Quantification of the contribution of processes in the ADAS beam model

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and many ADAS contributors

Motivation and areas of focus

High energy (E>50keV/amu) neutral beams are widespread in fusion plasmas:

- fueling the plasma – either deuterium or tritium.
- heating the plasma via collisions.
- shaping the current profile.
- enabling access to high confinement regimes (H-mode).

Neutral beams are extremely useful as diagnostic systems:

- finite in size and region of plasma probed is localized.
- emission from the NB atoms gives information on magnetic field via motional Stark effect (MSE) .
- interaction with local (thermal) plasma ions, via charge exchange (CXRS) give information on ion temperature, plasma rotation and impurity density profiles.
- probably the best/only method of determining the Helium ash content.

Modelling the beam is a straightforward application of collisional-radiative theory:

- mono-energetic beam and thermal plasma ions.
- ion impact is the dominant atomic process.
- lots of messy complications – halo, plume, nuisance lines, contamination from plasma edge, overlapping features from multiple beams and geometry effects.

Need for accurate/quantified accuracy data

JET has a ‘neutron deficit’ problem*:

- in JET neutrons are primarily from beam thermal reactions. ITER will hopefully be different.
- the measured neutron rate falls short of expectations based on ion orbit codes such as TRANSP, assuming only collisional fast ion orbit diffusion.
- many reasons suggested, all connected to fast ion-thermal reactivity:
  - fuel dilution – measurements from CXRS
  - NBI deposition – possibly overestimated
  - fast ion transport
  - plethora of geometry and mapping effects
- unfortunately still no resolution.

NBI deposition was not considered an explanation:

- power deposition with IR camera matches expectation.
- comparison of NUBEAM and ADAS atomic data differed by 2-4%

From our RCM viewpoint, is this because we ‘benchmark’ our data and models against what went before?

* H. Weisen *et al*, Nucl. Fusion, **57** (2017) 076029. doi:10.1088/1741-4326/aa6dcc

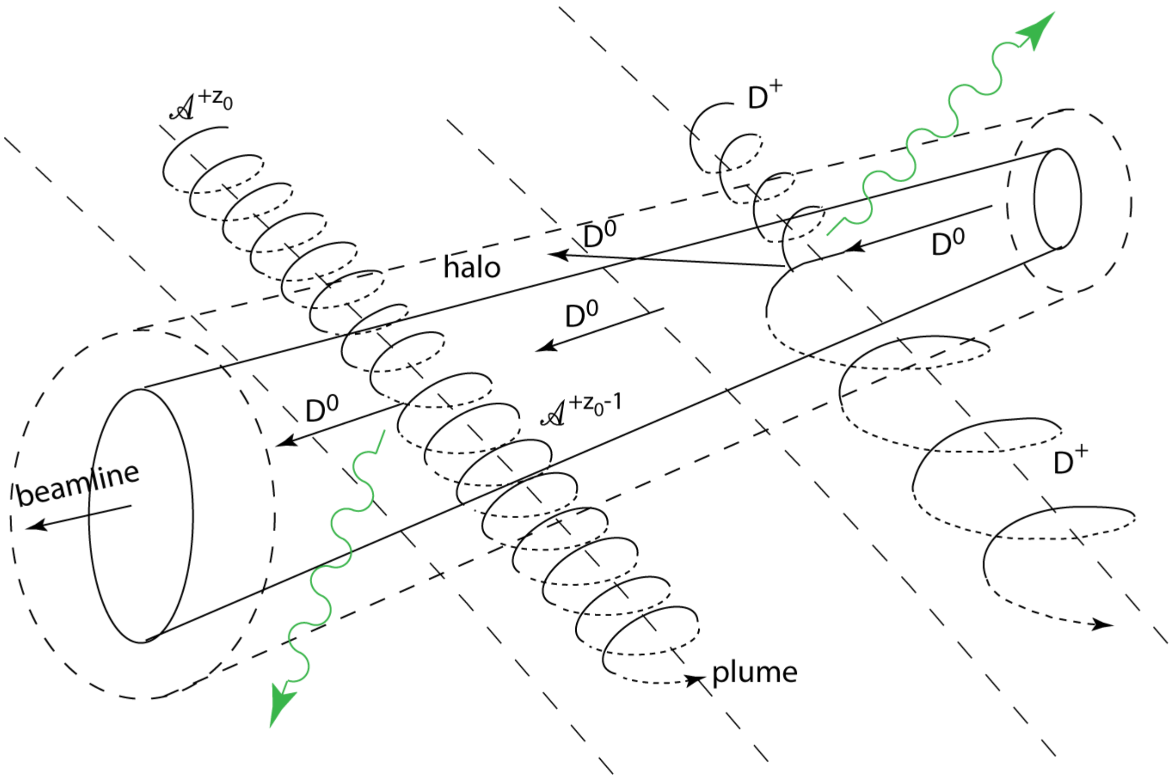
Beam-plasma environment

The injected neutral atoms, usually isotopes of hydrogen, have speeds comparable to the Bohr orbital speed (~25keV/amu).

Positive ion sources have acceleration voltages ~40-160keV. For hydrogen isotopes, the neutral beam contains three energy fractions, $E_{b,}$ $E_b/2$ and $E_b/3$ of varying proportions. These energies are well suited to CXRS.

^{2}D is the most commonly injected hydrogen isotope. Also ^{3}He and ^{4}He have been used, usually as minority admixtures to hydrogen. All can be handled with ADAS.

Negative ion sources (hydrogen isotopes) usually operate at acceleration voltages >200keV and give mono-energetic neutral beams. These energies are less suited to CXRS.



In the core plasma, with T_i ~6keV, a carbon nucleus has average energy 0.5keV/amu << E_b so the beam speed usually determines the collision speed of projectile (D^0 donor) and target(A^{+Z_0} receiver). This situation is reversed for electron collisions with both donors and receivers.

A^{+Z_0-1} is the CX emitter. The halo radius is an ionisation length. The key plume length is a radiative decay length.

