He II as a proxy for D I

Kerry Lawson

Joint IAEA-FZJ Technical Meeting
29 - 31 March 2021

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

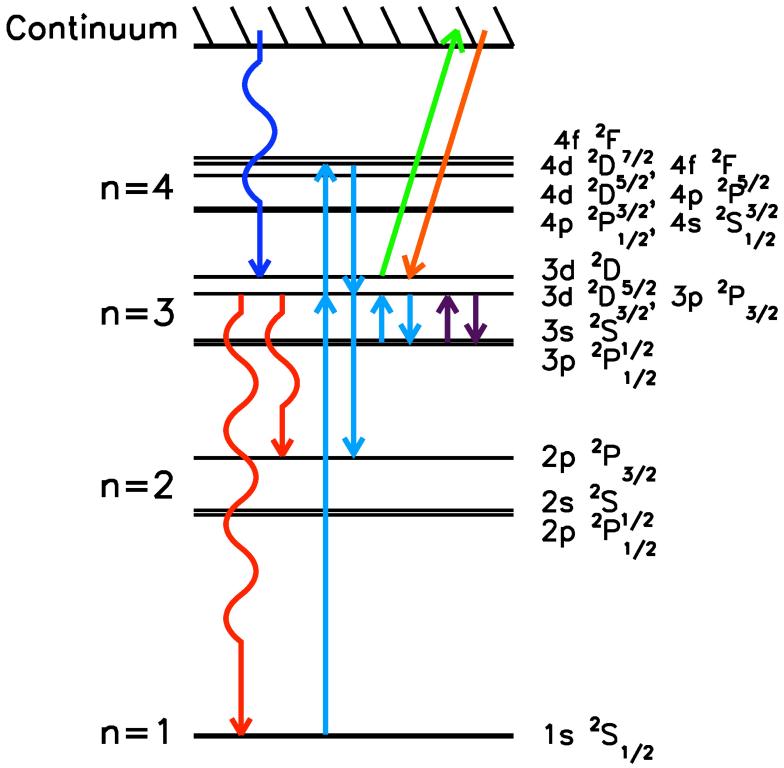
Acknowledgements

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

He II as a proxy for D I

- He atomic data, C-R models and edge transport simulations are of interest in their own right.
- He II can also be used as a proxy for D I – what is learnt for He II can inform the analysis of D I .
- He is to be used for the first non-nuclear phase of ITER, is used in JET, occurs as ash in DT plasmas and is used as a minority gas in various ICRH heating schemes.
- The atomic physics of H-like He (He II) is similar to D I, but more tractable – in particular heavy particle rates are more easily calculated, since the collisions are with ions rather than neutrals.
- The plasma behaviour of He II is similar to D I.
- However, He II avoids the complexities resulting from D molecules allowing the atomic physics to be investigated.
- A new He atomic database, the Culham He Model (CHEM), is described (Lawson et al. 2019, J. Phys. B, 52, 045001).
- A Collisional-Radiative model is derived from the CHEM database and is applied to EDGE2D-EIRENE edge transport simulations.
- In particular low temperature / high density simulations are considered – these have a shortfall in the simulated divertor radiated power.
- Finally questions regarding comparisons of the He II and D I line intensity ratio measurements with theory are raised.

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 $n \leq 16$.
- Heavy particle collisional rate coefficients were generated for this database.

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

He II atomic data

- Transition probabilities are available via the NIST database from :-
  Wiese and Fuhr, 2009, J. Phys. Chem. Ref. Data **38**, p565

  Data should be reliable and more accurate than collisional data.

- R-matrix electron collisional excitation rates from :-

  Aggarwal *et al*., 1991, J.Phys. B, **24**, p1757
  L-resolved, 15 level (n=1 to n=5), 0.43 – 8.6 eV, no fine-structure transitions.

  Callaway, 1994, ADNDT, **57**, p9, (ADAS 97)
  L-resolved, 15 level (n=1 to n=5), 0.5 eV – 10 keV, no fine-structure transitions.

  Kisielius *et al*., 1996, AA Supp. Ser. **118**, p157 (IRON project)
  j-resolved, 16 level (n=1 to n=4), 0.137 – 1.72 eV, with fine-structure transitions.

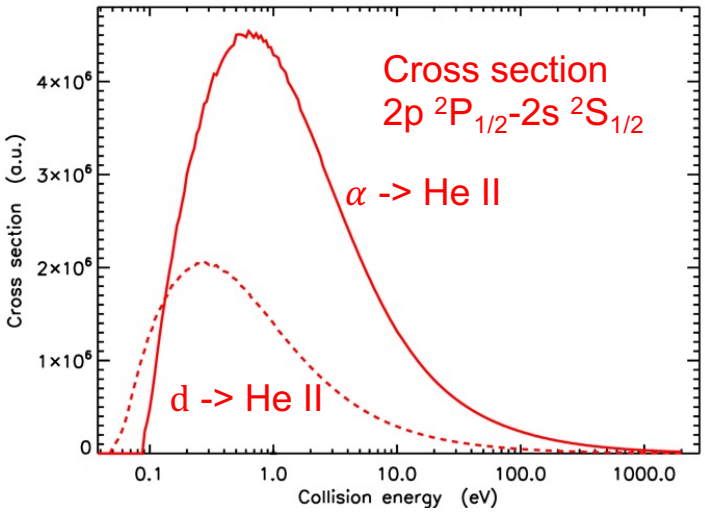
  Ballance *et al*., 2003, J.Phys. B, **36**, p3707
  L-resolved, 15 level (n=1 to n=5), 1.0 – 86.2 eV, no fine-structure transitions.

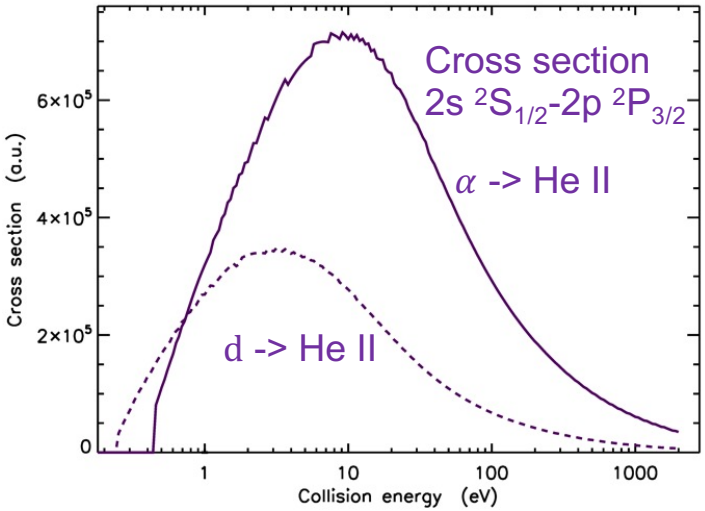
  Aggarwal *et al*., 2017, Atoms, **5**, p19
  j-resolved, 25 level (n=1 to n=5), 0.34 – 21.7 eV, with fine-structure transitions.

