EUROfusion

Atomic data required for fusion research

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13 – 15 April 2021

Atomic and Molecular Data needs for Plasma Applications

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement number 633053.
The views and opinions expressed herein do not necessarily reflect those of the European Commission.

JET

Acknowledgements

With particular thanks to Ivor Coffey, Gerard Corrigan, Mathias Groth, Derek Harting, Sheena Menmuir, Martin O'Mullane, Ewa Pawelec, Detlev Reiter, James Simpson and from Queen's University Belfast Francis Keenan and Kanti Aggarwal & JET Contributors

Atomic data required for fusion research

Introduction

- Consider the impurity and fuel elements for which we need atomic data using experience from the JET Tokamak.
- Highlight some of the atomic data needs through a discussion of these impurities.
- A user's perspective.
- Data required for a wide temperature range depending on the element – from < 1 eV to T_e ~15-20 keV and T_i ~20-30 keV
- Density ranges from ~10^{18} – 10^{21} m^{-3}

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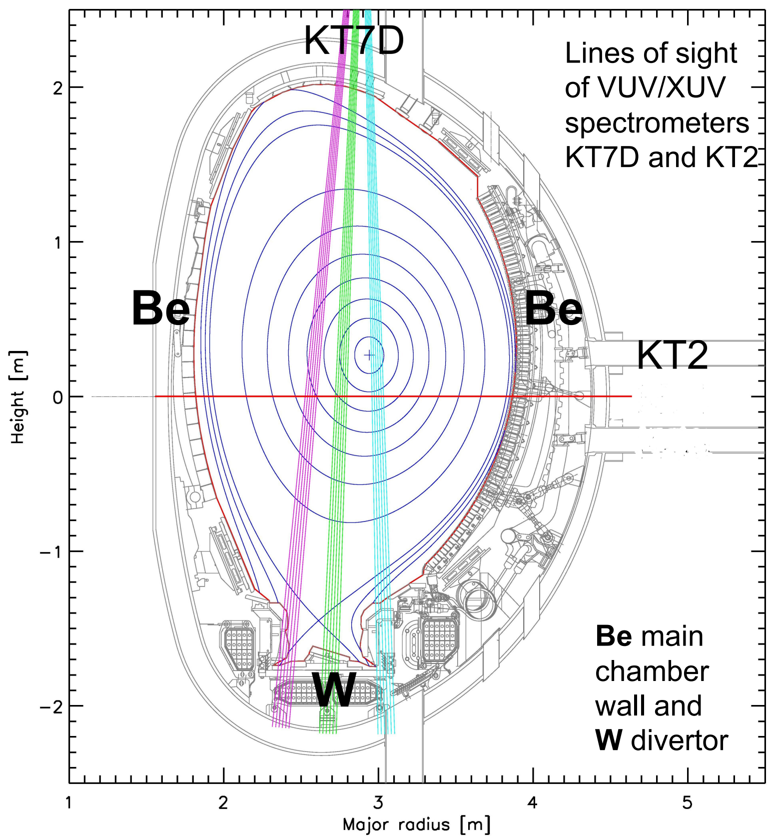
Which elements are important?

- The JET tokamak has an ITER-like wall of Be in the main chamber and W in the divertor.
- A recent study of divertor monitoring pulses (DiMPle) divided the impurities into two groups.
- The first includes gases introduced into the machine for particular experiments – N, Ne, Ar and Kr.
- The second group is of impurities released from the first wall – Be, C, O, Cl, Ti, Cr, Fe, Ni, Cu, Mo and W.
- In addition atomic data is required for the fuel – D or He.
- In machines that use boronizations B must be included.
- On JET spectroscopic observations are made in the visible, near-UV, the VUV / XUV and the soft X-ray spectral regions.



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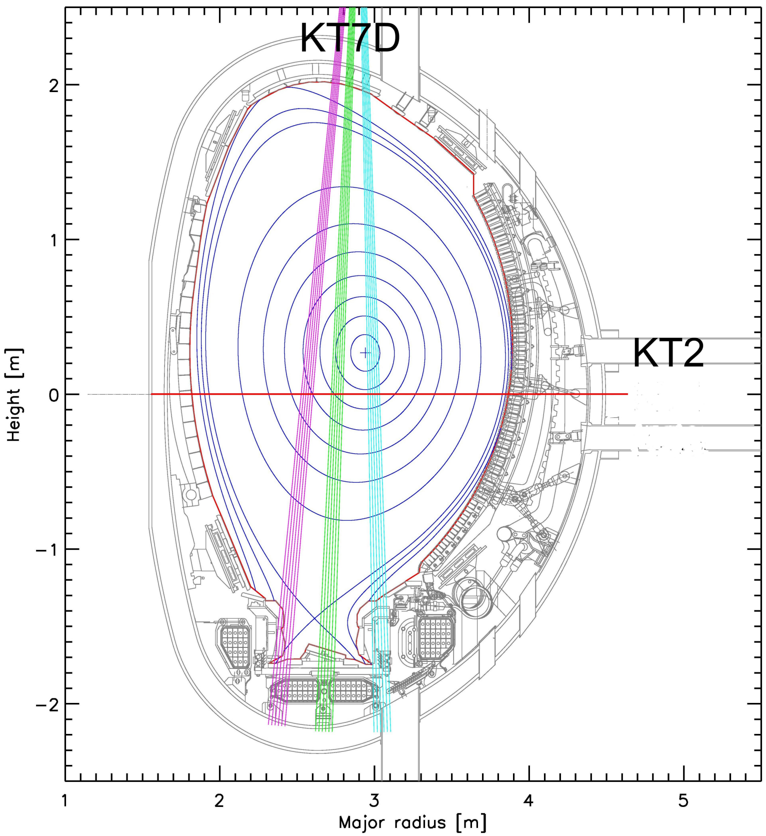
Which atomic data are important?

- In steady state applications processes determining the populations within an ionization stage are most important.
- Excited populations within an ionization stage adjust on a faster time scale than changes between ionization stages.
- The most important channels are radiative decay, electron collisional excitation and de-excitation, heavy particle collisional excitation and de-excitation, charge exchange, collisional ionization, radiative, dielectronic and three-body recombination.
- Rate coefficients for these various channels can be combined into a Collisional-Radiative model, which allows the excited level populations and, consequently, both line and total radiated powers to be determined.
- In time-dependent analyses, ionization and recombination are of crucial importance.
- They are usually reduced to effective ionization and recombination rate coefficients dependent on ground and metastable population densities.
- Ground and metastable populations depend on both the source of the impurities and their transport through the plasma.
- Measurements of line intensities therefore enable impurity transport studies.
- On JET and in many other fusion experiments wide use is made of ADAS which contains data for a large number of elements and processes (Hugh Summers and Martin O'Mullane).

KT7 and KT2 spectrometers



- The KT7 and KT2 spectrometers use SPRED instruments.
  - KT7 has a vertical line-of-sight, which can be varied.
  - KT7/1 covers 157 Å – 1480 Å with a spectral resolution of ~5 Å.
  - KT7/2 covers 140 Å – 443 Å with a spectral resolution of ~1 Å.
  - The highest time resolution is 11ms, although 20–50ms used routinely.
  - KT2 has a view along the horizontal midplane and observes 100 Å – 1100 Å with a spectral resolution of ~5 Å.

