A Validated Multi-Scale, Multi-Physics Modeling Approach to Predicting Erosion, Re-deposition & Gas Retention in Tokamak Divertors

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KNOXVILLE

A Validated Multi-Scale, Multi-Physics Modeling Approach to Predicting Erosion, Re-deposition & Gas Retention in Tokamak Divertors

With valuable contributions from:

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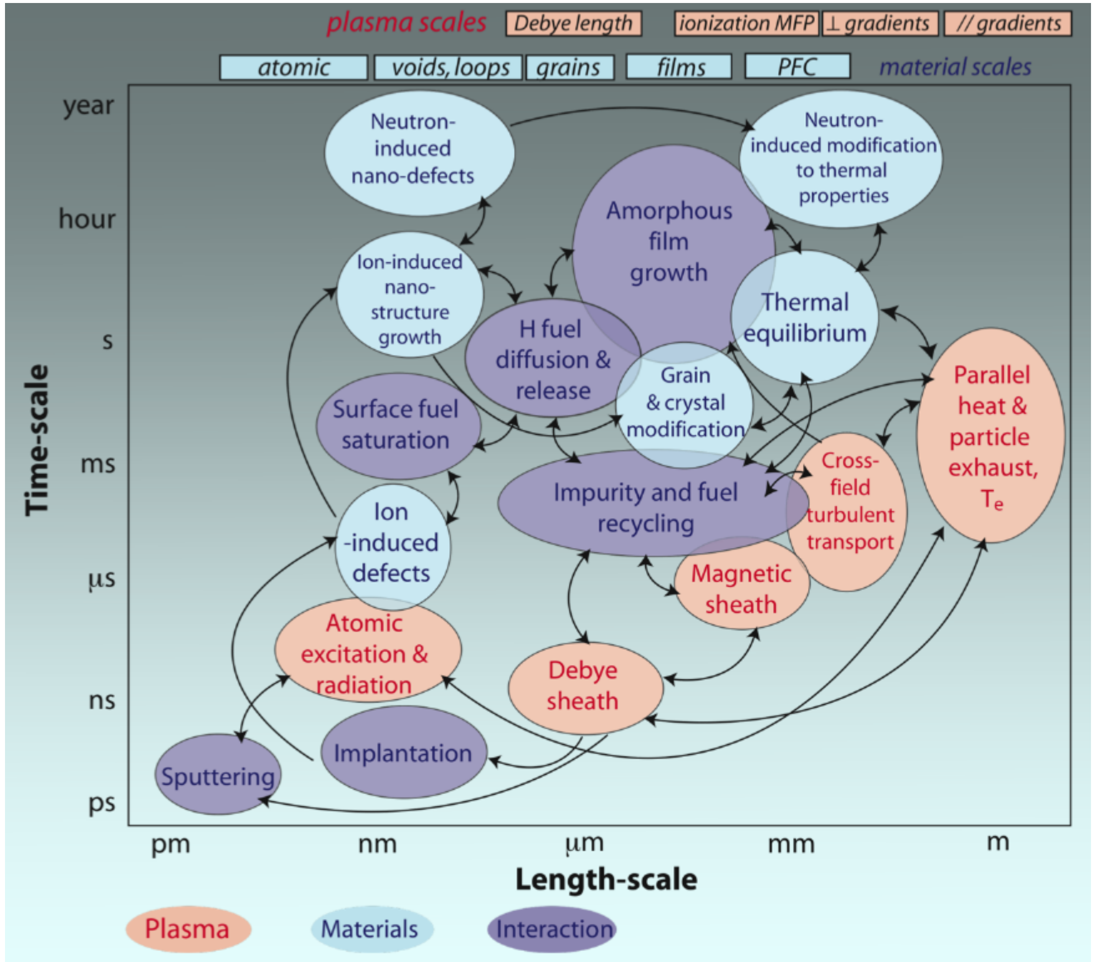
Plasma-material interactions (PMI) impact the performance of both material and plasma

- PMI compromise both material and plasma performance
  - Mutually degrade
  - Erosion, fuel trapping, morphology changes, etc.
- Critical for future fusion reactors, their wall design and material choice

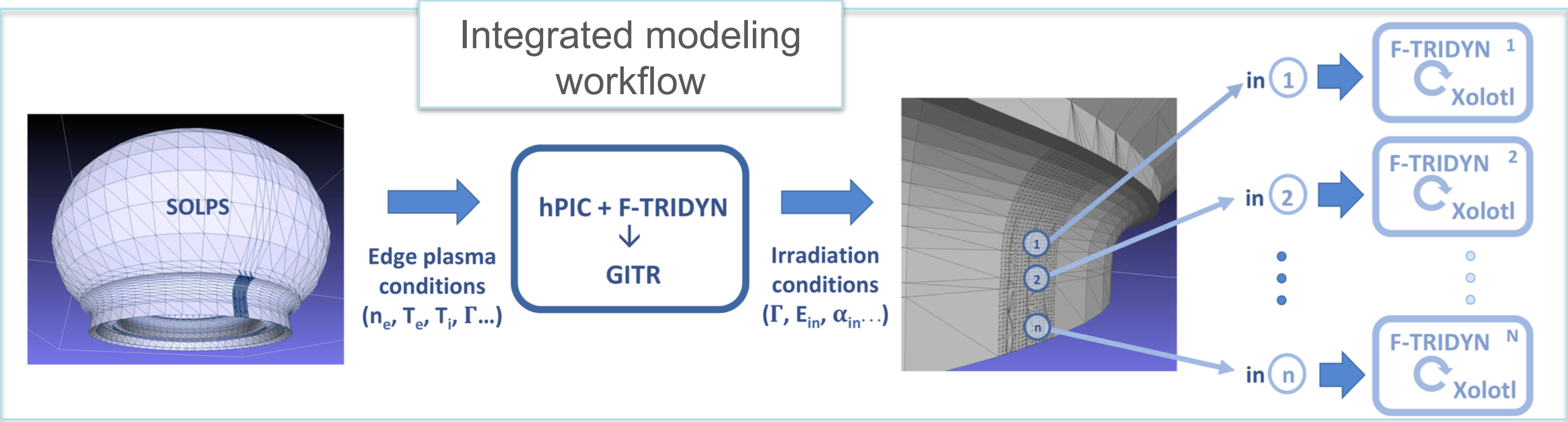
Plasma-material interactions (PMI) are multi-physics and multi-scale in nature

- PMI compromise both material and plasma performance
  - Mutually degrade
  - Erosion, fuel trapping, morphology changes, etc.
- Critical for future fusion reactors, their wall design and material choice
- It’s a multi-scale physics problem
  - We address it by integrating multiple, high-fidelity models



Wirth et al., *MRS Bulletin* **36** (2011)

The resulting integrated model is applied to simulate PISCES and ITER plasma exposures



OUTLINE

- The model was benchmarked against PISCES experiments
- We applied it to predict the evolution of the ITER divertor under He operation and burning D-T plasmas
- We use these tools to further examine the effect of He on hydrogenic retention
- We've applied the model to WEST experiments with He plasma

Model validation

Benchmarked against PISCES experiments

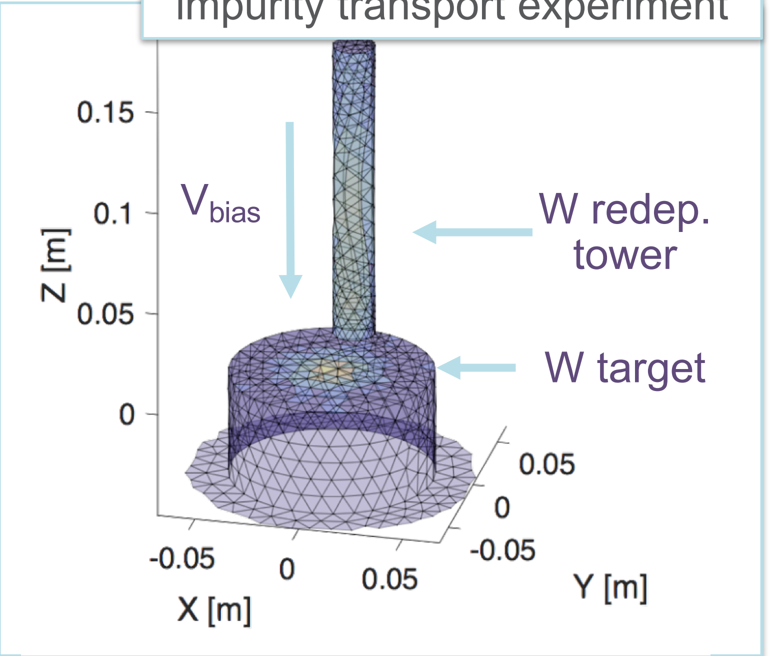
The integrated model was benchmarked against PISCES experiments

- Extensive comparison of impurity transport (GITR + F-TRIDYN) and sub-surface evolution (F-TRIDYN + Xolotl) predictions to experiments, across a range in
  - Flux: 0.5-5.4·10^{22} /m^2s
  - Biasing voltage: 75V, 250V
  - Plasma composition: 100% He,10%He-90%D

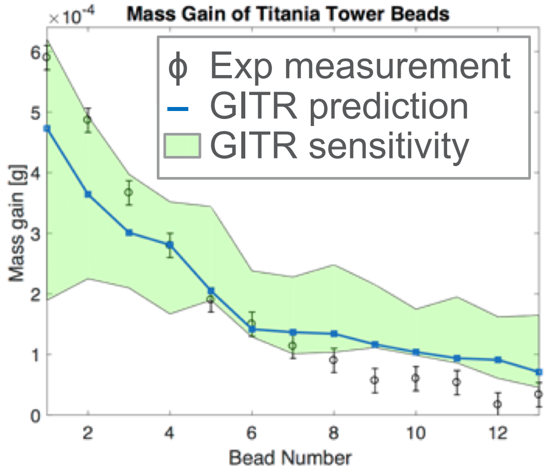
- Langmuir probe measurements provided the background plasma n_e, T_e

