EUROfusion

Lyman alpha discrepancy

Kerry Lawson **IAEA Technical Meeting**
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JET

Acknowledgements

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**See author list of J. Mailloux et al., 2021, Nuclear Fusion Special issue, 28th Fusion Energy Conf. (Nice, France, May, 2021)*

Particular thanks for discussions with Ursel Fantz and Stefan Briefi

Motivation

- To explain discrepancies between the JET D I and He II (He^+) Lyman series measurements and the Collisional-Radiative (CR) models describing their line intensities.
- To document pulses in which the Lyman line intensities ratios are observed to be near constant.

- It has been useful to describe the behaviour of data from a large number of pulses.

Background

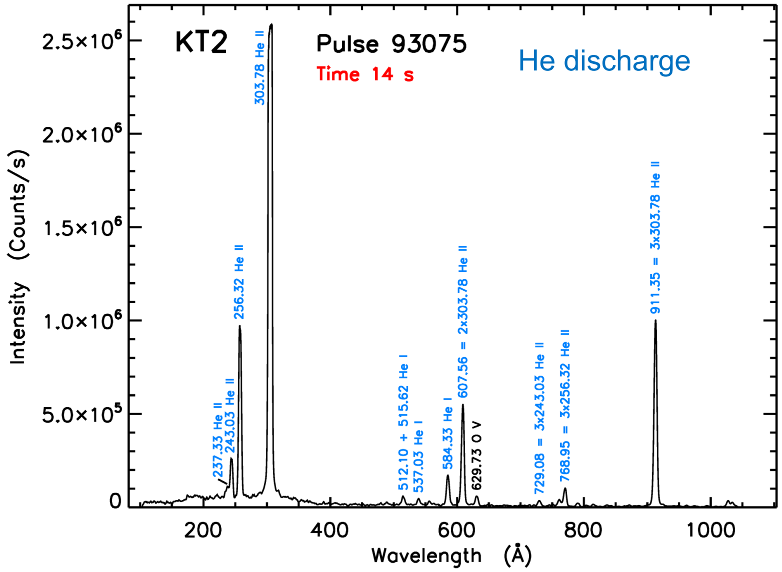
- Discrete spectral lines belonging to the Lyman series account for nearly all of the radiated power from the hydrogen-like D I and He II (He^+) ionization stages.
- For many analyses an understanding of the behaviour of the D or He fuel is essential.
- This is crucial for edge and divertor transport modelling used to predict plasma exhaust, surface erosion, etc.
- The Lyman series line intensities are described by well-established CR population models.
- Most JET observations of D I and He II cannot be explained by these CR population models.
- To gain understanding, measurements of Lyman series line intensities have been recorded and analysed.
- The most detailed study to date has been carried out for He II, although many features are common to both He and D.
- The He analysis is now being applied to a study of D discharges.
- Some observations of D line ratios have led to a rejection of the opacity model as an explanation of the Lyman alpha discrepancies.
- Nevertheless, the analysis has led to a much better understanding of the occurrence of opacity.

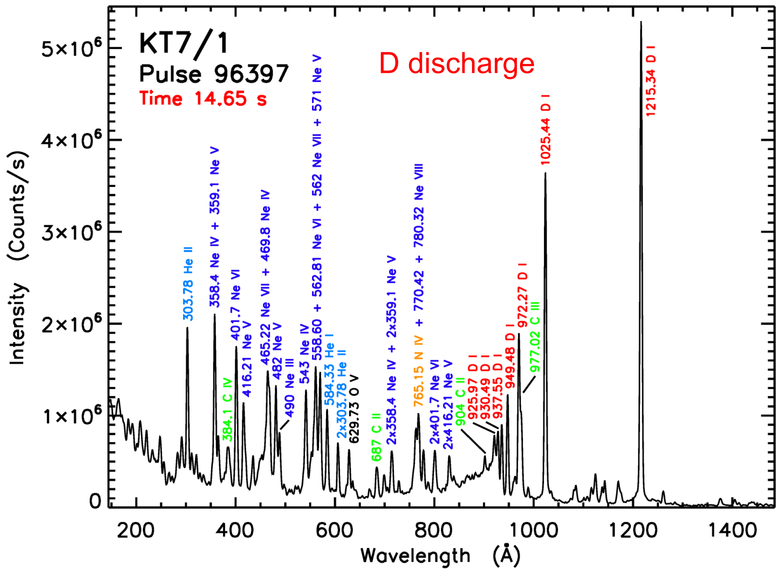
Overview

- JET measurements of He II Lyman series line intensities
  - He II (He$^+$) or D I ?
  - Brief outline of the JET observations - described in reports.
- Comparisons of measurements with Collisional-Radiative (CR) models
  - Stringent test of models.
  - Lyman alpha/beta discrepancy.
  - Discrepancy explained by opacity?
  - Opacity in He and D discharges.
  - Discrepancy explained by transient effects.
- Conclusions and further work

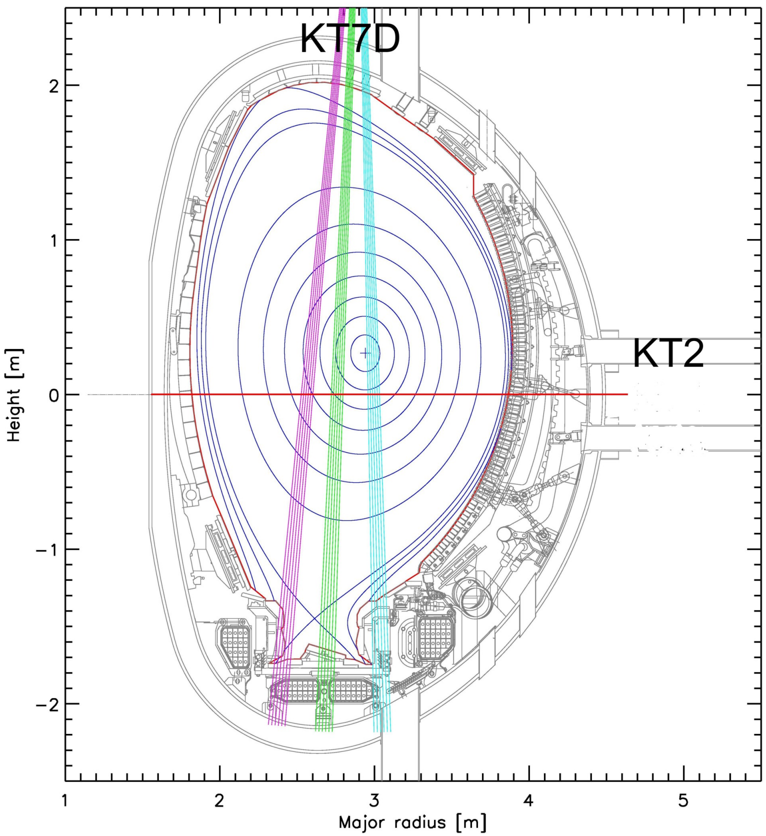
He II (He$^+$) versus D I?

- An understanding of both He II and D I models is required.
- Their atomic physics is similar so a study of either will contribute to an understanding of the other.
- He II (He$^+$) has advantages – simpler spectrum, accurate spectrometer calibration (relative ±10%), no molecular contributions, opacity effects expected to be smaller.
- Consequently, to date, most work has involved He II, with the study forming the basis of a study of D, which is in progress.