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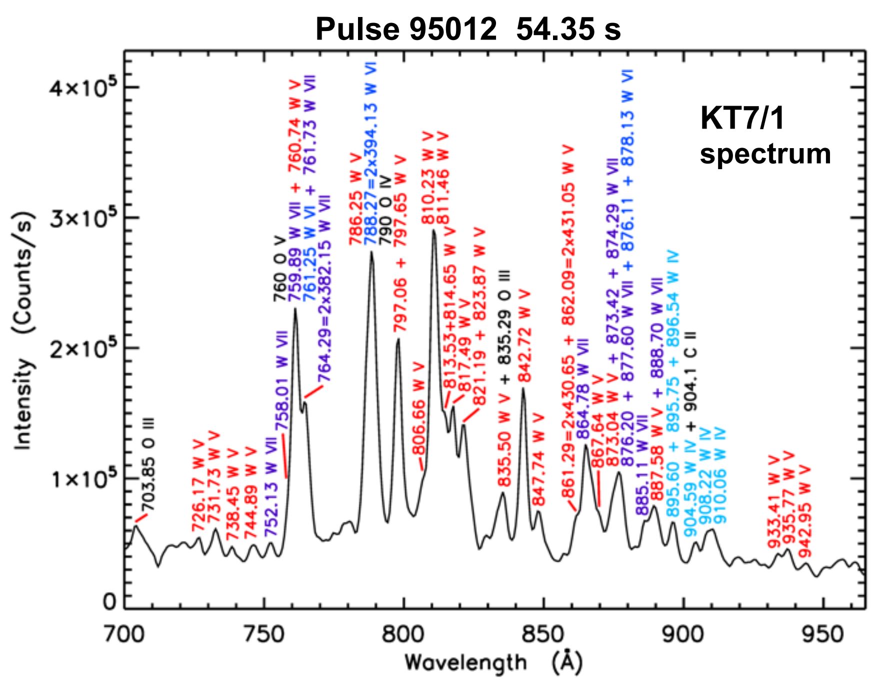
Tungsten (Z=74)

- W atomic data is required for all ionization stages (except perhaps the vey highest).
- Stages W XXVIII (W^{27+}) and above (>2-3 keV) are important for monitoring W, studying core W impurity transport and determining the power radiated by W.
- Stages W XIV (W^{13+})– W XXXI (W^{30+}) contribute to a VUV spectral feature which occurs at the plasma edge. Due to many Unresolved Transition Arrays (UTAs) quantitative measurements are difficult. Still useful as a relative monitor.
- The limitation of T_e in JET-ILW is not due to the reduction of low Z impurities or central impurity radiation. Radiation from the pedestal region is thought to be a contributing factor – W XVI (W^{15+}) – W XXVIII (W^{27+}) (Pawelec, 2017, Proc. of 44th EPS, Belfast, UK).
- W I is routinely used for influx measurements.

Tungsten (Z=74)

- However, the transport of neutrals and ions is very different, so the use of low ionization stages in transport studies is of particular value.
- W II and W III are only seen during extreme events. With a change of the line of sight of the KT7 VUV spectrometer it has been possible to observe discrete spectral lines from W IV-W IX.
- From these observations T_e of the emitting plasma region and W concentrations have been calculated using ADAS baseline data (Lawson, Pawelec, Coffey *et al.* In preparation).
- These suggest higher than expected concentrations and lower and more widely separated temperatures for neighbouring ionization stages than would be expected.



Electron temperature (eV)

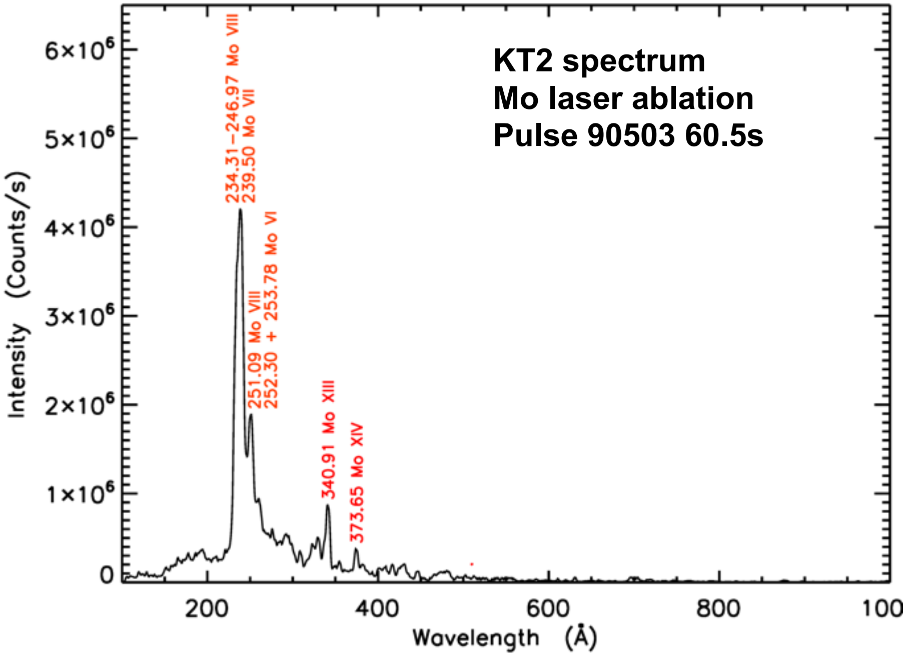
Pulse	94605	94645	95460	95463
W VI	3.9	3.5	3.9	3.9
W VII	9.7	9.5	9.1	9.0

W concentration

Pulse	94605	94645	95460	95463
W VI	0.1	0.07	0.03	0.03
W VII	0.004	0.002	0.002	0.002

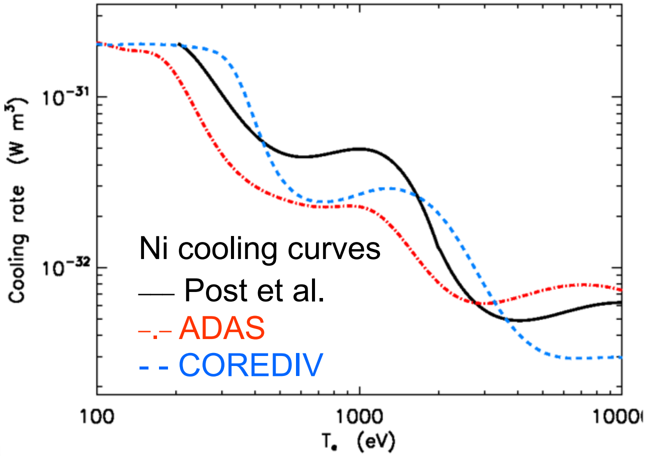
Molybdenum (Z=42)

