Impurity Migration Simulation of PISCES-A He Exposed Tungsten with GITR

Comparison of net erosion and volumetric transport

T. R. Younkin[1,2], D. L. Green[2], A. Lasa[2], J Drobny[3], D. Curreli[3], J. Canik[2], S. Blondel[1], R. P. Doerner[4], D. Nishijima[4] and B. D. Wirth[1]

[1] University of Tennessee, TN, USA
[2] Oak Ridge National Laboratory, TN, USA
[3] University of Illinois, Urbana-Champagne, IL, USA
[4] University of California, San Diego, CA, USA

THE UNIVERSITY OF TENNESSEE KNOXVILLE

s based upon work supported by the U. S. Department of Energy, Office ce of Fusion Energy Sciences and Office of Advanced Scientific earch through the Scientific Discovery through Advanced Computing ct on Plasma-Surface Interactions.

Simulating a linear device is a step towards modeling ITER Tungsten components

- Physics models to be evaluated with linear machine dedicated experiments:
  - Net erosion of materials exposed to He plasma.
  - Ionization and volumetric transport of impurities through the background plasma.
  - Redistribution of the eroded material.
- GITR is a component in a larger integrated simulation
  - High performance computing component for the impurity particle push.
  - Provided background plasma profiles, sheath model, surface model.
  - Traces particles through plasma and surface operators.

PISCES target and tower

GITR Uses Trace Impurity Model for Particle Track Simulation

Classical velocity change moments (Fokker-Planck)

Thermal gradient force correction

$$m_a \frac{\Delta \bar{U}}{\Delta t} = q_a(\bar{E} + \bar{U} \times \bar{B}) + m_a \left[\hat{U}_{\parallel} \frac{U}{\tau_s} \pm \hat{U}_{\parallel} \sqrt{\frac{U^2}{\tau_W \Delta t}} \pm \hat{U}_{\perp,1} \sqrt{\frac{U^2}{2\tau_D \Delta t}} \pm \hat{U}_{\perp,2} \sqrt{\frac{U^2}{2\tau_D \Delta t}} \right] + (\alpha \nabla_{\parallel} T_e + \beta \nabla_{\parallel} T_i)$$

Lorentz Force

Collisional Terms

$$\Delta \bar{x} = \bar{v} * \Delta t + \sqrt{D_{\perp} \Delta t} \cdot \widehat{e_{\perp}}$$

Anomalous perp. diffusion

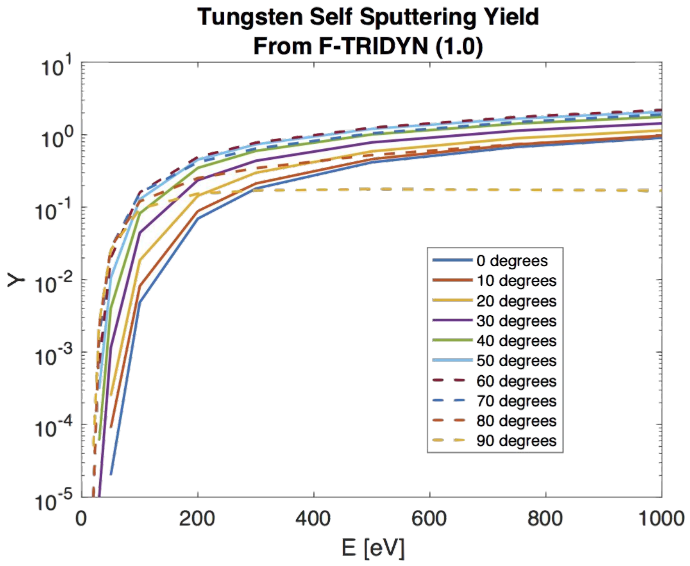
$$n_{Impurity} << n_{Background}$$

- Plus operators for ionization and recombination, multiple charge states, connected to ADAS.
- Particles hitting a material surface undergo operations to weight and re-sample the particle according to the process.

Sputtering Model Comes from Fractal-TRIDYN Output

- Fractal-TRIDYN is a BCA code that simulates a rough surface according to fractal dimension.
- Data for sputtering as a function of energy, angle, and surface roughness are compiled before GITR runs.
- With support of UIUC and the ATOM SciDAC, F-TRIDYN has been run in parallel on 5 nodes at NERSC making use of all processors.