ADAS beam model

The ADAS beam model is a bundle-n collisional-radiative calculation:

- n~100 included with assessed/recommended data for n=1-5 levels.
- impact parameter formulasims for electron and ion excitation and ionisation (Lodge, Percival-Richard, Van Regemorter, Burgess, Vainstein) are used when other data are available.
- H Anderson et al, PPCF, **42** (2000) p781 (doi:10.1088/0741-3335/42/7/304) or adas310 manual.

The isotope mass influences the beam speed. The fundamental collision cross-sections, as a function of relative collision speed are the same. So rate coefficients, for atom-ion collisions must use the correct speeds. Otherwise beam population and collisional-radiative modelling are the same.

Hydrogen isotope beams: collisionality is strong, the collision limit is typically ~n=4, l-sub-shells are strongly mixed. Bundle-n modelling is appropriate for the beam populations. The stopping coefficient is the $S_{CR,\,1s\,^2S}$ coefficient (including charge exchange losses) of the ground level. Excited beam populations are solved as

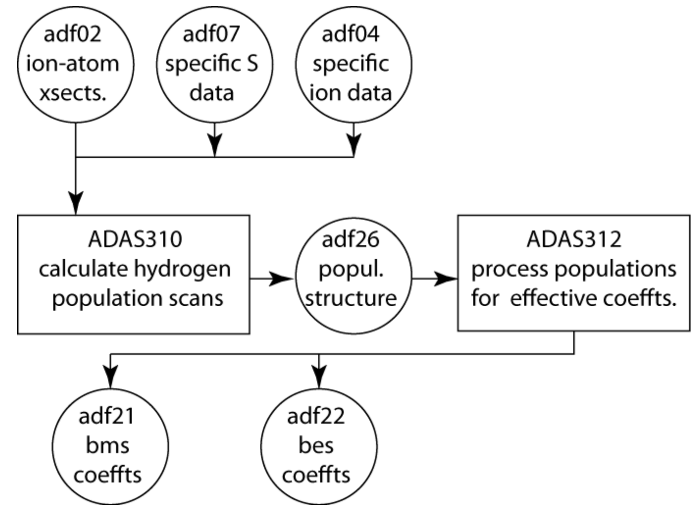
$$b_n = F_n^{(1)} \frac{N_1}{N_+} + \cancel{F_n^{(2)}} + F_n^{(3)} \cancel{\frac{N_H}{N_e}}$$

Helium isotope beams: collisionality is strong, the collision limit is typically n ~ 4, l-sub-shells are less strongly mixed. There are two effective metastables, the ground $1s^2\ ^1S$ and the triplet $1s2s\ ^3S$ (often $1s2s\ ^1S$ is also treated as metastable for consistency with other applications). The singlet and triplet sides behave like two almost independent beams with stopping coefficients $S_{CR,\,1s^2\,^1S}$ and $S_{CR,\,1s2s\,^3S}$. Bundle-nl modelling is appropriate. Excited populations are solved as

$$b_{nl^{2S+1}L} = FI_{(nlS)}^{(1)} \left(\frac{N_{1^1S}}{N_+}\right) + FII_{(nlS)}^{(1)} \left(\frac{N_{2^1S}}{N_+}\right) + FIII_{(nlS)}^{(1)} \left(\frac{N_{2^3S}}{N_+}\right) + \cancel{F_{(nlS)}^{(2)}} + F^{(3)} \cancel{\left(\frac{N_H}{N_e}\right)}$$

ADAS model data

For beam atom populations, collisions with impurity ions must be added to the rate equations and the beam translational speed added to collision dynamics to form the rate coefficients. In ADAS, adf02 provides the ion impact cross-section data. adf07 provides the most accurate electron impact direct ionisation coefficients.

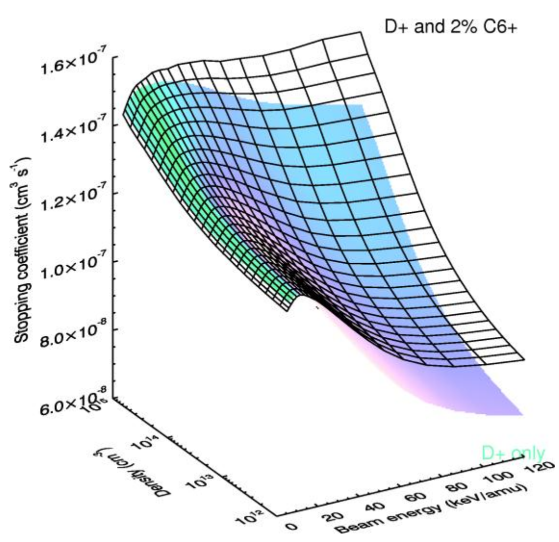


The ADAS data format adf21 and adf22 archive the beam stopping and beam emission coefficients. They are held in libraries for the different beam species in datasets for each individual impurity species which contributes to the stopping (see next viewgraph).

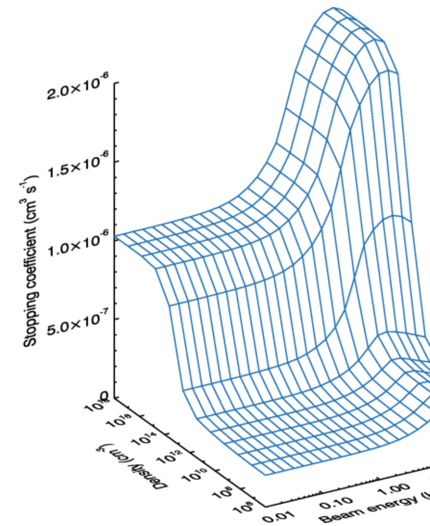
The beam energy and impurity number density are the primary parameters, with other secondary. This determines the organisation of the adf21 and adf22 archives.

Beam stopping by a composite of impurities and electrons is usually assembled as a linear superposition of pure stopping species.

The beam stopping coefficient is defined in terms of the electron density.



