Atomic and Molecular data for collisional radiative modelling relevant to fusion

D. Wünderlich and U. Fantz
Atomic and Molecular Data for fusion: Outline of the talk.

• Collisional radiative modelling for fusion
  • Atomic and molecular data for collisional radiative modelling
  • Application of collisional radiative models
Population models for fusion plasmas: Overview.

Tokamak plasma edge

Wide parameter range
\( T_e = 50 \text{ eV} \ldots \text{below 1 eV} \)
\( n_e = 10^{18} \text{ m}^{-3} \ldots 10^{21} \text{ m}^{-3} \)
Ionizing → recombining

NBI ion source plasma

Wide parameter range
\( T_e = \approx 10 \text{ eV} \ldots \approx 1 \text{ eV} \)
\( n_e = 10^{18} \text{ m}^{-3} \ldots 10^{17} \text{ m}^{-3} \)
Ionizing → recombining

Relevance of population models:

- Interpreting diagnostics results.
- Needed as input: atomic and molecular data.
Population models for fusion plasmas: Motivation and relevant species.

Low-temperature regions of tokamak plasma
- Operated in $\text{H}_2$, $\text{D}_2$ and/or $\text{T}_2$.
- High relevance of atomic and also molecular processes, especially in the detached case.
- Molecular assisted recombination.
- Impurity seeding ($\text{N}_2$, $\text{Ar}$, …) $\Rightarrow$ enhanced radiation losses.
- Optical thickness.

Ion source for neutral beam injection
- Operated in hydrogen or deuterium.
- Presence of caesium.
- Well defined transition ionizing-recombining plasma (created by a magnetic filter field).
- Optical thickness.

Picture by courtesy of D. Reiter, FZ Jülich
Population models for fusion plasmas: Collisional Radiative models.

Population models
- Predict population densities in dependence of plasma parameters ($T_e$, $n_e$, ground state densities).
- Main field of application: plasma diagnostics.

Collisional radiative models
Balance all relevant exciting and de-exciting reactions.

⇒ Needed: extensive data base of reaction probabilities.
⇒ Drastically increased complexity for molecules (vibrational and rotational excitation).

Error bar of model results directly correlates with the quality of the used input data.

Corona models

LTE

Relevance of processes including photons, e.g. self-absorption due to optical thickness

Collisional radiative models

Low collision rate

High collision rate

D. Wünderlich
IAEA Meeting, Vienna, 19.-21.11.2018
Population models for fusion plasmas: Yacora and available Collisional Radiative models.

Yacora is a flexible (0D)-solver for Collisional Radiative models:

- Used and improved for more than 16 years.
- Almost all available CR models are relevant for application in plasmas used for fusion:

<table>
<thead>
<tr>
<th>CR model for...</th>
<th># states</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>Electronic states only</td>
<td>33</td>
</tr>
<tr>
<td></td>
<td>Some vibrational states</td>
<td>214</td>
</tr>
<tr>
<td></td>
<td>Vib-rot resolved</td>
<td>&gt;626</td>
</tr>
<tr>
<td>H</td>
<td>44</td>
<td>Coupling to H⁺, H₂⁺, H₃⁺, H⁻, very well benchmarked</td>
</tr>
<tr>
<td>He</td>
<td>19</td>
<td>Very well benchmarked</td>
</tr>
<tr>
<td>Ar</td>
<td>16</td>
<td>Well benchmarked</td>
</tr>
<tr>
<td>Ar⁺</td>
<td>84</td>
<td>Only a collection of input data, not benchmarked</td>
</tr>
<tr>
<td>N₂</td>
<td>Electronic states only</td>
<td>6</td>
</tr>
<tr>
<td>C₂</td>
<td>Vibrationally resolved</td>
<td>80</td>
</tr>
<tr>
<td>CH</td>
<td>Vibrationally resolved</td>
<td>29</td>
</tr>
<tr>
<td>Cs</td>
<td>11</td>
<td>Includes MN H⁻ with Cs⁺, well benchmarked</td>
</tr>
</tbody>
</table>
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Atomic data in Collisional Radiative models: Situation for light atoms.

Collisional radiative modelling for light atoms:

- **Very good completeness and quality** of the available input data (for direct excitation).
- Some small adjustments were performed in the last years. Example: hydrogen.

Excitation of atomic hydrogen...

...in ionizing...

...and recombining plasmas

- **Attached divertor plasma**
- **Driver region of NBI sources**

- **Detached divertor plasma**
- **Expansion region of NBI sources**

Huge number of free parameters ⇒ Evaluation needs a lot of time and experience
Atomic data in Collisional Radiative models: Correction of literature data for the hydrogen atom.

Data by Janev et al:

- Compilation of recent calculations and measurements
- Low energies ($E_e<40$ eV): discontinuity between cross sections for $1\rightarrow 5$ and $1\rightarrow 6$
  - Reason: different primary data sources (R-Matrix, semi empirical modification of Born-Bethe)
  - Solution: fit of rate coefficients
  - Result: excellent agreement of measurement and model for ionizing plasma with known $T_e$ and $n_e$

Benchmarked set of rate coefficients for direct excitation

R. Janev et al, JÜL-4105, Forschungszentrum Jülich, 2003
D. Wünnerlich et al, JQSRT 110, 2009, 62
Molecular data in Collisional Radiative models:
Franck-Condon factors and Transition probabilities for $H_2$.