Sputtering yield parameterization

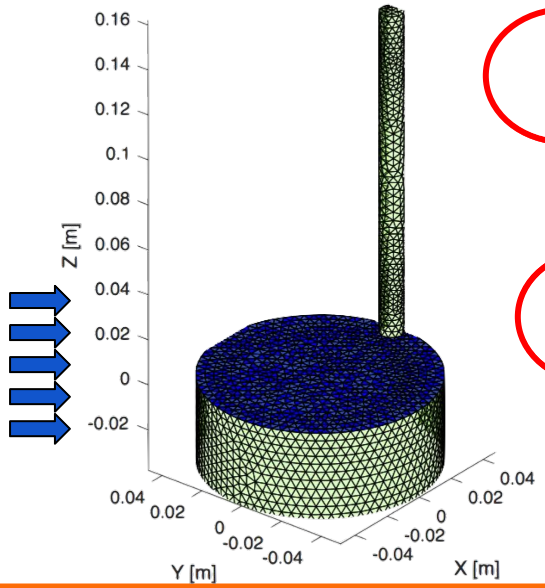


PISCES-A He on tungsten experimental setup is designed to measure impurity migration

- PISCES-A experiment exposes a tungsten target plate biased to -250 Volts to a helium plasma at an approximate flux of ~10^{22} $m^{-2}s^{-1}$ at temperatures of 400 to 600°C.

1

Axial array of W I spectroscopy to measure fall-off in neutral W signal - indication of ionization.



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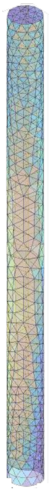
Mass gain of Ti collector tower beads - measure of longer range migration.



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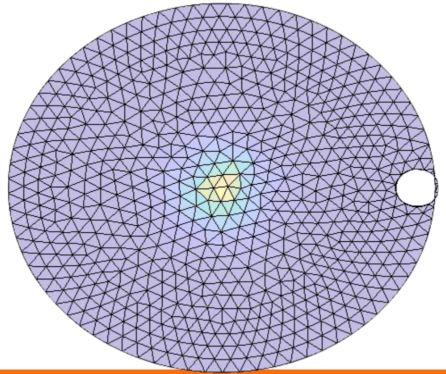
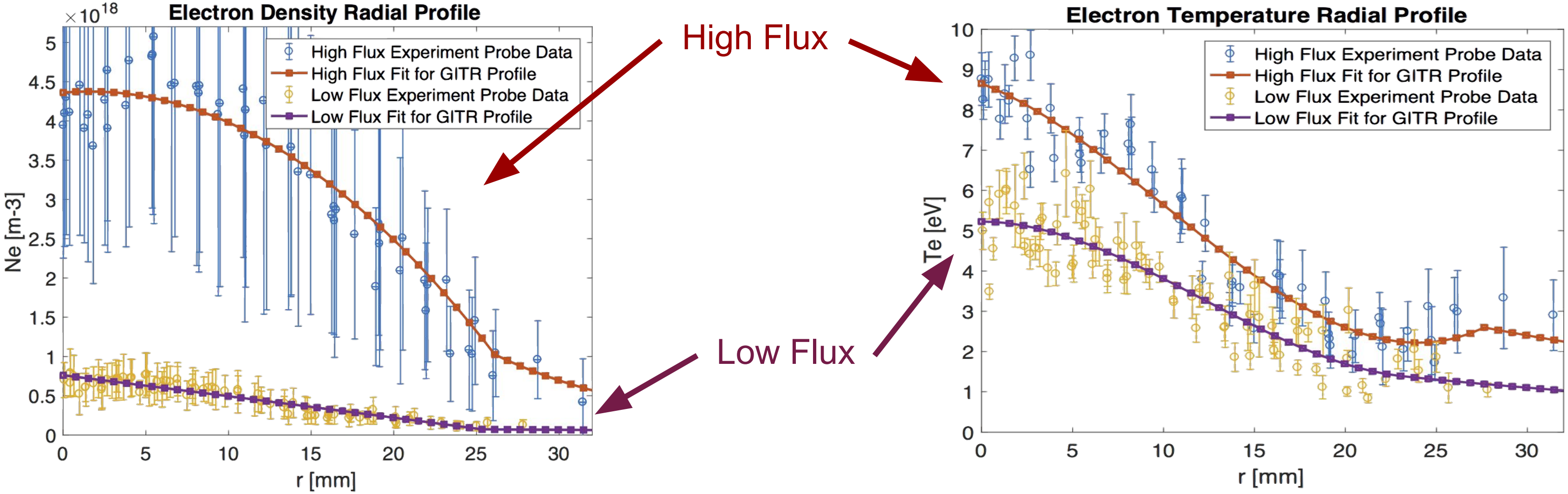
Mass loss of target plate - measure of erosion source and prompt redeposition.



