Simulations of Diffusive Lithium Evaporation onto the NSTX Vessel Walls*

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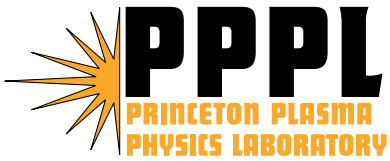


Poster presented at the 2010 Plasma Surface Interactions Meeting, San Diego, CA

*This work supported by U.S. DOE Contracts DE-AC02-09CH11466 and DE-AC05-00OR22725.

Abstract

NSTX is exploring and developing lithium (Li) conditioning of plasma facing surfaces. In the principal technique used thus far, Li is evaporated from the top of the vessel into a vacuum in the period between discharges and is primarily deposited on the lower divertor surfaces. Lithium coatings have reduced D recycling, improved confinement and suppressed ELMs. However, in the 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.

In this paper, we describe 3-D DEGAS 2 neutral transport modeling of Li evaporation into a helium filled vessel. With this technique, the Li diffuses throughout the vessel, coating a larger fraction of the graphite tiles. The mean free path of the Li atoms scales inversely with the helium pressure, so lower pressures coat the bottom of the vessel most effectively and higher pressures lead to thicker coatings at the top. A series of DEGAS 2 simulations is used to construct a sequence of evaporations at three pressures (corresponding to Li mean free paths of 0.5, 1.0, and 3.1 m) that provide a specified minimum Li coating at all locations in the vessel.

The data taken during the experimental implementation of this prescription will be used to validate the DEGAS 2 based model for Li evaporation and deposition, accounting for the effects of outgassing of molecular hydrogen (H_2, HD, and D_2) and other technical details. The corresponding DEGAS 2 simulations will utilize the measured vessel pressures and Li evaporation amounts and will be compared with quartz micro-balance (QMB) measurements of the actual deposition. Preliminary analysis of the QMB data indicates that the deposition rates do exhibit the expected qualitative variation with helium pressure.

NSTX Investigating Diffusive Li Evaporation to Reduce Sources of Impurities

- 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

- 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.
  - Resulting model can be applied iteratively to optimize coating procedure.
- Here: validate against evaporation experiments from 2009 NSTX campaign.