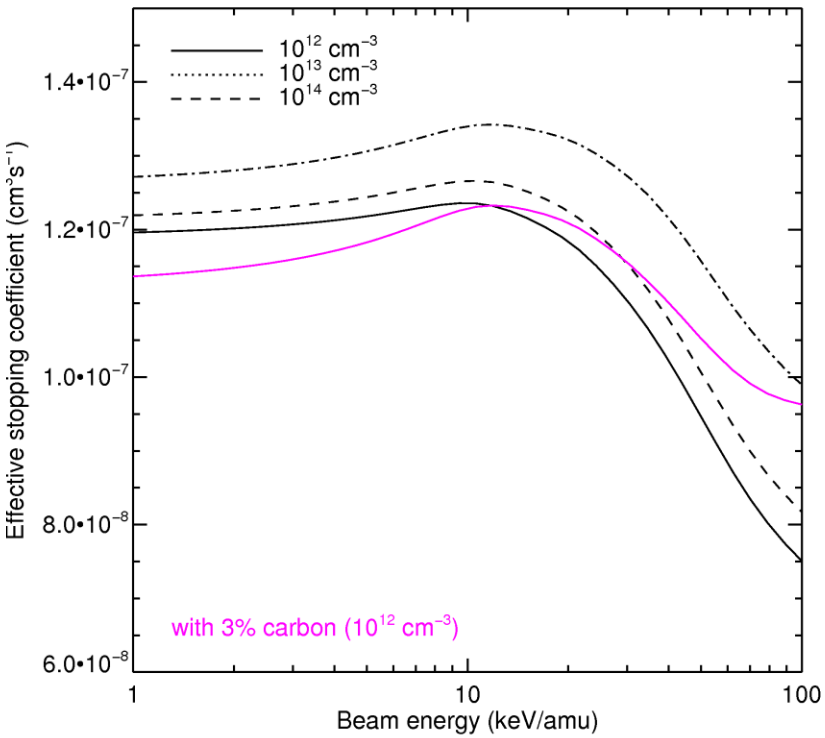
Stopping coefficient for D-beam in $2x10^3$ eV D^+ +2% C^{+6} plasma.

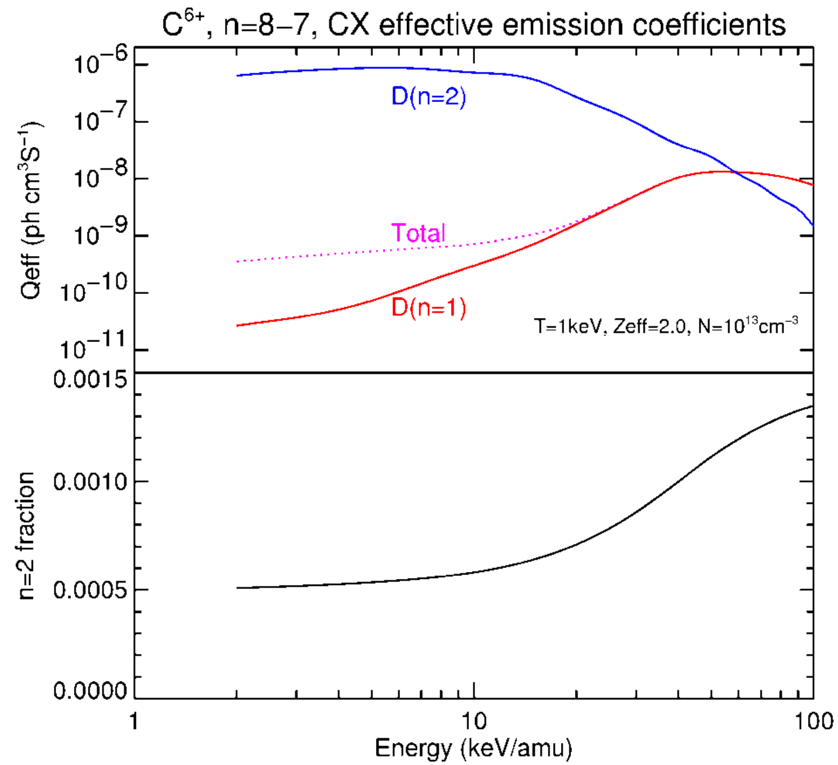


Stopping coefficient for the beam triplet metastable by a D+ plasma at $2x10^3$ eV.

University of Strathclyde Science

Missing physics / incorrect assumptions





Changing beam stopping – density, plasma impurity and excited beam atoms.

Revised data in 2010 – data problems

E Delabie et al, PPCF, **52** (2010) 125008 (doi:[10.1088/0741-3335/52/12/125008](10.1088/0741-3335/52/12/125008))