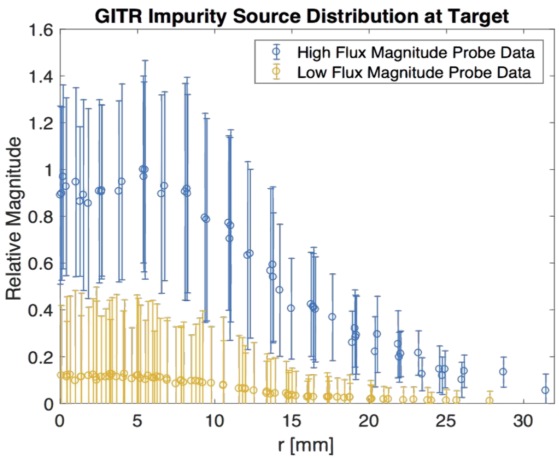
PISCES-A plasma profile measurements used as GITR input

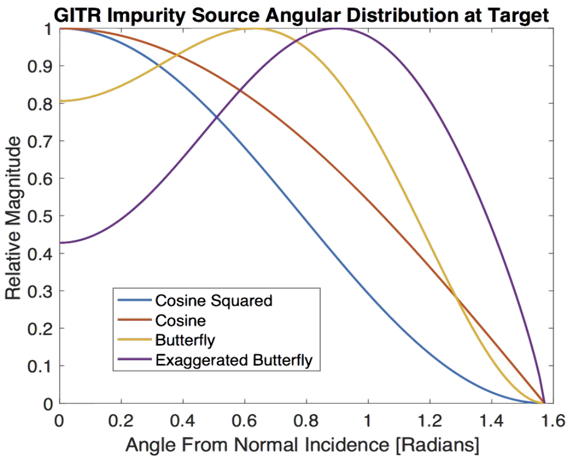
- 800 Gauss magnetic field perpendicular to W target minimizes sheath effects.
- Profiles with + and - 20% of Te and ne values were also used to investigate sensitivity.



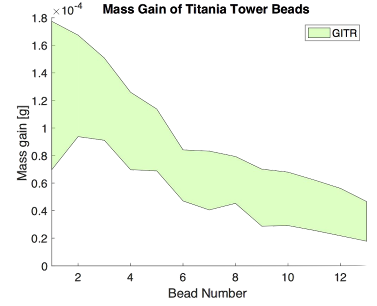
Spatial distribution of impurity source is known, but angular distribution is not

- Radial flux profiles were used to sample spatial distribution of He eroded W from the target.
- A variety of angular distributions were used to investigate sensitivity.
- Thompson energy distribution used with Es = 11.75 eV.