  Hamada *et al*., 2010, ADNDT, **96**, p9
  j-resolved, 25 level (n=1 to n=5) 0.86 – 8.62 keV, only fine-structure transitions.

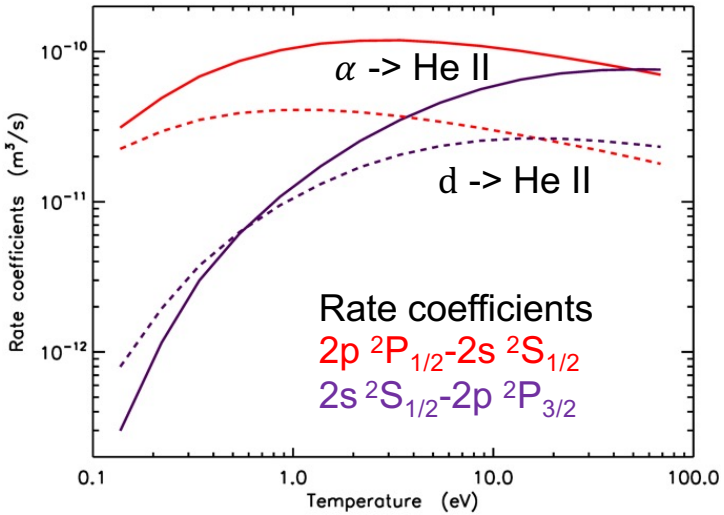
Spectroscopic nomenclature $nl\ ^{2s+1}L_j$

Heavy particle collisional excitation rate coefficients



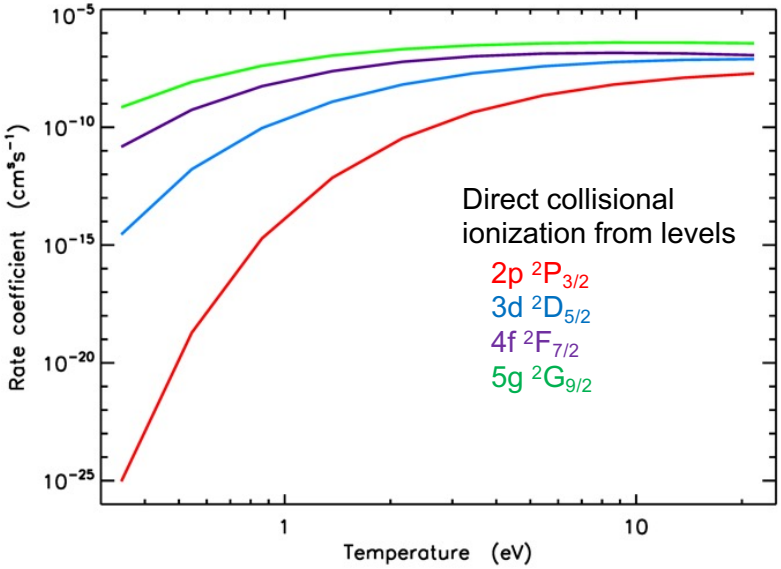


- There were no published heavy particle rate coefficients for He II (or D I).
- Implemented the method of Walling and Weisheit (1988), which is a semi-classical approach for bound-state excitation in ion-ion collisions extending the work of Seaton (1964).
- This allows cross sections of p, d, t and α-particle impact excitation of He II to be generated (Lawson et al. 2019, J. Phys. B, 52, 045001).

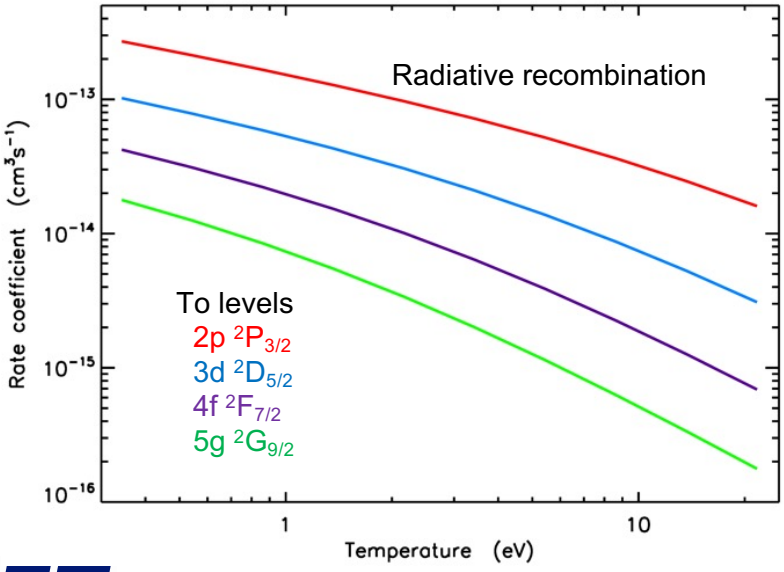


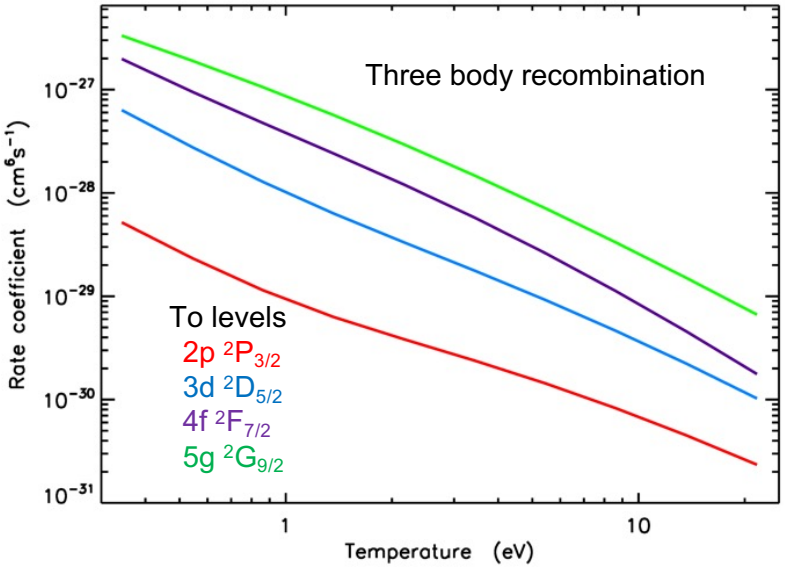
Walling and Weisheit 1988, Physics Reports, **162**, pp1-43; Seaton, 1964, Mon.Not. R. Astron. Soc., **127**, p191