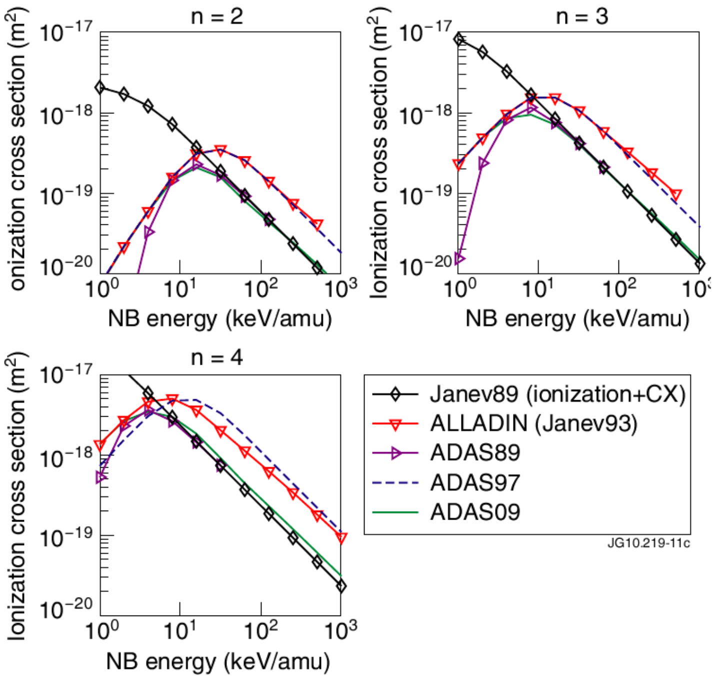
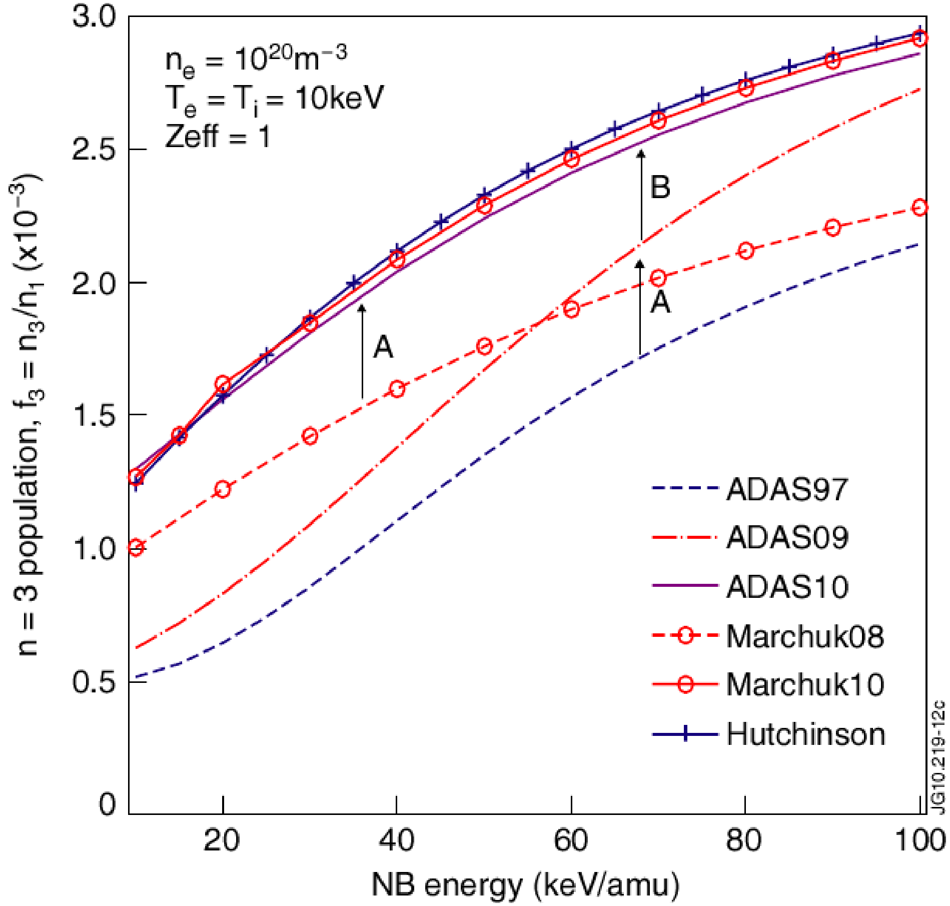


Figure 1. Proton impact ionization of excited states of the hydrogen atom. Recommended dataset (Janev89 [5] and Janev93 (as in the ALLADIN database) [21, 26]) and data used in the ADAS beam emission models are shown.



[13] M. B. Shah, D. S. Elliot, and H. B. Gilbody, J. Phys. B **20**, 2481 (1987).

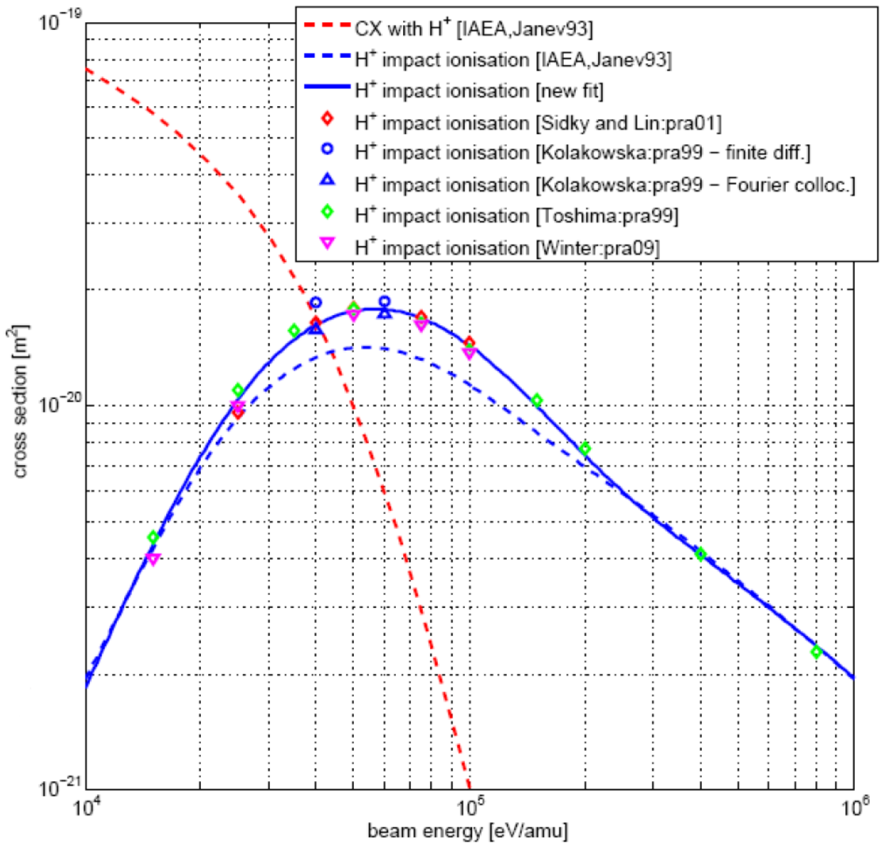
[14] M. B. Shah, D. S. Elliot, and H. B. Gilbody, J. Phys. B **20**, 3501 (1987).