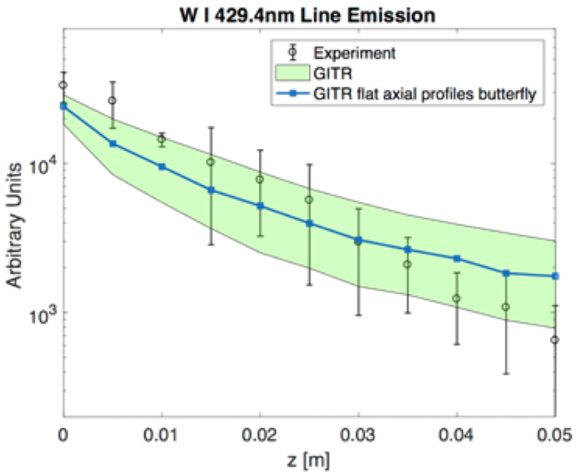
- Two sets of experiments
  - W I spectroscopy, target mass loss, tower mass gain for to measure W erosion and transport
  - Removable W targets to analyze with LIBS and LAMS

impurity transport experiment

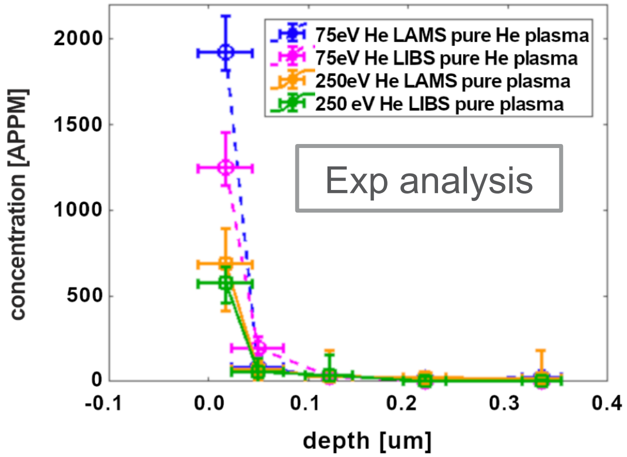


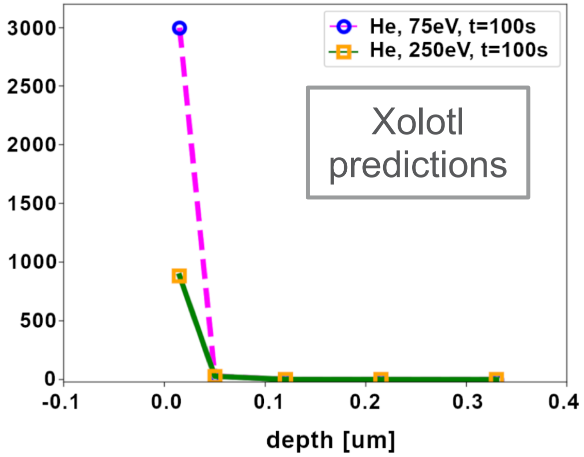
Xolotl and GITR show good agreement with experimental measurements





	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 reproduces experimentally measured mass loss, W I lines and Ti bead mass gains
- The experimentally measured He & D concentrations are fairly reproduced by Xolotl

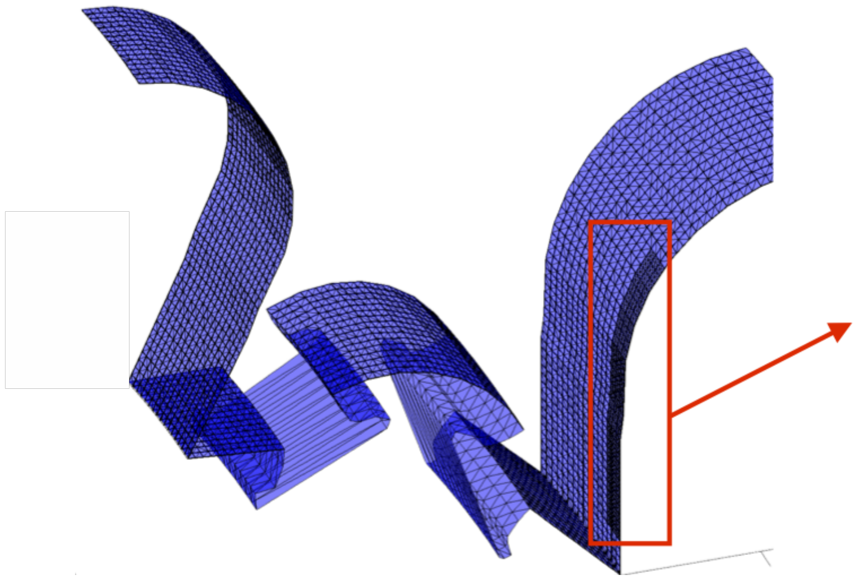
Model application

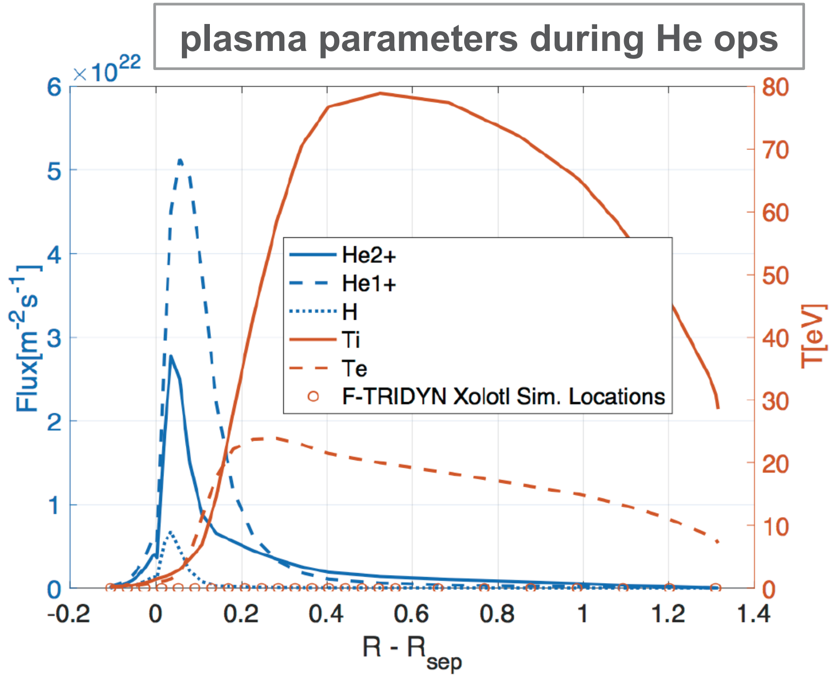
Predicting the evolution of the ITER divertor under He plasma and burning plasma operations

SOLPS predicts a partially detached divertor during He and burning plasma operations

- Standard strongly radiating, partially-detached scenario
  - Very low temperature (~1 eV), high flux near separatrix strike point
  - Higher temperature, lower density and flux away from strike point

- During BPO, nearly 75% of power is radiated,
  - mainly by Ne in the divertor; peak heat flux of ~7 MW/m^2



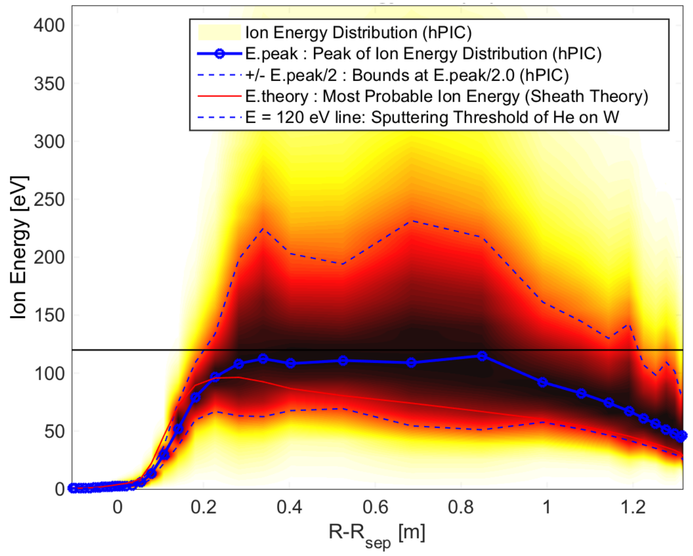


plasma parameters during He ops

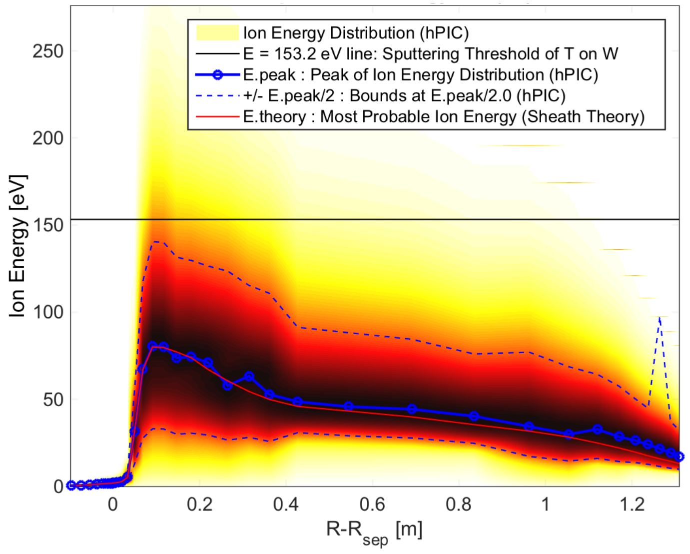
The high-energy tail of light species’ IEADs extends beyond the threshold for W sputtering

- hPIC shows that while much of the impact energy-angle distribution (IEAD) for light ions is below energy threshold for W sputtering,
- the high-energy tail extends well above sputtering threshold