Ionization and recombination

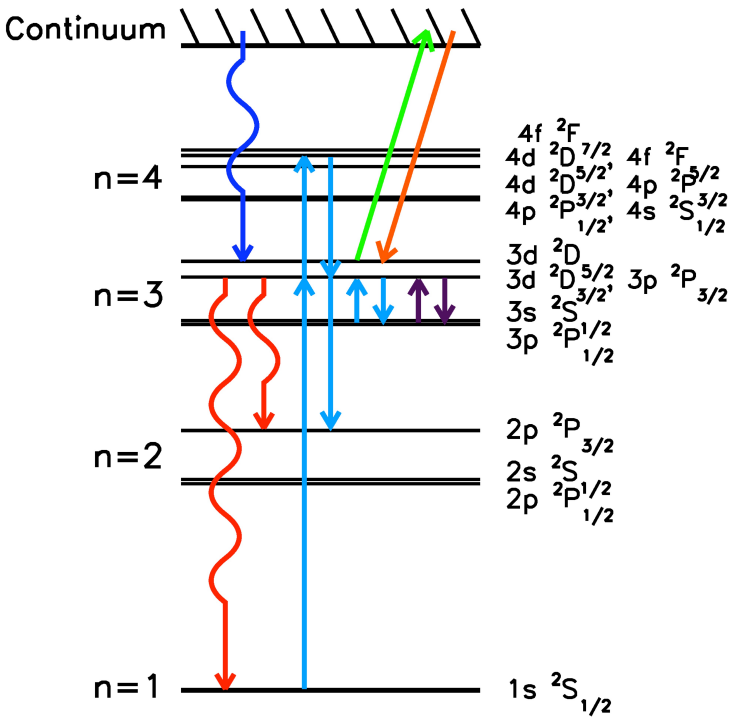


- Direct collisional ionization, radiative and three-body recombination rate coefficients were generated using the FAC code.
- Comparisons were made with CCC cross sections for collisional ionization (Bray, 'atom.curtin.edu.au/CCC-WWW').
- Good agreement was found with the ADAS radiative recombination rate coefficients.





Collisional-radiative population modelling



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.

EDGE2D simulations

- The CHEM database and its associated C-R model has been compiled for several reasons :-
- 1) To check the validity of branching ratio calculations for VUV spectrometer calibrations.
- 2) To compare with existing databases – for example, the high density behaviour of some D I and He II ADAS line intensity ratios is unexpected.
- 3) As a check on the atomic data being used by edge transport simulations, with particular focus on EDGE2D.
- How sensitive is the EDGE2D simulation to the atomic data used?
- Atomic data used in EDGE2D :-

  ionization balance + electron power loss

  In post-processing –

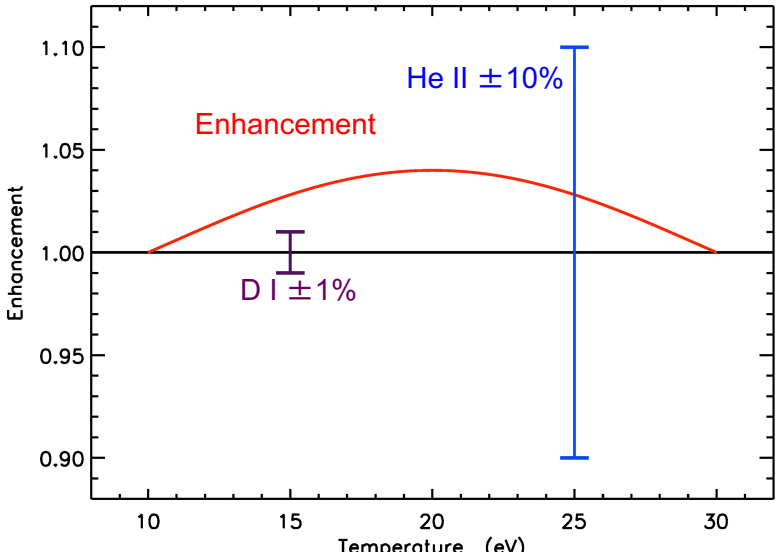
  radiated powers
- Question particularly relevant for low temperatures / high densities.

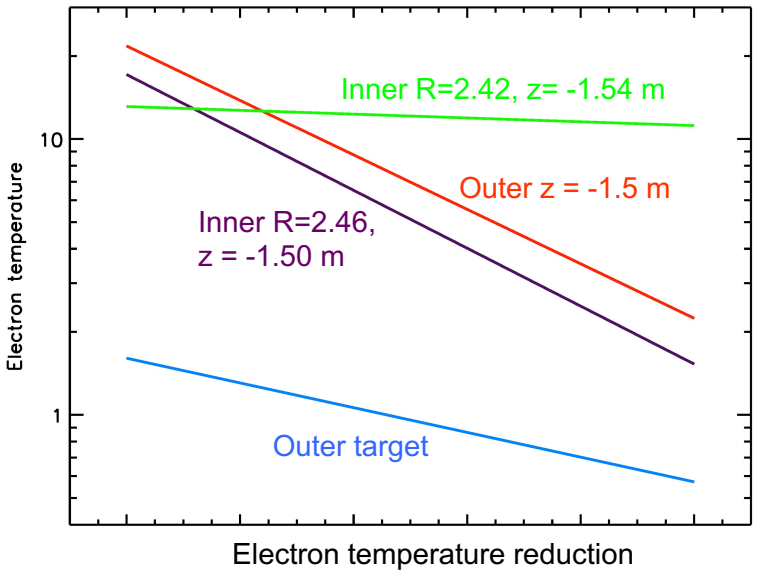
  There is concern that the simulations are not reaching sufficiently low temperatures – these are determined by the atomic physics.

Sensitivity to atomic physics

- Example from a D L-mode simulation
- The atomic power loss is artificially enhanced by <4% at temperatures of 10 – 30 eV.
- This is a 'worst case', but T_e is reduced by up to ×10 in some cells.
- Most of these cells have a low density and therefore do not contribute significantly to P_{rad}.
- Necessary to consider the simulation as a whole.