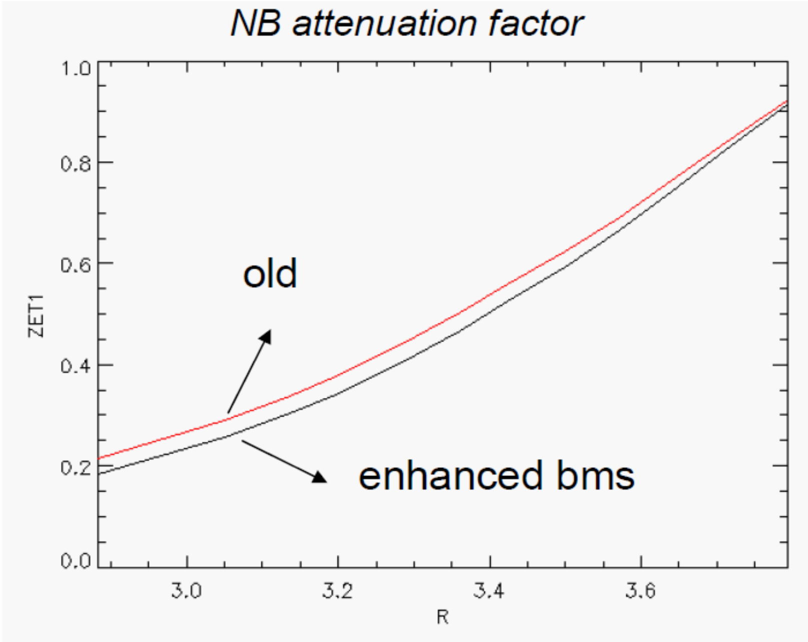
[15] The CDW-EIS cross section σ_2 presented here corrects the corresponding previous calculation from Fainstein *et al.*, J. Phys. B **21**, 287 (1988).

The correction

Ion impact is most significant process

- Beam stopping is an effective ionisation rate.
- The primary $H^0 + H^+ \rightarrow H^+ + H^+ + e^-$ controls the overall value.
- Many calculations since Janev compilation (1993).
- suggest an increase of ~10% at peak of cross section.





Should we change and how to manage the consequences?

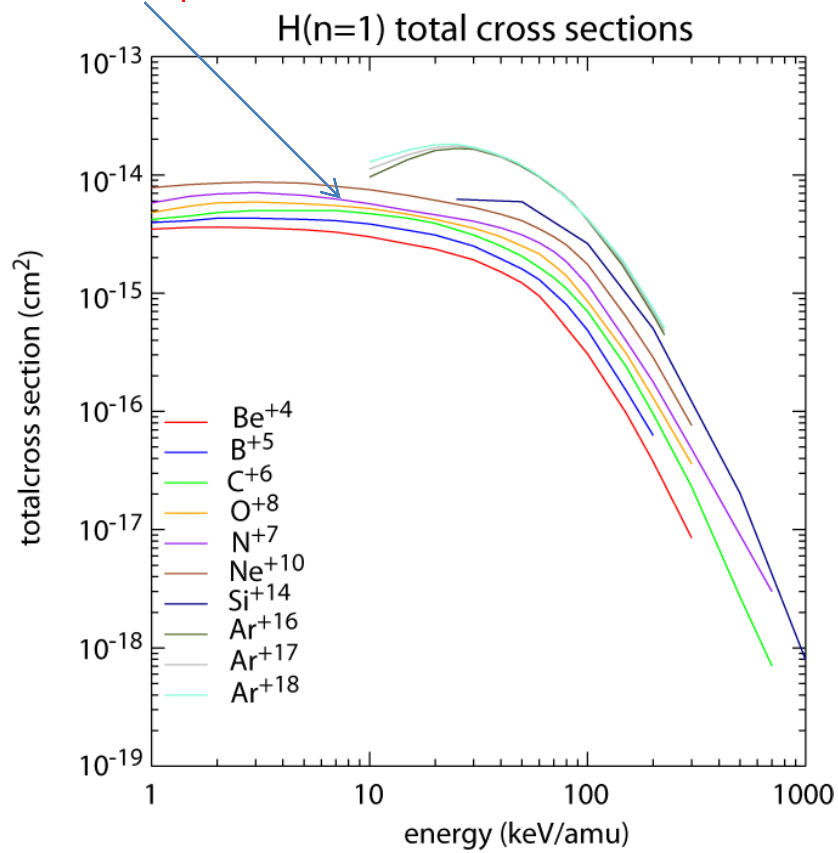
Z-scaling of total CX cross sections: H(1s) donor

For CX capture by heavier species into higher n-shells, the receiver core is passive. Only the receiver ion charge z_1 matters. The scaling su $n_{crit} \sim z_0^{3/4}$ led approach for the cross-sections.

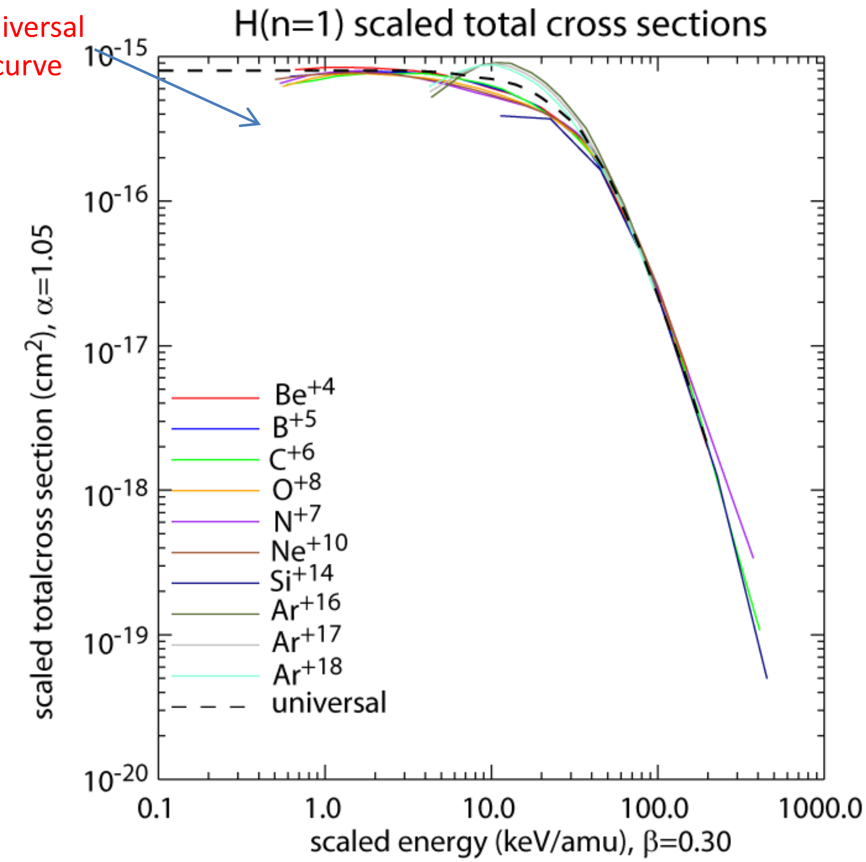
Introduce scaled energy $\bar{E}$ d scaled total cross-section as: $\bar{\sigma}_{tot}$

$$\bar{E} = E\, z_1^{-\beta} \qquad \bar{\sigma}_{tot} = \sigma_{tot} z_1^{-\alpha}$$

