Tungsten atomic data needs for ITER

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ITER Organization

with contributions from

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Categories of W data needed for ITER

- For plasma modelling and diagnostics:
  - Ionization and CX data for low ionization stages → Prompt redeposition rates
  - What spectral lines can be used to monitor the W content of the plasma?
  - W migration to main plasma: thermal and friction forces
  - Are charge bundling or average-ion simple models useful?
  - Sputtering and reflection yields for bulk/recrystallized/redeposited W
    - Effects of Be_xW alloying, other impurities, surface roughness, surface state, temperature, …
  - Vapour shielding during fast transients
- For materials modelling, including fuel retention issues:
  - Nature of hydrogen/helium traps in bulk W
  - Vacancy formation and diffusion rates
  - Blistering, cracking, fatigue, grain boundaries
  - IR emissivity, melting, evaporation
  - Not covered here!

Diagnostic measurements requirements

UID: WYWUMX

[55E3s1408-R] MP027, **W Influx** shall be delivered with the following specifications:

- Range: $10^{14} – 5.10^{17}\ m^{-2}.s^{-1}$
- Time Resolution: 10 ms
- Spatial Resolution: integral
- Accuracy*: 10% relative
- Diagnostics contributing:
  - 55.E2 H-Alpha (+ visible spectroscopy) - Primary
  - 55.E3 VUV (Main Plasma) - Supplementary
  - 55.ED X-Ray Crystal Spectrometer (survey) - Primary
  - 55.G1 IR Cameras, Vis/IR TV (Midplane) - Supplementary
  - 55.GA IR Cameras: Vis/IR TV (Upper) - Supplementary

[55E3s1409-R] MP028, **W Relative Concentration** shall be delivered with the following specifications:

- Range: $10^{-6} – 5.10^{-4}$
- Time Resolution: 10 ms
- Spatial Resolution: integral
- Accuracy*: 10% relative
- Diagnostics contributing:
  - 55.E3 VUV (Main Plasma) - Primary
  - 55.ED X-Ray Crystal Spectrometer (survey) - Primary

* Accuracy means measurement accuracy of impurity emission line itself (unit: photon/cm^2.s) and not density accuracy.

Diagnostic spectral ranges

- 55.E2: Visible spectroscopy: Will look at W^0 400.9 nm line with long integration times (>1s) and use the S/XB method (uncertainty quoted > 500%) (UID: TWRHG4)
- 55.E3: VUV spectrometer (main plasma) : 2.4 – 160 nm range, (W^{+46} 19.6 nm and W^{+44} 132.3 nm) (UID: 4BDN4T) [1]
- 55.EH: VUV spectrometer (edge): 17 – 32 nm
- 55.EG: VUV spectrometer (divertor): 15 – 32 nm
- 55.ED: X-Ray Crystal Survey Spectrometer (1-100 Å) (UID: SCSNQ3)
- 55.E4: Divertor Impurity Monitor (200 – 1000 nm) with dedicated hardware for the W^0 400.9 nm line (UID: RYRFCU)

[1] R. Barnsley and M. O'Mullane, Rev. Sci. Instr. **75**, 3743 (2004)