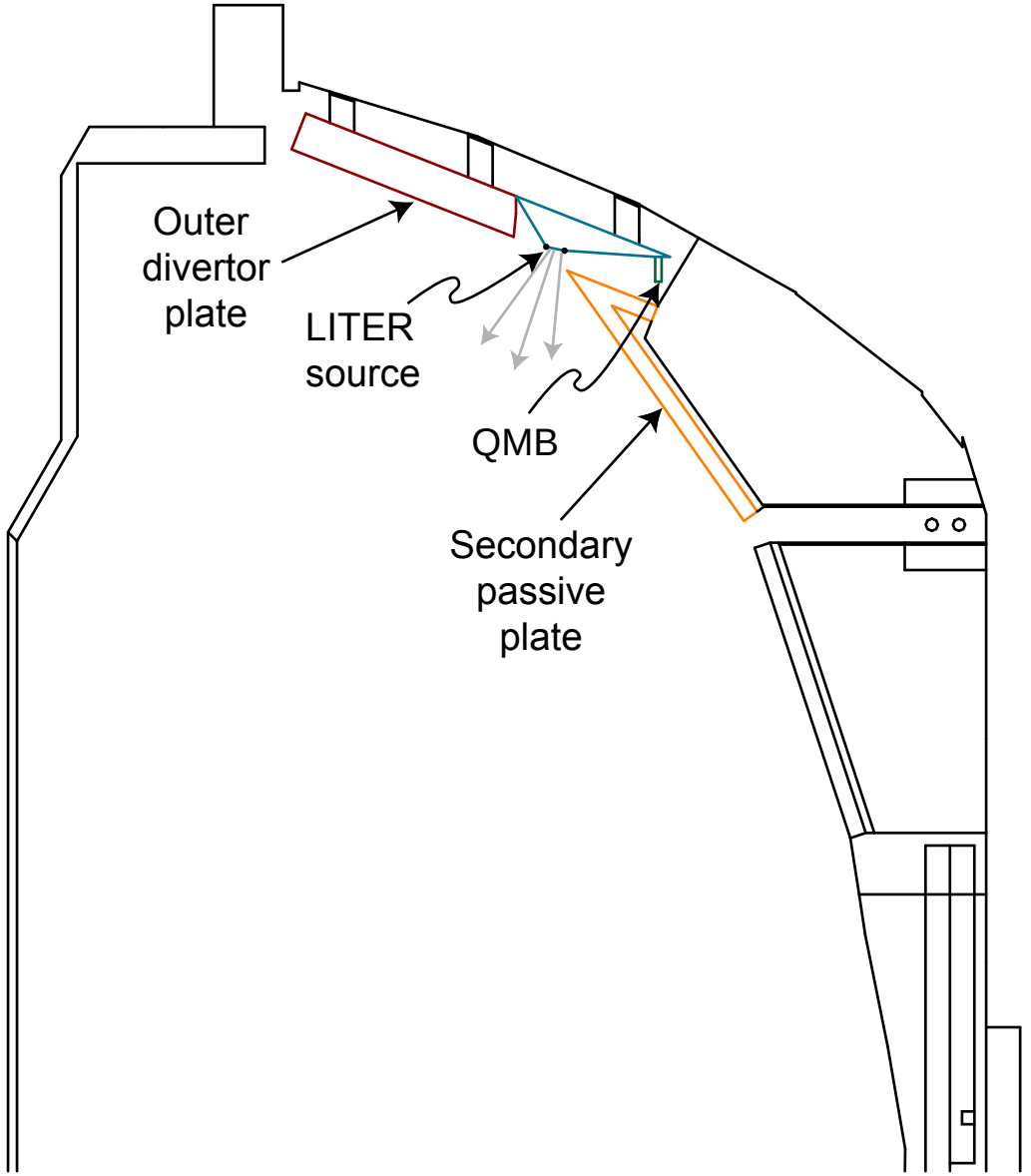
Model Consists of Small Set of Components

- 3-D description of NSTX vacuum vessel,
  - Including two LITERs,
  - And 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.
  - Here: operated at 640° C $\Rightarrow$ 60 mg/min total.
- Atomic physics processes: Li + He & Li + D_2 elastic scattering,
  - D_2 enters due to outgassing during evaporation,
  - 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.

