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

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With valuable contributions from:

Plasma-material interactions (PMI) impact plasma and material’s performance

• 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 & ITER plasma exposures

- 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
- Take a deeper look at the effect of He on hydrogenic retention

OUTLINE

Integrated modeling workflow

- SOLPS
- Edge plasma conditions ($n_e, T_e, T_i, \Gamma \ldots$)
- $\downarrow$
- hPIC + F-TRIDYN → GITR
- Irradiation conditions ($\Gamma, E_{in}, \alpha_{in} \ldots$)

1. F-TRIDYN
2. F-TRIDYN
   \[X_{\text{Xolotl}}\]
   \[X_{\text{Xolotl}}\]
   \[X_{\text{Xolotl}}\]
   \[X_{\text{Xolotl}}\]

\[\text{in} \quad 1 \quad \text{F-TRIDYN} \quad 1 \quad C_{\text{Xolotl}}\]
\[\text{in} \quad 2 \quad \text{F-TRIDYN} \quad 2 \quad C_{\text{Xolotl}}\]
\[\text{in} \quad \ldots \quad \text{F-TRIDYN} \quad \ldots \quad C_{\text{Xolotl}}\]
\[\text{in} \quad n \quad \text{F-TRIDYN} \quad n \quad C_{\text{Xolotl}}\]
Model validation

Benchmark against PISCES experiments
The integrated model was benchmarked against PISCES experiments

- We performed an 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 to measure erosion and transport (GITR)
  - Removable W targets to analyze with LIBS and LAMS (Xolotl)
Xolotl and GITR show good agreement with experimental measurements

- GITR reproduces experimentally measured mass loss, W I lines and tower mass gains
- 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 ops

- These are standard strongly radiating, partially-detached scenarios
  - 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/m²
Heavy impurities dominate sputtering when present, with contributions from the high-energy tail of light species

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
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
- heavy impurities dominate sputtering during BPO
  - W in the private flux region,
  - Ne elsewhere
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

![Gross & net erosion (GITR) during BPO](image)
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 ($T_i \sim$ eV) from shallow gas implantation, He-induced trap mutation and surface growth
- These processes affect less the locations with high impact energies ($T_i \sim$40eV, further up the target)
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 is \(~10\times\) less than at its peak value
  - 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
During BPO, heat fluxes increase the surface temperature by up to \(~200\text{K}\)

- For $P_{\text{in}}$, $\text{SOL} = 100\text{ MW discharge}$, $T_{\text{surf}}$ increases up to \(~200\text{K}\)
  - 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
Differences in gas diffusion correlated with the local heat flux

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

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

\[ R-R_{\text{sep}} = 0.025\text{m}: q \sim 5\text{MW/m}^2 \]
\[ R-R_{\text{sep}} = 0.19\text{m}: q \sim 1\text{MW/m}^2 \]
Gaining insight into the effect of He on hydrogenic retention

How pre-existing damage drives D&T content, as well as their depth-distribution
We now evaluate sequential exposure to He plasmas & ITER Burning Plasma Ops

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

- We use Xolotl to model the subsequent exposure to 100s of full power BPO, in 5 locations:
  - Peak in particle flux ($R-R_{\text{sep}} \sim 0.025$m)
  - Peak in heat flux ($R-R_{\text{sep}} \sim 0.05$m)
  - Peak in plasma temperature ($R-R_{\text{sep}} \sim 0.1$m)
  - 2$\textsuperscript{nd}$ peak in He flux ($R-R_{\text{sep}} \sim 0.2$m)
  - Further upstream ($R-R_{\text{sep}} \sim 1$m)
Gas content saturation depends on both vacancy content & their depth distribution

- In substrates pre-exposed in PISCES, T content stabilizes quickly, within fluences $O(10^{22} \text{ ion/m}^2)$
  - quick increase in D-T content due to localized near-surface V content
- Continues to grow in substrates pre-exposed to ITER He ops or initially undamaged
  - ITER He+BPO: larger increase in H on the long scale because of higher V concentration between 100 and 1000 nm
Pre-existing damage sets the saturation level of hydrogenic retention

- The amount of T contained in the PISCES pre-exposed material stabilizes at a fixed value for each $V_{\text{bias}}$
  - $1.4 \cdot 10^{20}$ at/m$^2$ at 250 V, $1 \cdot 10^{20}$ at/m$^2$ at 75 V

- These values are maintained over a wide range of parameters, although can be slightly altered e.g., by large presence of bursting

Exposed to peak particle flux during BPO

Exposed to peak in T$_i$ during BPO
He implantation in pre-existing vacancies leads to bursting

Implantation profile

Initial V size-depth distribution

Evolution of gas content

Implantation profile

Initial V size-depth distribution

Evolution of gas content

Implantation profile

Initial V size-depth distribution

Evolution of gas content
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)
He-induced damage modifies the depth-distribution of hydrogen species

• We observe 3 depth-ranges for gas accumulation:
  a) near-surface, present in all pre-exposed substrates & driven by He damage

![Graph showing T concentration over depth](image.png)
T remains closer to the surface in pre-damaged substrates

- We observe 3 depth-ranges for gas accumulation:
  a) near-surface, present in all pre-exposed substrates & driven by He damage
  b) mid-range, where the deepest post-PISCES exposure vacancies existed

![Graphs showing T and V concentration across depth](images)
T remains closer to the surface in pre-damaged substrates, while bulk content is higher for initially pristine ones.

- We observe 3 depth-ranges for gas accumulation:
  - a) near-surface, present in all pre-exposed substrates & driven by He damage, & mid-range, where the deepest post-PISCES exposure vacancies existed
  - c) deeper in the bulk (diffusion); consistently higher in initially pristine substrates
Even small concentrations of He can induce near-surface T trapping in the long term

- the surface grows because of net W re-deposition (x3 the sputtering rate)
- 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
Summary

• We’ve integrated and successfully validated our multi-physics PMI model

• Our predictions of ITER simulations reveal that:
  - 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
  - 80-90% 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 exposures to He plasmas and BPO reveal that D-T interact & bind with He-V clusters, modifying retention & permeation
  - 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

• We are experimentally validating our PMI model in all-metal devices (WEST), and expanding usage of our models to understand erosion-redeposition 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