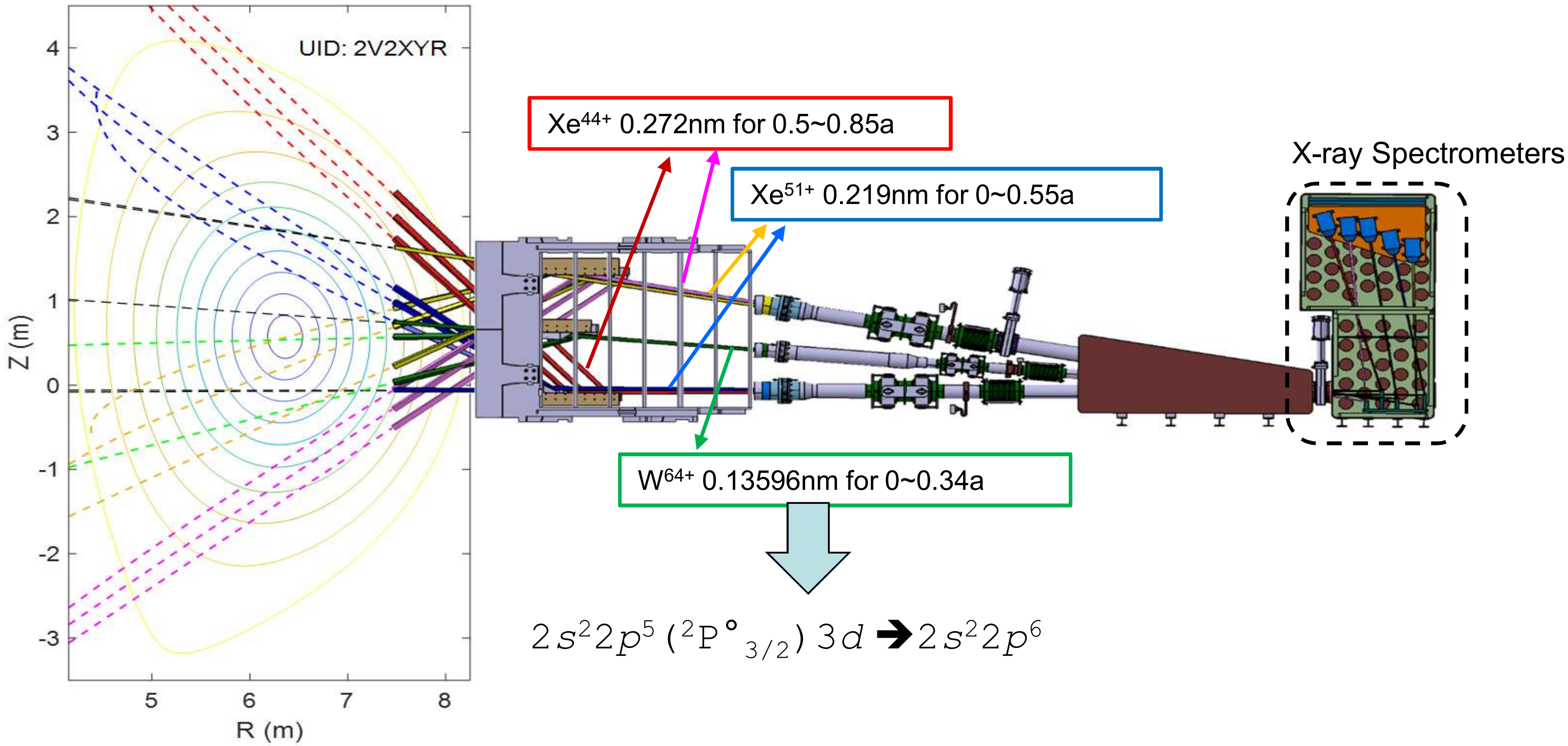
Important lines for VUV spectrometer (UID: 4BY2W7)

Ion	Wavelength (nm)	Rel. intensity	A_{ki} ($\times 10^8$ s^{-1})	f_{ik} ($\times 10^{-3}$)	S_{ik} (a.u. $\times 10^{-2}$)	Configurations
W VII	18.8159	800				$4f^{14}5p^6\ ^1S_0$ - $4f^{14}5p^5\ (^2P°_{1/2})\ 6s\ (1/2,1/2)^o_1$
W VII	21.6219	500				$4f^{14}5p^6\ ^1S_0$ - $4f^{14}5p^5\ (^2P°_{1/2})\ 5d\ (1/2,3/2)^o_1$
W VII	22.3846	300				$4f^{14}5p^6\ ^1S_0$ - $4f^{14}5p^5\ (^2P°_{3/2})\ 6s\ (3/2,1/2)^o_1$
W VII	26.1387	3000				$4f^{14}5p^6\ ^1S_0$ - $4f^{14}5p^5\ (^2P°_{3/2})\ 5d\ (3/2,5/2)^o_1$
W VII	28.9526	300				$4f^{14}5p^6\ ^1S_0$ - $4f^{13}(^2F°_{5/2})\ 5p^6\ 5d\ (5/2,5/2)^o_1$
W VII	29.4376	200				$4f^{14}5p^6\ ^1S_0$ - $4f^{13}(^2F°_{5/2})\ 5p^6\ 5d\ (5/2,3/2)^o_1$
W XLVII	19.1490	13				$3p^63d^94s\ (5/2,1/2)_2$ - $3p^63d^94s\ (3/2,1/2)_1$
W XLVIII	18.5780	20				$3p^63d^9\ ^2D_{5/2}$ - $3p^63d^9\ ^2D_{3/2}$
W LVI	16.3800					