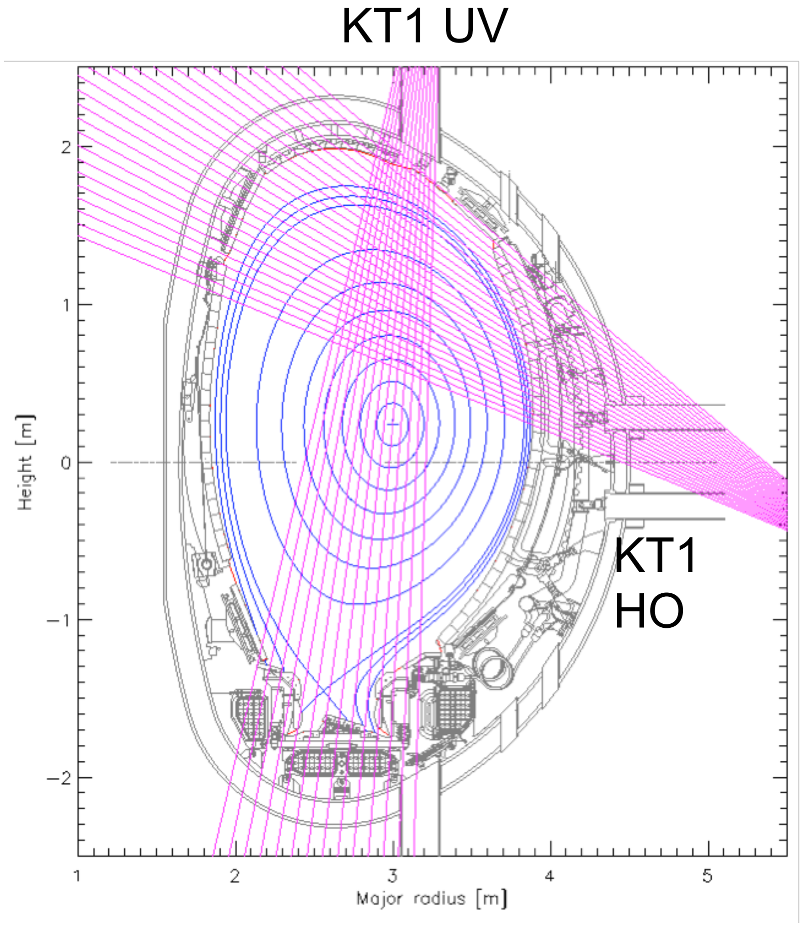
KT7 and KT2 spectrometers



SPRED :- Fonck *et al*., 1982, Appl. Opt., **21**, 2115

- The KT7 and KT2 spectrometers use SPRED instruments.
  - KT7 has a vertical line-of-sight, which can be varied. It has 3 detectors, results from the 2 SPRED instruments being used.
  - KT7/1 covers 157Å – 1500Å with a spectral resolution of ~5Å (used for D).
  - KT7/2 covers 140Å – 443Å with a spectral resolution of ~1Å (used for He II).
  - KT2 has a fixed horizontal line-of-sight along the vessel midplane.
  - KT2 covers 110Å – 1100Å with a spectral resolution of ~5Å (used for He II and D I).
  - The highest time resolution is 11ms, although 20–50ms used routinely.

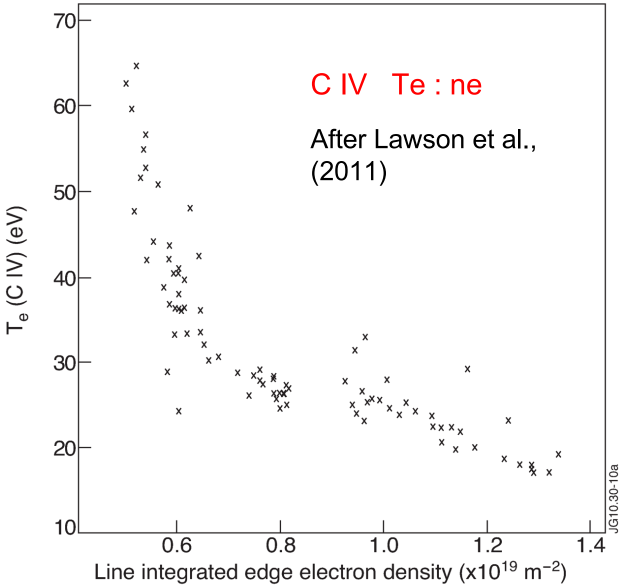
KT1 spectrometers

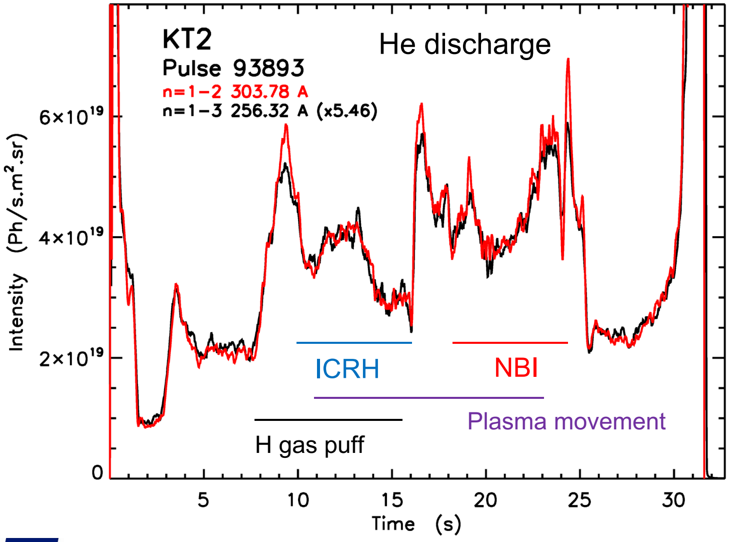


KT1 :- Lawson *et al*. 2012, RSI, **83**, 10D536

- The poloidally scanning KT1 spectrometers have both visible and VUV channels with a LOS across the divertor (KT1 UV) and along the upper inner wall (KT1 HO).
  - They are situated in the same toroidal location as KT7 and KT2 (Octant 6).
  - The scan is achieved using a small plane oscillating mirror outside the torus vacuum.
  - The visible KT1 collects light from close to the oscillating mirror and transmits this using optical fibers to spectrometers outside the biological shield.
  - The visible system is calibrated using an in-vessel calibration light source.
  - The VUV systems observe only 2 lines, one at short and one at long wavelengths.

What is expected?





- **Expect that the widely used existing CR models accurately describe the observations.**
- **However, no stringent test of either the D I or He II CR models found for JET plasmas.**
- Expect D I and He II to behave like impurities – in particular, a wide range of temperatures possible.
- Lyman series line intensities and intensity ratios are temperature dependent.
- However, found that Lyman series line intensity ratios are often near-constant, suggesting that the temperatures of the emission regions are similar.
- In the JET He pulse 93893 there are intensity changes due to gas puffing, NBI and ICRH additional heating and plasma position!

C IV : - Lawson *et al.*, 2011, PPCF, **53**, 015002

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What do we actually observe for He?

- Full details in reports by Lawson *et al.,* 2022, ‘He II Lyman series line intensity measurements in the JET tokamak’ and Lawson *et al.,* 2023 ‘He II VUV and visible line intensity measurements in the JET tokamak’. (On JET and CCFE pinboards)
- Data from 3 VUV spectrometers analysed, survey instruments KT7 and KT2 and the scanning spectrometer KT1.
- Lines-of-sight into the divertor, across the divertor, towards the divertor throat and a horizontal view through the core plasma.
- All pulse surveys carried out.
- Dependence of line intensity ratios on Lyman series spectral line intensities illustrated.
- Time histories of both equilibrium and non-equilibrium discharge phases presented.
- Data from 3 campaigns analysed
  - 1) JET-C, C27b He campaign, pulses 78907-79243, wide range of plasma parameters.
  - 2) JET-ILW, C38 He restart, pulses 93023-93089, limited range of parameters – no additional heating.
  - 3) JET-ILW, C38 He experiment, pulses 93847-93908, both NBI and ICRH used.