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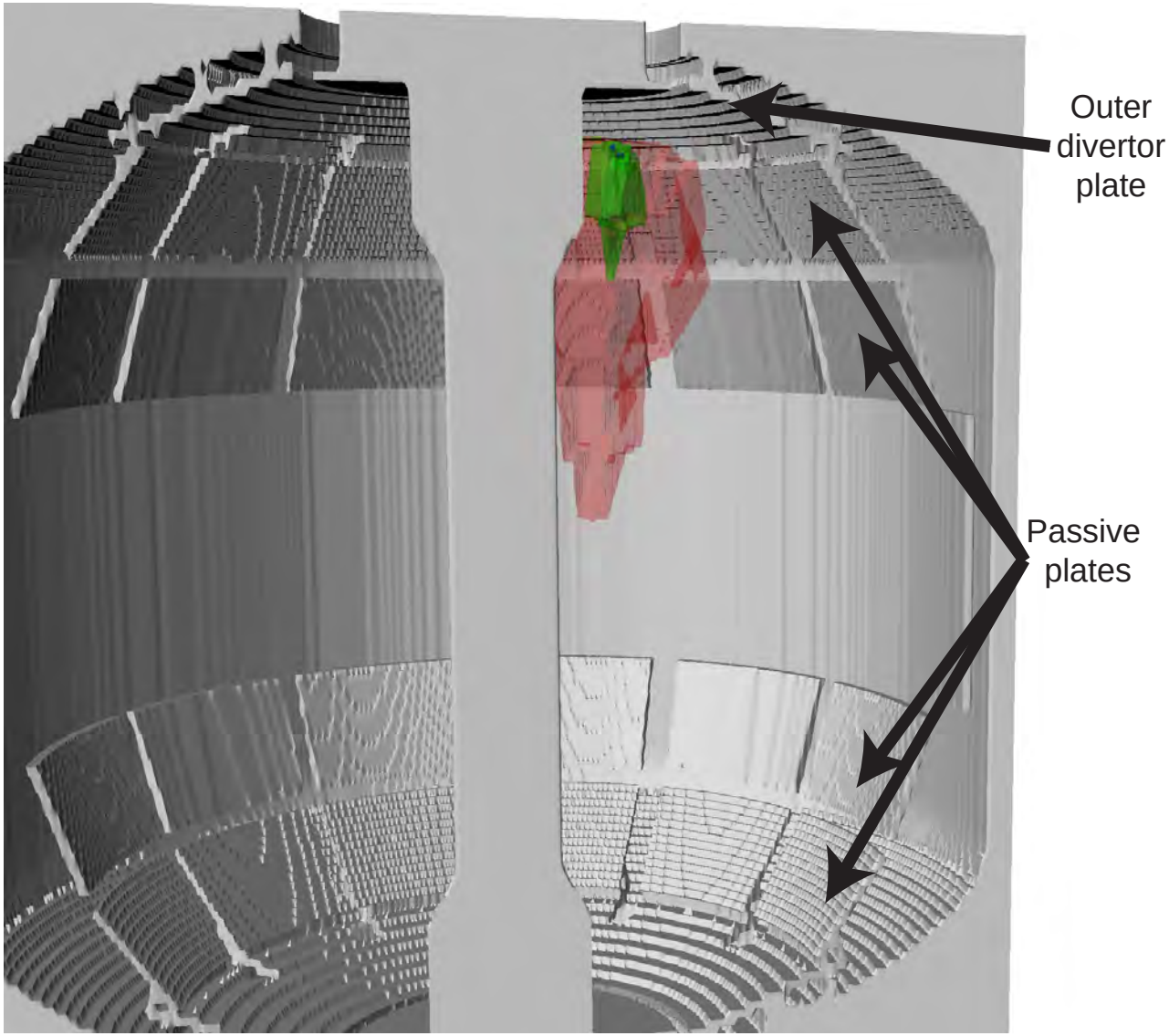
- Toroidal discretization adapted to provide specified toroidal widths of gaps & surfaces.
- LITERs at 45° (Bay K) & 195° (Bay F),
- Upper QMB at 225° (Bay E).
- Li density contours from Bay F LITER shown.



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:

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

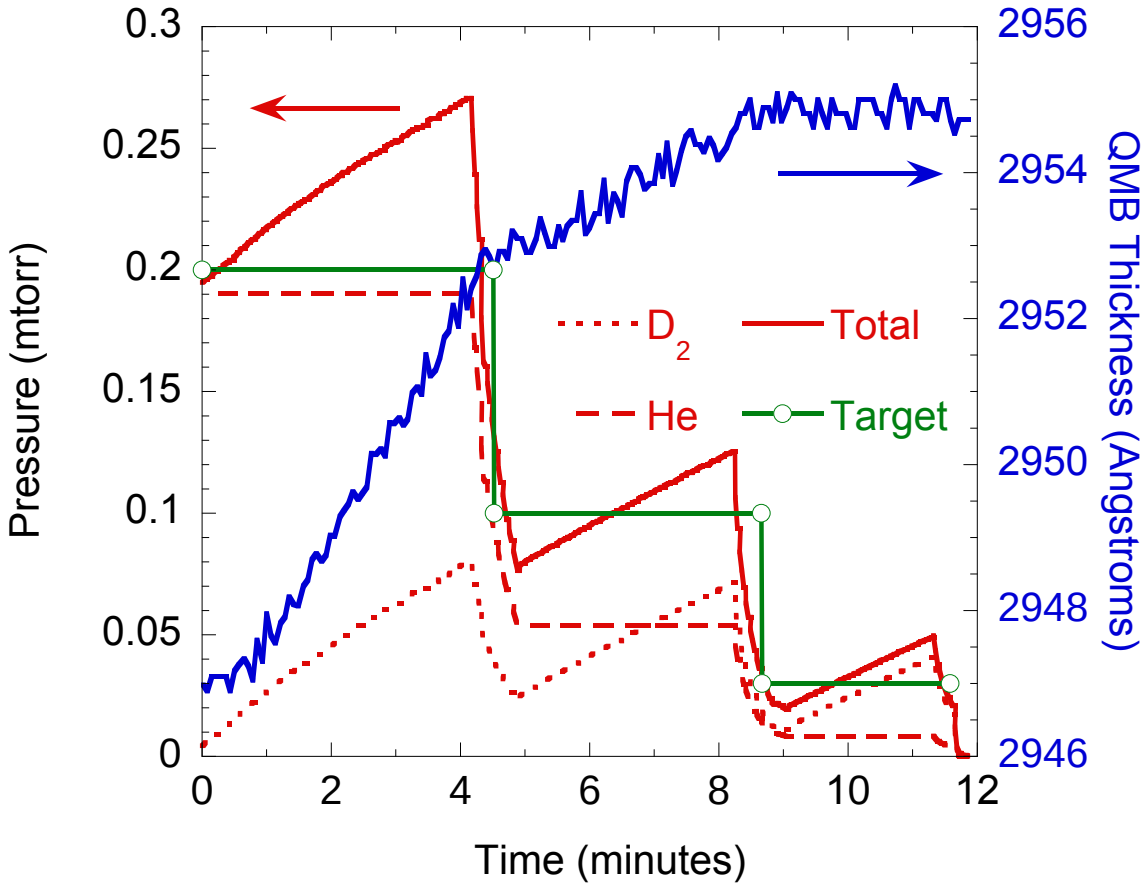
- Where $c_{\mathrm{D_2}} = 0.392$ & $c_{\mathrm{He}} = 0.186$.

- Assume:
  - All He after initial pump-down,
  - Subsequent pressure rise due to $\mathrm{D_2}$,
  - $P_{\mathrm{He}}/P_{\mathrm{D_2}}$ 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.
- He & D_2 pressures inferred from ionization gauge data,
- $P_{tot} = P_{He} + P_{D_2}$.
- 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 $\rightarrow$ number of atoms.
  - Usually converted to a thickness using a fixed density.
- Smooth data & take derivative $\rightarrow$ deposition rate.
- Normalize by LITER rate
  $\Rightarrow$ probability for evaporated Li atom to be deposited on QMB.

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	10%	Sensitivity run, angle $< 30^\circ$
QMB gap space ± 1 cm	10%	Data at adjacent segments
LITER position ± 6 mm	28%	Sensitivity runs
Cross section	50%	Variations @ low E_{cm}, unknown composition
Pressure	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: 71%.