Results from specific calculations



Best universal curve



Z-scaling of partial (nl) CX cross sections: H(1s) donor

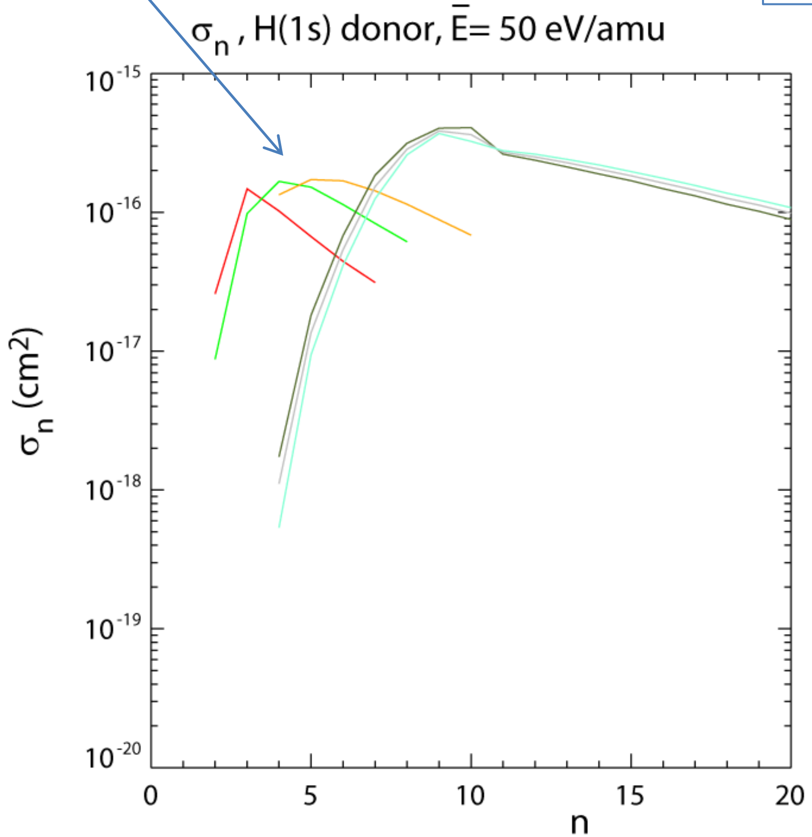
Likewise, the scaling $n_{crit} \sim z_0^{3/4}$ ests the same approach for the partial-n cross-sections.

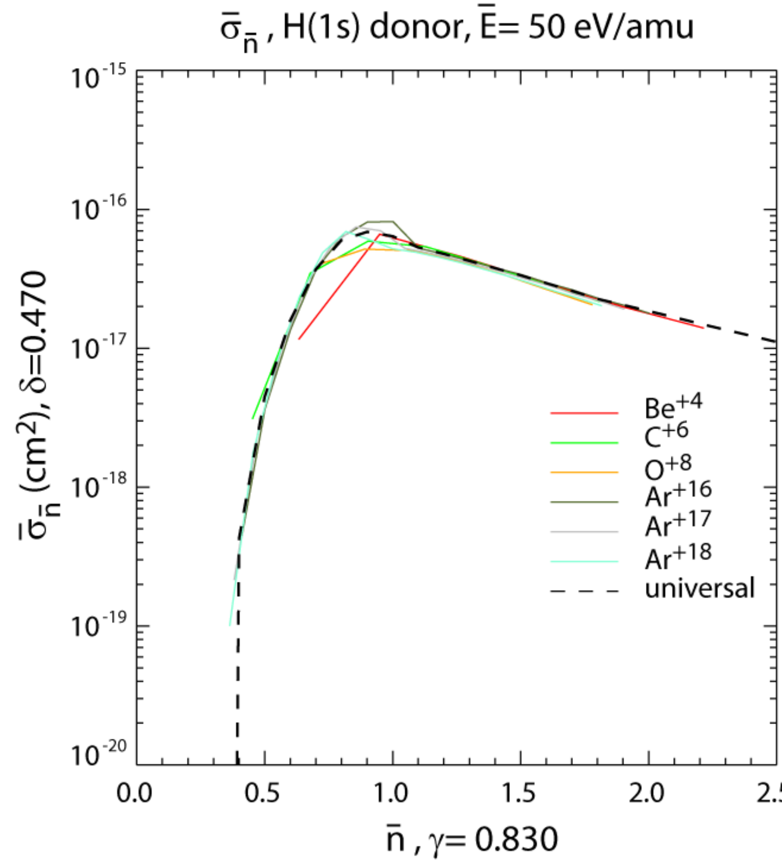
For each E that is at its corresponding , $\bar{E}$ ose z-scaling parameters γ and δ for best convergence for the different ions as:

$$\bar{n} = n\, z_1^{-\gamma(\bar{E})} \qquad \bar{\sigma}_n = \sigma_n z_1^{-\delta(\bar{E})}$$