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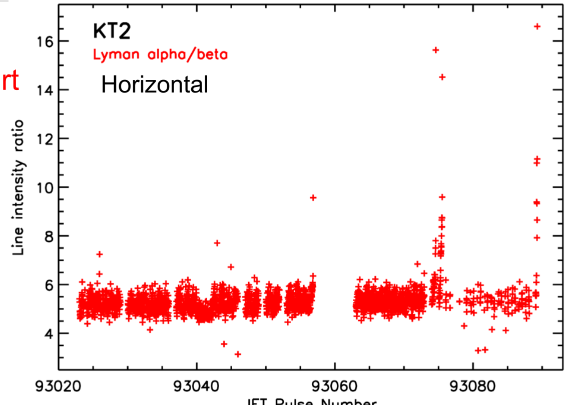
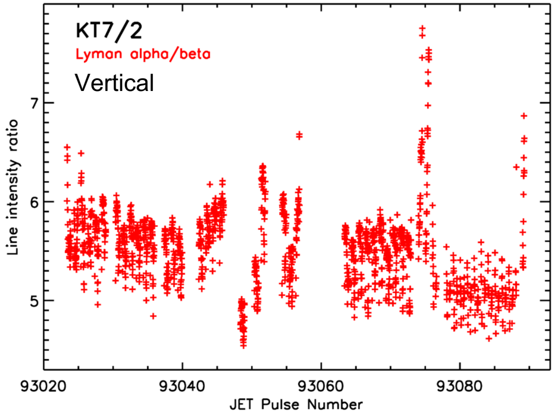
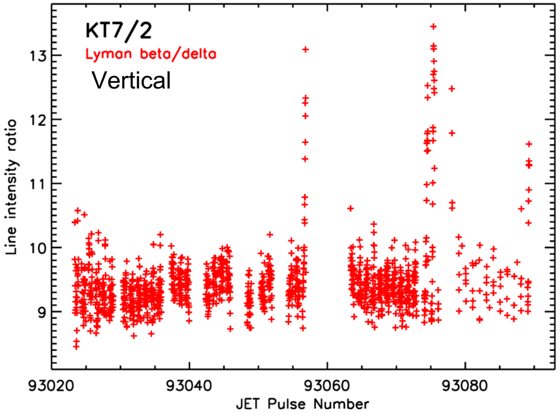
All pulse surveys for He (D more complicated!)

C38 He restart

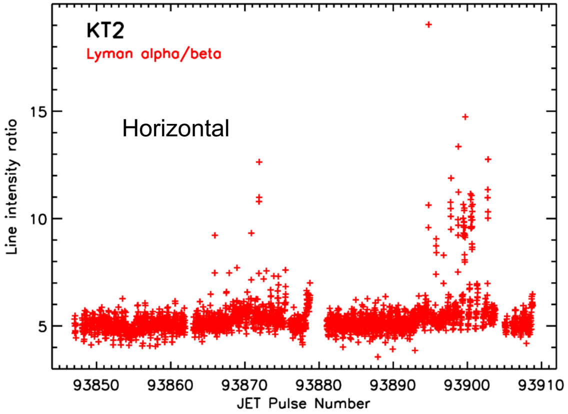






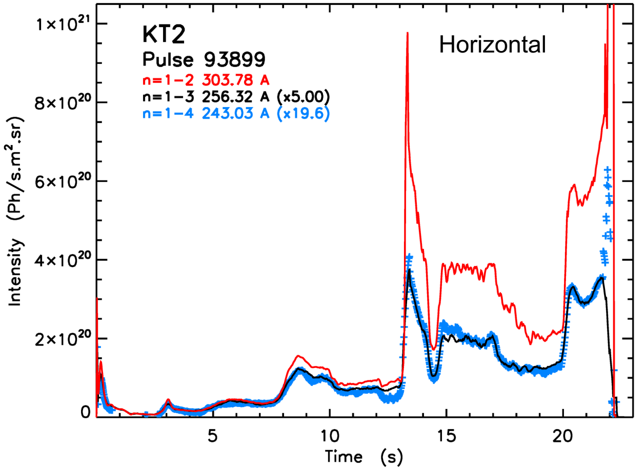
- **Temperature dependent** Lyman series line intensity ratios shown.
- Each point represents data averaged over 0.5s.
- For the equilibrium discharge phases, both horizontal and vertical LOS have similar ratios.
- ***NOT a feature of the divertor LOS.***
- Some excursions from the near-constant ratios – non-equilibrium phase.

C38 He experiment



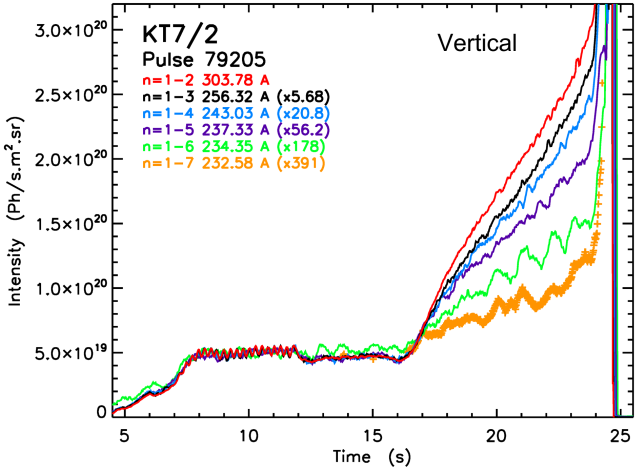
Intensity time histories (He) – non-equilibrium

JET-ILW C38 experiment

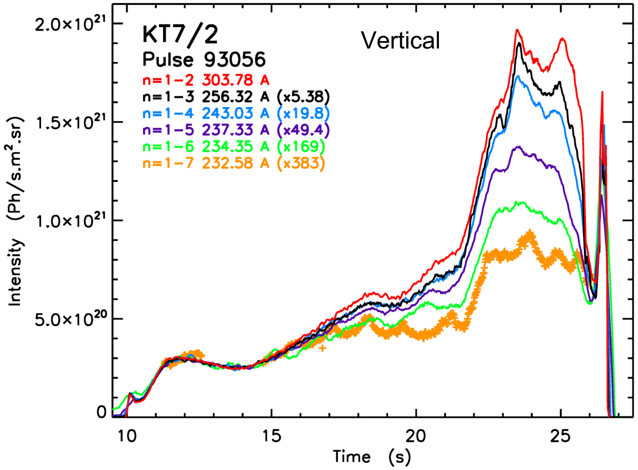


- During the non-equilibrium phases the Lyman series intensity ratios tend to increase.
- The higher spectral resolution of KT7/2 allows lines up to Lyman zeta (n=1-7) to be seen.
- The Lyman gamma intensity (KT2) and the Lyman zeta intensity (KT7/2) are obtained by line profile fitting.