Spectral lines for XRCS (UID: 3NQXBB)

Ground state	Excited state	Wavelengths (nm)
W^{+38} Kr-like		0.4705, 0.5964
W^{+44} Zn-like		0.4403, 0.4499, 0.4697, 0.5738
W^{+45} Cu-like		0.4300
W^{+64} Ne-like $2p^6\ ^1S_0$	$2p^5\ 3s^1\ ^1P_1$	0.1498
	$2p^5\ 3s^1\ ^3P_1$	0.1279
	$2p^5\ 3d^1\ ^3P_1$	0.1383
	$2p^5\ 3d^1\ ^1D_1$	0.1191
	$2p^5\ 3d^1\ ^3D_1$	0.1364
W^{+63} Na-like $3s^1\ ^3S_{1/2}$	$4p^1\ ^2P_{1/2}$	0.374
	$4p^1\ ^2P_{3/2}$	0.357

Core X-Ray Crystal Spectrometer Layout



$$2s^2 2p^5 ({}^2P^\circ_{3/2})\, 3d \rightarrow 2s^2 2p^6$$

Modelling needs

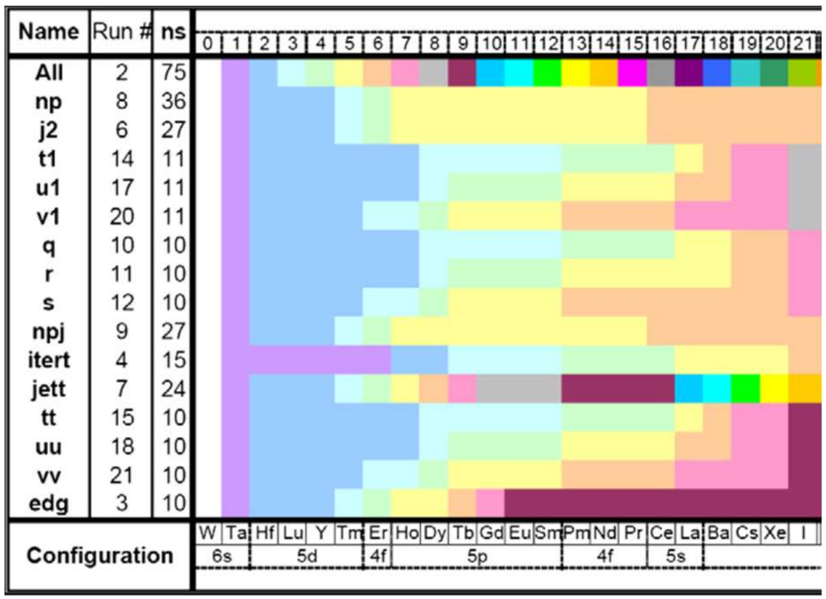
- Modelling must to be able to provide synthetic data to help in diagnostic and control system design
- Follow W atoms and ions as they sputter from the target
  - Radiation source from WI and WVII
  - Accurate ionization and CX rates to evaluate prompt re-deposition
  - W charge balance important for thermal force terms leading to migration upstream followed by core penetration
- Vapour shielding during fast transients
  - (Dielectronic) recombination rates and photon opacity
- Currently, the default SOLPS-ITER W data from ADAS is:

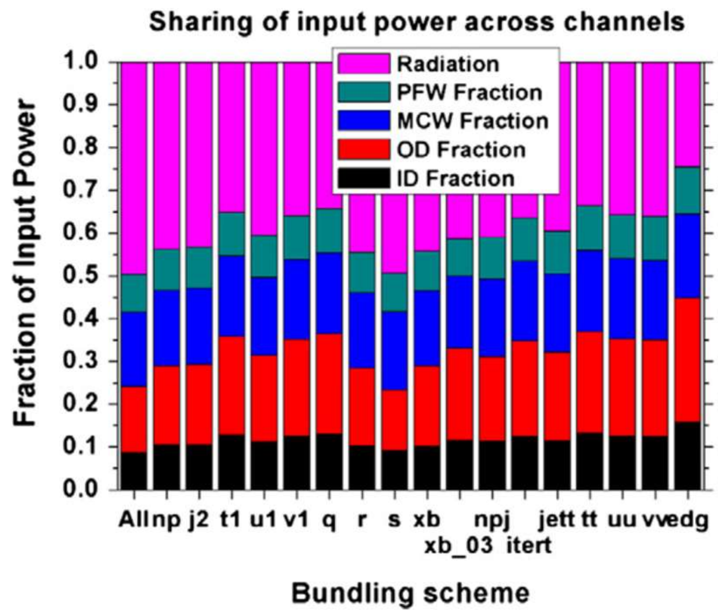
'50 '	'50 '	'89 '	'50 '	'42 '	'89 '	'89 '	'w '	
rec	ion	cex	prb	plt	zcd	ecd	es	[names in ratadas.F]
acd	scd	ccd	prb	plt	zcd	ecd		[directories in adas]

