A multi-physics modeling approach to predicting erosion, re-deposition and gas retention in fusion tokamak divertors A. Lasa, S. Blondel, T. Younkin, B.D. Wirth – U. Tennessee Knoxville D. Bernholdt, J.M. Canik, M.R. Cianciosa, W. Elwasif, D.L. Green, P.C. Roth – ORNL D. Curreli, J. Drobny – UIUC

#### INTRODUCTION

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



- PMI compromise both material and plasma performance
  - Mutually degrade
  - Erosion, fuel retention, morphology changes...
- It's a multi-scale physics problem
  - Address it with multiple, high-fidelity models

**GITR models the W migration in the ITER** divertor, showing strong local re-deposition

- Neon dominates surface sputtering, except near the strike point
- W erosion and re-deposition are strongly correlated: 93% prompt and local re-deposition
- Transport by local E fields and re-deposition in low T<sub>i</sub> results in net deposition around the strike point and net erosion further along the target.



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Similar surface height in Xolotl, with differences



#### We developed a new integrated model for PMI

- Steady state plasmas only  $\rightarrow$  oneway coupling
- Time-scale separation  $\rightarrow$  run codes sequentially
- Modest data exchange  $\rightarrow$  file-based coupling



#### The resulting integrated model is applied to simulate **PMI in the ITER divertor**

- The model was benchmarked against PISCES experiments
- It is here applied to exposure of the ITER divertor to He-operation and burning D-T plasmas
  - only the latter case presented here



# from sub-surface gas dynamics

- Higher surface growth around the strike point as modeled in Xolotl due to trap mutation and surface growth induced by He clusters
  - Larger growth in Xolotl around the strike point, due to He clustering & trap
    - mutation (low T<sub>i</sub> shallow He implantation)



- Surface height in Xolotl resembles that of GITR further along the target, as trap mutation is less likely (Ti~40eV, deep He implantation)

#### Heat fluxes increase the surface temperature up to 200K

- The thermal coupling between locations is negligible
  - We run multiple, independent 1D locations
  - May change in the full power operation of 500 MW
- For 100 MW discharge, increases in T<sub>surf</sub> of up to 200K, which affects sub-surface gas dynamics
  - No threat of melting-recrystallization (no transients)



#### T diffuses faster with increasing T<sub>surf</sub>, which is correlated with the local heat flux

- <u>SOLPS:</u> 2-fluid model of edge plasma + kinetic neutrals; D-T plasma + He, Ne, Be (CX-only); provides edge plasma profiles
- <u>hPIC:</u> 1D3V PIC code; multi-species (D, T, He, Ne); 36 locations across the divertor; outputs impact energy-angle distributions
- <u>GITR</u>: W sputtering, ionization & transport in the divertor; in 3D, 2.5M particles, O(10<sup>6</sup>) time-steps; calculates W re-distribution
- *F-TRIDYN*: binary collision approximation code; provides sputtering and reflection yields, and implantation profiles
- *Xolotl*: cluster dynamics code; evolves the surface height and sub-surface gas concentrations due to clustering, trapping...

#### RESULTS

#### **SOLPS-predicted plasma profiles are** representative of a partially detached divertor

- P<sub>in</sub>=100MW; P<sub>rad</sub>=73 MW, mainly by Ne, in the divertor; q ~7 MW/m<sup>2</sup> at the target
- The plasma profiles consistent with a partially detached divertor

#### **hPIC** reveals that light ions contribute to sputtering due



- The peak in concentration takes the value expected for  $T=T_{surf}(t)$
- Gases diffuse faster, mainly outgassing
- Results for D follow the trends of T, and are thus not shown here



#### **Pre-exposure to He forms a barrier for T**

permeation

At R-R<sub>sep</sub>=0.025m, q~5  $MW/m^2$ 

**Pristine W substrate** 

→ t = 0.01 s

W pre-damaged by He

- The pre-implanted He clusters, leaving Vclusters (voids) that refill with He and trap T (D)
- V and He clusters (which trap T) form a permeation barrier and limit the T<sub>surf</sub> dependence of the near-surface T concentration (in this T<sub>surf</sub> and *q* ranges)



### **Summary & Future Plans**

Integrated multiple, high-fidelity codes to model PMI to simulate 100 MW, burning plasma discharge, revealing:



#### to the high-energy tail

• Peak of hPIC's distribution is consistent with the most probable energy expected from classical sheath theory • Particles with E<sub>in</sub> in the high-energy tail, as predicted by hPIC, contribute to sputtering of W by light species

# **F-TRIDYN provides a high-resolution reduced**

model of sputtering and reflection

- To turn these fluxes and distributions into a W source, we build a reduced model for reflection and sputtering
- Based on O(10<sup>4</sup>) combinations of impact species, energy and angle



- Neon dominates both radiation and W erosion, although the high-energy IEAD tail contributes to erosion by light ions
- >90% local W re-deposition leads to net deposition near the strike point, net erosion at R-R<sub>sep</sub>>0.2m – with additional surface growth due to sub-surface gas dynamics in areas of low plasma temperature
- Hight heat flux (T<sub>surf</sub>) decreases near surface T concentration
- Pre-exposure to He plasma leads to increased near-surface T concentration (trapped in bubbles/voids), but also decreases T permeation
- Seeking opportunities to experimentally validate our PMI model
- Work towards understanding effects of **mixed materials**, e.g. W-Be & extending predictions of microstructure to thermal-mechanical properties
- Working in the SciDAC to include the **feedback** from PMI **onto plasma**; e.g. to Develop capability to model **ELMs**

#### **Further details:**

https://science.osti.gov/-/media/fes/pdf/program-documents/ FY2018\_PMI\_Theory\_Milestone\_Final\_Report.pdf



# NOIS

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