Simulations of Diffusive Lithium Evaporation onto the NSTX Vessel Walls*

D. P. Stotler, C. H. Skinner, W. R. Blanchard, P. S. Krstic[1],
H. W. Kugel, H. Schneider, and L. E. Zakharov,
Princeton Plasma Physics Laboratory
Princeton University
Princeton NJ 08543

[1]Oak Ridge National Laboratory, Oak Ridge, TN

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Abstract

The evaporation of lithium (Li) onto the NSTX divertor plates has reduced D recycling, improved confinement, and suppressed ELMs. However, in plasmas with suppressed ELMs, the core carbon and medium-Z metallic impurity concentrations increase in the latter part of a discharge. To the extent that these impurities are the result of sputtering from the graphite tiles and other surfaces, increased coverage of the plasma facing surfaces with Li should reduce the impurity sources. This increased coverage can be achieved by evaporating the Li into a helium (He) filled vessel and exploiting the fact that the mean free path of the Li atoms scales inversely with the He pressure. Thus, higher (lower) pressures preferentially coat the top (bottom) of the vessel. A model for predicting and optimizing this process has been developed and validated against an initial set of deposition experiments. The model is found to agree with the data to within the estimated errors over a range of He pressures. The most significant uncertainties in the model have been identified and more discriminating validation tests are planned.

NSTX Investigating Diffusive Li Evaporation to Reduce Sources of Impurities

NSTX

- NSTX using Li coating to improve performance & provide density control,

- Primarily deposited by LITER evaporation into vacuum between discharges,
  - $\Rightarrow$ Reduces D recycling, improves confinement, suppresses ELMs,
  - However, ELM suppression leads to core accumulation of C & metallic impurities.

- To extent that these impurities due to sputtering, increased coverage of surfaces with Li should reduce them.

- $\Rightarrow$ investigating diffusive evaporation into He filled vessel.

Simulating Diffusive Evaporation Requires 3-D Kinetic Calculations

NSTX

- Diffusive evaporation seen before with He glow discharge cleaning.
- Li mean free path $\lambda_{\mathrm{Li-He}} \propto 1/P_{\mathrm{He}}$,
  - $\Rightarrow$ low P_{He} coats bottom of vessel,
  - High P_{He} coats surfaces close to LITERs at top of vessel.
- 3-D problem $\Rightarrow$ optimal strategy for coating all surfaces not obvious,
- Moreover, need $\lambda_{\mathrm{Li-He}} \simeq R \Rightarrow$ Monte Carlo treatment of collisions required.
- Use 3-D Monte Carlo neutral transport code, DEGAS 2.
  - Run multiple times for different $P_{\mathrm{He}} \Rightarrow$ fluxes to PFCs,
  - Compile optimized procedure as set of evaporation intervals at specified P_{He}.
- Here: validate against evaporation experiments from 2009 NSTX campaign.

Model Consists of Small Set of Components

NSTX

- 3-D description of NSTX vacuum vessel,
  - Including two LITERs,
  - And quartz micro-balance (QMB) $\Rightarrow$ deposition data used for comparison.