- At IO, the recommended set is the ‘year42’ ADAS dataset

Charge state bundling for W

Code speed-up ⟷ Result variability

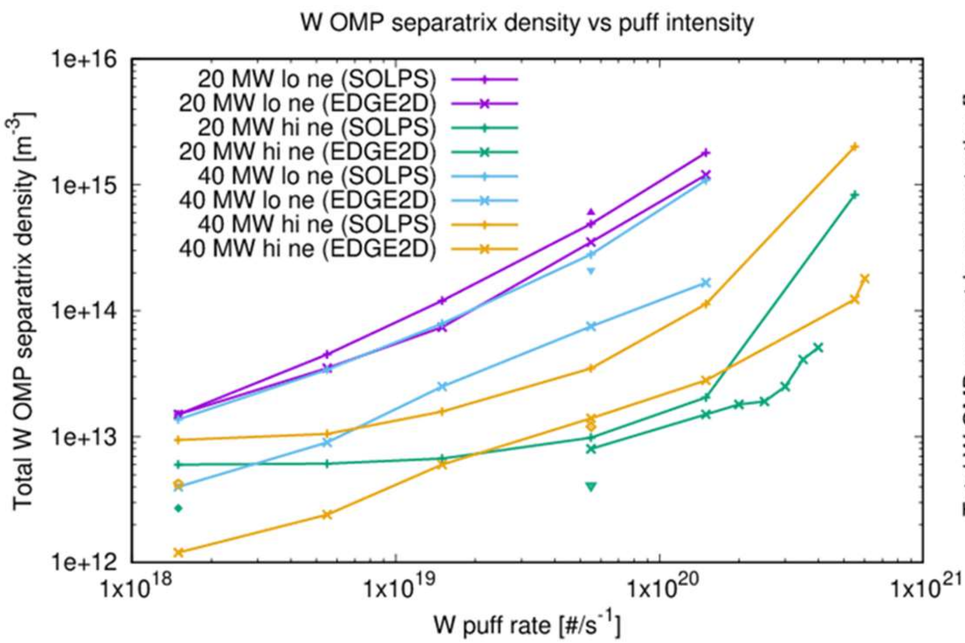


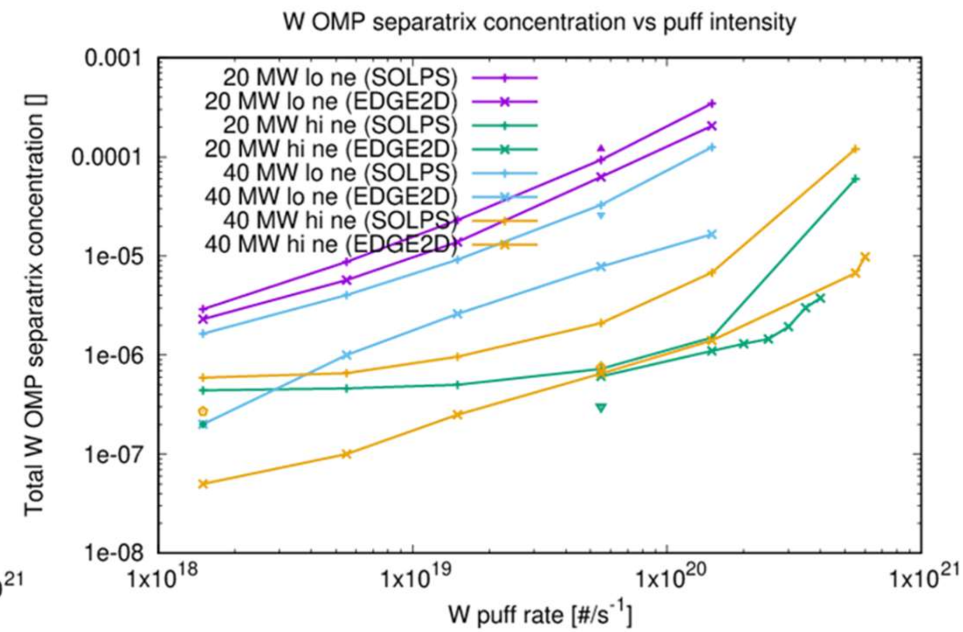


SOLPS5.1 AUG benchmark study
Bundles based on ‘year89’ data
CPU effort scales ~ $\mathcal{O}$(ns)