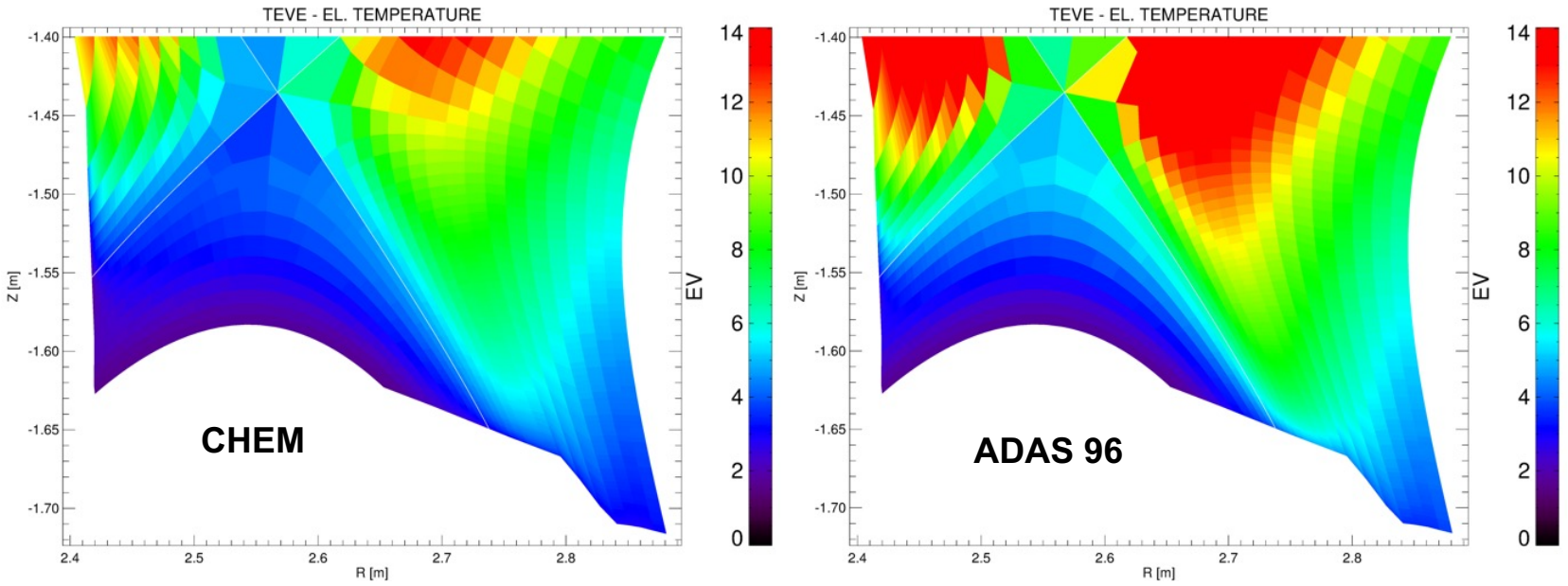
(For D I see Benda and Houfek, 2018, ADNDT, **119**, 303 and Aggarwal *et al.* 2018, Atoms, **6**,37)





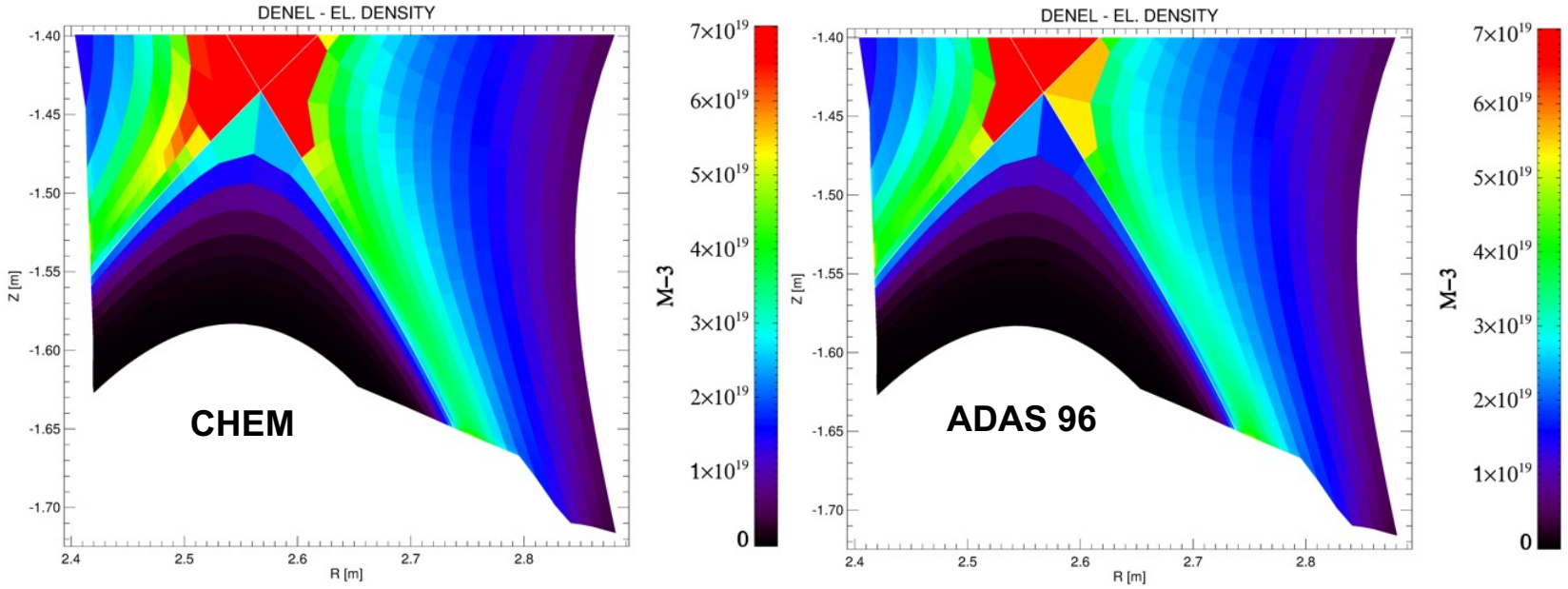
He EDGE2D-EIRENE simulation

- 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.

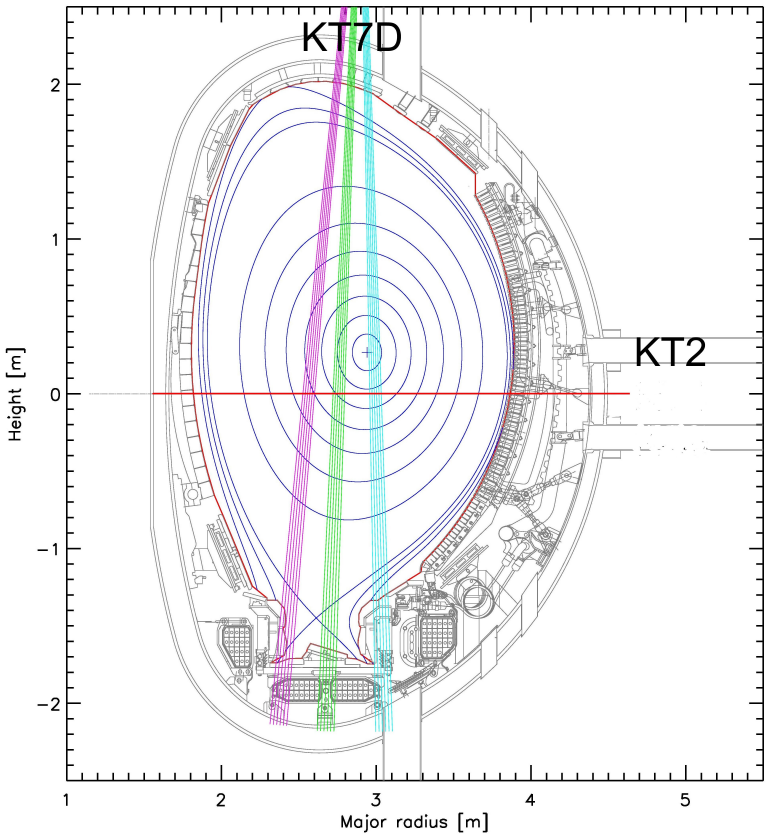


- The simulations are not compared with measurements to date.
- Demonstrates the importance of the atomic physics.
- If the temperature can be lowered further, this will lead to an increase in P_{rad} and may explain the shortfall in the simulated divertor radiation (~30% in He simulations).