IEADs for He$^+$, He ops



IEADs for T$^+$, BPO

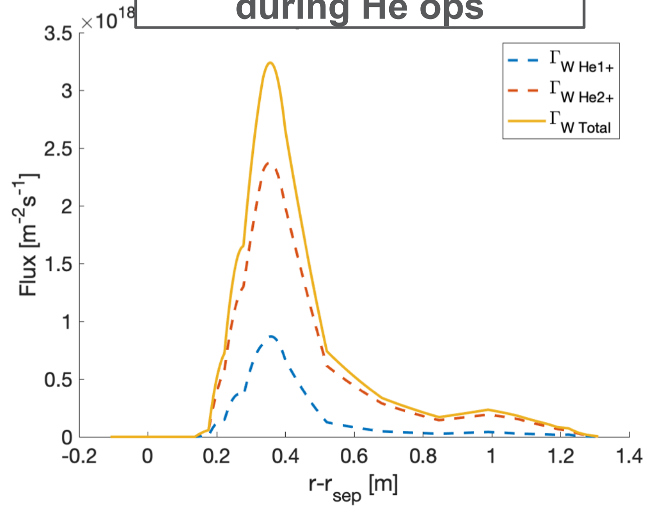


Heavy impurities dominate sputtering when present, with contributions from the high-energy tail of light species

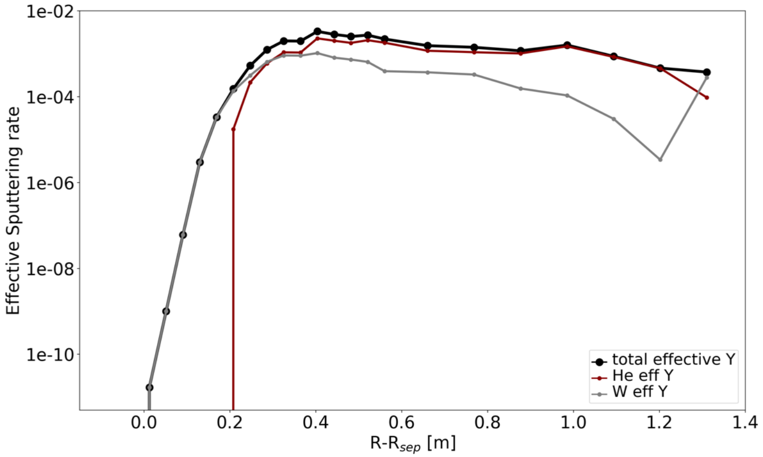
Accounting for sputtering and reflection rates provided by F-TRIDYN, integrated impurity transport calculations predict

- He^{2+} is the main impurity source during He plasma operations (W in near the strike point)
- heavy impurities (Ne) dominate sputtering during BPO (W in the private flux region)

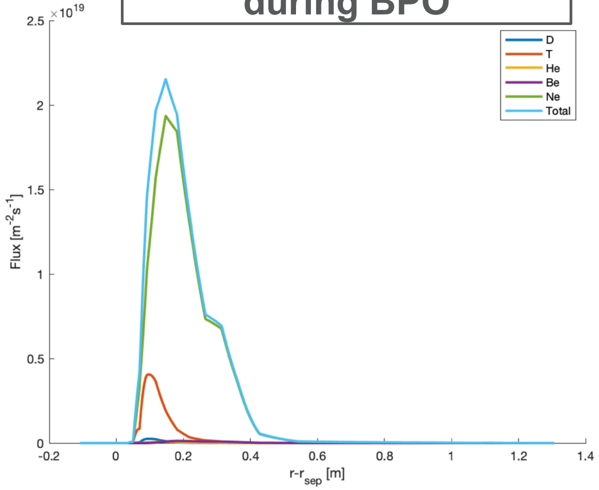
W erosion contributions during He ops



Sputtering rate during He ops



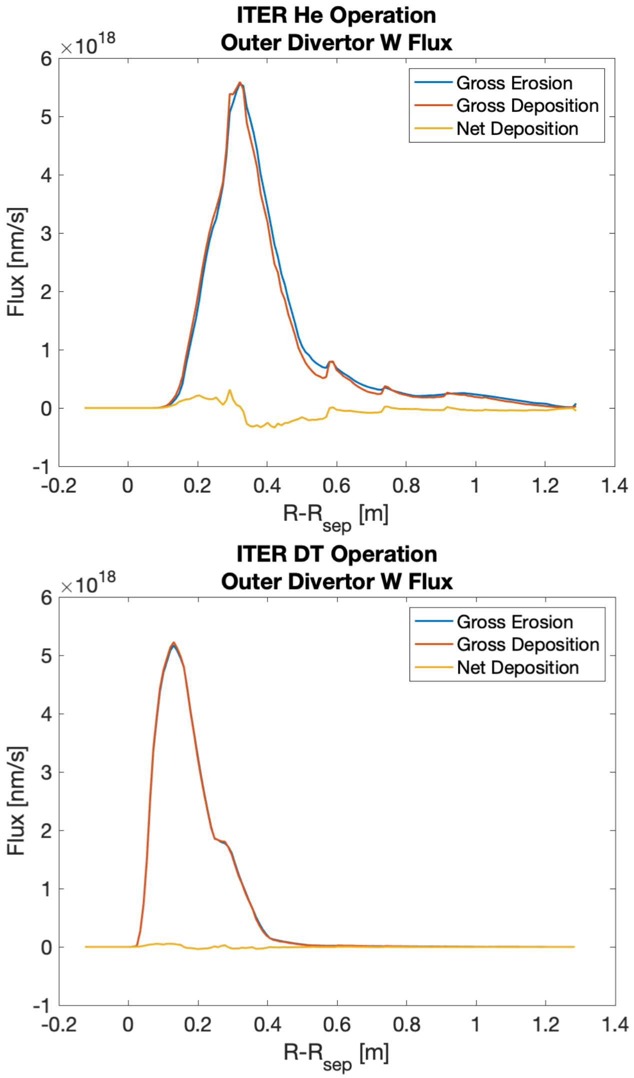
W erosion contributions during BPO



GITR predicts strong local re-deposition, with net deposition around the strike point

Impurity transport calculations of GITR predict

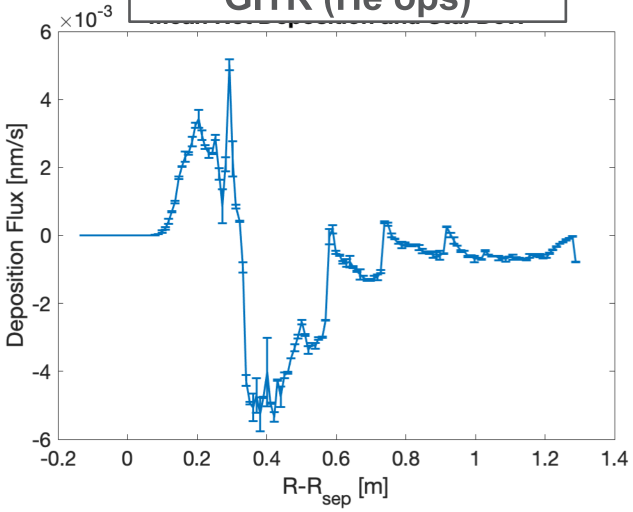
- strong (>95%) prompt or local re-deposition of the eroded W
  - strong drag forces that push impurities back to the surface
- net deposition around the strike point
  - transport by local E fields
  - higher deposition rate at lower T_i
- net erosion further along the target



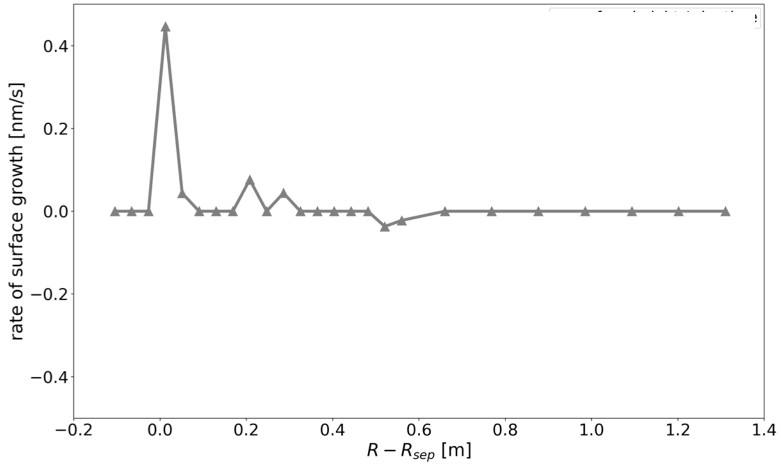
Surface height in Xolotl is similar to GITR, with enhanced, He-induced surface growth

- The same surface height pattern is predicted by GITR and Xolotl
- Differences arise around the strike point (T_i~eV) from shallow gas implantation, He-induced trap mutation and surface growth
- These processes affect less the locations with high impact energies (T_i~40eV, further up the target)

GITR (He ops)



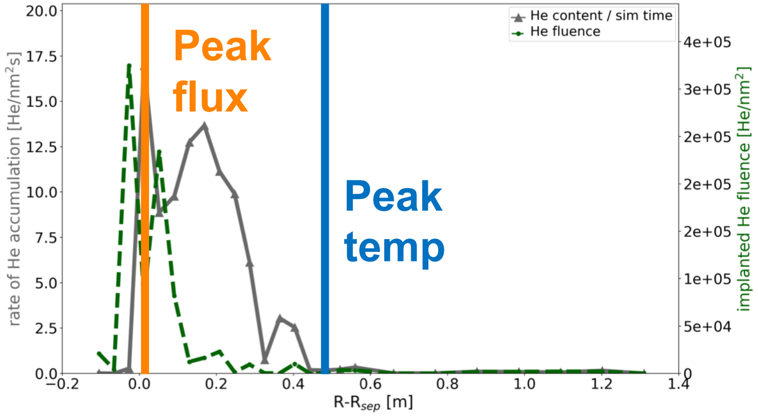
Xolotl (He ops)