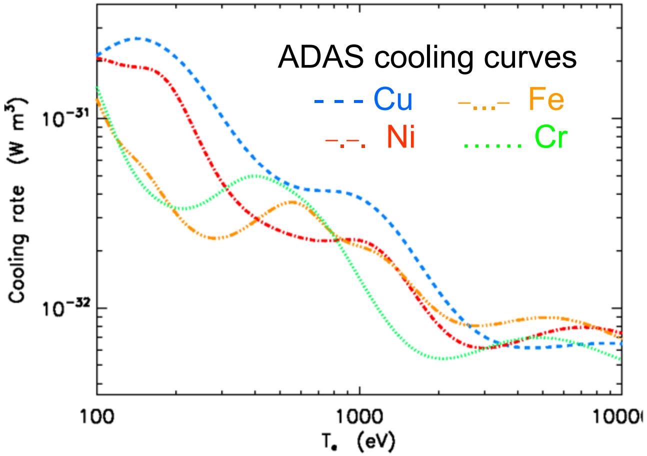
- Mo is used in fusion research, for example, in plasma machines such as Alcator C-Mod, the MIT tokamak that achieved particularly high magnetic fields.
- It has been used on JET for laser ablations in which a small quantity is injected into the plasma to study the impurity transport of mid- to high- Z elements.
- It was also seen in JET plasmas from 2013 being identified by Mo V to Mo VII features in VUV spectra immediately following a plasma disruption.
- At the time it appears to have come from the substrate of W coated divertor tiles.
- In the last few years, there have been Mo influxes from the injectors during Neutral Beam heating.
- It is now routinely observed in JET spectra and in some pulses will make a significant contribution to the radiated power.
- Good atomic data required for Mo.



Mid-Z metals – Cr, Fe, Ni and Cu (Z=24-29) (Ti and Mn)

- The mid-Z metals, Cr, Fe, Ni and Cu, are routinely seen in JET originating in the INCONEL of the vacuum vessel (Cr and Ni), the heating systems (ICRH Fe, Mn and Cu; LHCD Fe; NBI Cu) and other in-vessel stainless steel components.
- Ti influxes come from an ageing coil; no recent observations of Mn.
- DiMPle pulses give relative concentrations – Cr : Fe : Ni : Cu
  0.12 : 0.21 : 1.00 : 0.46
- The atomic physics of these mid-Z elements is similar.
- ADAS atomic data successfully used for core impurity transport studies, often involving Ni laser ablation.
- Ni and Cu can dominate the impurity radiation and so the total radiated power is important.
- A significant variation between different calculations and for different elements is seen.
- Accurate total radiated power calculations for these elements required.

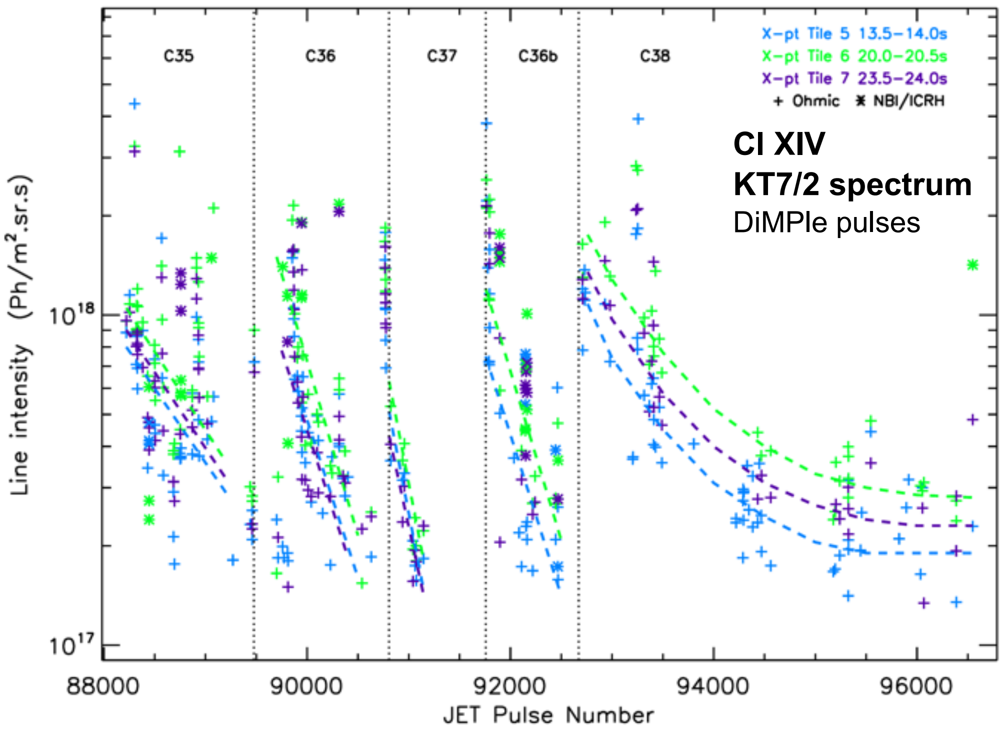




Chlorine and Argon (Z=17 and 18)

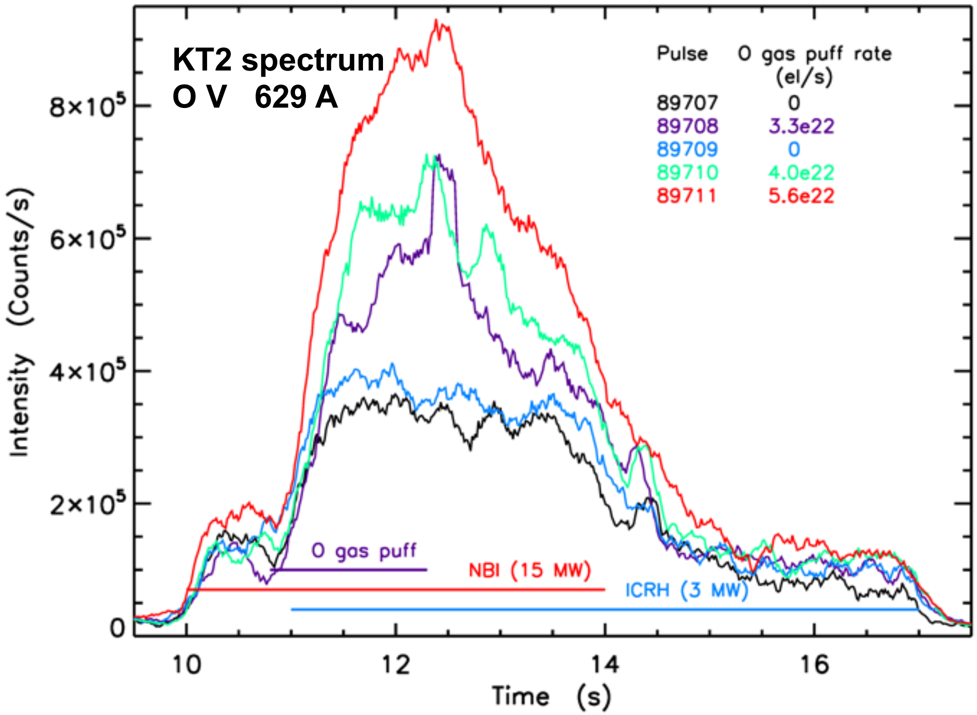
- Although Cl and Ar have very different chemical properties, they are neighbouring elements in the periodic table with similar atomic physics properties.
- Ar gas-puffing used for various experiments after which it rapidly decays.
- Cl retained in vessel walls – released particularly after shutdowns after which decays – its chemical properties lead to long term retention in the torus

- Good atomic data for Ar required if it is to be used as a divertor gas.