He II (and D I) line intensity ratios

- A *preliminary analysis* has not found agreement between measured and theoretical line intensity ratios.
- Not due to sensitivity calibrations – some uncertainty with D but known to ± 10 % in the case of He.
- Does not appear to be due to the errors in the atomic data – necessary to change data very significantly without acceptable agreement being achieved.
- Ratios similar for both vertical LOS into the divertor and along a horizontal midplane LOS.

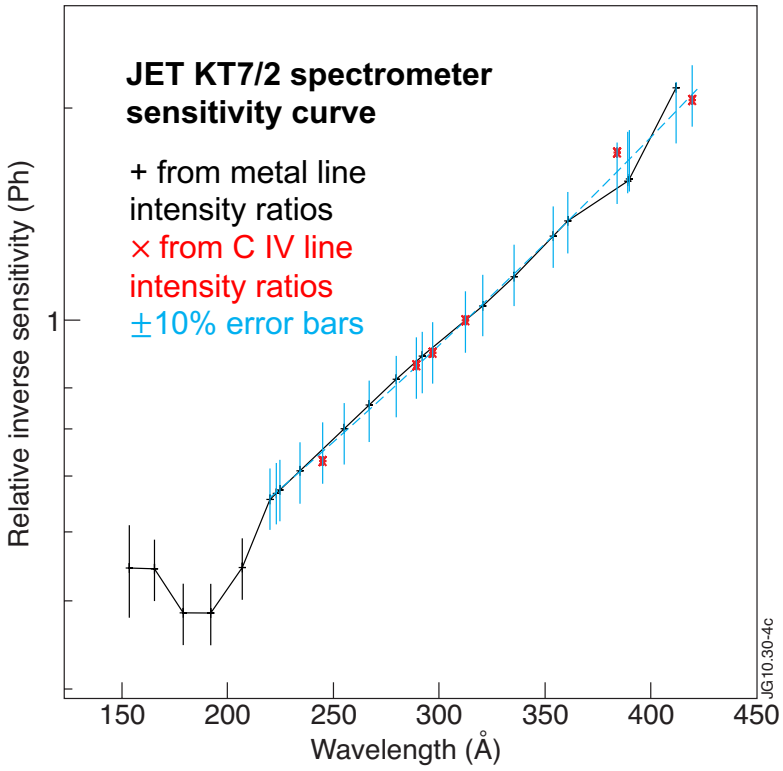
KT7 and KT2 spectrometers



- 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 (used for D).
  - KT7/2 covers 140 Å – 443 Å with a spectral resolution of ~1 Å (used for He II).
  - The highest time resolution is 11ms, although 20–50ms used routinely.
  - Measurements of opacity made using the divertor (green) view.
  - KT2 has a view along the horizontal midplane and observes 100 Å – 1100 Å with a spectral resolution of ~5 Å.

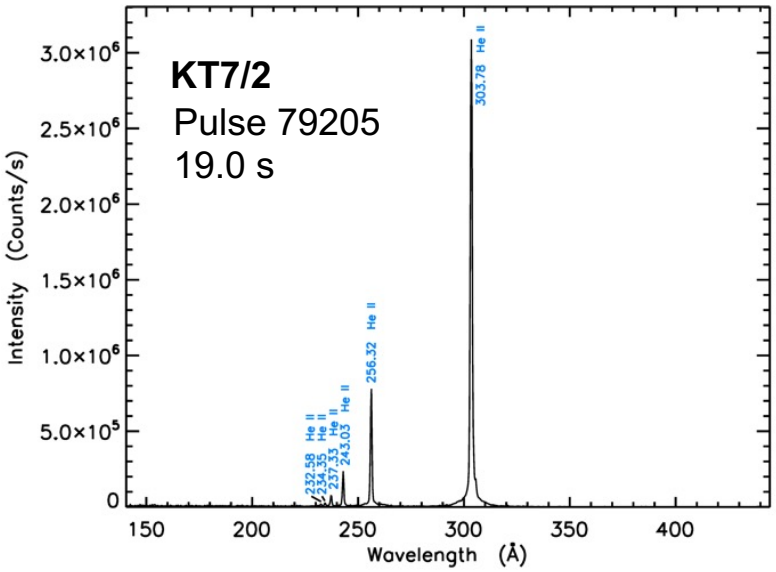
.

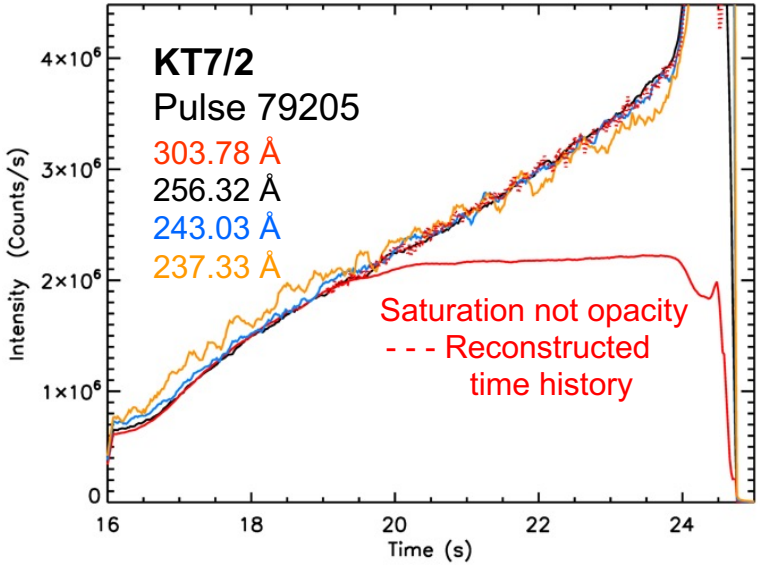
Excellent agreement for C IV



- 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).
- C IV atomic data of Aggarwal and Keenan (2004, Phys. Scr., **69**, 385).
- C IV a simpler system than He II or D I.
- In tokamaks C IV in the low density limit – collisions between excited levels can be neglected (although radiative cascading included).