Prepare extension of cross section database

Collect and prepare eigenvalues of electronic wave functions (=potential energy curves)

⇒ Vibrational eigenvalues
⇒ Vibrational wave functions
⇒ Franck Condon Factors

... for $H_2$ and $H_2^+$ (and its isotopomers)
Molecular data in Collisional Radiative models: Franck-Condon factors and Transition probabilities for H$_2$.

Prepare extension of cross section database

Collect and prepare eigenvalues of electronic wave functions (=potential energy curves)

⇒ Vibrational eigenvalues

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... for H$_2$ and H$_2^+$ (and its isotopomerses)

Collect and prepare dipole transition matrix elements

⇒ Einstein coefficients

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Molecular data in Collisional Radiative models: State-resolved ionization cross sections for \( \text{H}_2 \).

Literature: virtually no data for ionization of excited states in \( \text{H}_2 \)

- Performed calculations based on the Gryzinski method.
- Dissociative and non-dissociative channel.

\( \text{H}_2(\text{X}^1) \): Comparison with existing data (experimental and theoretical)

- Perfect agreement for non-dissociative and dissociative ionization.
- Reason: removing one electron easy to be described by simplified methods.

D. Wünderlich, Chem. Phys. 390, 2011, 75
Molecular data in Collisional Radiative models:
Relevance of the isotope effect.

Isotope effect mainly caused by:

- More tight vibrational and rotational energy level spacing in D$_2$.
- Impact on wave functions and threshold energies.

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Molecular data in Collisional Radiative models: Excitation cross sections: lack of data for H₂ (and its isotopes!).

Excitation processes in the H₂ molecule:
- Data collections by Tabata (2000) and Yoon (2008): only a few reactions.
- Calculations by Celiberto (2001): only a few transitions, but isotope effect.
- Miles: semi empiric cross sections, 1972.

Significant inconsistencies

T. Tabata et al, ADNDT 76, 2000, 1
R. Celiberto et al, ADNDT 77, 2001, 161
Molecular data in Collisional Radiative models: Excitation cross sections: lack of data for H₂ (and its isotopes!).

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- Miles: semi empiric cross sections, 1972.
- New consistent data set: CCC (Convergent Close-Coupling), 2017 and ongoing.

Significant inconsistencies

T. Tabata et al, ADNDT 76, 2000, 1
R. Celiberto et al, ADNDT 77, 2001, 161
W.T. Miles et al, J. Appl. Phys. 43, 1972, 678
M.C. Zammit, Phys. Rev. A 95, 2017, 022708
Molecular data in Collisional Radiative models: Example: Determine the ratio $n(H)/n(H_2)$.

Models using Miles, Janev and CCC data:

- Differences in population densities directly mapped onto diagnostics results
- Up to now: model almost non-usable due to inconsistencies in the input data.
- CCC cross sections in between results based on Janev than Miles.

New CCC data may enable performing dedicated extensions:

- Excited state-excited state reactions (high relevance in the triplet system).
- Isotope effect ($H_2$, $D_2$, $T_2$)

Significant step towards (finally) a correct description of emission from $H_2$.
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Application of population models: Vibrational-rotationally resolved corona model for H₂.

Werner ($C^1\Pi_u \rightarrow X^1\Sigma_g^+$) and Lyman ($B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$) bands

- Resonant transitions in the VUV/UV
- Overlap between Werner and Lyman $\Rightarrow$ high relevance for the interpretation of measured spectra
  $\Rightarrow$ Important role of model (e.g. scaling measurement to the full band)
- Position of the lines and general structure well described by the model
- Next step: investigate influence of cascades on the vibrational and rotational population (steps toward a CR model needed?)

Very good results of ro-vibrational Corona models for Werner and Lyman H₂
Determination of power radiated by photons and ratio fluxes photons/atoms/ions:

- ICP (f=13.56 MHz), P<600 W, p<10 Pa
- Plasma parameters from Balmer lines and CR model
- Emission from defined wavelength windows:
  - Werner: 117-130 nm
  - Lyman: 130-190 nm
  - Fulcher: 600-640 nm (diagonal bands)

Thus, apply ro-vibrationally resolved corona models to deduce total emission or for predictive modelling.

- Up to 21 % of P_{RF} measured as radiant power, mostly VUV/UV
- Photon fluxes ≈ ion fluxes, atomic fluxes much higher
Application of Collisional Radiative models: Yacora on the Web.

Yacora on the Web provides online access to selected Yacora CR models

Aims and features of Yacora on the Web

• Making public collisional radiative models based on Yacora in a user friendly environment.

• Available up to now: models for H, H₂ and He.

• Very simple registration (self registration).

• Extensive documentation available (also for anonymous users).

• Web application based on Plone and Python.
Conclusions

Input data set for population models of low-temperature plasmas
- Collected from different literature sources for different particle species.
- Extended and corrected where necessary and possible.

Yacora CR models for different particle species relevant for fusion
Relevance of processes including photons and the isotope effect $H_2 - D_2 - T_2$.

Thorough benchmark at different plasma experiments
- Low-temperature region ($T_e < 10\text{eV}$) of fusion machines.
- Ion sources for NBI.
- Lab-scale experiments.