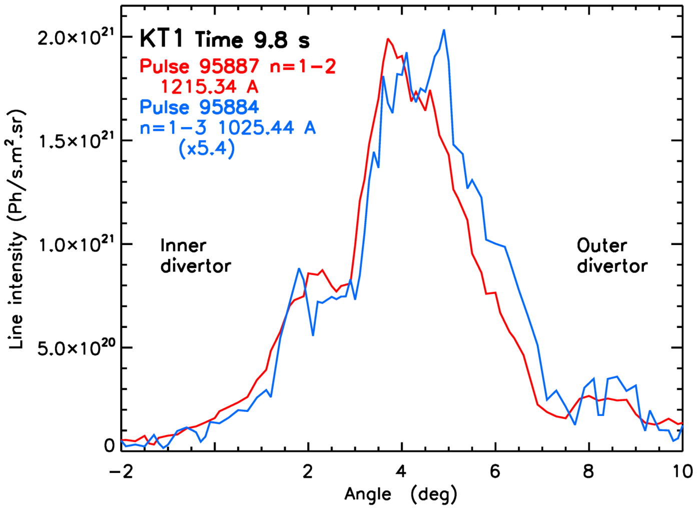
JET-C C27b campaign

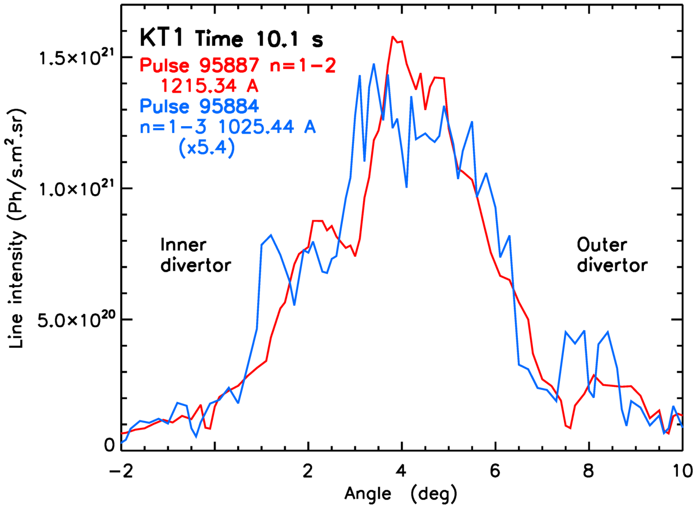


JET-ILW C38 restart



D I example from KT1 - equilibrium





- The near-constant Lyman series ratios first observed for D I.
- Pulse 95884 and 95887 are similar D fuelled L-mode discharges.
- Poloidal scans of emission across the divertor of the Lyman alpha and Lyman beta intensities overlay showing that their ratio is approximately constant.

- **SUMMARY**
- **He II Lyman line intensity ratios for the equilibrium discharge phases are near-constant and do not depend on the line-of-sight or observing spectrometer.**
- **This suggests localized regions of emission having the same electron temperature.**
- **D I ratios show a similar behaviour within a pulse, but greater differences between dissimilar pulses.**
- **Confirmation that when higher series (Balmer or Paschen) lines seen the VUV Lyman series line is observed.**

Comparisons with Collisional-Radiative models

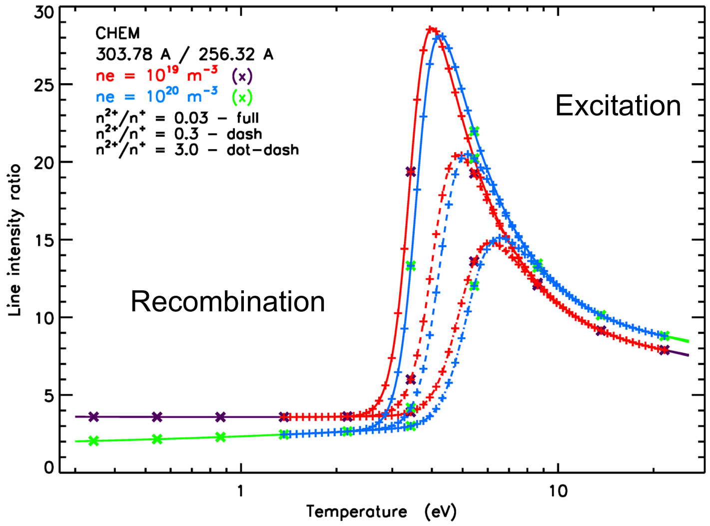
- The JET observations allow a stringent test of the CR models.
- The CHEM (Culham He Model, Lawson *et al.*, 2019, J. Phys. B, **52**, 045001) and ADAS CR models are used.
- In the VUV, relative sensitivity calibrations are known more accurately (for He II lines to within $\pm 10\%$) than absolute sensitivity calibrations.
- Hence, line intensity ratios used.
- The IDL CONSTRAINED_MIN routine minimizes the sum of the squared modelled – measured fractional differences,

$$\sum_i w_i \left(\frac{R_{mod,i} - R_{meas,i}}{R_{meas,i}} \right)^2 ,$$

where $R_{mod,i}$ is the modelled intensity ratio for the ith ratio and $R_{meas,i}$ the corresponding measured ratio, with w_i a weighting for the ith ratio to account for the differences in accuracy of the measurements.

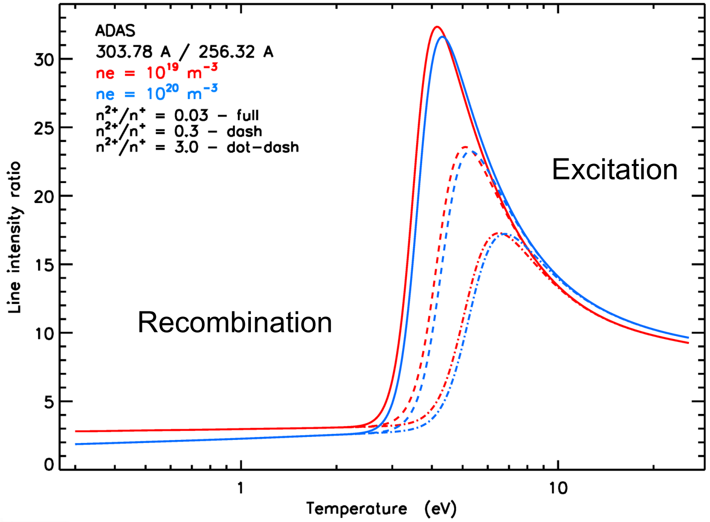
Line intensity ratios (He II)

Lyman alpha / beta - CHEM

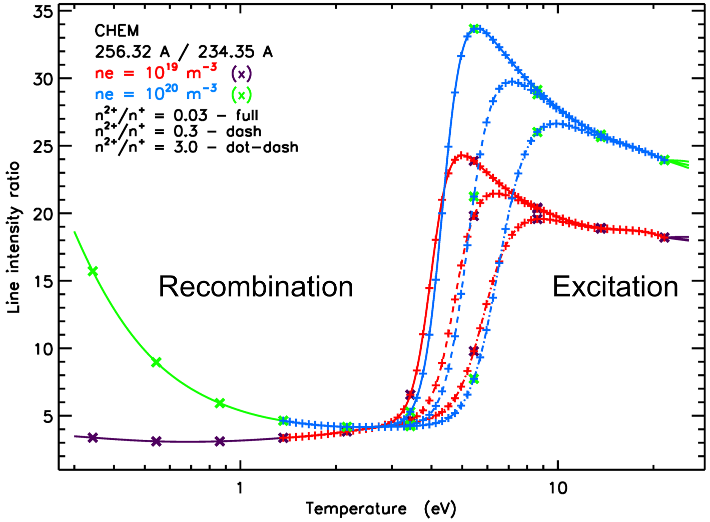


- ADAS and CHEM line intensity ratios similar.
- At high temperatures (>9 eV) populations driven by excitation from the ground state.
- At low temperatures (<2 eV) populations result from recombination.
- In between is a transition region where both excitation and recombination are important.