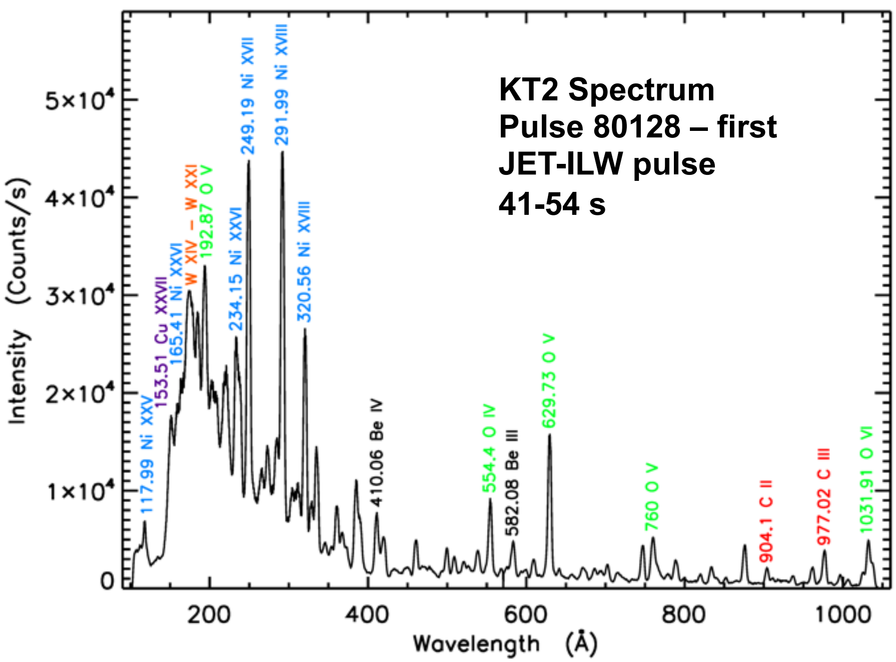
Oxygen (Z=8)

- Oxygen is always present in the plasma and almost always ignored.
- The use of Be either through Be evaporations or Be first wall components significantly improves machine operation, but there is a greater retention of O in a Be machine than a C one. C is more efficient at removing O.
- In 2016, O was gas-puffed with rates similar to those used in N radiative divertor experiments (Sebastijan Brezinsek).
- The VUV signals were ~ doubled. Although wall and gas-puffing sources differ, it does show that O should not be neglected – good atomic data required.

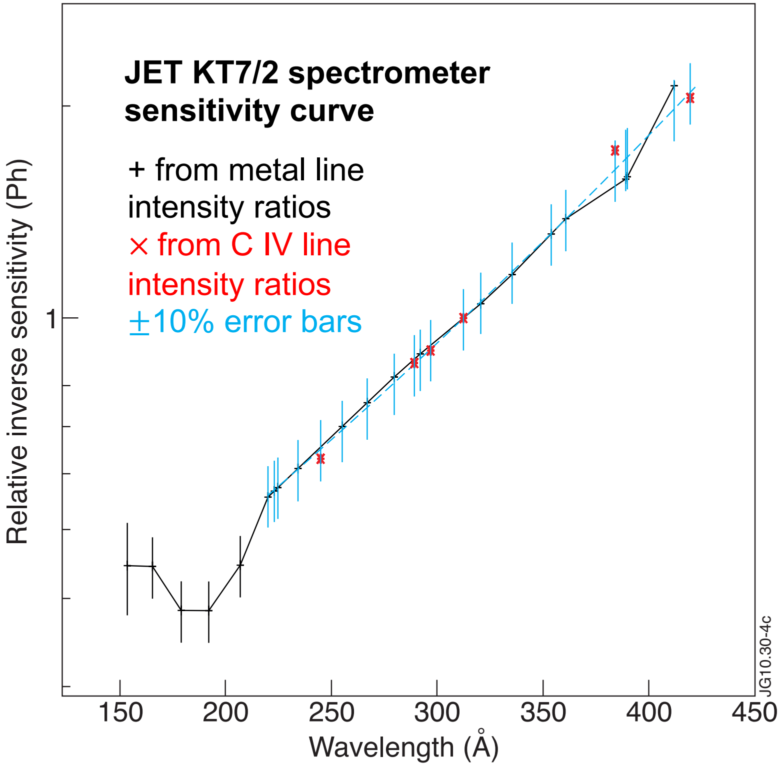


Carbon (Z=6)

- Carbon was used in JET for the main plasma facing surfaces before the installation of the Be and W tiles and is used in many other machines.
- With a Be first wall and W divertor there should be no C in JET.
- However, ‘*C is present in all plasma machines*’. This includes JET-ILW, although at significantly reduced levels.
- Good atomic data for C is essential.
- An analysis of C IV spectra of JET-C pulses shows the atomic data requirements for some of the low-Z elements.
- C IV is a simple ‘one-electron’ system with no metastable levels.
- In tokamak plasmas it is in the low density limit – collisions between excited states are unimportant.
- However, radiative cascading should be included in population modelling.



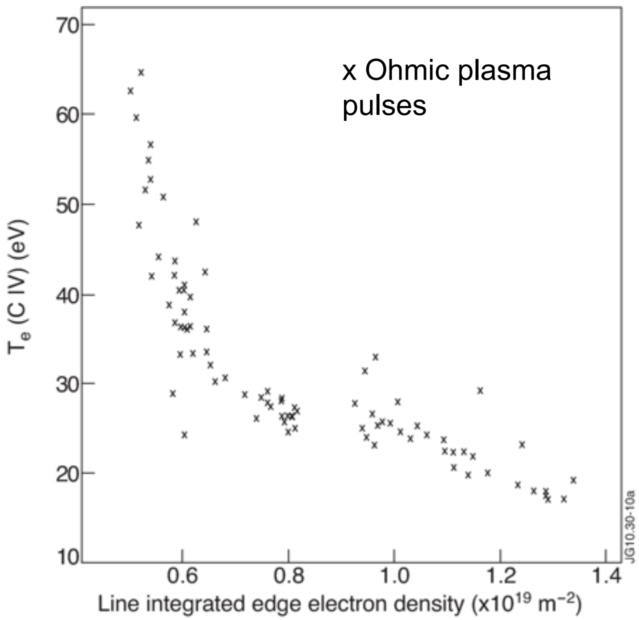
Carbon (Z=6)