[1] X. Bonnin and D. Coster, J. Nucl. Mater. **415**, S488 (2011)

W core influx sensitivity

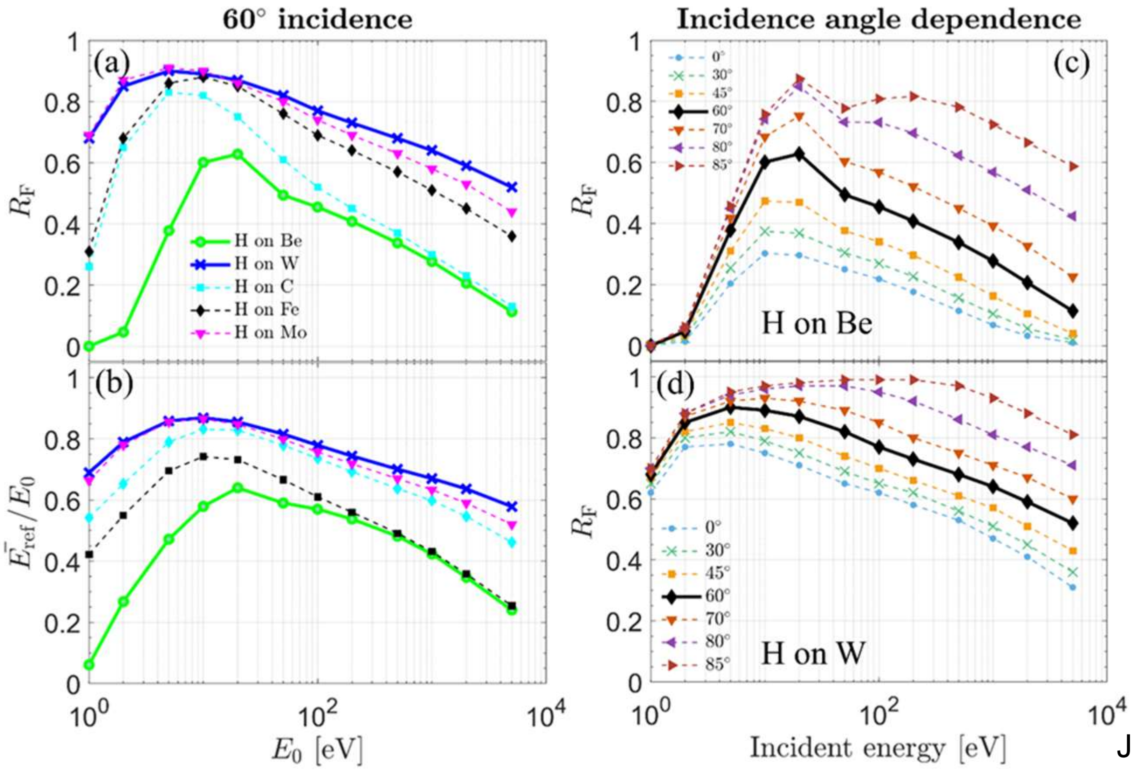




- This comparison with EDGE2D uses a more recent set of bundles, using 7 stages, based on ‘year42’ data (SOLPS-ITER data available as IMAS #103077-80/13-24)