Lyman alpha / beta - ADAS



Lyman beta / epsilon - CHEM



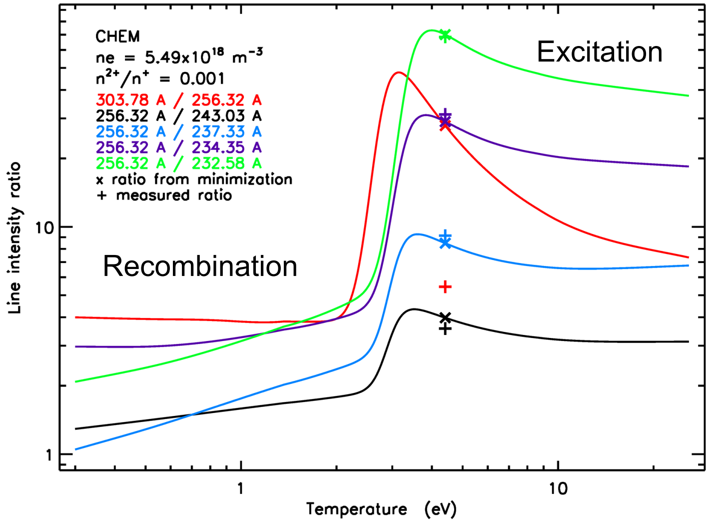
Lyman alpha discrepancy (He II)

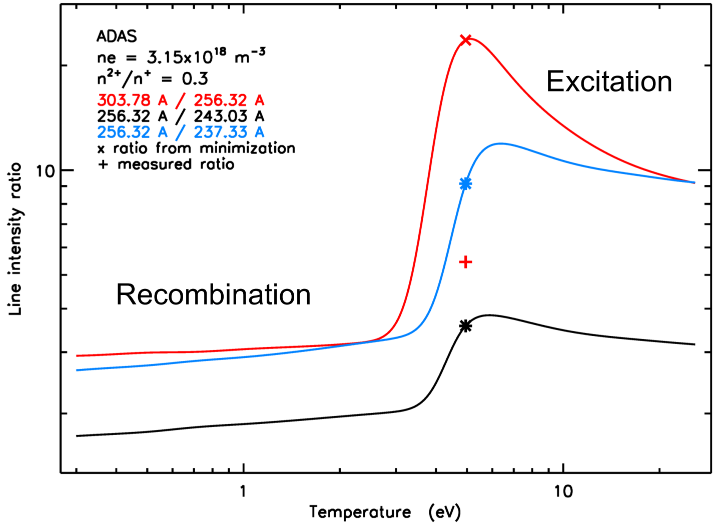
- T_e, $\mathrm{Log}_{10} n_e$ and n^{2+} / n^{+} are varied in the minimization.
- Including the Lyman alpha intensity gives poor agreement.
- The measured Lyman alpha intensity is × 3-5 smaller than predicted!
- Ratios taken with the Lyman beta line.

Parameter	**Initial value**	**Upper and lower bounds (measured)**	**Including alpha/beta**		**Excluding alpha/beta**	
			CHEM	ADAS	CHEM	ADAS
T_e (eV)	4.0	0.2-25.0	4.01	4.25	4.41	4.95
$\mathrm{Log}_{10}(n_e)$ (m^{-3})	19.0	18.0-21.0	18.0	18.0	18.74	18.50
n^{2+}/n^{+} ratio	0.1	0.001-3.0	3.0	3.0	0.001	(0.3)*
Alpha / beta		(5.45)	6.14	5.85	27.9	23.6
Beta / gamma		(3.57)	2.26	2.21	3.98	3.57
Beta / delta		(9.15)	3.64	3.85	8.47	9.15
Beta / epsilon		(31.2)	5.37	-	29.0	-
Beta / zeta		(68.4)	7.68	-	70.1	-
RMS fractional difference			0.56	0.39	0.075	0.001

*In the ADAS case in which the Lyman alpha to beta ratio is excluded the n^{2+}/n^{+} ratio is fixed.

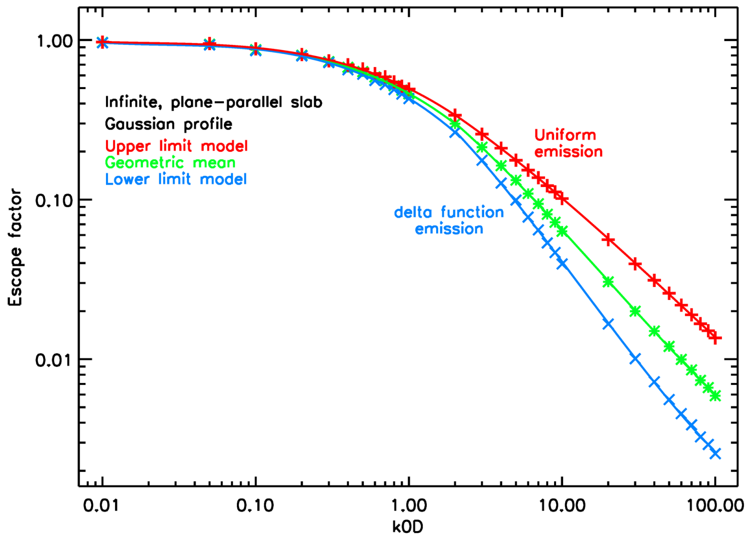
Lyman alpha discrepancy (He II)


Lyman line intensity ratios - CHEM


Lyman line intensity ratios - ADAS

- Measured and modelled data on curves of line intensity ratios for minimizations *excluding* Lyman alpha/beta ratio.
- Measured ratios close to the peaks of the ratios.
- Measured Lyman alpha / beta ratio (+) low!

Inclusion of opacity in CR models



After Figure 1 of F E Irons (1979)

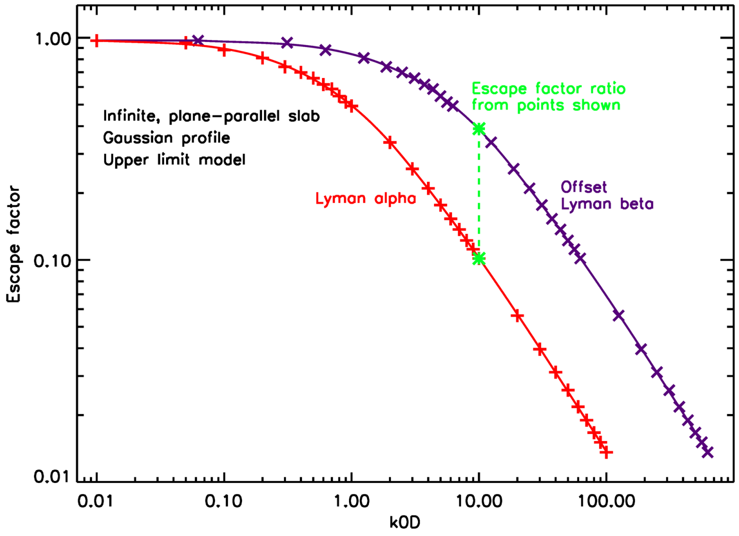
k0 Is the absorption coefficient, D distance

$$k_0 = \frac{\lambda_0^3 n^+ \, g_2 \, A}{8\pi^{3/2} g_1 \, v}$$

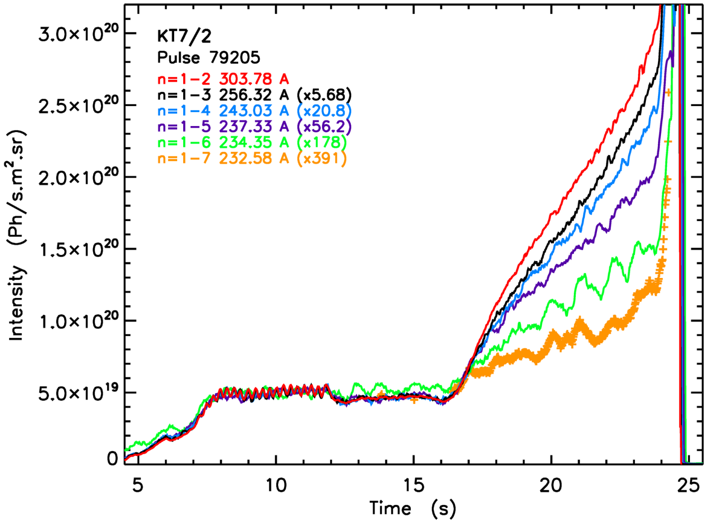
$$\text{where the velocity is } v = \left(\frac{2kT_e}{m}\right)^{1/2}$$

Lyman beta escape factor curve offset by ratio of absorption coefficients, x6.236