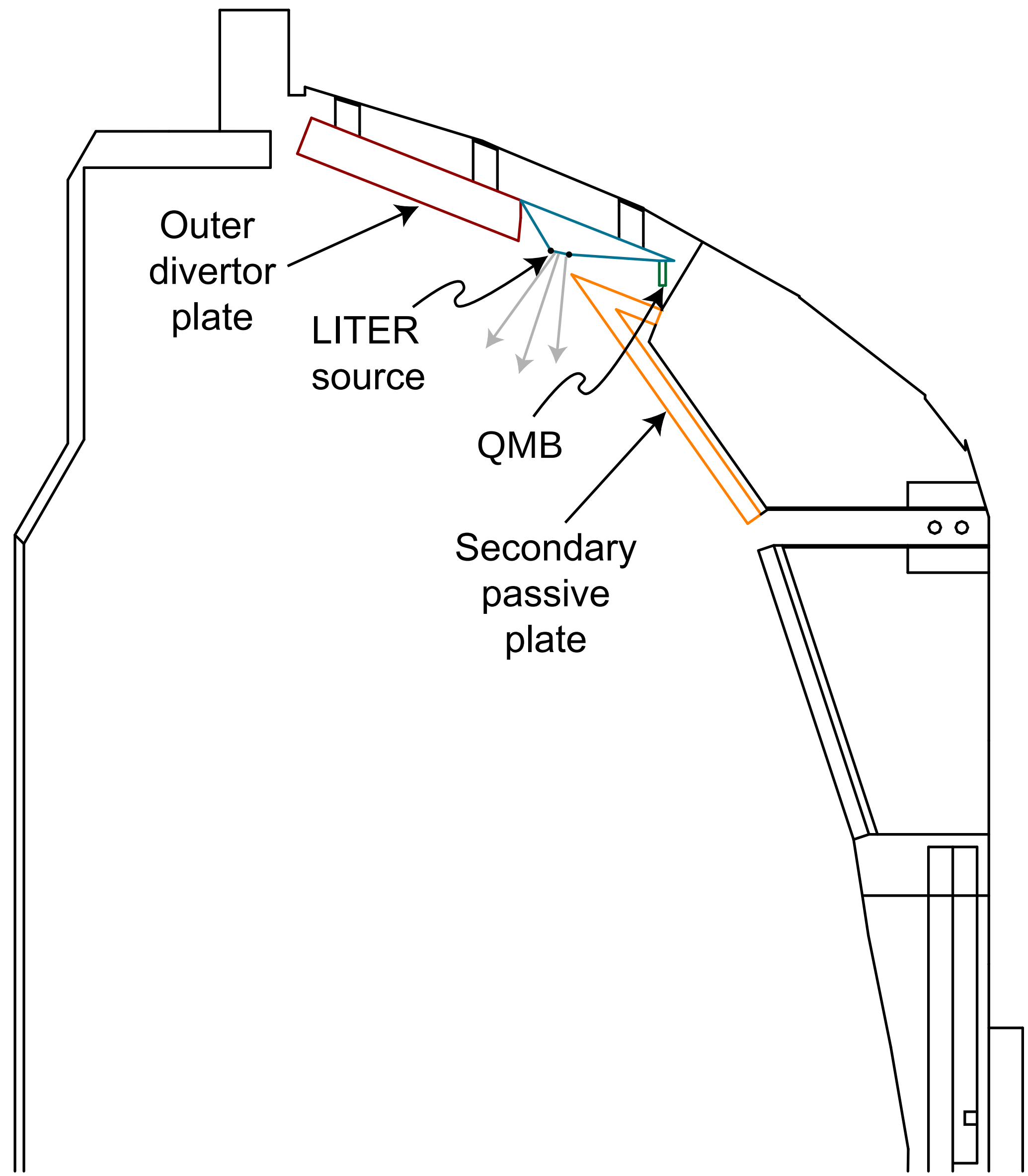
- Angular distribution of Li atoms from LITER,
  - Measured in laboratory,
  - Agrees well with molecular flow simulations using `Cbebm` code [Zakharov],
  - $\Rightarrow$ spline fit used to characterize source in DEGAS 2.
  - Thermal energy distribution at $T = 900$ K.

- LITER evaporation rate,
  - Oven temperature computer controlled $\Rightarrow$ Li vapor pressure,
  - Rate determined using molecular flow conductance.
  - Confirmed with laboratory data.
  - These experiments: operated at 910 K $\Rightarrow$ 60 mg/min total.
- Atomic physics processes: Li $+$ He & Li + D_2 elastic scattering,
  - D_2 enters due to outgassing during evaporation experiments,
  - Differences in He & D_2 mean free paths $<$ uncertainties in either,
  - And masses same $\Rightarrow$ treat as single background,
    * With $P_{\mathrm{tot}} = P_{\mathrm{He}} + P_{\mathrm{D_2}}$.
  - $\Rightarrow \lambda_{\mathrm{Li-He}} = 9.92 \times 10^{-2} / P_{\mathrm{tot}}(\mathrm{mtorr})$ m.
- Assume Li sticks to all surfaces with 100% probability,
  - Or is same everywhere.