Reflection data

From TRIM data set with dedicated W runs

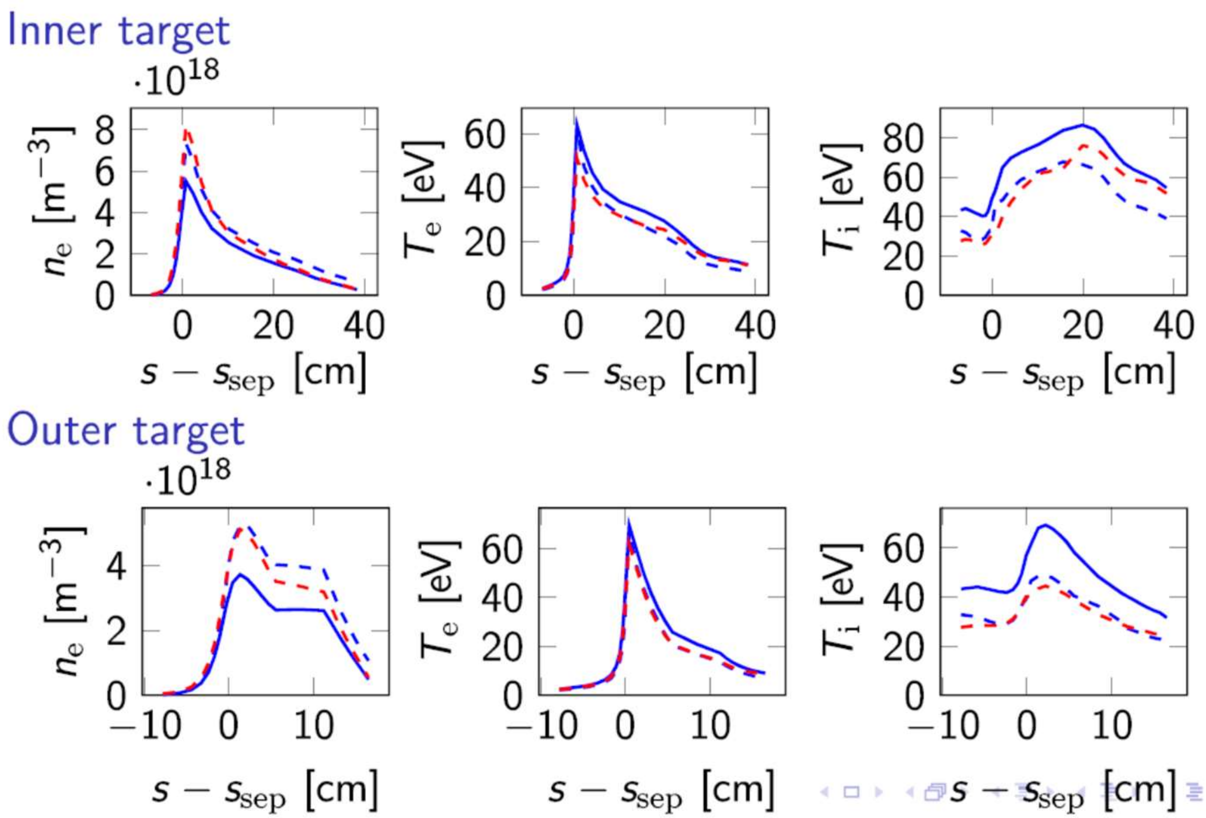


EIRENE assumes that Hydrogen isotopes that are not backscattered ("fast reflection" rate R_F) are recycled as "thermal" molecules

TRIM data loses accuracy at low energy (of the order of the surface binding energy [~5 eV], which itself varies accordingly to W crystallographic surface state)

J.-S. Park *et al.*, Nucl. Fusion **61**, 016021 (2021)