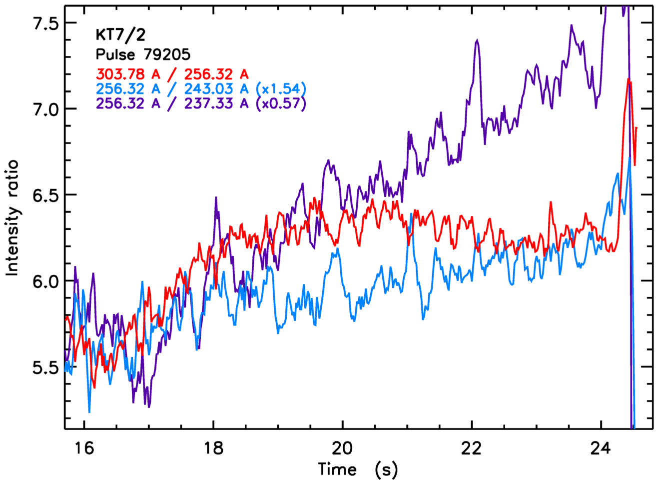
- Opacity included in CR models using escape factors summarized by Irons (1979, J. Quant. Spectrosc. Radiat. Transfer, **22**, 1).
- The escape factor is the reduction in the transition probability (A-value) to account for the self-absorption of radiation.
- The opacity model used is for an infinite, plane-parallel slab, with a Gaussian spectral line profile.
- Matches well the use of line intensity ratios, since the *ratio of absorption coefficients* is independent of T_e and n_e.
- This allows the ratio of the escape factors for the Lyman series ratios to be determined and included in the CR model.

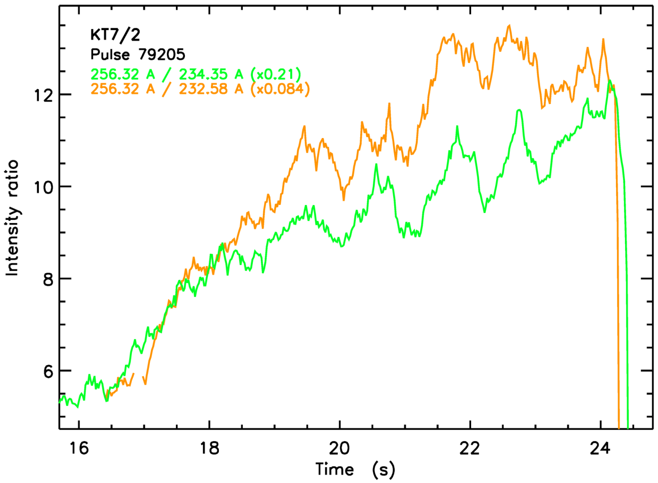


Use of opacity to explain He II Lyman alpha discrepancy

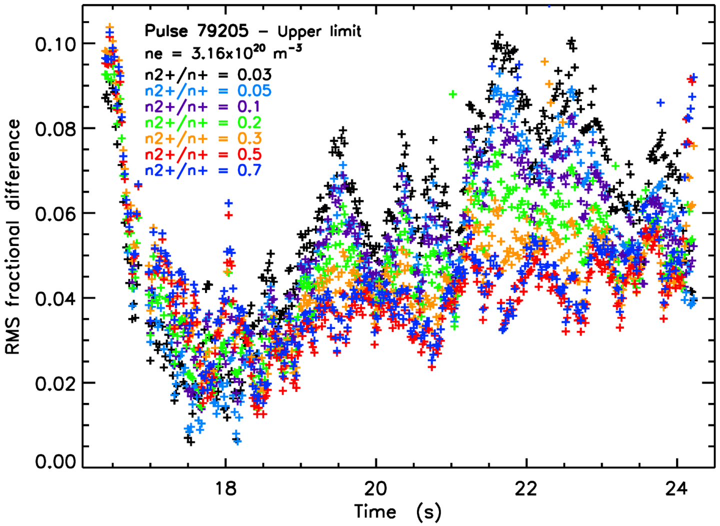


- Pulse 79205 used as example:- Ohmic 2.3 T, 2.4 MA density limit pulse from the JET-C C27b He campaign.
- The lowest 6 Lyman series members are reliably measured in this pulse, the Lyman zeta (*n*=1-7) line by line profile fitting.
- Details given in report Lawson *et al.*, 2023 ‘Comparison between He II Lyman series line intensity measurements in the JET tokamak and collisional-radiative models’.

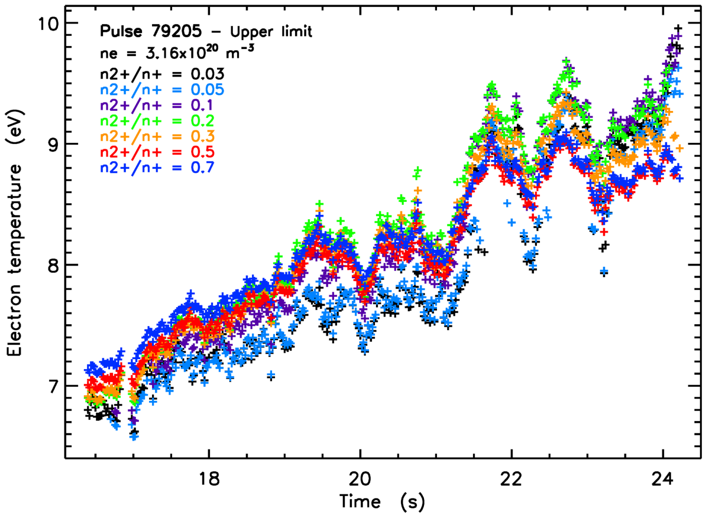


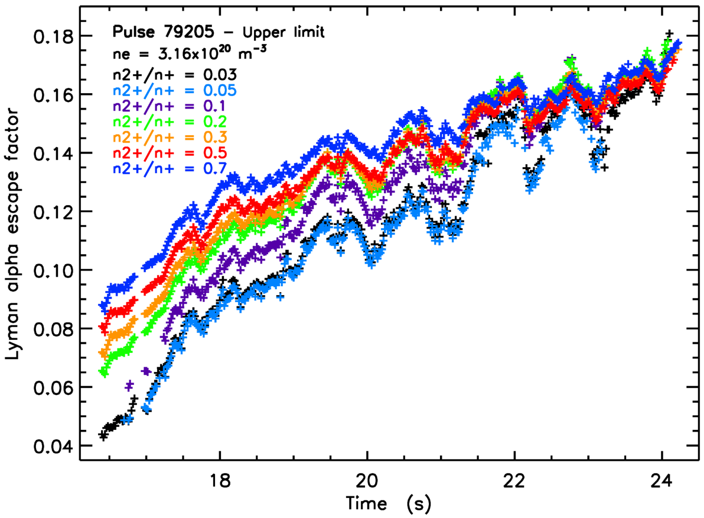


Use of opacity to explain He II Lyman alpha discrepancy



- The Lyman alpha escape factor is ~0.1!!





