Integrated peturbative and non-perturbative collisional calculations underpinning magnetically-confined plasma diagnostics, with propagated uncertainties

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Outline

- Motivation
- Baseline and Monte-Carlo Collisional Radiative Models
- Secondary derived atomic parameters that are temperature and density dependent
  (Effective ionisation/recombination/excitation)
  => ionisation fraction,
  => SXB impurity influx
  => radiative power loss
- Challenges (Near Neutral W and Mo)
Motivation: High-Z materials are leading candidates for first wall materials in future fusion energy devices

- Reactor temperatures and heat flux will require new high-Z materials
  - High melting point and thermal conductivity
  - Reduced sputtering
  - Tritium retention is reduced
  - First wall lifetime is increased

- Tungsten (W) is a leading candidate for the divertor material for ITER

- Mo is presently being used on NSTX-U as the first wall material

“There is an urgent need in the fusion energy community to understand the rate of high-Z material erosion presently – DIII-D 5 year plan”
Motivation: High-Z materials are leading candidates for first wall materials in future fusion energy devices

- **Allowable impurity concentration lower for high-Z materials**
  - High-Z materials radiate much more than previously used materials
  - Radiation significant enough to denigrate plasma performance
    - Concentration needs to be less than ~1E-4 (Putterich)
  - Need to accurately quantify and minimize erosion of wall
We categorize the problem into 2 groups:

- **Baseline** uncertainty data to give an indication of the parameter space
- **Method sensitivity** uncertainty data with tighter and more realistic error bars.

- The approach is valid for both astrophysical and tokamak plasma regimes.
Baseline vrs Monte-Carlo

**Baseline Studies**
- Uncertainty is quantified as the difference between different theoretical approaches.
- Representative of differences in the literature.
- Quickly provides a generous uncertainty on an atomic dataset, while providing the correct temperature and density trends of more elaborate calculations.
- May not reflect the tighter constrained uncertainties derived from more elaborate calculations.
- Fundamental atomic structure and collisional rates remain uncorrelated.

**Sensitivity Studies**
- Uncertainty is determined from the sensitivity of the calculation to key input parameters.
- Can produce fully correlated uncertainties.
- The objective choice of variation in the input parameters that reflects meaningful physical values remains difficult.
- Does not determine the absolute uncertainty between methods.
- More time and resource intensive.

**Monte-Carlo Collisonal Radiative Modeling**

- Emissivities
- Uncertainties
  - Monte-Carlo line ratio diagnostics

- Uncertainties
  - Effective ionization and recombination
  - Uncertainties on Te and Ne
  - Uncertainties on abundances and ionization age

- Monte-Carlo ionization balance
Monte-Carlo RMPS approach

Initially, we shall require complete data sets for the lighter fusion related elements, before moving to the heavier Tungsten-like elements.

To do list: For every ion stage

a) Electron-impact (de-)excitation between every level/term, then convoluted with a Maxwellian

b) Ground and meta-stable ionisation

c) Ground and meta-stable recombination (RR, DR, 3 body)

(This has been scripted: Structure → Collisional rate)

But although a concern, our TDCC, our many hundred term CCC and RMPS calculations do this pretty well!
However, it is not these but the secondary derived quantities, that provide diagnostics or interface with transport codes (and are density/temperature dependent).

The generalized ionization rate coefficients are given by:

\[ S_{\beta \rightarrow \gamma} = I_{\beta \rightarrow \gamma} - \sum_j I_{j \rightarrow \gamma} \sum_{j'} (C_{j j'}^{\gamma})^{-1} C_{j' \beta}^{\gamma}, \]

For example, let us consider an effective ionization rate (temperature/density dependent).

It will be a function of the ground and excited state ionisation. The contribution from the excited states, requires knowledge of the excited state populations relative to the groundstate; in effect the solution to collisional radiative problem. Therefore, our problem is now an explicit function of the atomic structure (A-values), the excitation/de-excitation rates, maybe even the ionisation/recombination of the neighbouring ion stages.
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SXB ratio dependence on the effective ionisation rate
Quantifying wall erosion with passive spectroscopy