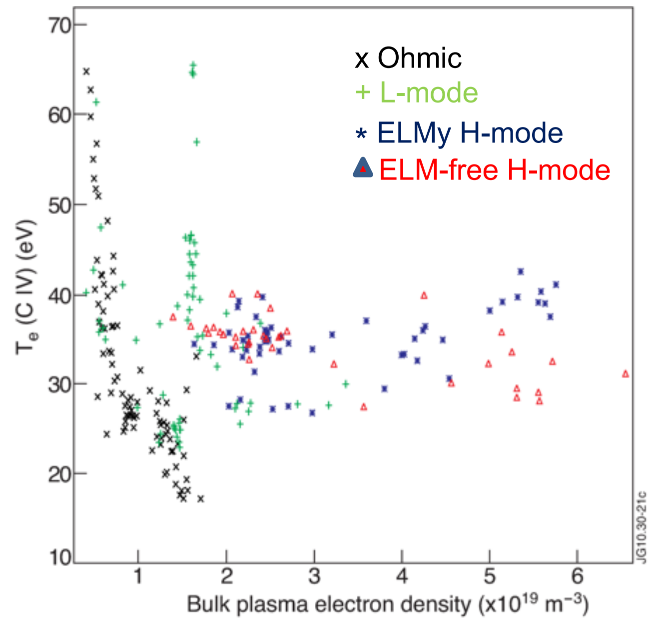


- KT7/2 VUV sensitivity calibrations derived from Na- and Li-like metal line intensity ratios that are temperature insensitive (+).
- Points (×) derived from C IV line intensity ratios lie on the calibration curve showing excellent agreement between measured and theoretical line intensity ratios (Lawson *et al.* 2011, PPCF, **53**, 015002).
- The electron collisional rate coefficients from Aggarwal and Keenan used (2004, Phys. Scr., **69**, 385).

Carbon (Z=6)

- Temperatures of the C IV emitting region can be calculated.





- The analysis shows that the electron collisional excitation rate coefficients are important – RMPS calculations of Griffin *et al*. (2000, J. Phys. B, 33, 1013) are less successful.
- For steady state modelling of level populations within an ionization stage free electron recombination is not important, although *l* - or *J* - resolved charge exchange data is required.

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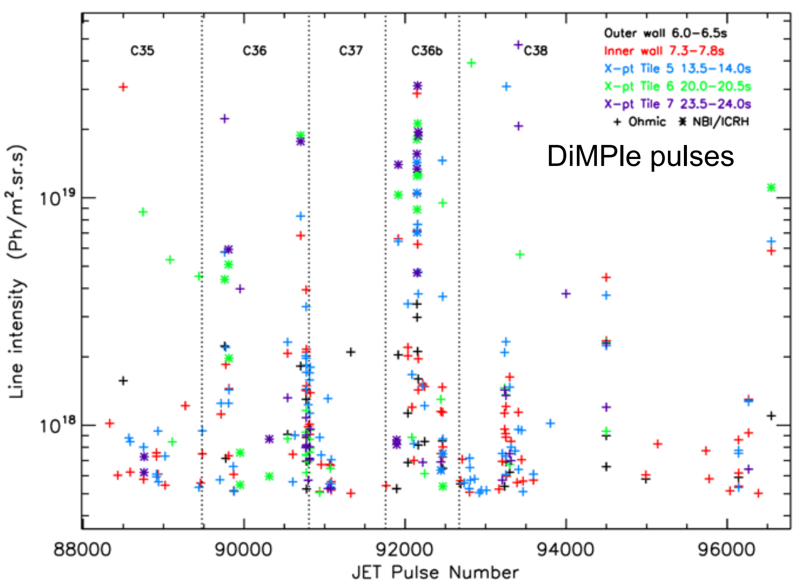
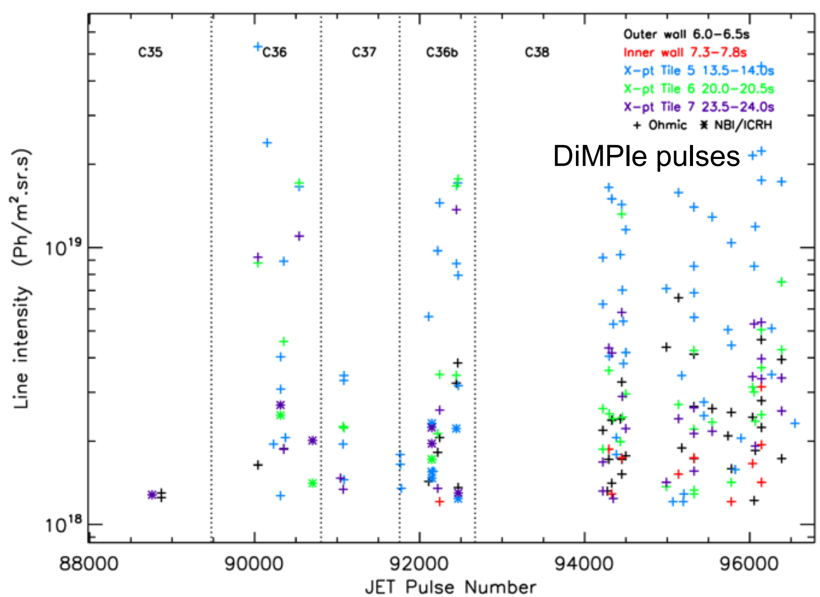
Nitrogen and Neon (Z=7 and 10)

- N used in particular experiments such as radiative divertor experiments.
- It appears immediately after its use and rapidly decays.
- It is unlikely to be used routinely in ITER because of the production of ammonia making the exhaust gas collection problematic.
- Ne behaviour was similar until it was used extensively for charge exchange measurements. It was increasingly retained in the vessel and became part of the background spectrum.
- D charge exchange data in ADAS was only available for C IV.
- Charge exchange data is essential for the analysis of N V and Ne VIII (and for C III, N IV, and Ne VII) spectra and desirable for any ionization stage being studied.

N IV KT2

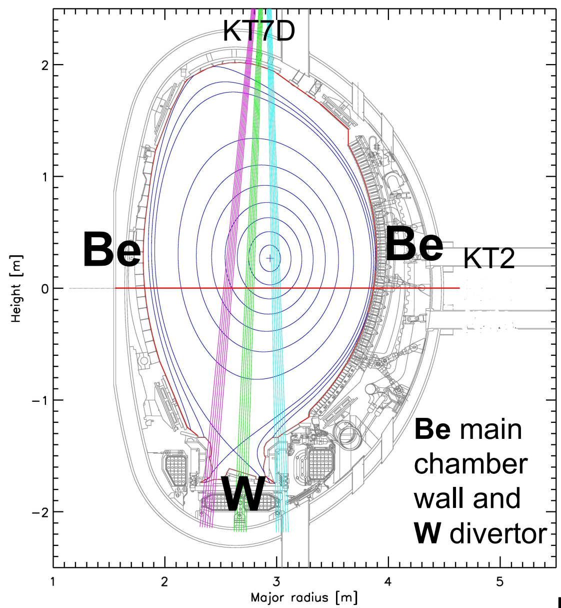


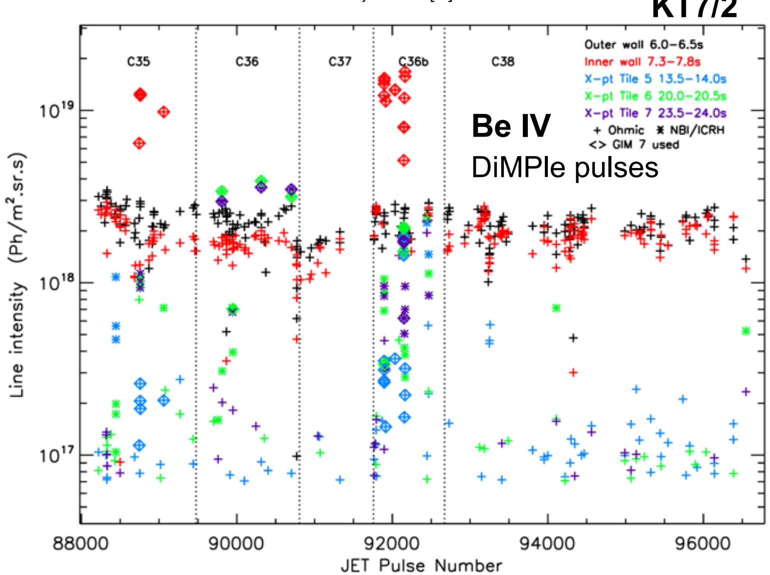
Ne VIII KT2



Beryllium (Z=4)

