New Molecular Collisional-Radiative Model in ADAS

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ADAS Workshop 24 – 25 September 2012
Outline

1. Motivation

2. Molecular ADAS routines: ADAS900
   - General view
   - Molecular Data
   - CR Model

3. Results

4. Summary
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Motivation

- Molecules desorbed from the wall contribute to the neutral density and influence the divertor physics.
- ADAS 900 series main objective is to extend ADAS Database to molecular data.
- We want to provide molecular data tools to use in plasma edge and divertor calculations and experiments.
Steps to follow for a Molecular CR model

1. Compile a database. Structure it and provide readings tool for it. Do maxwellian integration of cross sections to obtain rates (Boring part).

2. There are gaps!. Fill the gaps with estimation of molecular processes. Automatic process is needed due to the big number of states.

3. Solve CR model for all molecules and all dissociation products.
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ADAS 900

Fundamental Molecular Data → mdf02 FILE → 902 & 903 GENERATION ROUTINES

FC FACTORS A−VALUES mdf00

MOLECULAR FORMAT FILE ν−ν resolved mdf04

ADAS904 CR MODEL

EFFECTIVE COEFFICIENTS → POPULATIONS

SPECTROSCOPY PARAMETERS PECS, SXB, DXB
Molecular ADAS routines: ADAS900

- **mdf00** General information. Vibrational energies. FC factors. A-values.
- **mdf02** Cross sections and rates obtained from external sources or calculations.
- **mdf33/34** ADAS902 product. Rates (upsilons and \( cm^3 s^{-1} \)) obtained from maxwellian integratrion of mdf02.
- **mdf04/14** ADAS903 product. Maxwellian rates completed with EIQIP and EICIP to be used in population models.
- **mdf11** ADAS904 product. Molecular effective coefficients.
- **mdf15** Molecular PEC, SXB, DXB.
- **mdf25** Mapping Central ADAS adf and mdf formats correlation.
- **mdf38** Autoionization and predissociation rates.
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Molecular Data: H$_2$

- **Excitation data**: There is available data$^1$ that have been checked to be in good agreement with the fitting formulas from Janev.

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- **Attachment**: Fitting formulas from Celiberto$^2$ for fitting calculations. Vibrational excitation through resonant attachment.

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ADAS903 matrix completion

- EIQIP\(^4\) (bound-bound collisional IP) is used for excitation inside a molecular specie.
- ECIP\(^5\) (bound-free collisional IP) has been used for ionization (dissociative and non-dissociative) and dissociative excitation. It is needed a better optimization for the extension to molecules.
- Calculation are performed over vibronic levels and summed in case of electronic resolution.
- EIQIP uses A-values to calculate the oscillator strengths so Franck-Condon factors unitarity is fullfilled.
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ADAS903: filling the matrix

INPUT & RULES → READ MDF33 FILES → LOOK FOR NEW PROCESSES

LOOP IN PROCESSES

MDF33

LOOP IN PROCESSES

DIPOLAR RULES

IP CALCULATIONS

ORDER MATRIX DISCHARD O'S

MDF04
Why filling the matrix?

Maxwellian time constant: \( \tau = \frac{1}{n_e \langle \sigma v \rangle} \)

\[
\begin{align*}
H_2(X, \nu = 0) & \rightarrow H + H \\
H_2(X, \sum \nu \nu) & \rightarrow H + H
\end{align*}
\]

Processes from excited vibrational levels are needed.
Motivation

ADAS904: Solving CR

- Dissociative processes are all that go to dissociation (diss. excitation, ionisation, CX, recombination ...).

- Metastables are always vibrationally resolved $\rightarrow 150 \times 150$ maximum dimension of metastable matrix.

- Autoionisation and predissociation are included at this stage from *mdf38* format data.

- Atomic dissociation products equilibrium ionisation balance is included in the CR model.
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Molecules CR model

\[
A^{q-1} \leftrightarrow A^q \leftrightarrow A^{q+1}
\]

\[
M^q \leftrightarrow M^{q+1} \leftrightarrow \ldots \leftrightarrow M^{q+n}
\]

\[
A^q \leftrightarrow A^{q+1} \leftrightarrow \ldots \leftrightarrow A^{q+n}
\]
ADAS904: The population model

\[
\frac{dN_X}{dt} = \begin{pmatrix}
H_2 & \sim 0 & 0 \\
\neq 0 & H_2^+ & 0 \\
\neq 0 & \neq 0 & H(n), H^+
\end{pmatrix} \times \begin{pmatrix}
N_X \\
\Gamma_{in}
\end{pmatrix}
\]

\[
\begin{pmatrix}
\cdots \\
\text{states} \\
\cdots
\end{pmatrix}
\]

\(\Gamma_{in}\) can correspond to the collisional terms from constant populations.
ADAS904: CR model

1. **INPUT & RULES**
   - Read MDF04 files

2. **MDF04**
   - Loop in (Te, Ti), Tm, Ne
   - Fill the matrices

3. **MDF04, MDF11**
   - Eff. coeffs.
   - Write eff. coefficients

4. **CALCULATIONS OF POPULATIONS**
   - Effective coeffs.
   - Output

5. **OUTPUT**
   - SxB, PEC, DXB

6. **LOOP IN PROCESSES**
   - MDF11, MDF15
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Effective coefficients

CR dissociation from ground state

CR ionization from ground state to ground state
Population

\[ T_e = 25 \text{ eV} \]
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- New molecular collisional-radiative tools have been developed and will be soon available.

- The tools can be extended to other diatomic molecules other than H₂.

- Molecular data are the main problem in building such a model.

- Checking and developing of method of calculations under way.

- Easy implementation of results in models (ADAS structure).