Use of opacity to explain He II Lyman alpha discrepancy

- The same explanation of the Lyman alpha discrepancy is required for D I and He II.
- In searching the JET database, agreement has been found for a few *high density*, JET-ILW D pulses along a view towards the divertor throat.
- The latest KT7/1 relative calibration is used with a correction for a line intensity affected by a blend with a third order C IV line.
- **Using opacity to explain the discrepancy is not consistent with D I observations.**

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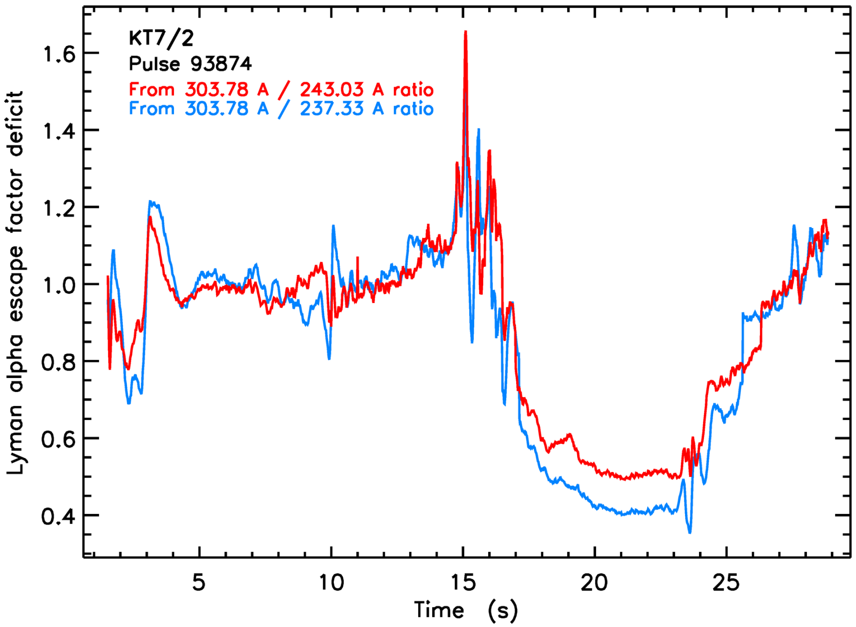
Opacity in He discharges

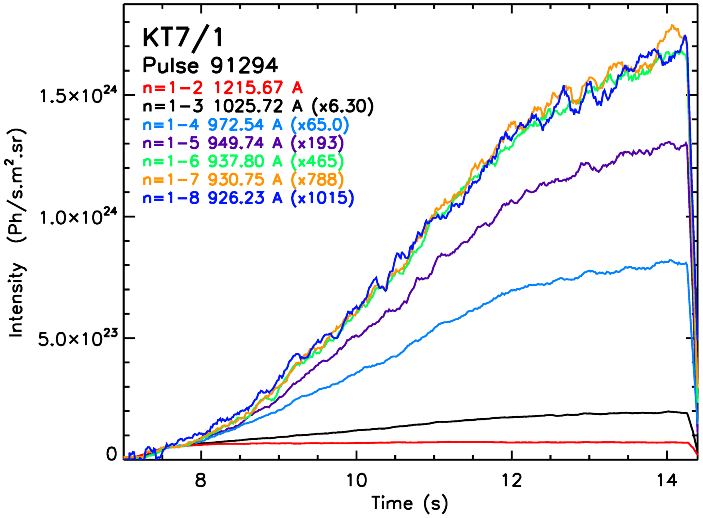
- Analysis of He II pulses has led to an understanding of opacity in JET He discharges.
- Relatively few He pulses affected by opacity.
- Pulse 93874 studied the L-H mode transition in He and shows significant opacity after 15s.
- The treatment of opacity in He discharges would not appear to be a priority, only occurring in a limited number of extreme cases with very intense He emission.

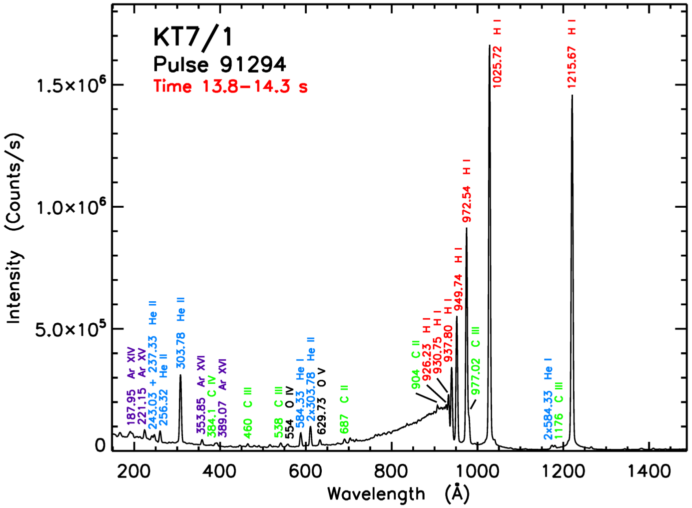


He Campaign	Pulses	No. of plasma pulses	No. of pulses with significant opacity	No. of pulses with marginal opacity
JET-C C27b	78907-79243	244	11 (4.5%)	17 (7.0%)
JET-ILW C38 restart	93023-93089	54	-	1 (1.9%)
JET-ILW C38 experiment	93847-93908	59	9 (15.3%)	9 (15.3%)

The escape factor is the reduction in the transition probability (A-value) to account for the self-absorption of radiation. (Irons, 1979, J. Quant. Spectrosc. Radiat. Transfer, **22**, 1).

Opacity in H / D discharges





- In contrast, opacity is more important in hydrogenic discharges.
- Pulse 91294 is a 2.5 T, 2.4 MA, Ohmic density limit pulse with H fuel reaching a maximum density of 1.1×10^{20} m^{-3}.
- The *n*=1-6, 1-7 and 1-8 Lyman lines overlay.
- Based on the analysis of He II and other H and D pulses, it is expected that the *n*=1-2, 1-3, 1-4 and 1-5 lines should follow the same trajectory as the *n*=1-6, 1-7 and 1-8 lines.
- The shortfall in the *n*=1-2, 1-3, 1-4 and 1-5 line intensities appears mainly due to opacity.
- **It is essential that photon transport is included in H / D transport simulations (Groth *et al.*).**

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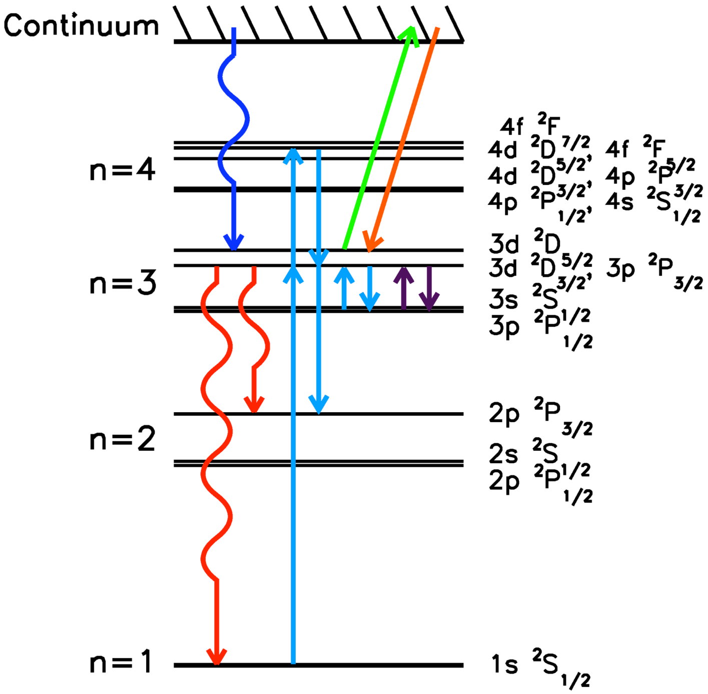
D I and He II Collisional-Radiative (CR) models



The CHEM CR model includes the main populating channels in a hydrogen-like species, **H** :-