- Be has been used extensively in JET both through Be evaporations for gettering O and as a limiter material.
- Its release into the plasma from plasma facing surfaces is less efficient than that of C, although it is clearly seen in discharges which are limited by Be surfaces (the inner and outer walls).
- Consequently, in many X-point experiments it contributes little to the radiation, although will play a role in diluting the plasma fuel.
- During plasma operations it has been distributed throughout the vessel, being retained on W surfaces (Krieger *et al.*, 2013, J. Nuc. Mater., **438**, S262; Lawson *et al.*, 2013, Proc. 40th EPS Conf., Espoo, Finland).
- ADAS data was used in Be impurity transport simulations.
- Understanding the erosion of Be limiting surfaces and its effect on W divertor plates are the most important challenges.



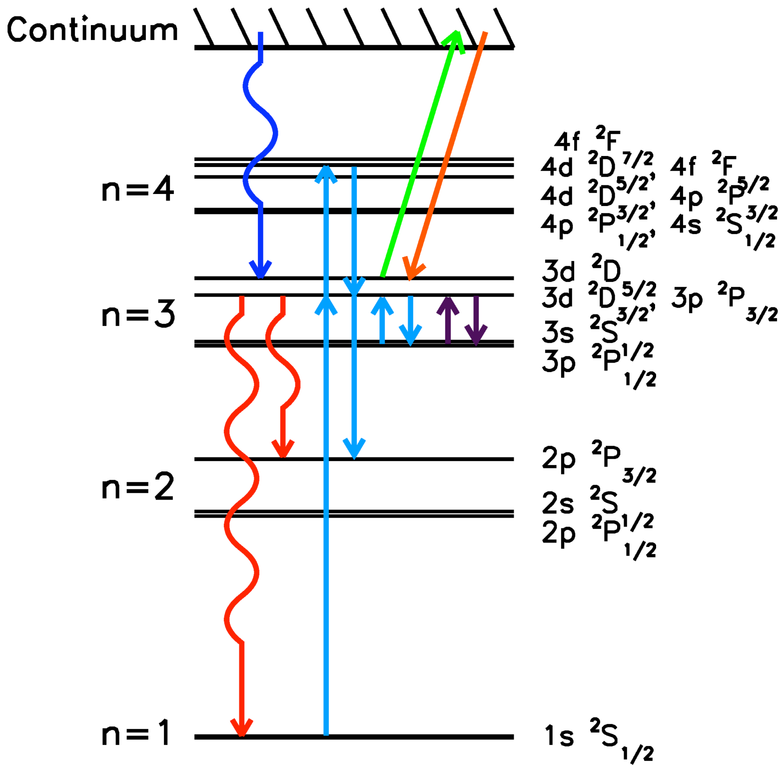


JET

Helium - Hydrogen / Deuterium / Tritium (Z=2 and 1)

- He is important in its own right. It is to be used as a fuel in the first non-nuclear phase of ITER, is a product of DT reactions and is used as a minority gas in some Ion Cyclotron RF heating experiments.
- He II can also be used as a proxy for D, since their atomic physics and behaviour in the plasma are similar.
- Importantly, a study of He II avoids the complications of D molecules, so that the atomic physics alone is better understood.
- The atomic physics of He II is also more tractable, in that heavy particle collisions are with ions rather than neutral atoms.
- To date, transport modelling of the divertor has not been able to reproduce the measured radiated powers which is crucial for ITER predictions. Shortfall of ~50% in D plasmas (Groth *et al*., 2013, Nuc. Fus., **53**, 093016; Jarvinen *et al*., 2015, JNM, **463**, 135), 25-35% in He (Canik *et al*., 2017, Phys. of Plas., **24**, 056116).
- This appears to be due to the simulations not reaching low enough electron temperatures, ~1 eV for D and ~2 eV in He.
- In the first instance it is the atoms that determine the simulation temperature. In D plasmas molecules only become important at low divertor temperatures.
- How sensitive are the simulations to the atomic physics?

CHEM database for He II



The CHEM database for He II includes atomic data for the main populating channels in a hydrogenic species :-

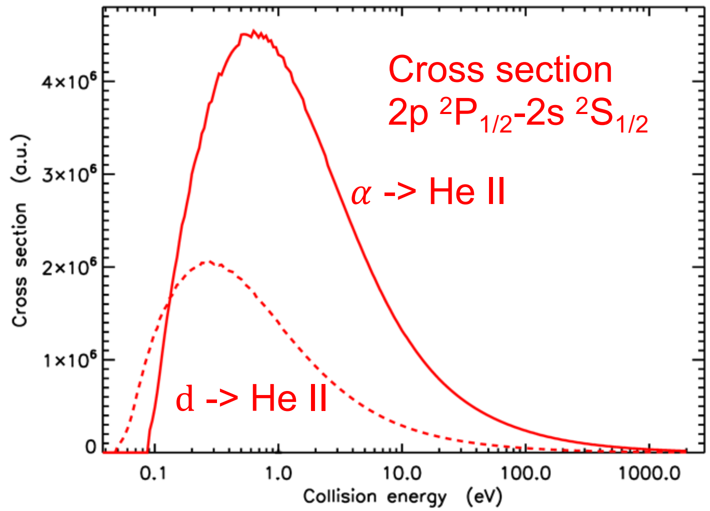
1. Electron collisional excitation and deexcitation
   $e + A \leftrightarrow A^{*} + e$
2. Heavy particle collisional excitation and deexcitation
   $\alpha\ (d,p,t) + A \leftrightarrow A^{*} + \alpha\ (d,p,t)$
3. Radiative decay
   $A^{*} \rightarrow A + h\nu$
4. Direct electron collisional ionization
   $e + A^{z+} \rightarrow A^{(z+1)+} + e + e$
5. Radiative recombination
   $e + A^{(z+1)+} \rightarrow A^{z+} + h\nu$
6. Three-body recombination
   $e + e + A^{(z+1)+} \rightarrow A^{z+} + e$