He II VUV spectrum and line intensity ratios



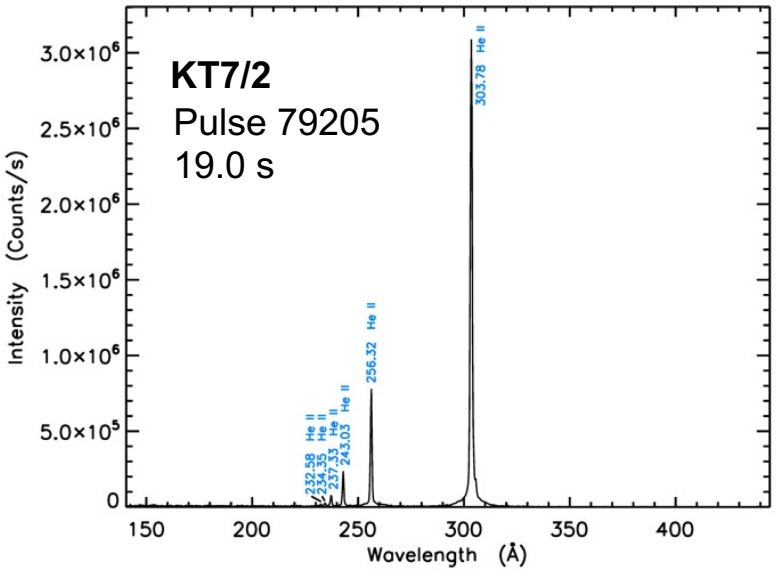


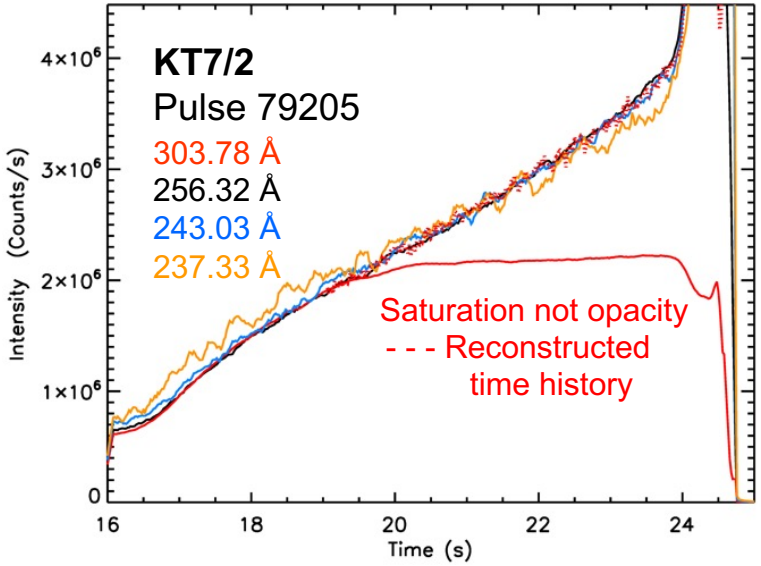
- Pulse 79205 is a 2.3 T / 2.4 MA He fuelled Ohmic density limit pulse run during JET-C.
- No evidence of a T_e dependence in the line ratios.
- Note – no evidence of opacity in He discharges.

Ratio	Measured		Theoretical
	KT7/2	KT2	
256Å/304Å	0.17-0.19	0.15-0.16	0.28/0.38
243Å/304Å	0.044-0.052	0.035	0.16/0.31
237Å/304Å	0.015-0.018	-	0.13/0.19

Theoretical ratios at T_e = 2.2 eV, $n_e = 10^{13} / 10^{14}$ cm^{-3}

He II VUV spectrum and line intensity ratios



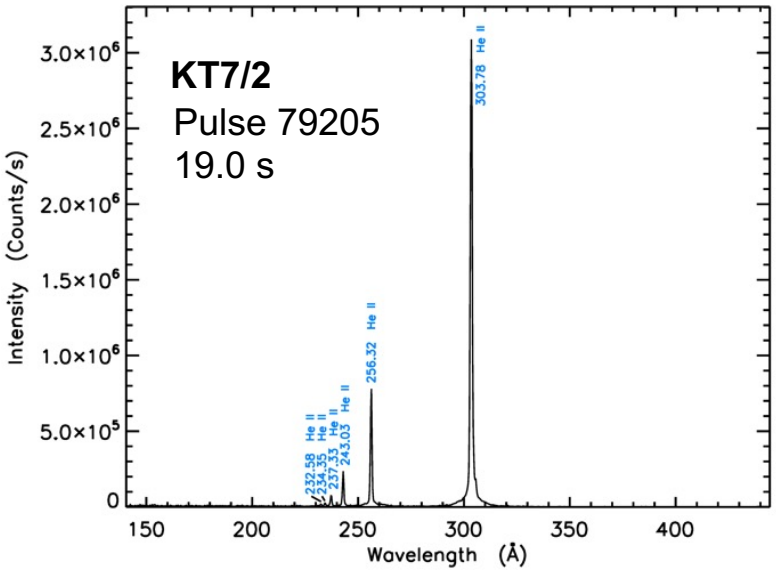


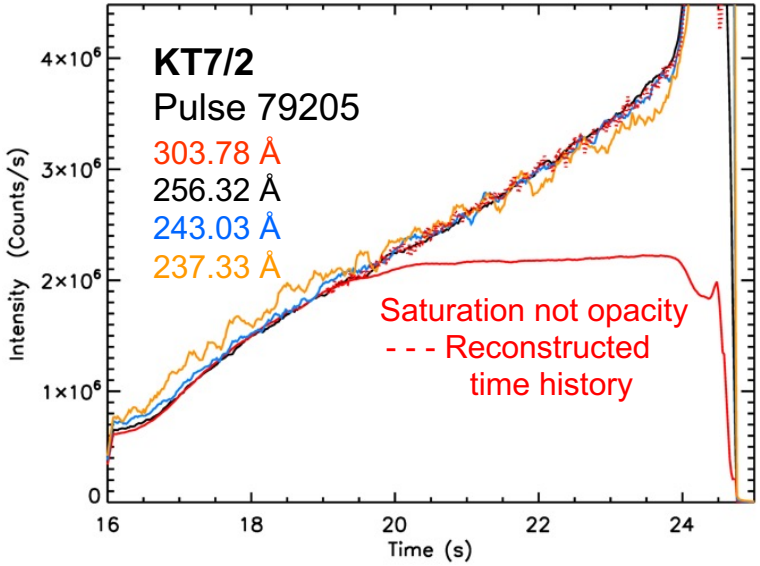
- Pulse 79205 is a 2.3 T / 2.4 MA He fuelled Ohmic density limit pulse run during JET-C.
- No evidence of a T_e dependence in the line ratios.
- Note – no evidence of opacity in He discharges.

