound dissociation energy have on results?

- Elements entrained in compounds require more energy to sputter, since the molecular bonds must be broken as well
  - Toy model: SBEs = Constant SBEs + 5.0 eV
  - SBE_{Li}=6.64 eV, SBE_C=12.37 eV, SBE_O=7.58 eV
- Huge effect on concentration results!
- SBE changes due to compound formation require further study



Future work – Model improvements



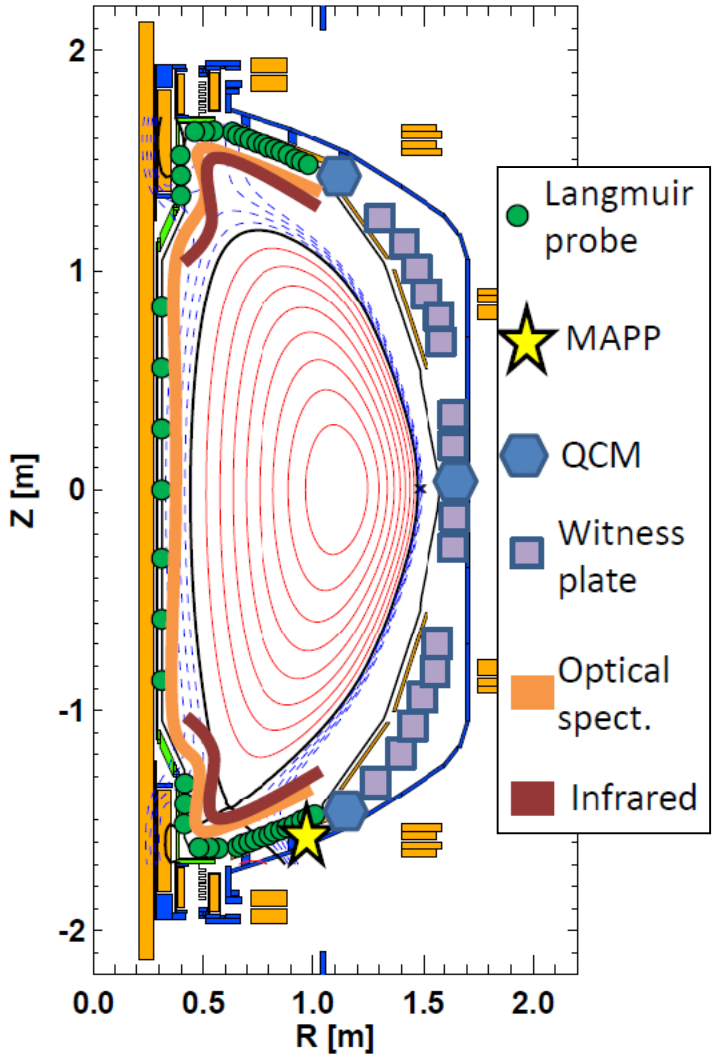


- Extended plasma grids are being incorporated into the NSTX-U WallDYN workflow
  - DIVIMP cannot accurately launch particles from the main wall on standard grids due to the large gap between grid and wall
  - Far SOL will be filled with short, isothermal flux tubes
  - Will also provide more accurate D^+ flux to main wall
- Surface model
  - Constrain mixed-material SBEs in SDTRIM.SP via comparison to test stand XPS data
  - Relax assumption that $SBE_{C\text{-}Li}=SBE_{Li\text{-}C}$, etc.
  - Explore and quantify sputtering changes due to the presence of Li_2O, Li_2CO_3, Li_2C_2, etc. in test stand experiments and MD/DFT surface codes
  - Add diffusion/intercalation and thermal effects

Future work – Experiments

- Experiments are planned on NSTX-U to quantify material migration and benchmark WallDYN model
- Will utilize extensive suite of PMI diagnostics on NSTX-U
  - Materials Analysis and Particle Probe (MAPP) will provide first-of-its-kind inter-shot, *in vacuo* surface concentration data

    (*see Lucia GP12.109, Bedoya GP12.97*)
  - Complementary campaign-integrated surface data from witness plates
  - Wide-angle spectroscopic coverage provides gross erosion data
- Extended Langmuir probe coverage will enhance accuracy of plasma reconstructions



Conclusions

- The global mixed-material migration model WallDYN has been applied to NSTX to couple plasma impurity transport with surface erosion and deposition
- An analytic Li-C-O surface sputtering/reflection model has been developed by parameterizing the output of SDTRIM.SP
- A sensitivity scan of unknown parameters in the surface model has shown that modifications to the carbon surface binding energy correlate most strongly to observable migration results
- Compound formation also appears to have a strong influence on migration results and requires further study

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