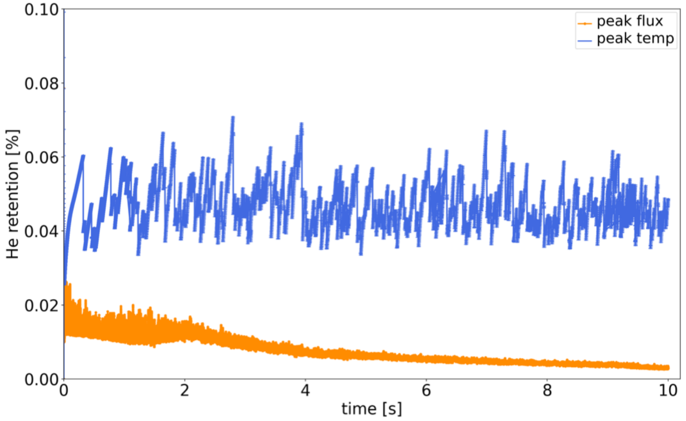
During He ops, He accumulation & retention are a balance between implantation rate & energy

- He accumulation largely follows the flux profile, with larger retention where T_i is high,
  - even though flux & fluence are order(s) of magnitude less than at the peak
  - Shallow implantation at low T_i leads to higher outgassing rates and more frequent, small bursts; thus lower He retention
  - Deeper implantation at high T_i leads to less outgassing and larger, less frequent bursts; thus higher He retention
- Consistent with results from PISCES

He accumulation



He retention

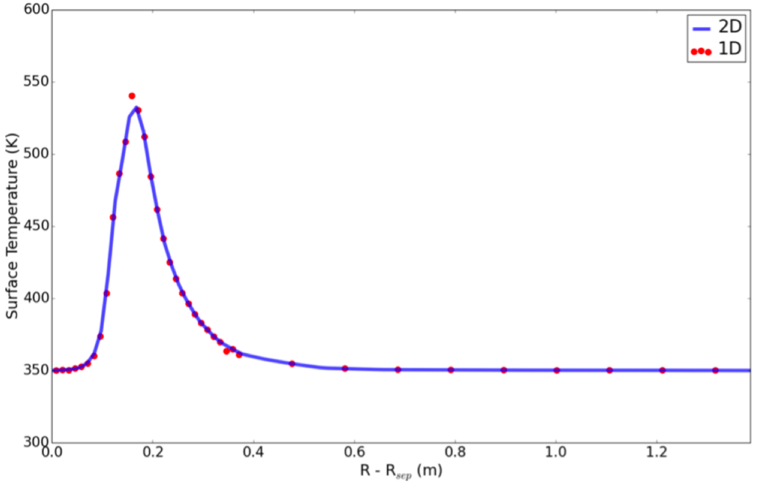


During BPO, heat fluxes increase the surface temperature by up to ~200K

- For $P_{in,\ SOL}$= 100 MW discharge, T_{surf} increases up to ~200K
  - While this is no threat of melting or recrystallization (no transients included)
  - It does affect gas dynamics

- The thermal coupling between locations is negligible
  - We model multiple, independent 1D locations

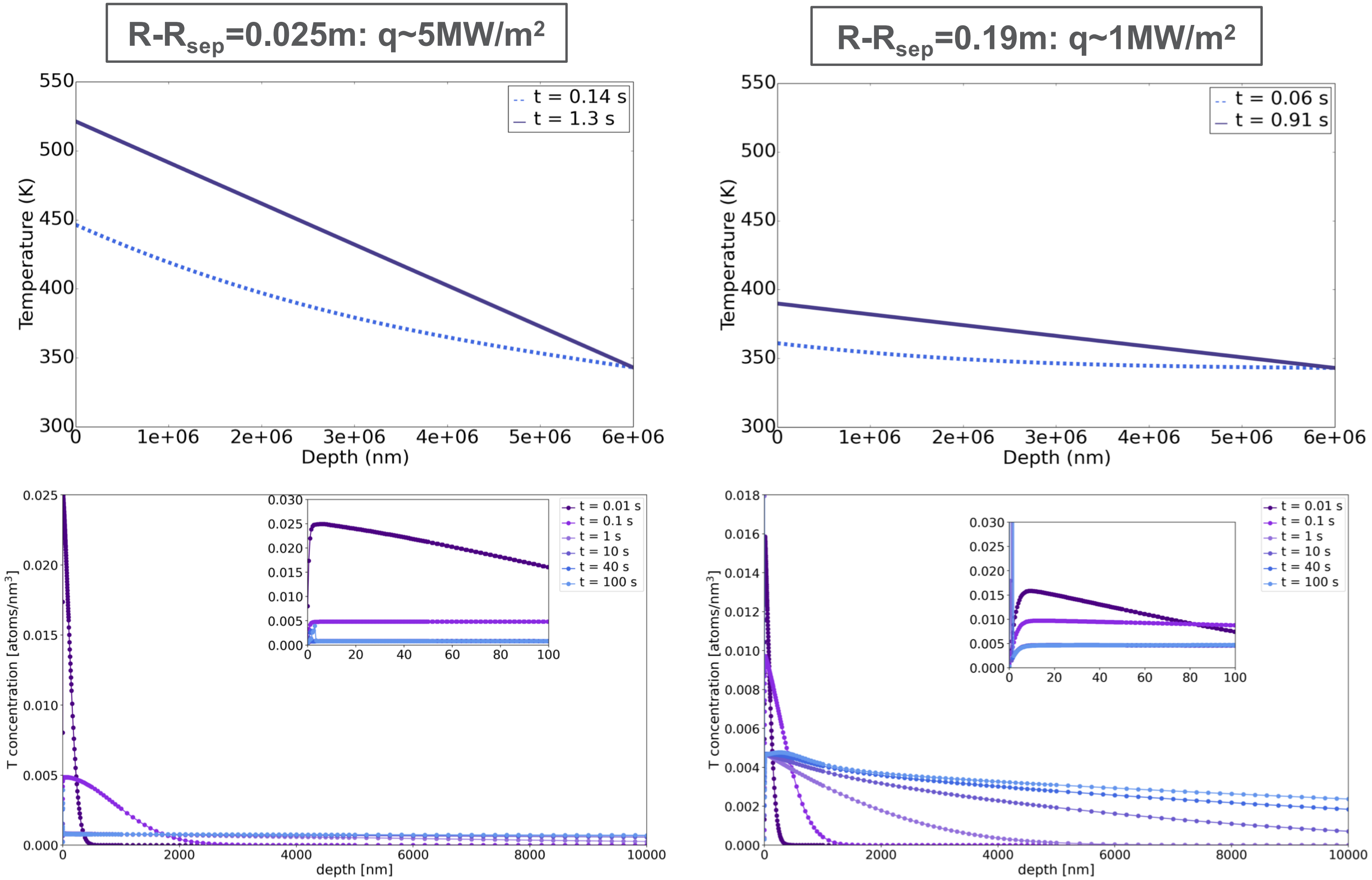
Surface temperature



Differences in T_{surf}, and thus in gas diffusion correlated with the local heat flux

- Tritium diffuses faster with increasing surface temperature (T_{surf}), mainly outgassing

- The peak in hydrogen concentration takes the value expected for $T_{surf}=T_{surf}(t)$



$R-R_{sep}=0.025m$: q~$5MW/m^2$

$R-R_{sep}=0.19m$: q~$1MW/m^2$

Gaining insight into the effect of He on hydrogenic retention

How pre-existing damage drives the depth-integrated T content, as well as its depth-distribution

We now evaluate sequential exposure to He plasmas and ITER Burning Plasma Operations

- For each of the 3 substrate compositions (in He-V clusters), resulting from exposure to:
  - 100s of He plasma in PISCES, at V_{bias} ~ 75 V
  - 100s of He plasma in PISCES, at V_{bias} ~250 V
  - 10s of early ITER He ops

Higher He fluence

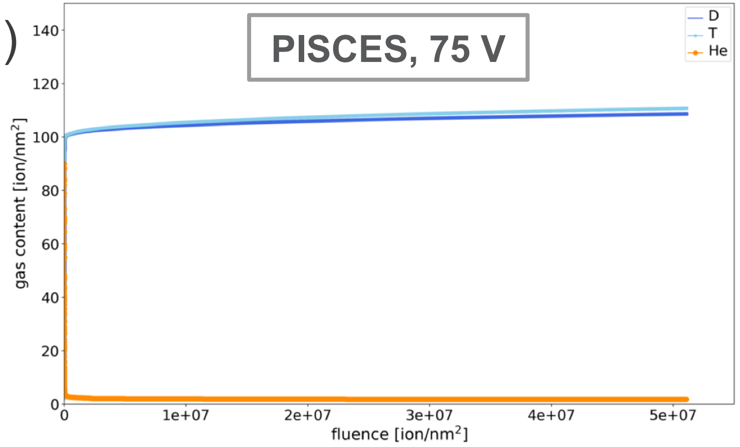
Realistic He spectrum

- We model the subsequent exposure to 100s of full power BPO in 5 locations:
  - Peak in particle flux ($R-R_{sep}$~0.025m)
  - Peak in heat flux ($R-R_{sep}$~ 0.05m)
  - Peak in plasma temperature ($R-R_{sep}$~ 0.1m)
  - 2nd peak in He flux ($R-R_{sep}$~0.2m)
  - Further upstream ($R-R_{sep}$~ 1m)

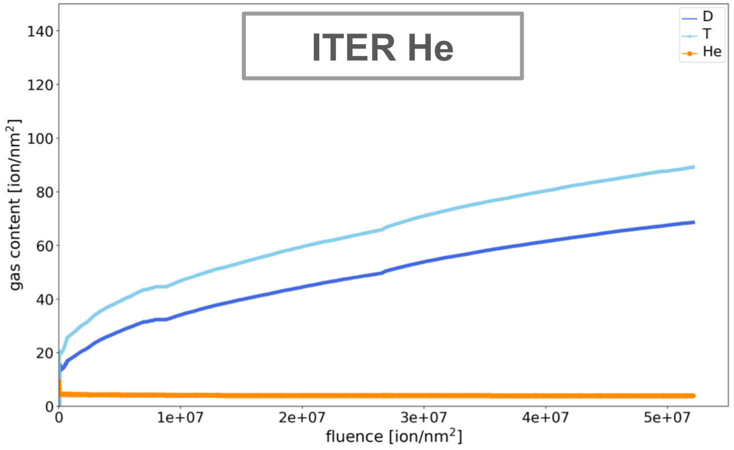
Gas content saturation depends on both the vacancy content and their depth distribution