Vessel Structures Represented in DEGAS 2 as Plane Surfaces

- Coordinates for tiles from NSTX design & construction drawings.

- Lower divertor tile surface & gaps measured during last opening.



Toroidal Variation Specified in DEGAS 2 via "Pie Slice" Model

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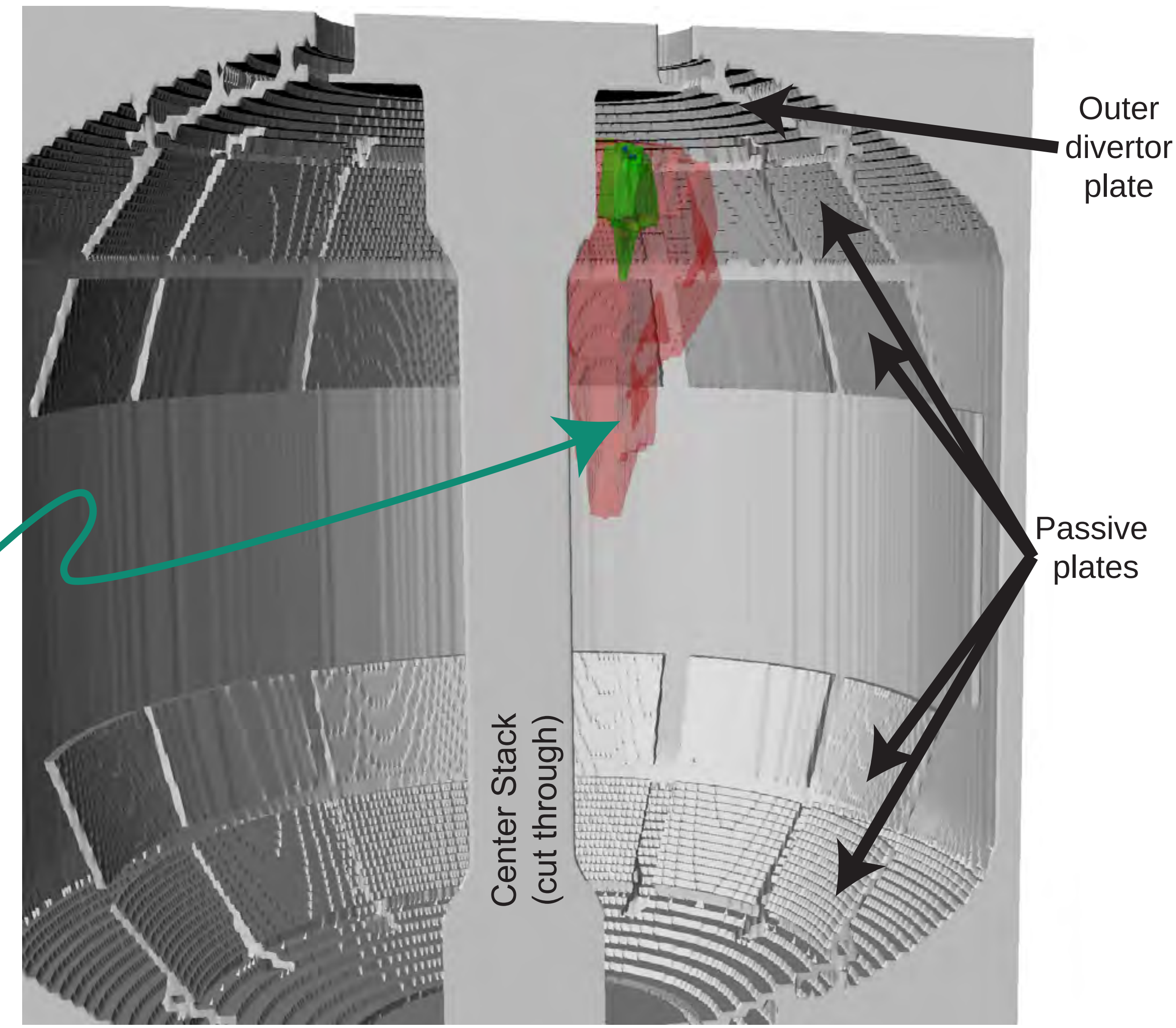
- Toroidal discretization adapted to provide specified toroidal widths of gaps & surfaces.
- LITERs at 45° (Bay K) & 195° (Bay F),
- Upper QMB at 225° (Bay E).
- Li density contours from Bay F LITER shown.