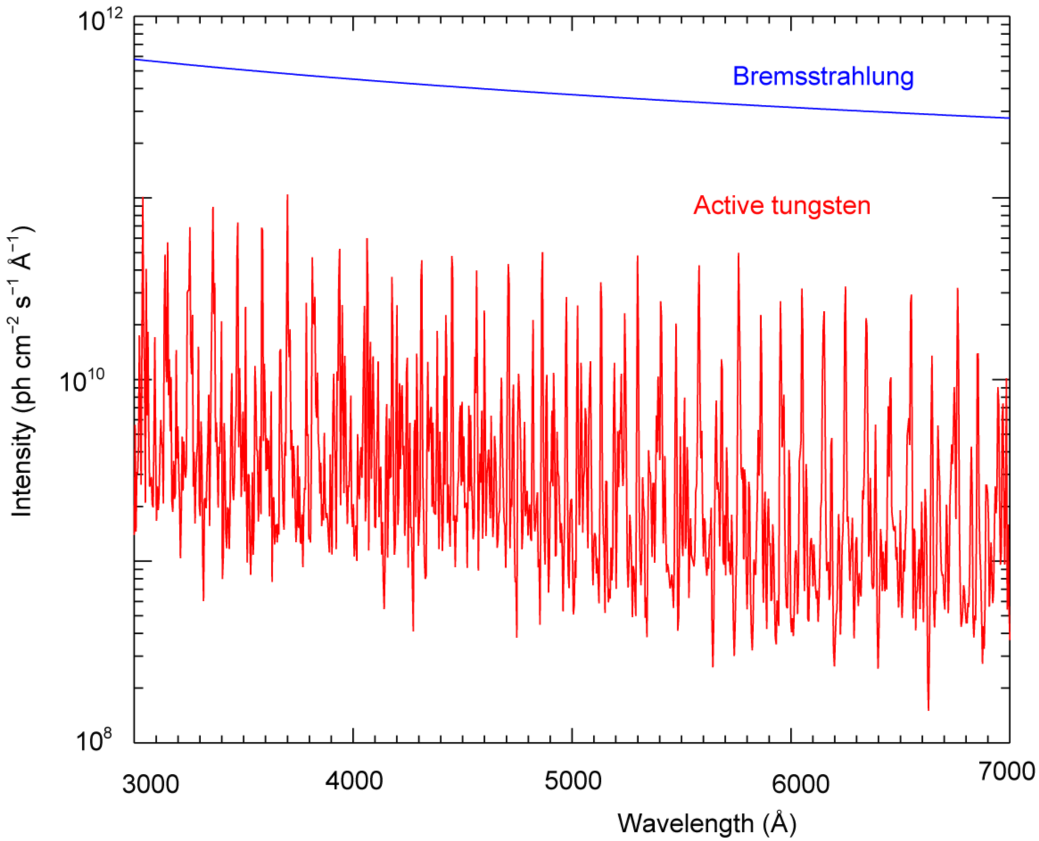
Results from specific calculations

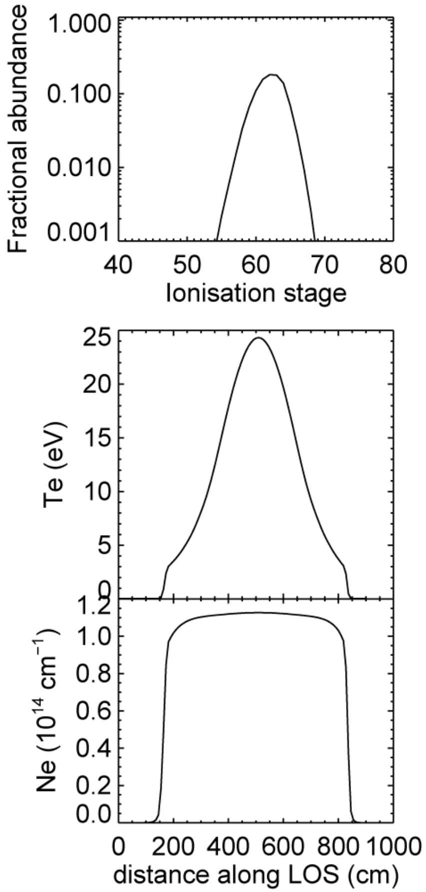
Note: non-integral





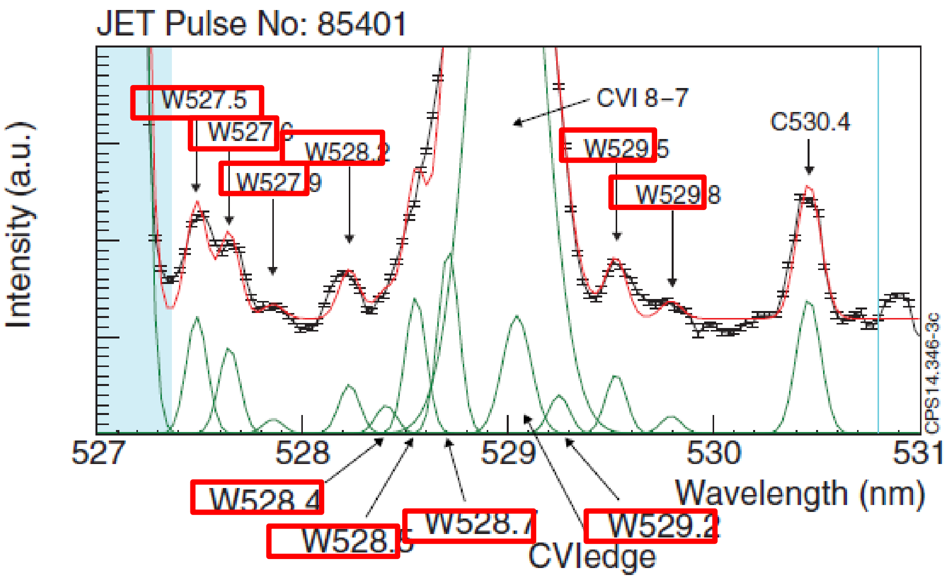
ITER: tungsten CX emission compared with Bremsstrahlung





- 50 keV/amu D beam (diagnostic NB), JNBI=300A/m2, INBI=60A
- Using ITER scenario 2 (Te=24keV core, Ne=1x10^{14}cm^{-3})
- No transport – steady state ionisation balance
- Assume looking vertically down on the beam at the core.
- No beam attenuation effects taken into account.
- W concentration = 1x10-6 of N_H