- In substrates pre-exposed in PISCES, T content stabilizes within *O*(10^{22} ion/m^2)
  - quick increase in D-T content due to initial near surface V content
- continues to grow for initially pristine substrates & pre-exposures to ITER He ops
  - ITER He+BPO: larger increase in H on the long scale because of higher V concentration between 100 and 1000 nm

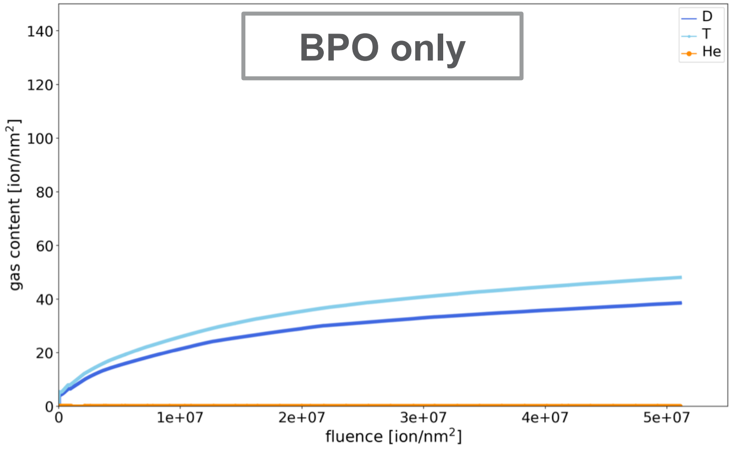
a)



b)



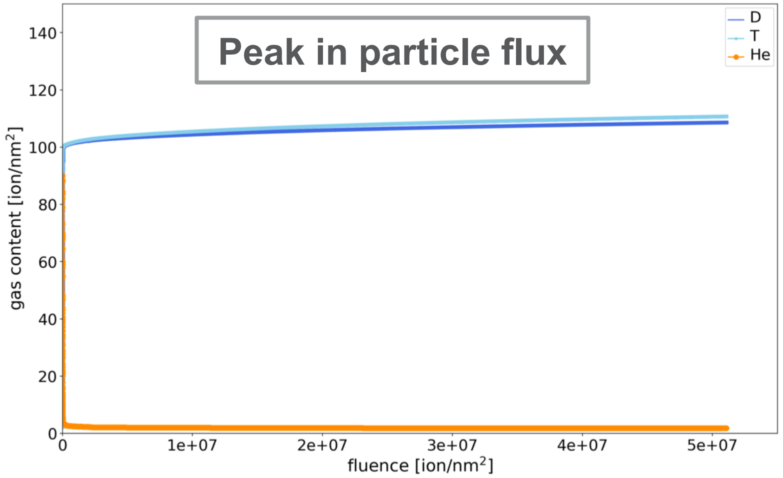
c)



Pre-existing damage greatly determines the saturation level of hydrogenic retention

- The amount of T contained in the PISCES pre-exposed material stabilizes at a fixed value for each V_{bias}
  - 10^{20} atoms/m^2 (75 V) and $1.4 \cdot 10^{20}$ atoms/m^2 (250 V)
- These values are maintained over a wide range of other parameters, although can be altered e.g., by a large presence of bursting

a)



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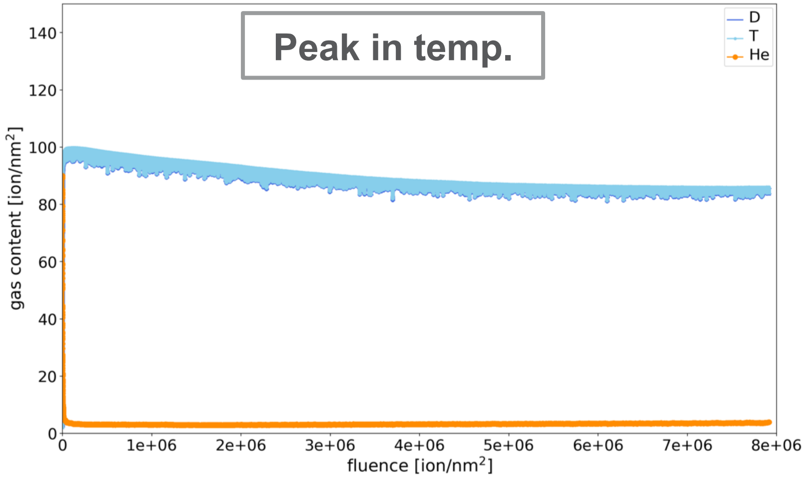


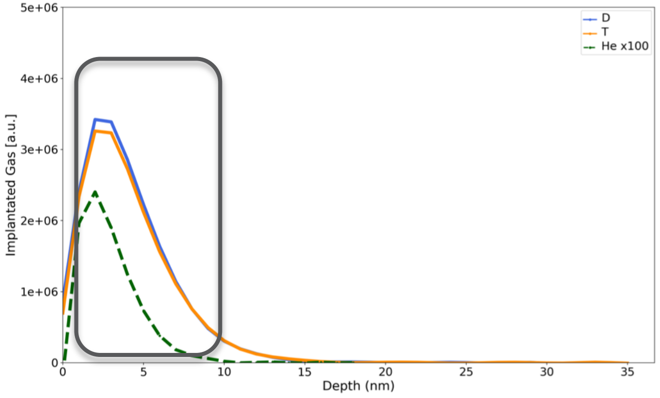
He implantation in pre-existing vacancies leads to bursting

Implantation profile

Initial V size-depth distribution

Evolution of gas content

peak in temp



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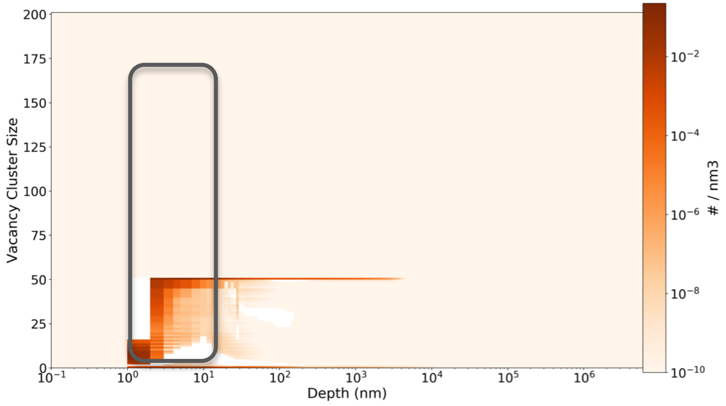

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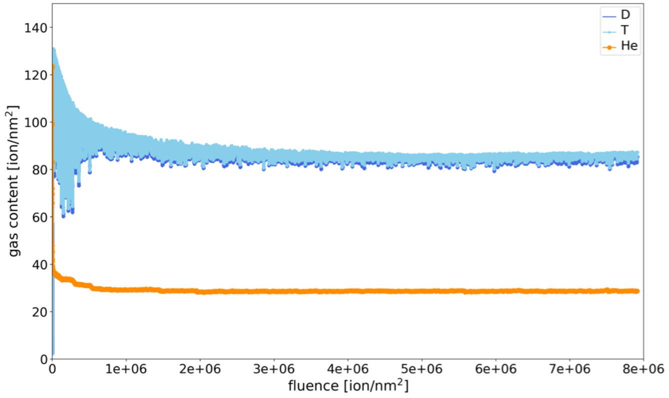
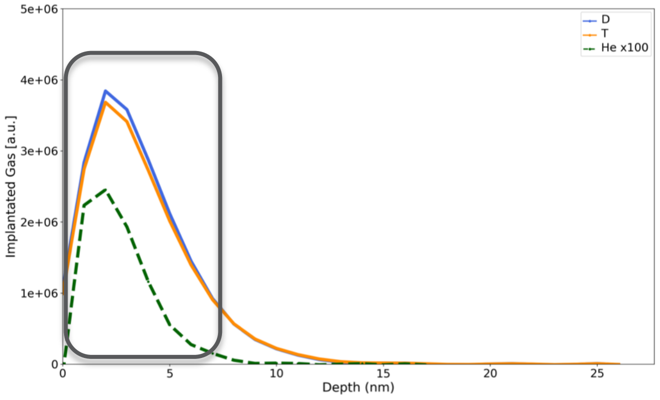


peak in heat flux



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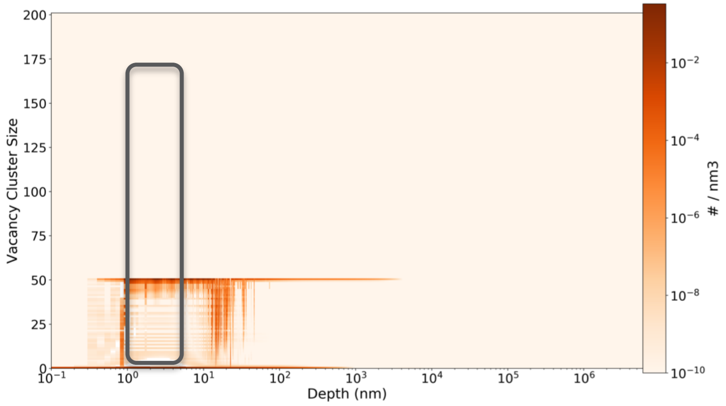