Ratio	Measured		Theoretical
	KT7/2	KT2	
256Å/304Å	0.17-0.19	0.15-0.16	0.11/0.13
243Å/304Å	0.044-0.052	0.035	0.047/0.066
237Å/304Å	0.015-0.018	-	0.028/0.036

Theoretical ratios at T_e = 4.4 eV, $n_e = 10^{13} / 10^{14}$ cm^{-3}

He II VUV spectrum and line intensity ratios





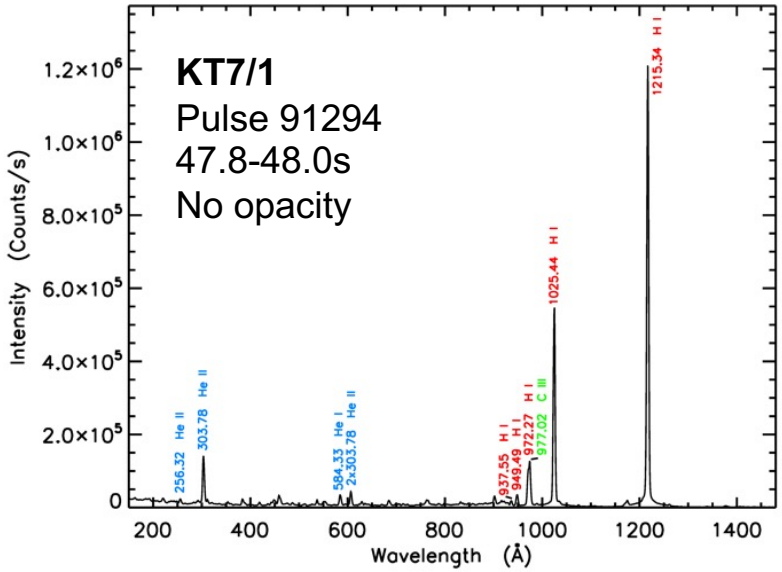
- Pulse 79205 is a 2.3 T / 2.4 MA He fuelled Ohmic density limit pulse run during JET-C.
- No evidence of a T_e dependence in the line ratios.
- Note – no evidence of opacity in He discharges.

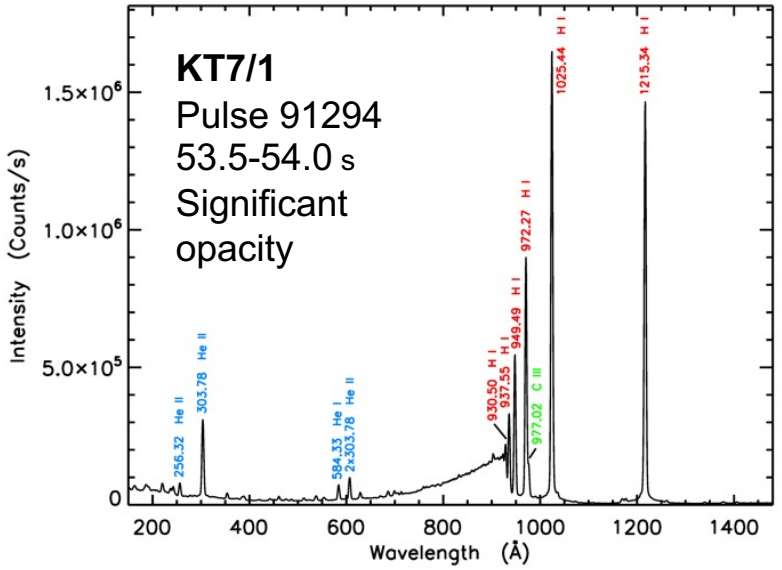
Ratio	Measured		Theoretical
	KT7/2	KT2	
256Å/304Å	0.17-0.19	0.15-0.16	0.082/0.075
243Å/304Å	0.044-0.052	0.035	0.025/0.019
237Å/304Å	0.015-0.018	-	0.012/0.0061

Theoretical ratios at T_e = 8.6 eV, $n_e = 10^{13} / 10^{14}$ cm^{-3}

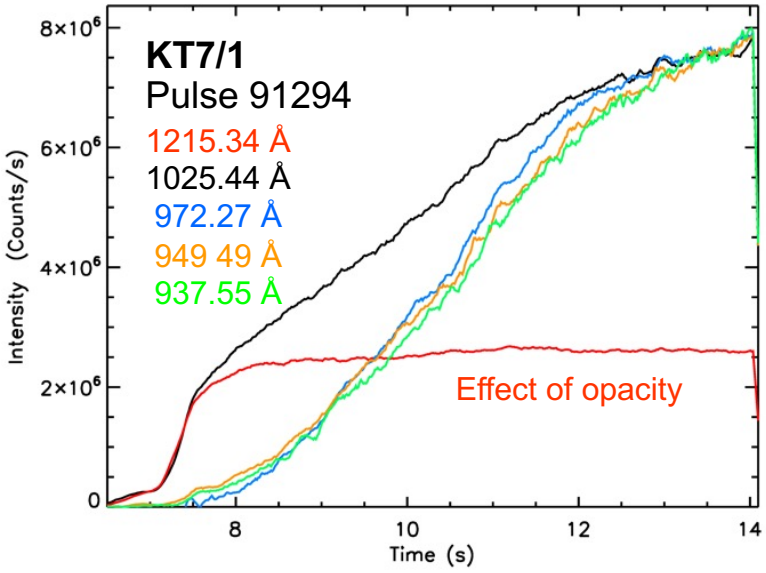
Theoretical ratios temperature and density dependent

H I VUV spectra and measured line intensity ratios





- Pulse 91294 is a H fuelled Ohmic density limit pulse at 2.5 T / 2.4MA.
- Opacity is seen to be important reducing Ly_α by ~55% and Ly_β by ~6%.
- The T_e dependence suggested by all the theoretical intensity ratios is not observed.