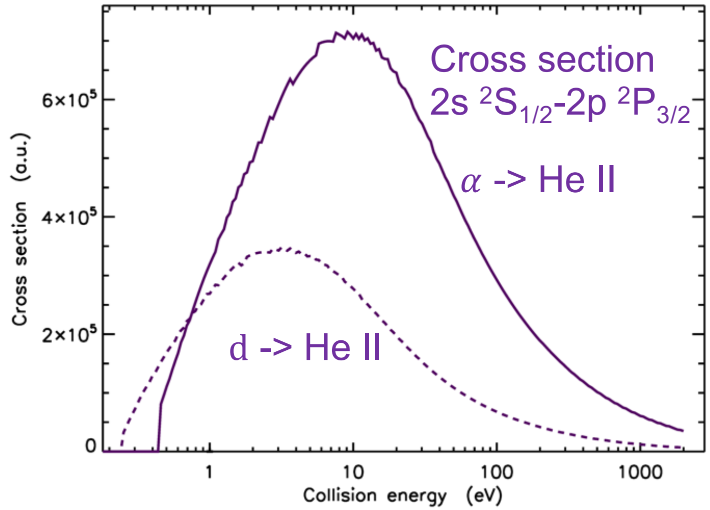
- The most recent atomic data is used covering a temperature range of 0.2 – 30 eV with particular attention being paid to the lowest temperature data.
- *J*-resolution is used for the spectroscopic levels (n = 1-5), *n*-resolution for $n \leq 16$.
- Electron collisional excitation rates were taken from Aggarwal *et al*. (2017, Atoms, **5**, 19).

Spectroscopic nomenclature $nl\ ^{2s+1}L_j$

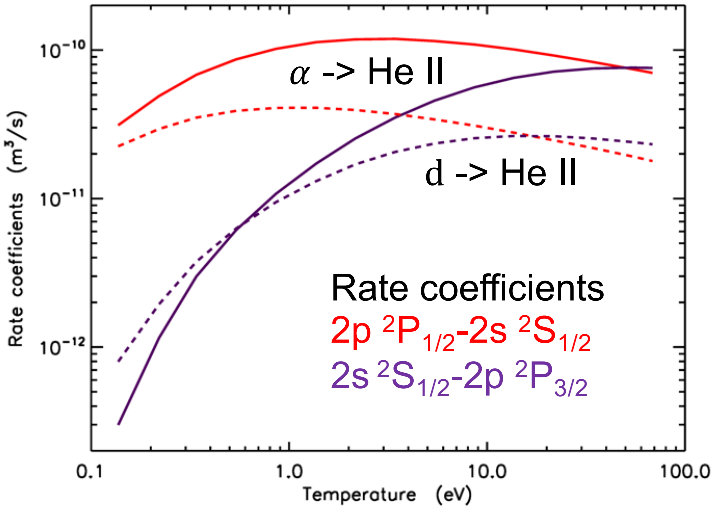
JET

CHEM database for He II



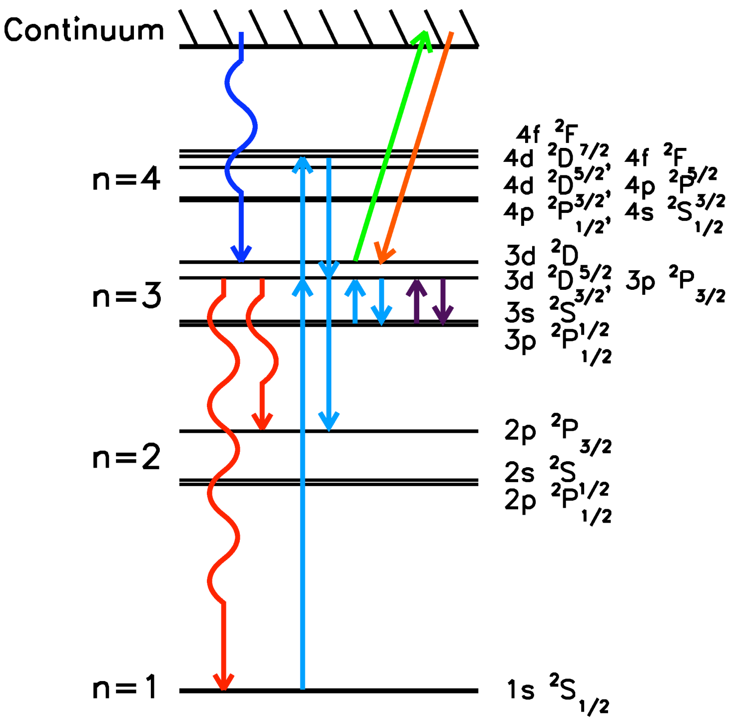


- No published heavy particle rate coefficients for He II (or D I). Generated using method of Walling and Weisheit (1988), which is a semi-classical approach for bound-state excitation in ion-ion collisions, this extending the work of Seaton (1964).
- Rate coefficients of p, d, t and α-particle impact excitation of He II listed by Lawson *et al.* (2019).
- Direct electron collisional ionisation, radiative recombination and three body recombination rate coefficients generated using Gu's (2008) Flexible Atomic Code (FAC).



Walling and Weisheit 1988, Physics Reports, **162**, pp1-43; Seaton, 1964, Mon.Not. R. Astron. Soc., **127**, p191
Lawson *et al*. 2019, J. Phys. B, **52**, 045001; Gu, 2008, Can. J. Phys., **86**, 675

Collisional-radiative population model



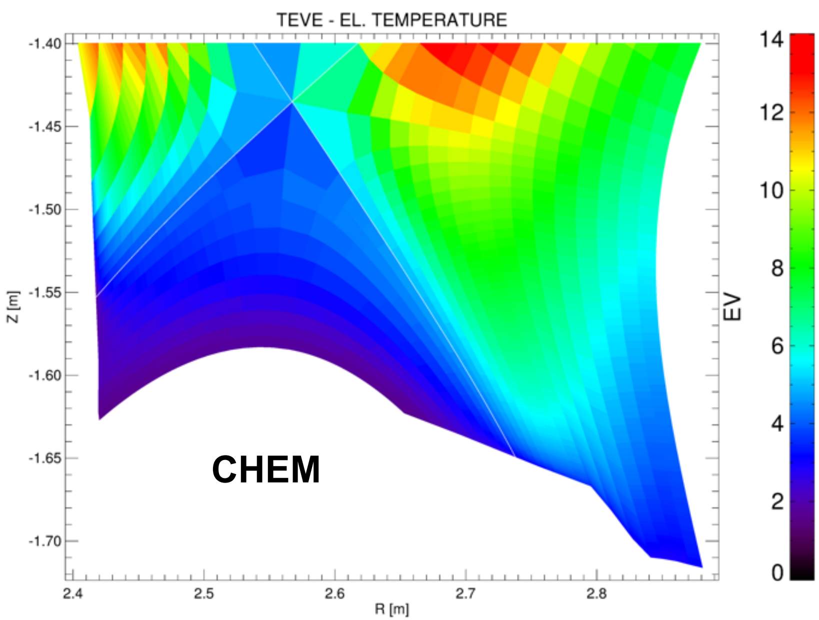
Spectroscopic nomenclature $nl\ {}^{2s+1}L_j$