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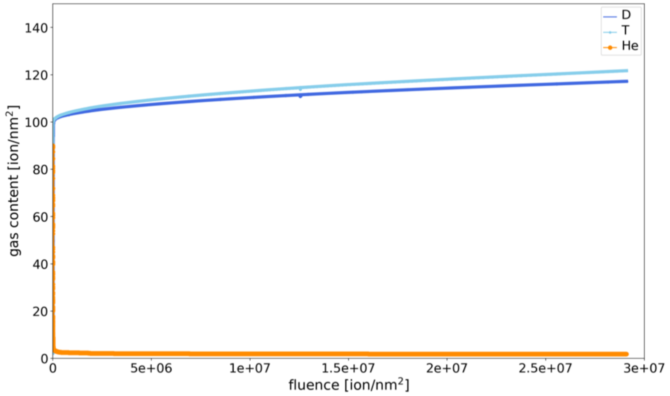
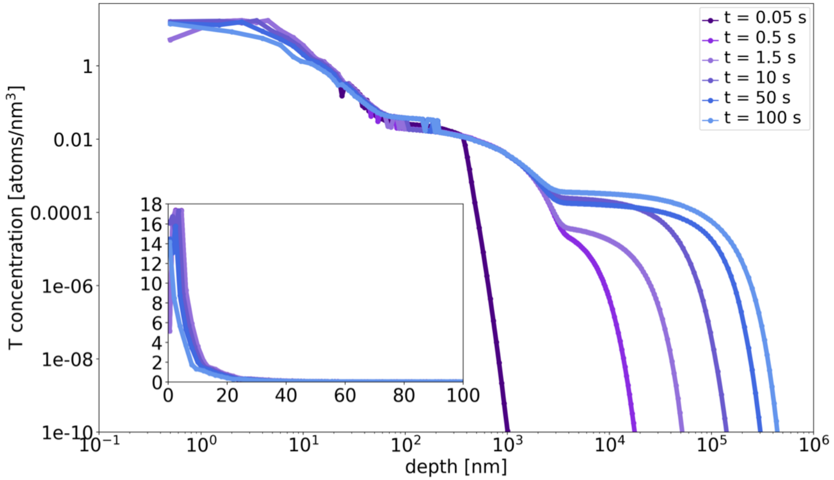


Substrates with pre-existing damage show a reduced temperature sensitivity

- Heat-flux induced temperature variations (~200K) are insufficient to de-trap T from He-V clusters (present in all pre-damaged substrates)

T concentration, peak heat flux, PISCES 250 V

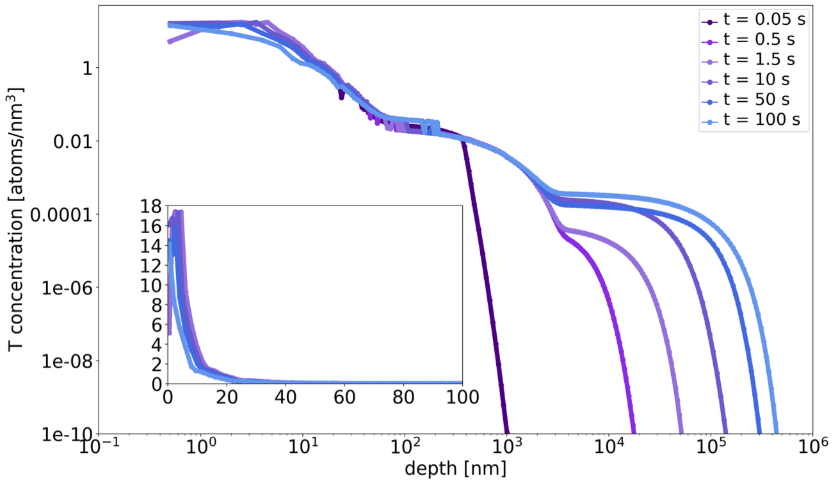


T remains closer to the surface in pre-damage cases, while bulk content is higher for initially pristine ones

- Over all, we observe 3 depth-ranges for gas accumulation:
  a) near-surface (10-100nm), present in all pre-exposed substrates & driven by He damage

(a)

T concentration, peak heat flux, PISCES 250 V



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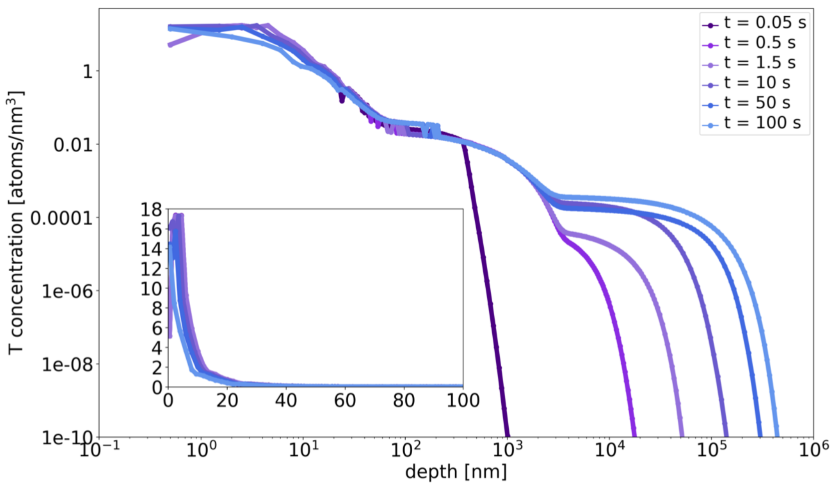
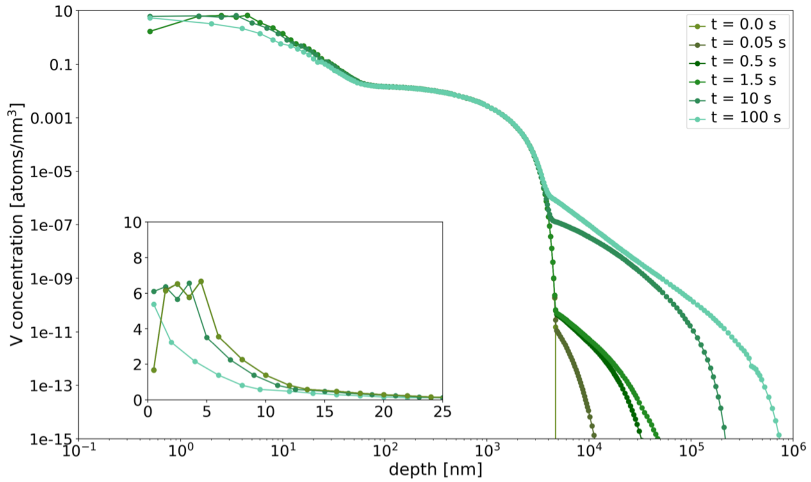
  b) mid-range (100nm-10um), where the deepest post-PISCES exposure vacancies existed

(a) **T concentration, peak heat flux, PISCES 250 V**



(b) **V concentration, peak heat flux, PISCES 250 V**



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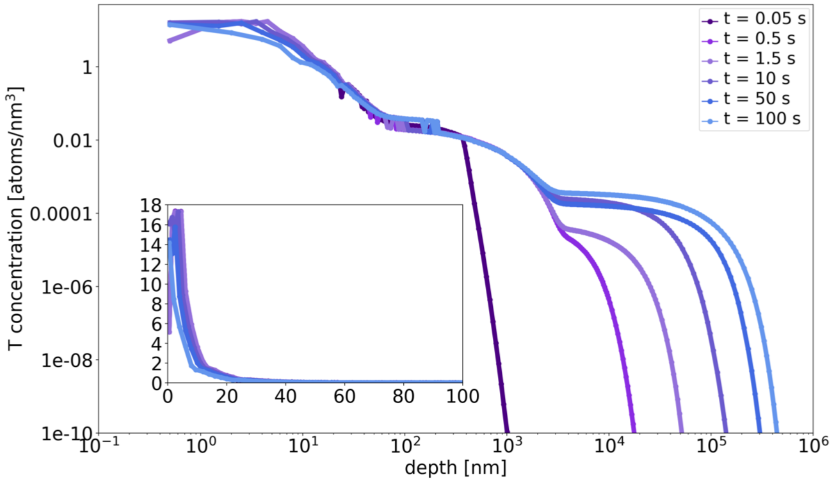
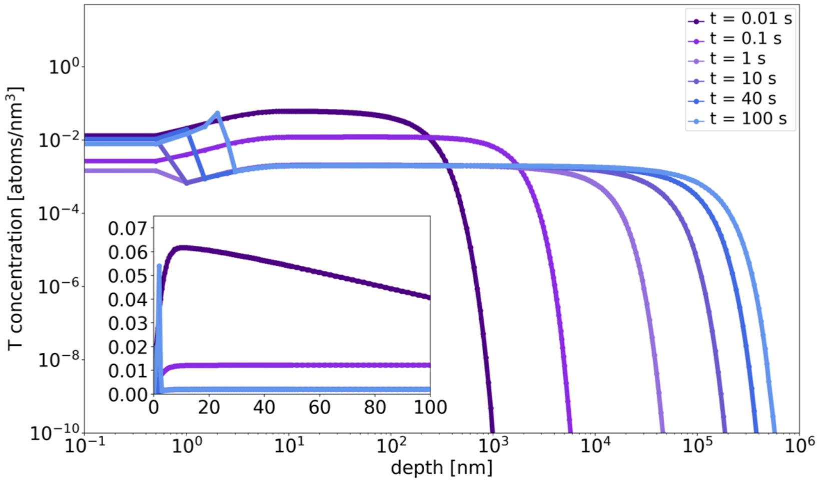
- Over all, we observe 3 depth-ranges for gas accumulation:
  a) near-surface (10-100nm), present in all pre-exposed substrates & driven by He damage
  b) mid-range (100nm-10um), where the deepest post-PISCES exposure vacancies existed
  c) deeper in bulk (>10um), consistently higher in initially pristine substrates

(a), (b) **T concentration, peak heat flux, PISCES 250 V**

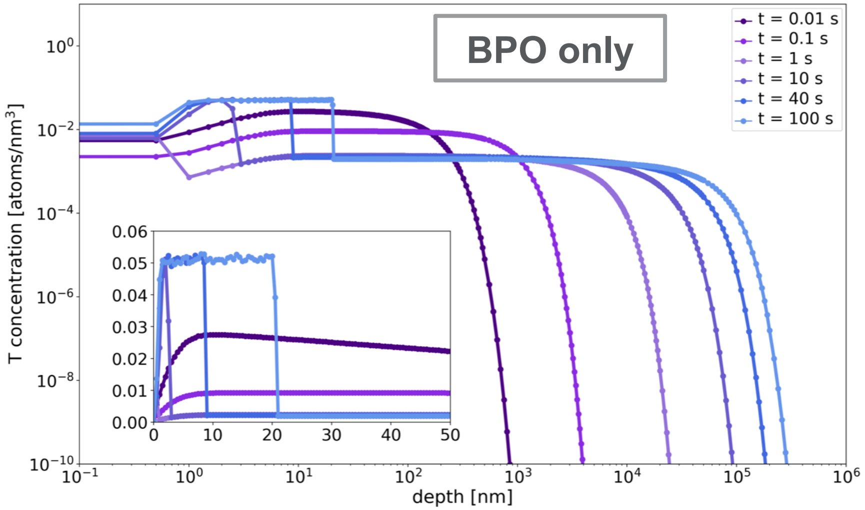


(c) **T concentration, peak heat flux, pristine W**



Even small concentrations of He can induce near-surface T trapping in the long term