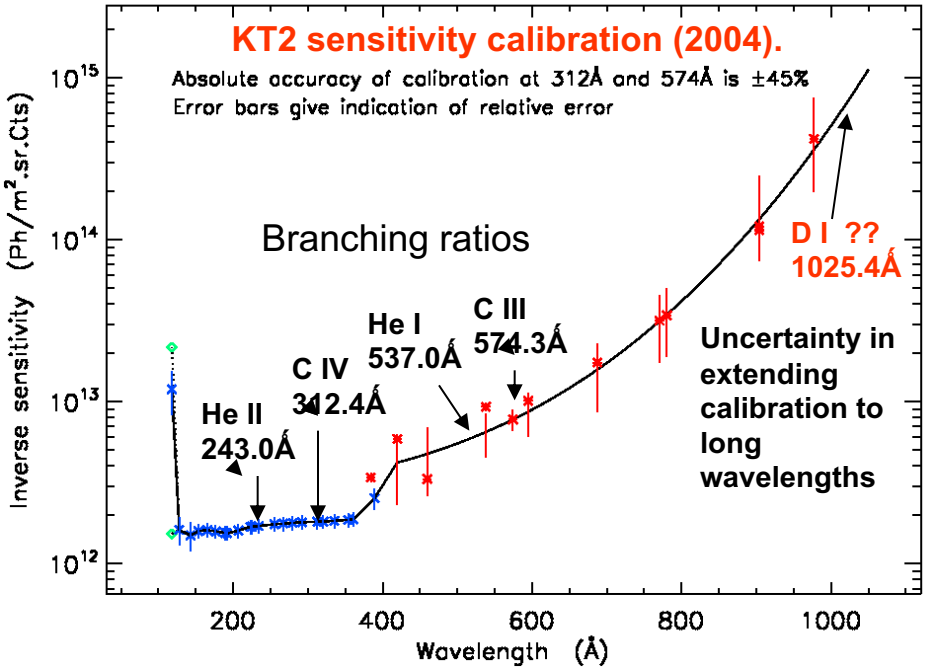
Conclusions

- The CHEM database for hydrogen-like He (He II) has been compiled using the most recent atomic data, paying particular attention to that at the lowest temperatures.
- Data for all significant populating channels is included.
- Heavy particle collisional excitation and ionization data and radiative and three body recombination rate coefficients have been generated for the database.
- A collisional-radiative population model has been generated from these data.
- The population model has provided He II atomic data to EDGE2D-EIRENE He simulations, a comparison being made with simulations in which ADAS atomic data is used.
- The simulations in which the He II data is from the CHEM database achieve lower temperatures than those using only ADAS data, demonstrating the importance of atomic data in determining the simulated temperatures.
- To date measured He II (and H I / D I) line ratios have not been explained by any of the theoretical models.

Back-up slides

KT2 sensitivity calibrations

- VUV sensitivity calibrations consist of a relative calibration with wavelength and an absolute calibration to fix the level of the relative calibration. The absolute calibration can be obtained using branching ratios from calibrated visible spectra.



A new analysis involving recently compiled C III and N IV atomic datasets suggest ~x10 lower S^{-1} at the longest wavelengths. These datasets produced in the previous 'Call for Analysis'

C III :- K M Aggarwal and F P Keenan, 2015, MNRAS, 450, 1151

N IV :- K M Aggarwal *et al.*, 2016, MNRAS, 461, 3997

1025.4Å / 6561.0Å D I 'branching ratio' crucial for fixing the long wavelengths

A branching ratio is a ratio of transitions with the same upper electronic state or level. The intensity ratio is given by the transition probabilities, $I_{ij} / I_{kj} = A_{ij} / A_{kj}$ – no population modelling is required and independent of T_e.

Collisional-Radiative Model (1)

Collisional-Radiative Model for hydrogen-like species

K.D. Lawson

The collisional-radiative model used for hydrogen-like species uses a set of rate equations, which for the rate of change of the population of the *i*th level is

$$\frac{dn_i}{dt} = -\left(n_e \sum_{j\neq i} q_{ij} + \sum_{j<i} A_{ij} + n_e s_i\right) n_i + \left(n_e \sum_{j\neq i} q_{ji} + \sum_{j>i} A_{ji}\right) n_j + n_e\left(\alpha_i^r + n_e \alpha_i^{3b}\right) n^+$$

where n_e, n_i, n_j and n^+ are the electron density, those of the *i*th and *j*th levels and the fully stripped ions, q and s are the collisional excitation and direct collisional ionization rate coefficients, A the Einstein spontaneous transition probability and α^{rr} and α^{3b} the radiative and three-body recombination rate coefficients.

The set of equations can be written in matrix form as

$$\begin{pmatrix} \dot{n}_g \\ \vdots \\ \dot{n}_i \\ \vdots \\ \dot{n}_j \end{pmatrix} = \begin{pmatrix} -C_g & \cdots & C_{ig} & \cdots & C_{jg} \\ \vdots & & \vdots & & \vdots \\ C_{gi} & \cdots & -C_i & \cdots & C_{ji} \\ \vdots & & \vdots & & \vdots \\ C_{gj} & \cdots & C_{ij} & \cdots & -C_j \end{pmatrix} \begin{pmatrix} n_g \\ \vdots \\ n_i \\ \vdots \\ n_j \end{pmatrix} + \begin{pmatrix} \alpha_g \\ \vdots \\ \alpha_i \\ \vdots \\ \alpha_j \end{pmatrix} n^+,$$

where g and + represent the ground and fully ionized states. c_i is the loss of population from the *i*th level

$$c_i = n_e \sum_{j\neq i} q_{ij} + \sum_{j<i} A_{ij} + n_e s_i$$

and c_{ji} includes populating channels from level j to level i. If j > i

$$c_{ji} = n_e \sum_{j\neq i} q_{ji} + \sum_{j>i} A_{ji}$$

and if j < i

$$c_{ji} = n_e \sum_{j\neq i} q_{ji}$$

In the recombination term

$$\alpha_i = n_e\left(\alpha_i^{rr} + n_e \alpha_i^{3b}\right).$$

Collisional-Radiative Model (II)

Excited level populations within the ion reach equilibrium on a much faster time scale than changes in the ionization balance and hence

$$\dot{n}_i = 0.$$

Rewriting as

$$\begin{pmatrix} \dot{n}_g \\ 0 \end{pmatrix} = \begin{pmatrix} M_g & M_{Qg} \\ M_{gQ} & M_Q \end{pmatrix} \begin{pmatrix} n_g \\ n_Q \end{pmatrix} + \begin{pmatrix} R_g \\ R_Q \end{pmatrix} n^+,$$

where

$$M_g = -c_g, \qquad M_{Qg} = \left(c_{ig} + \cdots + c_{jg}\right), \qquad R_g = \alpha_g,$$

and

$$M_{gQ} = \begin{pmatrix} c_{gi} \\ \vdots \\ c_{gj} \end{pmatrix}, \qquad M_Q = \begin{pmatrix} -c_i + \cdots + c_{ji} & \vdots \\ \vdots & \\ c_{ij} + \cdots - c_j & \end{pmatrix}, \qquad n_Q = \begin{pmatrix} n_i \\ \vdots \\ n_j \end{pmatrix}, \qquad R_Q = \begin{pmatrix} \alpha_i \\ \vdots \\ \alpha_j \end{pmatrix}.$$

Therefore,

$$n_Q = \frac{-1}{M_Q}\left(M_{gQ} n_g + R_Q n^+\right)$$

and

$$\dot{n}_g = \left(M_g - M_{Qg} M_Q^{-1} M_{gQ}\right) n_g + \left(R_g - M_{Qg} M_Q^{-1} R_Q\right) n^+.$$

Defining the effective ionization and recombination coefficients, S_{eff} and R_{eff}, respectively, by

$$\dot{n}_g = S_{eff} n_g + R_{eff} n^+$$

it follows that

$$S_{eff} = M_g - M_{Qg} M_Q^{-1} M_{gQ} \qquad R_{eff} = R_g - M_{Qg} M_Q^{-1} R_Q.$$