Comparison of Measured & Simulated Deposition

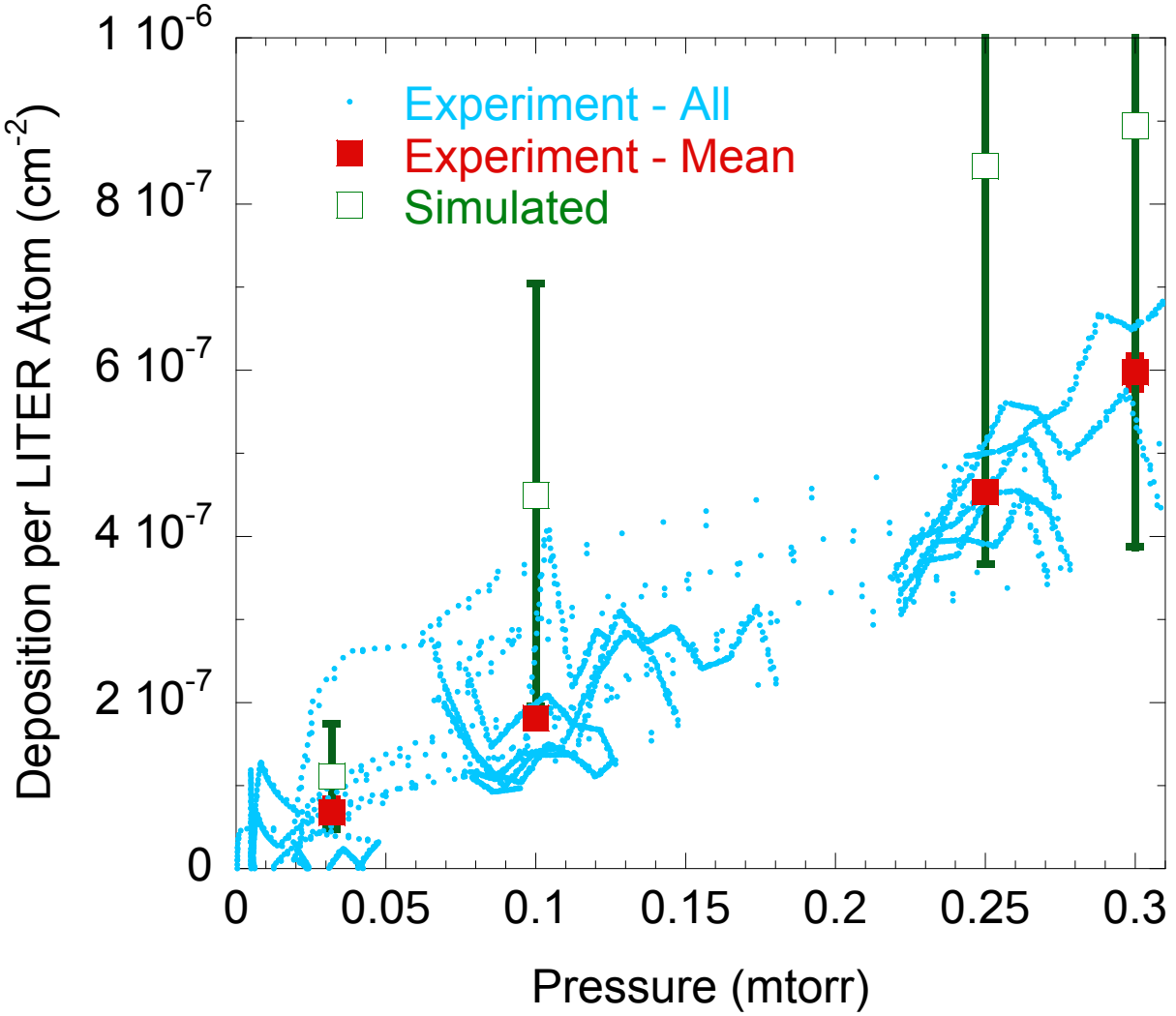
- Simulation error bars: $(2/\pi)^{1/2}$ x 71%.

- Combine experimental data in 0.01 mtorr bins,

  - Compute 90% confidence intervals,

  - N ~ 100 $\Rightarrow$ too small to see!

  - But, errors NOT normally distributed.



Discussion

- Simulations agree with experimental data within estimated uncertainties,
- But, consistent 50% discrepancy & tracks in data suggest systematic errors.
- Future work will focus on reducing uncertainties.
- Also, perform dedicated experiments to decouple model components,
  - Operate LITERs separately,
  - Use QMBs in other parts of vessel,
  - Run LITERs at lower temperatures.