- the surface grows because of net W re-deposition
- modified trap mutation (TM) creates He-V clusters near the surface, which move as the surface grows
- when the surface moves up, the He gets implanted where the HeV had been created (implantation at 1-5 nm), trapping directly with the HeV clusters and generating bubbles large enough to burst



- after bursting, the He outgasses and V's remain; the cavity is refilled with D-T, the main plasma species, which saturate the bubble

- Similar effects have been observed experimentally

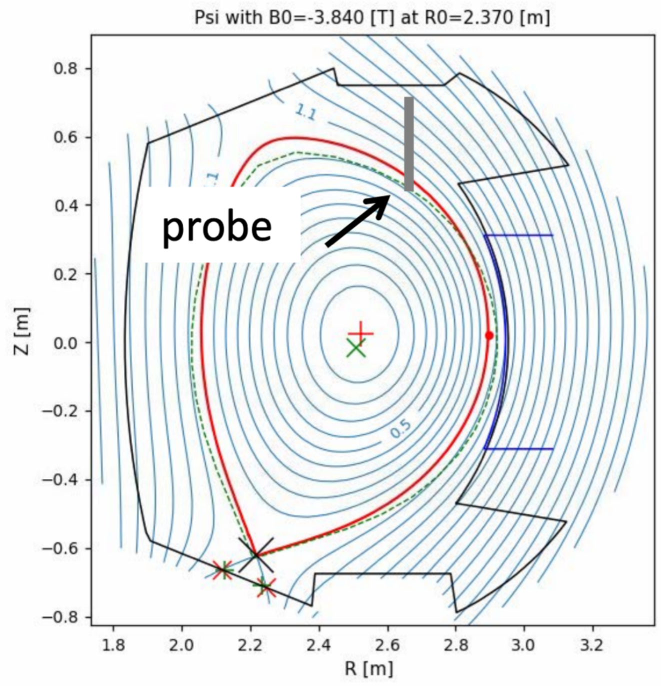
V.K. Alimov et al., JNM 399 (2010)
K. Kayatama et al., FST, 54:2 (2008)
M.J. Baldwin et al, NME 23 (2020)

Application of our model to simulating WEST experiments

We’ve applied similar workflows as for ITER simulations to interpreting WEST He plasma experiments

This was a great opportunity to benchmark our codes against existing, all metal tokamak experiments

- Unfortunately we’ve faced the reality of working with tokamaks (high O concentrations)



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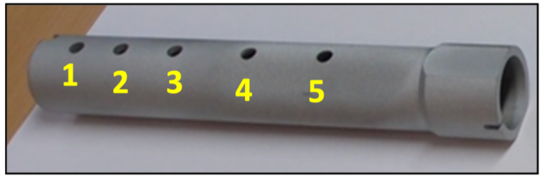

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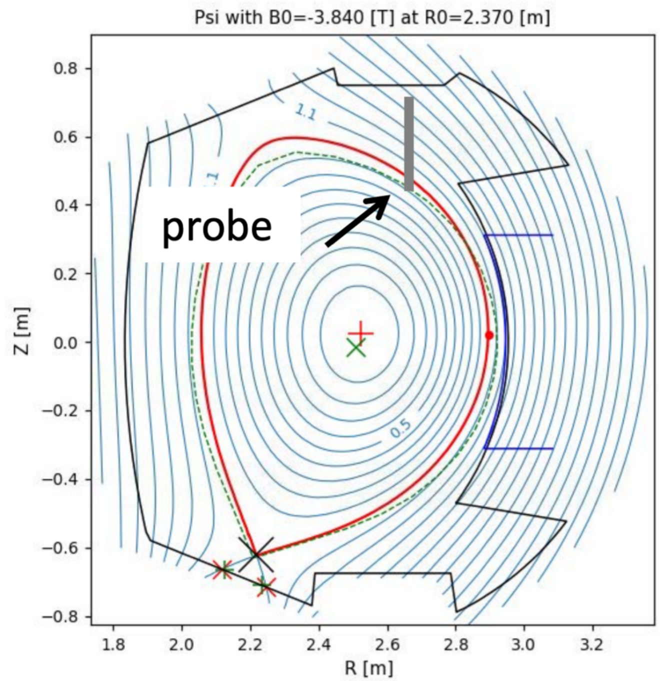
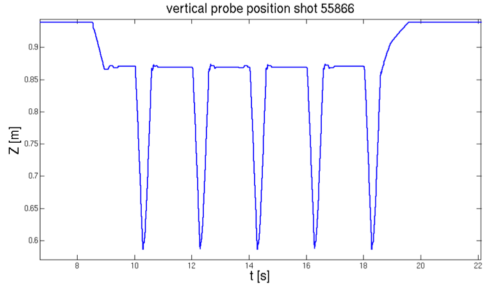


We’ve followed two different workflows:

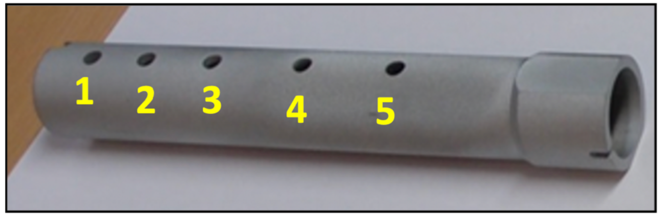
- ITER-like flow to study erosion-transport of W off the divertor
- A simplified sequence to study the evolution of samples in the collector probe

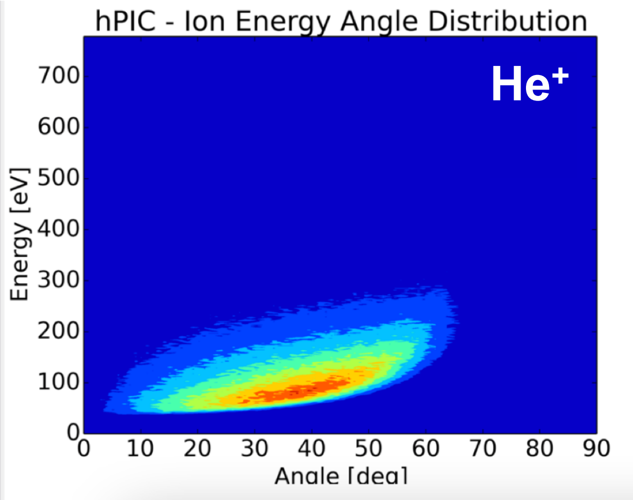
SOLPS (n, T, …) → **hPIC (IEADs)** → **RustBCA (spY, implantation)** → **Xolotl (matl. evolution)**

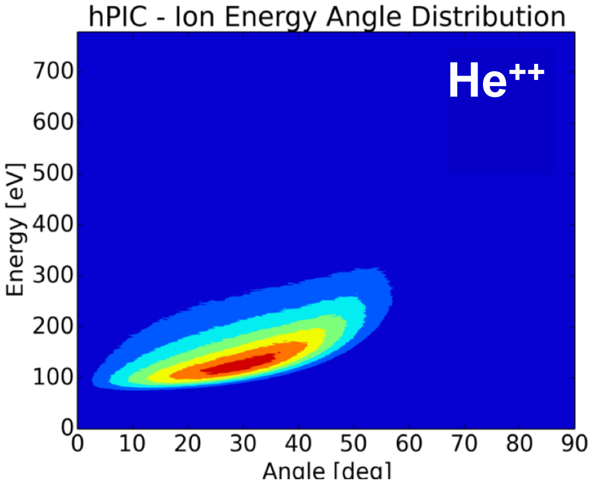


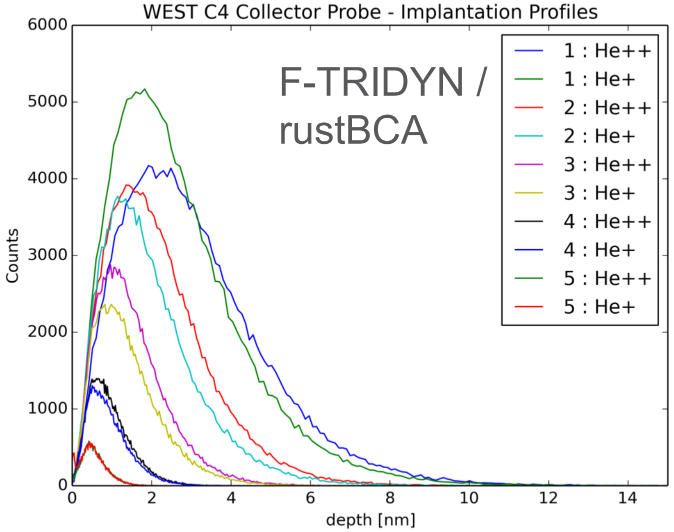
The plasma and sheath near the probe are characterized by SOLPS & hPIC simulations

For a background plasma characterized by SOLPS, we've calculated the IEADs at the different locations of the probe