Need to model edge nuisance lines also



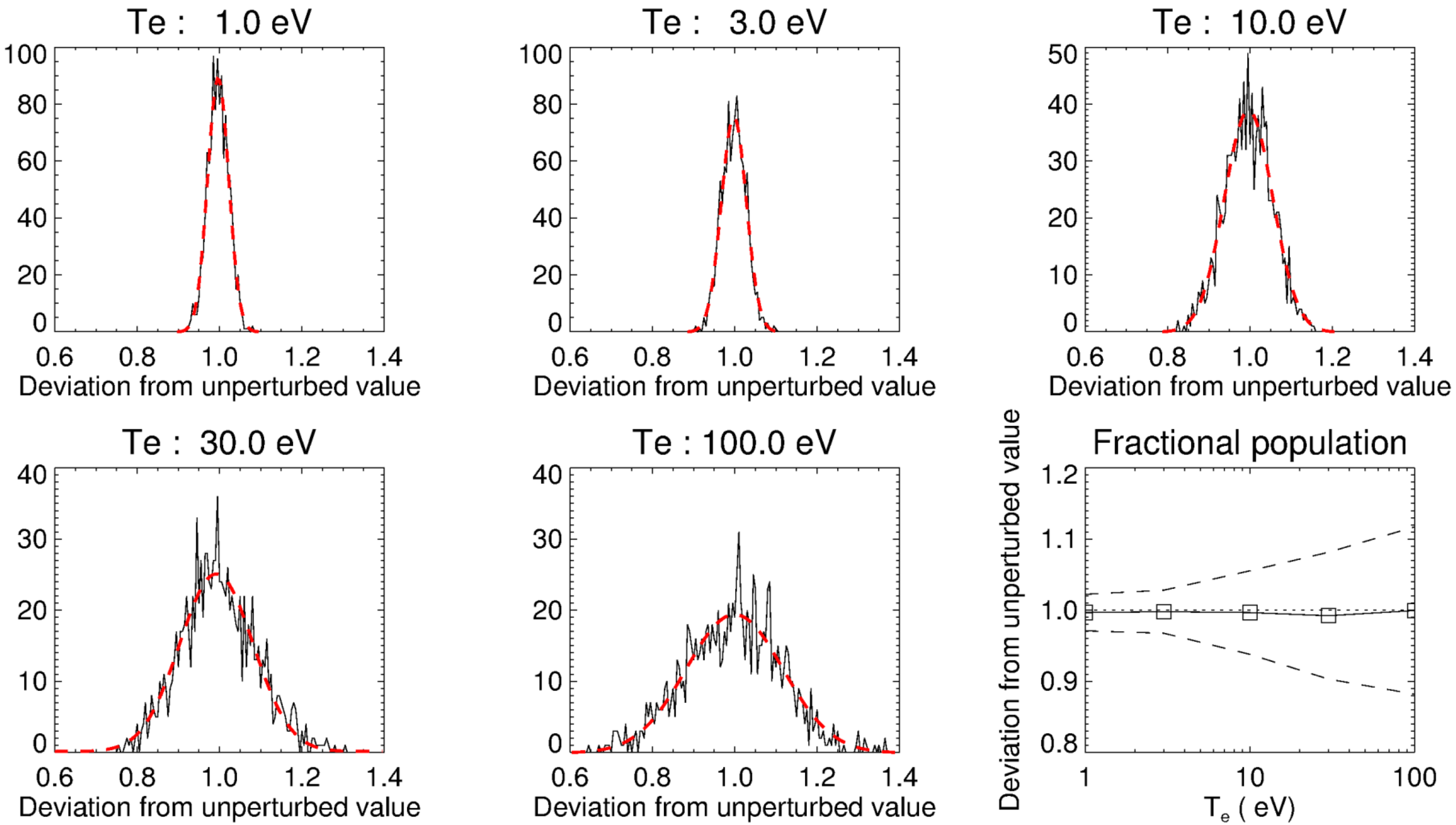
Wavelength (nm)	Description	Fig. 3 relative intensities
525.586	**BeII**	**2.6**
525.724	CII	1.0
525.966	CII	0.7
526.153	**BeI**	**0.3**
527.063	BeII	(Not fitted)
527.478	**WI**	**0.4**
alt. 527.553	**WI**	
527.645	*?W (no W in NIST here)*	*0.8*
527.858	**WI**	**0.3**
527.981	**WI**	**...**
528.229	*WI (528.265 in NIST)*	*0.6*
528.408	**WI**	**0.4**
528.552	**WI**	**1.8**
528.712	**WI**	**2.4**
528.83	*WI (528.850 in NIST)*	*...*
529.059 (free)	CVI 8-7 (the CX line)	236
529.059 (free)	CVI passive	...
529.059 (fixed)	CVI edge	3.9
529.249	**WI**	**0.4**
529.525	**WI**	**1.0 (ref.)**
529.79	*WI (529.858 in NIST)*	*0.6*
530.238	**WI**	**...**
530.462	CIII	1.0

S. Menmuir et al, Rev. Sci. Instrum. **85**, 11E412 (2014)

- Primary nuisance lines were identified as coming from W^{0+} emission
- W^{7+} or W^{11+} at 527.32nm identified by E-bit spectroscopy (R. Hutton)

Error estimation by Monte-Carlo algorithm

Thermal helium – population of excited level due to an ascribed uncertainty in every transition. Apply this technique to beam population model. Need the errors!



Data/model uncertainty, provenance and usage

- ADAS is a numerical database – the aspiration is to have a *.err* file for every *.dat* file.
- New tooling and tracking methods needed – doi/url reference method.
- Open access and data+model tracking is one driver for enhanced trackability.
- Big issue is getting the 'with errors' atomic data into wider use.

There are a number of assessments that will be done as part of the CRP.

1. Rank the importance of the various process to the final stopping coefficient For a number of representative target plasmas. This can act as a guide to which data needs dedicated effort.
2. Explore in-built assumptions such at Te=Tion and the data reduction choices.
3. Ascribe a realistic error bar to each quantity/process and propagate these uncertainties through the beam population model. Check the effect on the attenuation/deposition profiles.
4. Explore the effect of beams with significant birth populations in excited states. The ADAS model can be adapted to give relevant cross coupling coefficients. Explore the effect of these on the attenuation profiles.
5. Evaluate the model at MeV energies. Test whether the high energy asymptotic regime leads to better constrained attenuation profiles.