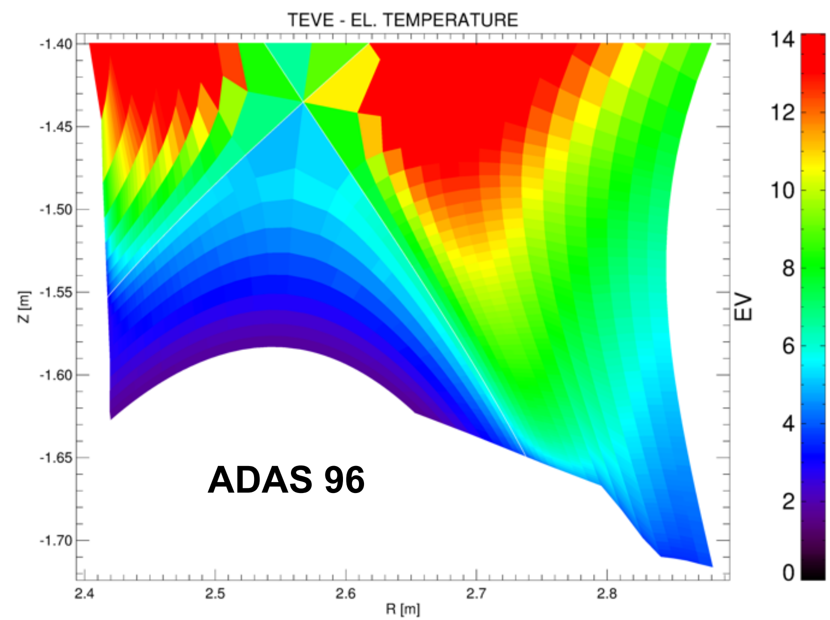
- The CHEM database has been used in a C-R model for He II.
- The electronic energy levels are populated by electron collisional excitation and de-excitation, radiative decay, direct collisional ionization, radiative recombination, three body recombination and, within an n shell, heavy particle collisional excitation and de-excitation.
- The model is derived from rate equations that include these populating channels following the treatment of Burgess and Summers (1976, MNRaS, **174**, 345), also described by Zholobenko *et al*. (Juel-4407).
- The model is linear with populations depending on the He II ion ground state density and the fully stripped He density.
- It covers a temperature range of 0.2-30 eV and all densities of interest.

- The C-R model is versatile giving all components to the radiated power with different channels easily switched on and off. Total power and line radiation can be compared with experiment.

He EDGE2D-EIRENE simulations

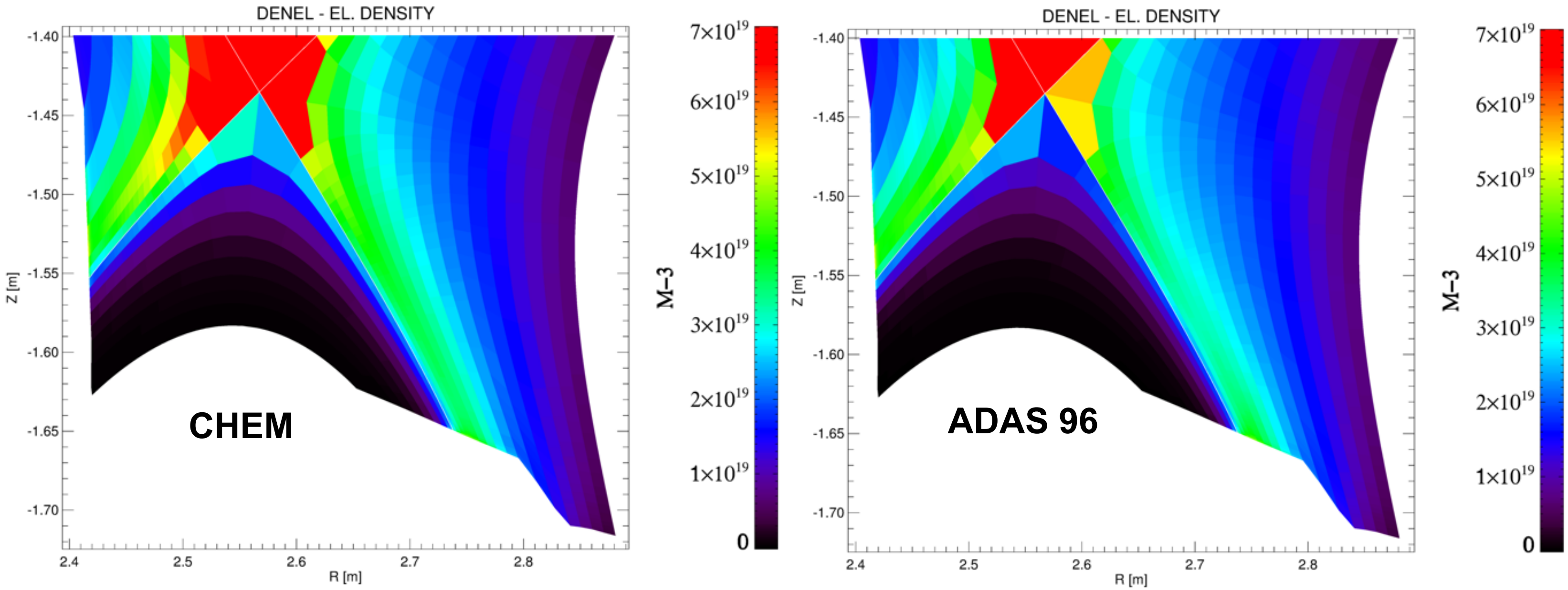
- Comparison of high density He simulations (D fuel ~4%) with JET geometry.
- CHEM data used for He II (T_e ~0.2-30 eV) compared with ADAS 96 data; otherwise the simulations are the same.
- Atomic data for He I from the AMJUEL database (through EIRENE).
- T_e ~2 eV reached in the inner divertor and ~3 eV in the outer divertor in the CHEM case.
- 2 eV is the temperature at which radiation due to recombination becomes important.
- In some cells (T_e ~2 eV) the radiated power increases by ~70% for He I and ~40% for He II, although overall there is a reduction in the radiated power.





He EDGE2D-EIRENE simulation

- n_e is found to be somewhat higher in the CHEM simulation.



- To date, the simulations have not been compared with measurements.
- Demonstrates the importance of the atomic physics and that the highest quality data is essential.
- This study justifies reassessing the atomic data for He I and for D I.
- If this leads to a further lowering of the temperature, this may help to explain the shortfall in the simulated divertor radiation (~30% in He simulations).

Conclusions

- Impurity studies on JET have been used to suggest which are the most important elements for fusion research.
- These include the fuel gases D/H/T and He and impurities Be (B), C, N, O, Ne, Ar, mid-Z metals Cr, Fe, Ni and Cu and Mo and W.
- Atomic data required for a wide range of temperatures, from <1 eV in the divertor to many keV in the core plasma, this depending on the element and ionization stage.
- These studies highlight the need for the most accurate electron collisional excitation rate coefficients.
- Heavy particle collisional excitation rate coefficients may also be required.
- For low Z elements charge exchange data are important in modelling level populations.
- Accurate 'cooling curves' for all elements are essential to allow prediction of the total radiated power.