Evaporation Experiments Based on Initial Pressure Prescription from DEGAS 2 Model

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Pressure (mtorr)	λ_{Li-He} (m)
0.032	3.1
0.1	1.0
0.2	0.5

- 0.032 mtorr for 1 time unit, 0.1 & 0.2 for 2 time units.

- Total time chosen to allow several shots to be run during allotted time.

Pressure Values Unfolded from Ionization Gauge Data

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- Ionization gauge calibrated for air
  & requires calibration factors when used with other gases.

- Use here:

$$P_{\mathrm{ig}} = c_{\mathrm{He}} P_{\mathrm{He}} + c_{\mathrm{D_2}} P_{\mathrm{D_2}},$$

- Where $c_{\mathrm{D_2}} = 0.392$ & $c_{\mathrm{He}} = 0.186$.

- Assume:

  – All He after initial pump-down,

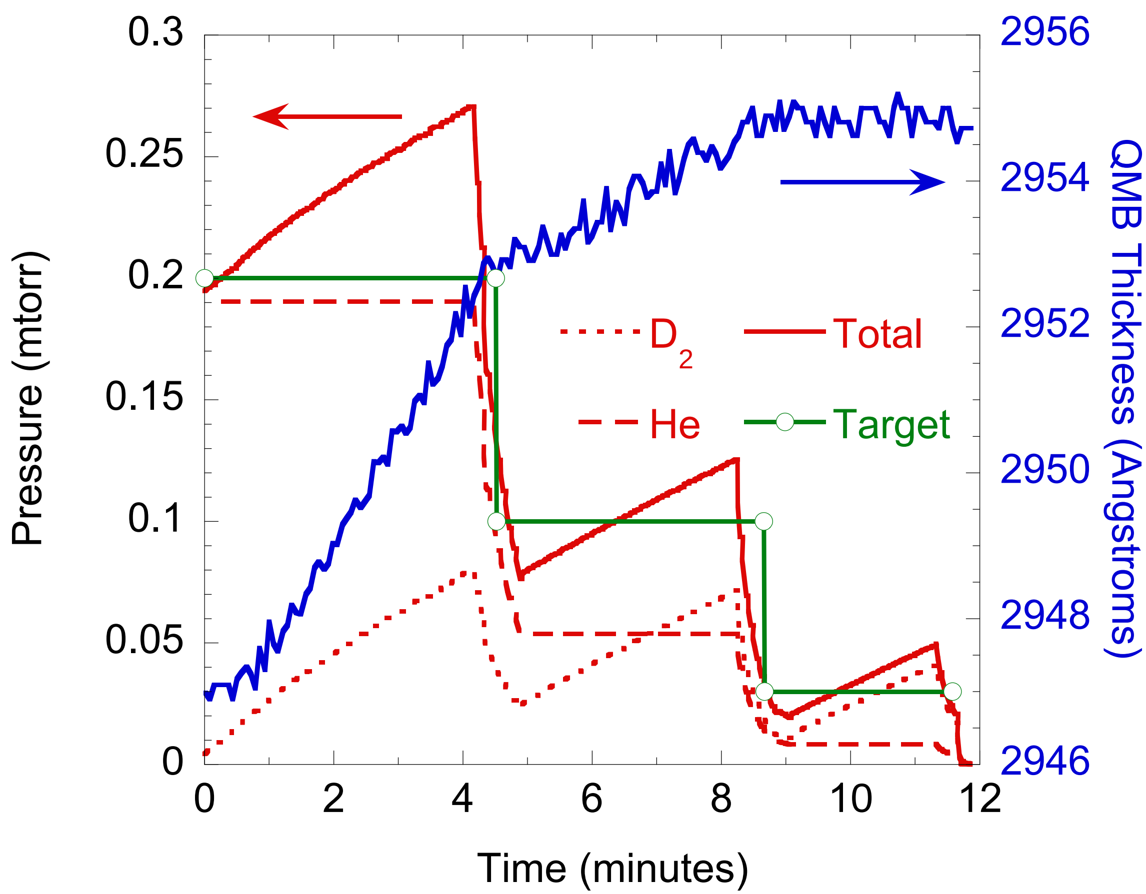
  – Subsequent pressure rise due to D_2,