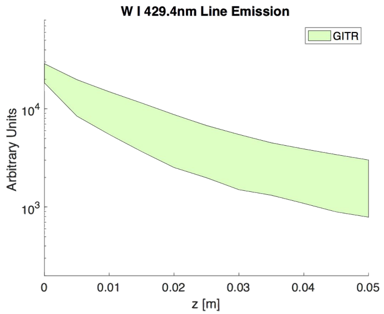




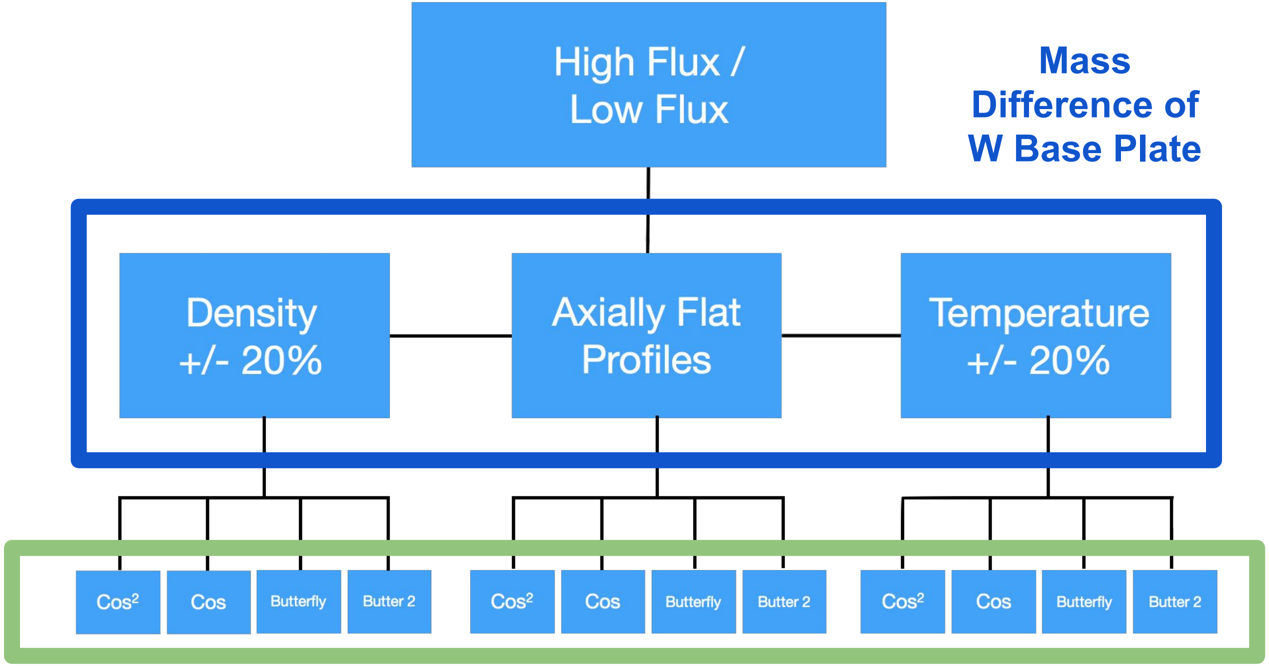
A scan in several parameters will display the sensitivity of the model



Mass Difference of Tower Beads



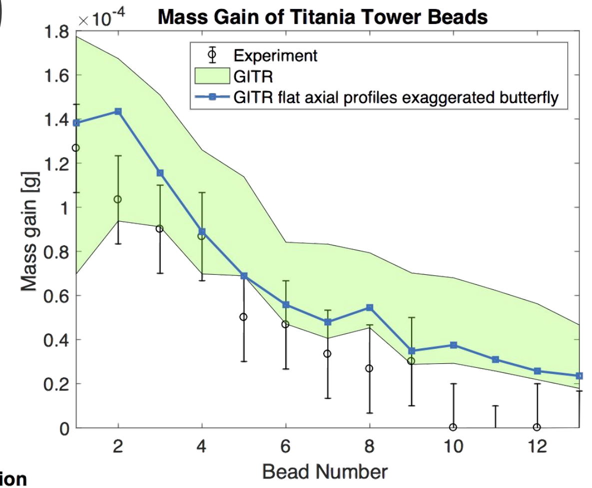
W I Synthetic Diagnostic



Mass Difference of W Base Plate

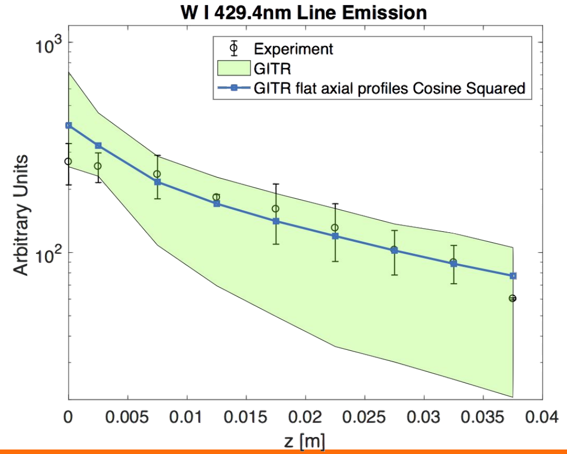
Results for low flux exposure (10,000s)