- The intensity of a spectral line can be related to its influx rate [Behringer PPCF 31 2059 (1989)]
- The number of ionizations per photon (S/XB) is directly proportional to the impurity influx

\[ \Gamma = \int_0^\infty N_e N^z S^{z \to z+1} dx \]
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\[
\Gamma = \int_0^\infty N_e N^z S^{z\to z+1} \, dx = \int_0^\infty N_e \frac{S^{z\to z+1}}{A_{i\to j} N_i / N^z} \left( A_{i\to j} \frac{N_i}{N^z} \right) N^z \, dx
\]
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\]

\[
= \int_0^\infty N_e S X B_{i \rightarrow j}^Z \left( A_{i \rightarrow j} \frac{N_j}{N^Z} \right) N^Z \, dx
\]

where \(S X B_{i \rightarrow j}^Z = \frac{S^{z \rightarrow z+1}(N_e, T_e)}{A_{i \rightarrow j} \frac{N_i}{N^Z}(N_e, T_e)}\)

Note electron temperature and density dependence
Heavy species: Molydebnium and Tungsten

(Theory can provide a predicative capability, verified by experiment)
ADAS predicts spectral emission of W I to be predominately at UV wavelengths (it is not just the 400.9 nm line)

- Predicted lines in synthetic spectra should match real spectra
- ADAS predictions motivated installation of UV spectrometers
- Purpose was to find other strong W I lines as erosion diagnostics
- Presently the 400.89 W I lines solely used to diagnose W erosion
  - There are concerns about this line being blended with W II
  - Ideal erosion diagnostic lines would be isolated
- Other high-Z also predicted to be strong in the UV
Molybdenum calculations completed and benchmarked using C-Mod tokamak spectral measurements
(The need to filter Gbs of data, for good candidates)

• ADAS provides a good match with measured spectrum
• Relative line heights are not strongly density dependent
• Two lines were strongly temperature dependent
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  • Ratio of the two lines can be used for electron temperature diagnostic
• S/XB dependent on temperature
  • eliminates the need for independent temperature diagnostic
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Molybdenum line ratios allow for plasma temperature in the edge to be calculated

- Ratio of Mo II 284.8 nm and Mo II 286.67 nm
- Ratio of lines not density dependent but strongly temperature dependent
- Predicts a reasonable electron temperature of 1.5 eV
Back to Tungsten
Auburn UV survey spectrometers Installed on DIII-D: Spectrometers

- Three Stellarnet USB spectrometers installed with different spectral ranges:
  - Spectrometers with 200-300 nm, 300-400 nm, and 200-400 nm ranges
  - Compact concave grating spectrometers ~20 cm length
  - Integration times of 30 to 2000 ms utilized

- Two viewing chords available simultaneously:
  - Lenses were located at a port slightly above the midplane
  - Ability to measure emission from lower divertor floor & shelf simultaneously
  - 5 m fused fibers were used to minimize UV absorption

- Spectrometers housed in radiation shield boxes
  - Neutrons and x-rays
  - Stronger magnetic and electric fields
A typical spectrum for the 200-300 nm spectrometer is shown.

200-300 nm spectrometer viewing the lower divertor shelf.

W lines small compared to other impurities.

- Consistent with low sputtering rates.

ELMing H mode plasma 4 MW injected power (medium power shot).

First UV survey spectral measurements in DIII-D, multiple W I lines observed.
New W I candidate lines found to use for W erosion measurements

- W I 265.65 nm observed to be on the order of the widely used 400.89 line:
  - Atomic calculations using ADAS confirm that W I 265.65 nm is strong for divertor temperatures and densities $\sim 1 \times 10^{19} \text{ m}^3 \sim 10 \text{eV}$
- Multiple W I lines in the region around 265.65 region:
  - High density of lines in this region motivates higher resolution spectrometer/instrument
300-400 nm spectrometer also identified additional W I spectral lines to the 400.89 line

- 300-400 nm spectrometer view of the shelf
- L mode plasma 3.8 MW injected power (medium power)
Summary and future work

Promising new W I lines identified for erosion measurements:

- Erosion measurements (….. mmmm) can be done after absolute calibrate to be done Nov 5th
- Further benchmarking of W I spectra will be completed on CTH

- New R-Matrix W I (QUB) atomic calculations in the process of being calculated will compare to experiment
- New R-matrix Mo I (QUB) atomic calculations in the process of being calculated will compare to experiment

Perl/Python scripting of R-matrix calculations now feasible, but need to include RMPS ionisation / recombination aspects