  – $P_{\mathrm{He}}/P_{\mathrm{D_2}}$ constant during pump-down.

- $\Rightarrow$ can determine P_{tot}.

Pressure & QMB Data from Shot 135697

- "Target": prescribed He pressure.
- Pressure rise to D_2 outgassing,
  - RGA mass 2 & 4 saturated.
- He & D_2 pressures inferred from ionization gauge data,
- $P_{tot} = P_{He} + P_{D2}$.
- Corresponding QMB data on right axis.



Compute Normalized Deposition Rate from QMB Data

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- QMB measures frequency $\propto$ deposited mass,
  - Calibration factor must be corrected for temperature changes.
- If deposits all have same mass $\longrightarrow$ number of atoms or molecules.
  - Usually converted to a thickness using a nominal density.
- Smooth data & take derivative $\longrightarrow$ deposition rate.
- Normalize by LITER rate
  $\Rightarrow$ probability for evaporated Li atom to be deposited on QMB.
- Baseline assumption is that deposits are pure Li,
  - But, RGA indicates $> 10^{-6}$ torr of H_2O during evaporation,
  - H_2O flux $> 10\times$ Li flux; is deposit LiOH?
  - $\Rightarrow$ Assume: deposited mass between Li & LiOH.

Simulations & Uncertainties

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- Simulations done at 0.032, 0.1, 0.25, & 0.3 mtorr.

Quantity	Deposition Rate Uncertainty	Basis
QMB depth ± 1 cm & angle	25%	Sensitivity runs
QMB position in gap ± 1 cm	10%	Data at adjacent segments
LITER position ± 6 mm	28%	Sensitivity runs
Cross section	50%	Variations @ low $E_{\rm cm}$, unknown composition
Effect of pressure uncertainty on rate	40%	Vary He / D_2 fractions in model

- LITER may not be in molecular flow regime,
  - Evaporation rate could be larger by $2\times$ or more,
  - But, angular distribution could be more peaked.
  - Due to magnitude & complexity, leave out of analysis.

- $\Rightarrow$ total rms uncertainty: 75%.