- Mass loss of target plate is near experimental values.
- Mass gain of collector beads is accurate with slight overprediction far from the target plate.
- Shape of line emission curve shows fair agreement with considerable sensitivity to scanned parameters.



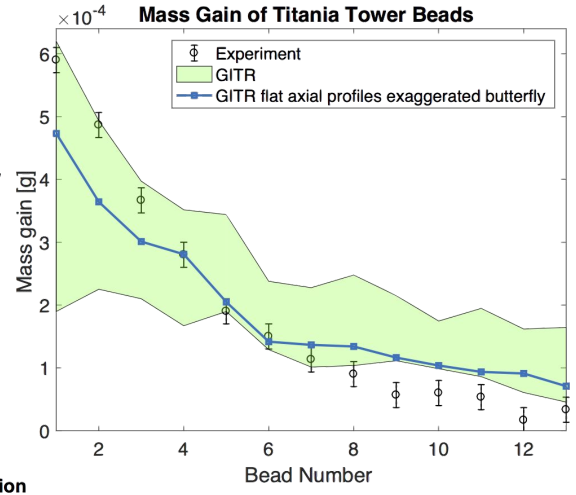
Mass Difference of W Base Plate

	Mass Loss [g]	%Eroded Material Returned to Target
Experiment	0.01883	-
GITR flat profiles	0.0152 - 0.0188	57 - 65
GITR +/- Te	0.0146 - 0.0295	32 - 67
GITR +/- ne	0.0145 - 0.0208	52 - 67



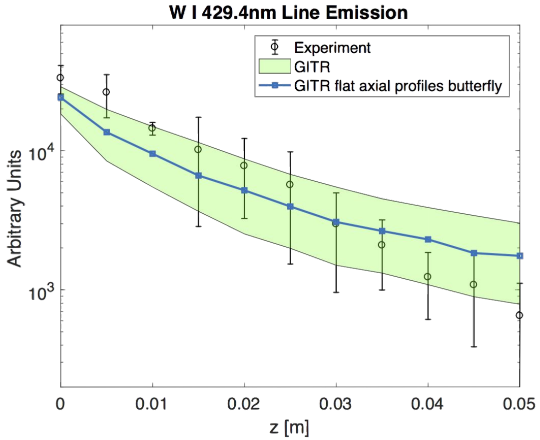
Results for high flux exposure (5,000s)

- Higher percentages of prompt redeposition compared to low flux case.
- Mass gain of bead collectors agrees well with experimentally measured values.
- Variability in synthetic diagnostic profile.



Mass Difference of W Base Plate

	Mass Loss [g]	%Eroded Material Returned to Target
Experiment	0.079533	-
GITR flat profiles	0.0563 - 0.0737	70 - 77
GITR +/- Te	0.0475 - 0.0888	65 - 81
GITR +/- ne	0.0475 - 0.0888	65 - 81



GITR Performance And Numbers

- GITR running on single node of a GPU development machine - 2 NVidia Tesla K80s.
- 28,000 triangular face boundary elements.
- The hashing algorithm removes the simulation run time dependence on the number of mesh elements used to represent the material surface.
- 10^5 particles per run
- dt = 1e-8s for 10,000 steps
- run time is ~ 66 seconds

Conclusions and future work

- GITR trace impurity model predictions of W erosion, ionization, and deposition agree well with the three experimental observables.
- Initial sensitivity study on variations in sputtered W angular distributions as well as background plasma temperature and density provide a prediction band reasonably consistent with experimental error bars.
- More formal uncertainty quantification planned for future.
- He/D mixed plasma experiments are planned for PISCES.
- Revisit calculations with improved coupling to assess Fractal TRIDYN input for the sputtered W energy and angle distributions.