Importance of surface reflection data choice



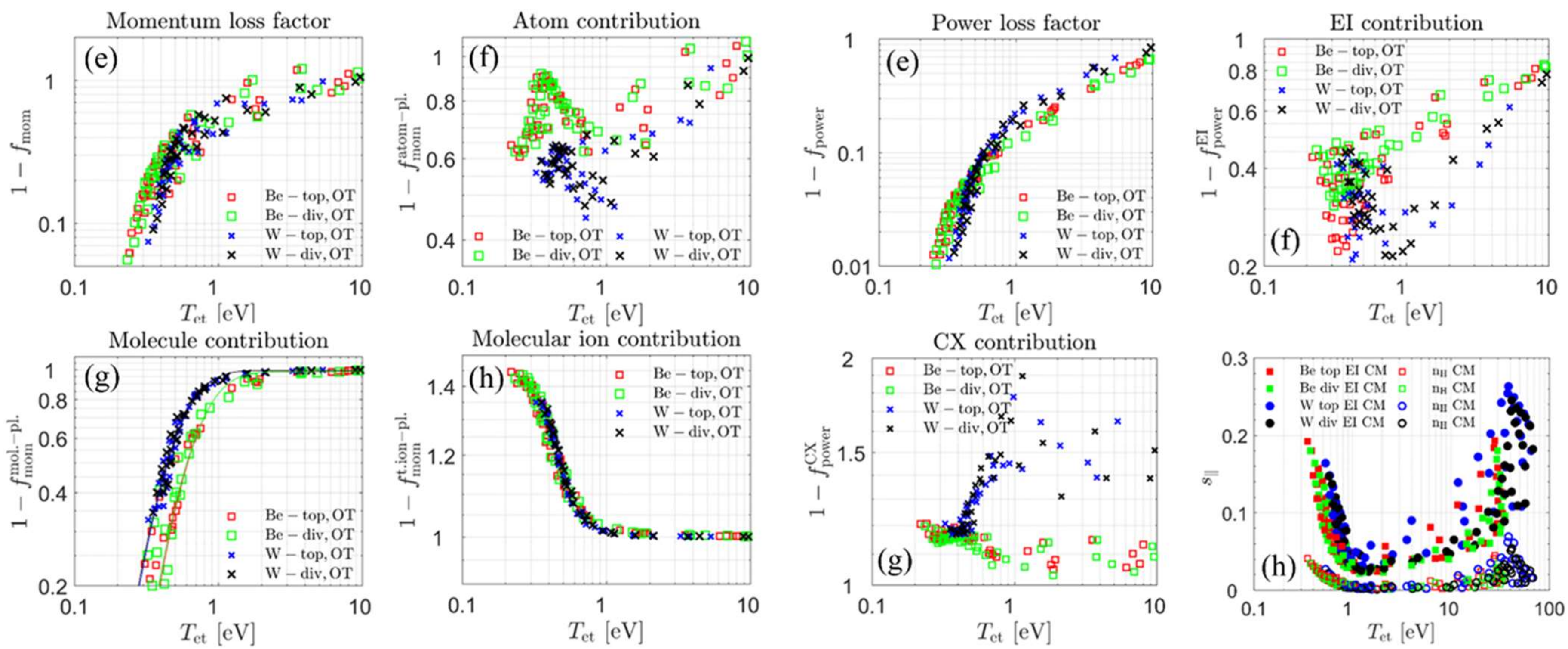
JET comparison case
- D only, attached conditions

SOLPS 3.0.7 (blue solid line)
SOLPS 3.0.6 (blue dashed line)
EDGE2D-Eirene (red dashed line)

Difference was tracked to use of older default TRIM dataset by Eirene for SOLPS 3.0.6 and EDGE2D (with extrapolated W reflection data), while SOLPS 3.0.7 uses a new TRIM dataset with dedicated W reflection data

Courtesy of N. Horsten (Aalto U.)

Atom/molecule mix influence



J.-S. Park *et al.*, <u>Nucl. Fusion</u> **61**, 016021 (2021)

On-going work to refine our models

- Extensive study of the impact of divertor surface material (Be vs W):
  - J.-S. Park *et al.*, *Assessment of ITER divertor performance during early operation phases*, Nucl. Fusion **61**, 016021 (2021)
- Improvement to physics model to compute thermal and friction forces on impurities:
  - E. Sytova *et al.*, *Comparing N versus Ne as divertor radiators in ASDEX-Upgrade and ITER*, Nuclear Materials & Energy **19**, 72-78 (2019)
  - E. Sytova *et al.*, *Derivation of the friction and thermal force for SOLPS-ITER multicomponent plasma modelling*, Phys. Plasmas **27**, 082507 (2020)
  - S. Makarov *et al.*, submitted to Phys. Plasmas (2021)
- Revisiting W bundling schemes in SOLPS-ITER
  - S. Gao *et al.*, accepted for publication in AIP Advances (2021)

Summary of data needs

- Improved S/XB ratio accuracies for all spectral lines of interest
  - Critical to climb back from photon emission rates to W plasma concentration
  - Need to cover range from W^0 to at least W^{+64}
- Refinement of reflection data at low energies
  - Dependencies on W surface state, incident angle, incident hydrogen isotope, …
- Detailed sputtering yields
  - As functions of temperature, surface roughness, other impurities present…
- Fast and reliable prompt redeposition model
- Improvement of accuracy of ionization, recombination, radiation, and CX rates
  - Reliable charge distribution to deduce upstream W migration and core penetration