Comparison of Measured & Simulated Deposition

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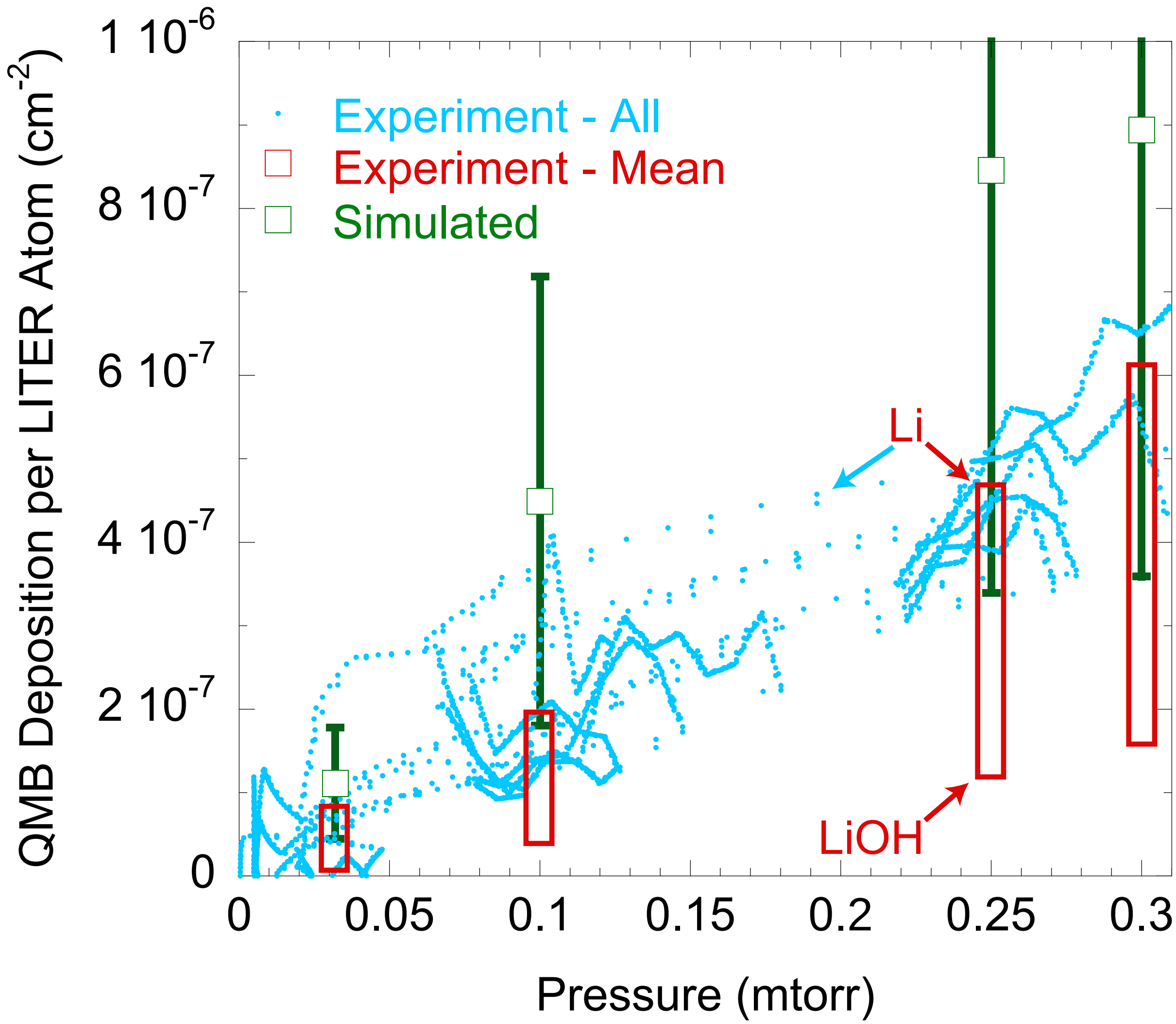
- Simulation error bars: $(2/\pi)^{1/2}$ x 75%.

- Combine experimental data in 0.01 mtorr bins,

  - Rectangles are mean values,
  - Upper end: pure Li,
  - Lower end: pure LiOH.



Discussion

- Simulation error bars overlap experimental rectanges,
- But, consistent 50% discrepancy & tracks in data suggest systematic errors.
- Plan dedicated experiments to decouple model components:
  - Operate LITERs separately,
  - Use QMBs in other parts of vessel,
  - Run LITERs at lower temperatures,
  - Evaporate with pumps on & maintain P_{He} via leak valve,
  - Post-mortem ex-vessel analysis of QMB to quantify hydration.
- Also, reduce other uncertainties with more in-vessel measurements.