1. Electron collisional excitation and deexcitation

   $e + H \leftrightarrow H^* + e$

2. Heavy particle collisional excitation and deexcitation

   $d\ (p,t,\alpha) + H \leftrightarrow H^* + d\ (p,t,\alpha)$

3. Radiative decay

   $H^* \rightarrow H + h\nu$

4. Direct electron collisional ionization

   $e + H^{z+} \rightarrow H^{(z+1)+} + e + e$

5. Radiative recombination

   $e + H^{(z+1)+} \rightarrow H^{z+} + h\nu$

6. Three-body recombination

   $e + e + H^{(z+1)+} \rightarrow H^{z+} + e$

- The population n_i of the *i*th level is given by the rate equation :-

$$\frac{dn_i}{dt} = n_e \sum_{j\neq i} n_j q_{ji} - n_e \sum_{i\neq j} n_i q_{ij} + \sum_{j>i} n_j A_{ji} - \sum_{i>j} n_i A_{ij} + n_e n_{con} \alpha_i^{rr} + n_e^2 n_{con} \alpha_i^{3b} - n_e n_i s_i$$

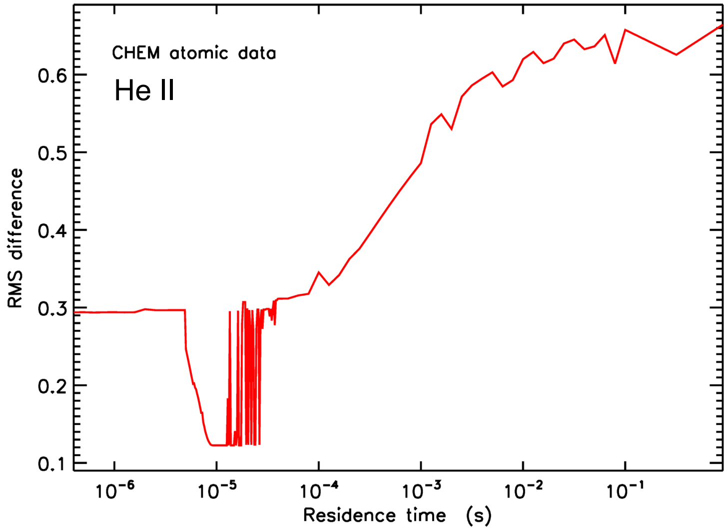
where *q* are the collisional rates, *A* the A-values and α^{rr}, α^{3b} are radiative and three-body recombination rates, *s* the electron collisional ionization rates and n_{con} the continuum population.

Transient explanation of the Lyman alpha discrepancy

- In hydrogen-like species the excited populations, n_i, *are* usually a small fraction of the ground state population, n_1.
- The ground state population changes due to transport, recycling and gas puffing, whereas the excited populations rapidly reach a distribution determined by the temperature and density of the surrounding plasma.
- Consequently the excited populations are assumed to be in steady-state where

$$\frac{dn_i}{dt} = 0.$$

- *However, some of the populating channels are slow.* Does their inclusion in the CR model make a difference to the calculated populations?



- Comparisons made between the He II equilibrium measurements and the CHEM CR model.
- As before the sum of the squared (modelled – measured) fractional differences minimized.
- Progressively the slowest populating channels (determined by a characteristic time ~ 1 / A_{ij} or 1 / n_e×rate) were removed from the CR model.
- Reasonable agreement is found for a cut-off time of ~10 μs.

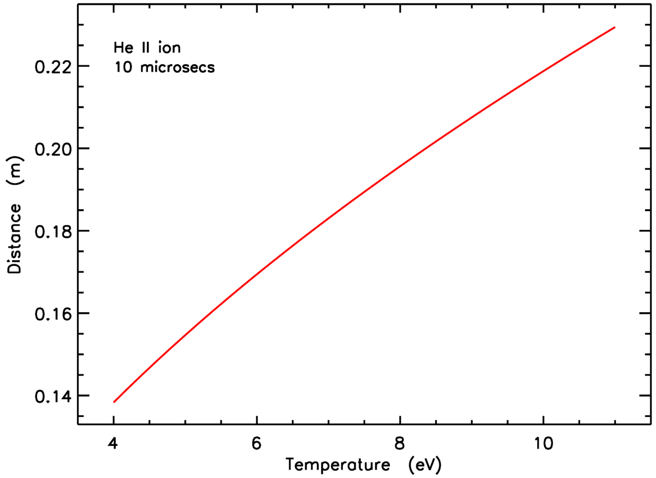
Transient explanation of the Lyman alpha discrepancy

Parameter	Initial value	Upper and lower bounds / (Measured values)	Without cut-offs	With cut-off at 10 μs
			CHEM	CHEM
T_e (eV)	4.0	0.2-25.0	4.01	9.49
$\text{Log}_{10}(n_e)$ (m^{-3})	19.0	18.0-21.0	18.00	20.74
n^{2+}/n^{+} ratio	0.1	0.00-3.0	3.0	0.00
Alpha / beta % frac. diff.		(5.45)	6.14 12.6	5.45 0.1
Beta / gamma % frac. diff.		(3.57)	2.26 -36.8	3.20 -10.4
Beta / delta % frac. diff.		(9.15)	3.64 -60.2	10.8 18.1
Beta / epsilon % frac. diff.		(31.2)	5.37 -82.8	24.7 -20.8
Beta / zeta % frac. diff.		(68.4)	7.68 -88.8	69.2 1.2
RMS fractional difference			0.562	0.123

T_e, $\text{Log}(n_e)$ and n^{2+}/n^{+} varied in the minimization.

- The minimization results with all populating channels (no cut-offs) and with those slower than 10 μs excluded from the CHEM CR model.

Transient explanation of the Lyman alpha discrepancy



- **Excluding slow populating channels from the He II CHEM CR model makes a significant difference and can give better agreement with experiment.**
- The best agreement is with a cut-off of ~10μs, this corresponding to the residence time of the He II ion in the emission region of the plasma.
- The distance that a He II ion travels in ~10μs corresponds roughly to the size of the expected He II emission region.

- Radiative decay, electron collisional *deexcitation,* electron collisional ionization and heavy particle collisions have little effect on the RMS difference.
- The improved agreement results from removing the slow electron collisional excitation and recombination (both radiative and three body) channels.
- Electron collisional excitation channels particularly from the ground state tend to be slow.
- At T_e > 1 eV *all* recombination channels have a characteristic time slower than ~10μs.
- Hence, excitation from the ground state and recombination will have a limited effect on the populations during the ions transit through the emission region. The populations are far from steady-state!
- These results involve switching populating channels on and off in the existing CHEM CR model. They are not from a fully time-dependent CR model – *illustrative calculation*.

Conclusions

- Extensive measurements of the He II VUV Lyman emission from JET are given in the report 'He II Lyman series line intensity measurements in the JET tokamak'.
- The measurements show that most He II emission originates in plasma regions with similar electron temperatures (~6-7 eV), the temperature-dependent line intensity ratios being near-constant. The intensity ratios do not depend on the line-of-sight or observing instrument.
- The report 'He II VUV and visible line intensity measurements in the JET tokamak' confirms the reliability of the VUV Lyman measurements by making comparisons with Balmer and Paschen series members.
- There is a significant discrepancy (~x3-5) between measured He II Lyman alpha/beta line intensity ratios and those predicted by Collisional-Radiative models, both ADAS and CHEM.
- Although including opacity in the Collisional-Radiative model does give an explanation of the JET He II observations, extending the analysis to D I measurements shows this explanation to be unsatisfactory.
- The analysis has allowed an understanding of opacity in He fuelled discharges and would suggest that it effects only a limited number ($\leq 15\%$) of discharges.
- In contrast, opacity is found to be more significant in hydrogenic fuelled discharges and should be included in transport simulations and other analyses.
- An alternative explanation of the Lyman alpha discrepancy is suggested, since inclusion of slow populating channels affects the CR model. A 10μs residence time of the He II ions in the emitting plasma is estimated, which does not allow the level populations to reach a full equilibrium.
- This will not only affect the modelling of the VUV Lyman line intensities, but all (including visible) hydrogen-like line intensities.
- A fully time-dependent CR model is being constructed and the analysis of the more challenging D fuelled discharges continued, with their more complex spectra and in which molecular channels affect the D I energy level populations.