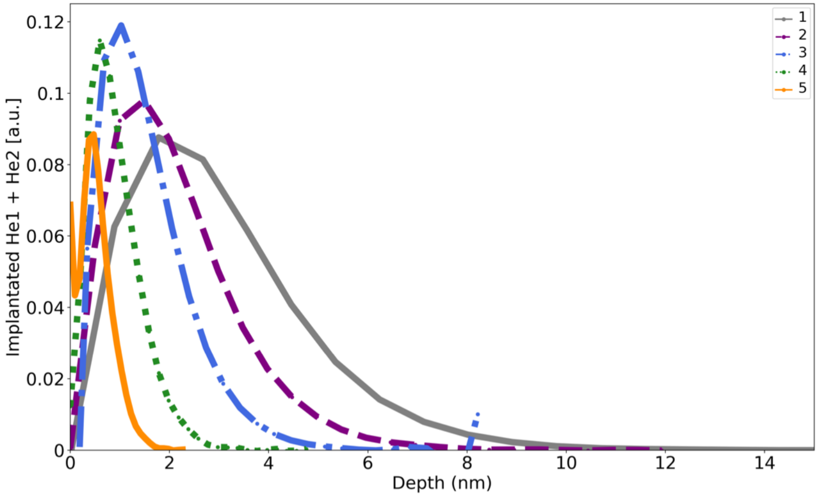


We model the substrate evolution using Xolotl

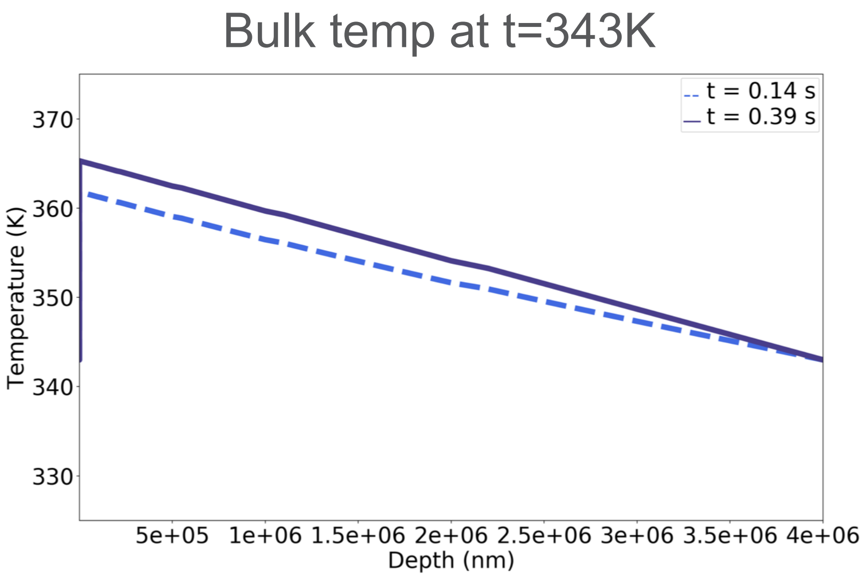
With these IEADs, we've modeled the evolution of the collector probe samples in Xolotl, exploring different assumptions for heat fluxes and surface temperatures

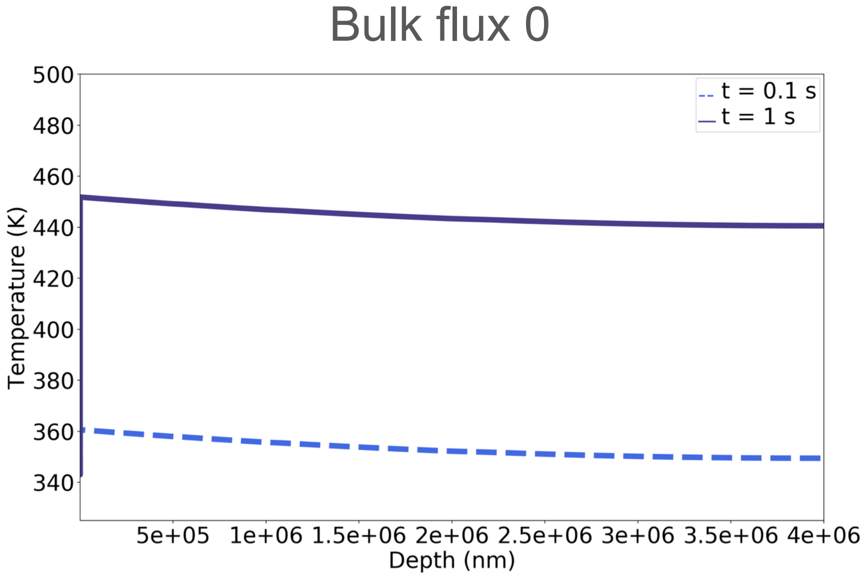
- Particle flux ~ $7.8 \cdot 10^{22}$ He/m^2
- Heat flux ~ 1MW/m^2
- Bulk boundary condition: fixed temp (343K) or reflective
- Depth ~ 4mm
- Simulated time = 1s
- Sp Yield=$4.4 \cdot 10^{-3}$

He+ and He++ implanted as a single flux



The temperature evolution changes with the boundary conditions in the bulk



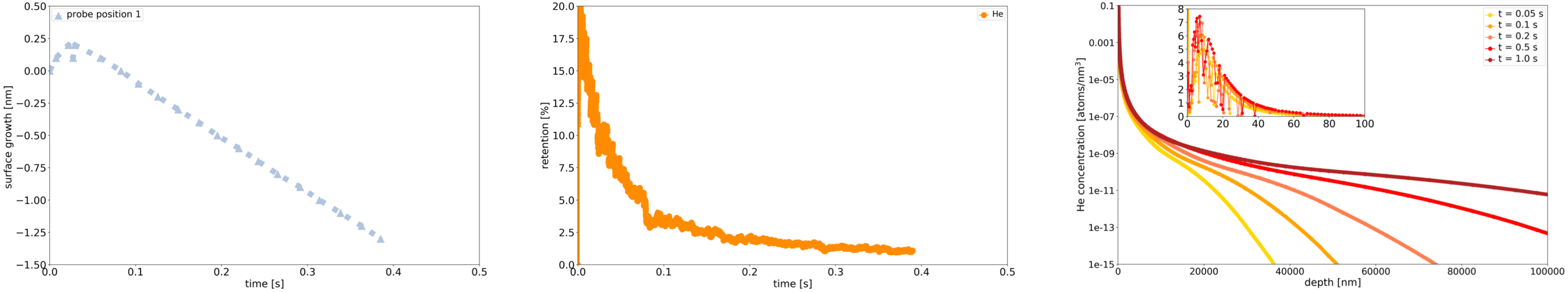


Clearly different temperature profiles,

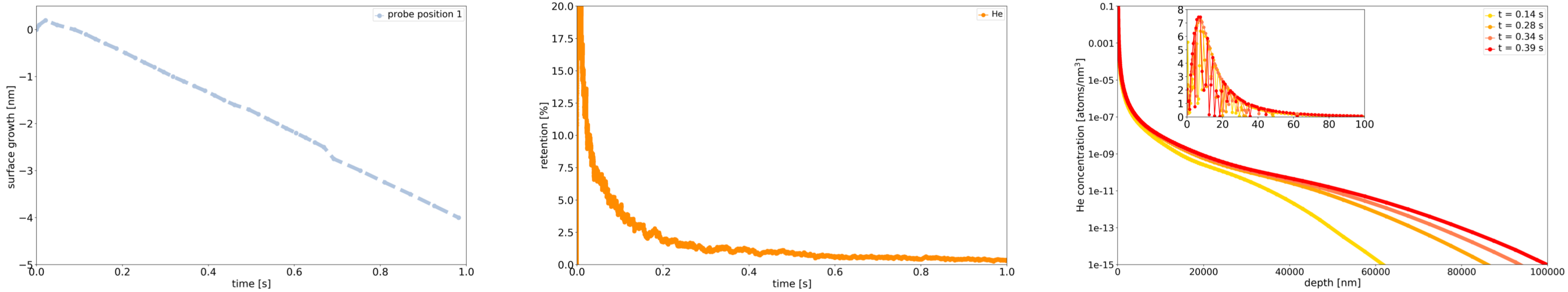
- especially in shape (slope vs flat)
- 80-110K difference in temperature range as well (surface & bulk, respectively)

However, that doesn’t seem to significantly affect He retention, surface growth, depth profiles

Bulk temp at t=343K



Bulk flux 0



Lack of temperature effect in this range due to…

No effect in He retention

- Because content is driven by trapping in V's (created by TM) → He-V binding stronger than this 80K difference

No effect on surface growth because:

- after the initial phase, dominated by sputtering
- the change in temperature (smallest in the near-surface) isn't sufficient to affect the TM
- transition in TM models of Xolotl is outside this range

And so, depth profiles neither change with the bulk boundary condition

Note: All these conclusions are based on simulations of up to 1s (experimental range)

Summary

- We’ve integrated and successfully validated multiple high-fidelity codes to model PMI
- Our predictions of ITER simulations reveal:
  - The edge plasmas are representative of partially detached divertors
  - Heavy impurities dominate erosion when present, with contributions from light ions due to the high-energy tail of IEADs
  - >95% of eroded W is locally or promptly re-deposited
  - sub-surface gas dynamics leads to additional surface growth in areas of low T_i
  - High heat flux decreases near surface T concentration
- Subsequent He - BPO exposures show that hydrogenic species interact (& bind) with He - V clusters, which will modify the tritium retention/permeation behavior
  - Gas content stabilizes in substrates pre-exposed in PISCES, at levels set by pre-existing V’s, while continues to grow in substrates initially pristine or pre-exposed ITER He plasmas
  - Bursting occurs when gases implanted in pre-existing vacancies
  - T remains closer to the surface in pre-damage substrates, while the bulk content is higher for initially pristine cases

Outlook

- **Experimentally verify** hydrogenic retention in growing W layers
- Evaluate the impact of pre-damage beyond plasma ops, e.g. in **maintenance phases** (baking temperature and duration)
  - Need for further parametrization of the H-He-V system for mainly hydrogenic, non-over-pressurized bubbles

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- Continue **experimentally validating** our PMI model in all-metal devices (WEST), and **extend usage** of our models to interpret /predict erosion-redeposition and H-trapping/W sub-surface evolution experiments (DIII-D)

- Extend the models to self-consistently treat **seeded impurities** (e.g., neon), the effects of **mixed materials (**W-Be) and evolving **thermo-mechanical properties**
- Transition into dynamic simulations; e.g., to model ELMs

Thank you for your time and attention!