Molecules in fusion plasmas

Hydrogen molecules and molecular ions (H₂⁻, H₂⁺)

\[ \text{plasma kinetics} \]

H₂⁺ \rightarrow H + e⁻, \quad \text{H}_2 \rightarrow 2H + e⁻

Recombination coefficient \( f(\text{material}, T, \text{H}_2, \text{ablation}) \)

Vibrationally excited molecules

Dissociative recombination

Molecular Assisted Collisional Radiative model

Relevance of molecules in the transition regime towards detachment

Achievement of the recombining regime by atoms and / or molecules?

Electron Ion Recombination EIR

H⁺ + e⁻ + \* \rightarrow H + H + \* charge exchange with

\[ n_e = 10^{20} - 10^{21} \text{ m}^{-3}, T_e < 1.5 \text{ eV} \]

Divertor of ASDEX Upgrade (carbon machine): modelling & diagnostics

Molecular Assisted Recombination MAR

H⁺ + e⁻ + \* → H + H + \* dissociative recombination

\[ n_e = 10^{19} - 10^{20} \text{ m}^{-3}, T_e = 2 - 10 \text{ eV} \]

Role of molecules in the Balmer line analysis

Collisionsal radiative model for H with coupling to different particle species: Yacora

\[ n(p) = R_n(p) n_e + R_m(p) n_e + R_n(p) n_e \]

Many free parameters!

Molecules in fusion plasmas

Cold plasma edge:

SOL and divertor region

Wide parameter range

\[ T_e = 50 \text{ eV} \rightarrow \text{few eV} \rightarrow \text{below 1 eV} \]

Ionising plasma \( \rightarrow \) Recombining plasma

- Different recycling regimes
- Similar to laboratory plasmas
- Low temperature, low pressure plasmas
- Relevance of diagnostics and modelling

Relevance of molecules in the transition regime towards detachment

Linear plasma device: cascaded arc at TU/e Eindhoven

Plasma parameters from Thomson scattering, probes, OES, ...

Role of molecules in the Balmer line analysis

Collisionsal radiative model for H with coupling to different particle species: Yacora

\[ \text{Many free parameters!} \]
**Role of molecules in the Balmer line analysis**

**Collisional radiative model for H with coupling to different particle species: Yacora**

- **Data sets for dissociative recombination**
  - $H_2^+ + e \rightarrow H(n) + H$
  - $H_2^+ + \gamma \rightarrow H(n) + H$

- **Fixed branching ratio**
  - $m_1 = 0.1$
  - $m_2 = 0.2$
  - $m_3 = 0.3$

- **Energy [eV]**
  - $10^{-1}$ to $10^{1}$

- **Electron temperature [eV]**
  - $10^{-1}$ to $10^{1}$

- **Volume**
  - $10^{-19}$ to $10^{-16}$

- **Molecules in negative hydrogen ion sources**

- **Ion sources for negative hydrogen ions:**
  - Linear plasma device: cascaded arc at TU/e Eindhoven
  - RF source performance

- **Plasma Generation**
  - Driver
  - Expansion Chamber

- **Molecules in negative hydrogen ion sources**

- **Ion sources for negative hydrogen ions:**
  - Surface process via volume process
  - $H_2^+ + e \rightarrow H(n) + H$
  - $H_2^+ + \gamma \rightarrow H(n) + H$

- **Volume**
  - $10^{-19}$ to $10^{-16}$

- **Energy [eV]**
  - $10^{-1}$ to $10^{1}$

- **Volume processes**
  - Electron stripping
  - Mutual neutralisation
  - Associative detachment (non-associative)

- **Data set changed**

- **Branching ratio**
  - Well known

- **Open issue:**
  - Data for dissociative recombination of $H_2^+$

- **Role of molecules in the Balmer line analysis**

- **Collisional radiative model for H with coupling to different particle species: Yacora**

- **Data for dissociative recombination of $H_2^+$**
  - $H_2^+ + e \rightarrow H + H + e$

- **Fixed branching ratio**
  - $m_1 = 0.1$
  - $m_2 = 0.2$
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- **Energy [eV]**
  - $10^{-1}$ to $10^{1}$

- **Volume**
  - $10^{-19}$ to $10^{-16}$

- **Molecules in negative hydrogen ion sources**

- **Ion sources for negative hydrogen ions:**
  - Linear plasma device: cascaded arc at TU/e Eindhoven

- **Mixed reactors:**
  - Driver
  - Expansion Chamber

- **Molecules in negative hydrogen ion sources**

- **Ion sources for negative hydrogen ions:**
  - Volume production
    - $e + H_2 \rightarrow H_2(B,C) + e$ or $H_2(v) + e$ or $H_2 + hv$

- **Vibrational excitation**
  - $H_2 + e \rightarrow H_2(v) + e$

- **Dissociative attachment**
  - $H_2 + e \rightarrow H + H + e$

- **Concept of a tandem source**

- **Problems:**
  - High ion extraction current
  - Pressure and thus stripping losses in accelerator
  - $H_2 + e \rightarrow H_2 + H + e$

- **Low ion current for low pressure**

- **Ion sources for negative hydrogen ions:**
  - Ionising – recombinating plasma

- **Volume production**
  - $H_2 + e \rightarrow H_2 + H + e$ or $H_2 + e + H + e$

- **Partitioning**
  - $H_2$ generation
    - Recombining plasma
      - $T_e = 1$ eV
      - $n_e = 5 \times 10^{22}$ m$^{-3}$
      - $H_2$ generation
      - Recombining plasma
        - $T_e = 1$ eV
        - $n_e = 5 \times 10^{22}$ m$^{-3}$

- **Cs evaporation**
  - Low work function
Balmer line analysis in negative hydrogen ion sources for fusion

Collisional radiative model for H with coupling to different particle species: Yacora

![Graphs showing ionizing and recombining plasma](image)

Relevance of H and H₂

![Graphs showing the density ratio H/H₂](image)

Molecular emission in negative hydrogen ion sources for fusion

Collisional radiative model for H and for H₂; Yacora

![Graph showing the density ratio H/H₂ obtained from the intensity ratio H₂/H₁ Fulcher band](image)

Important parameter: density ratio H/H₂ obtained from the intensity ratio H₂/H₁ Fulcher band

Example: data base in triplet system

Benchmark with experiments: better agreement for the semi-empiric Miles data but uncertainty of a factor of 3 remains

![Graph showing the density ratio H/H₂](image)

Beam Emission Spectroscopy (BES): analysis of Doppler-shifted Hg line

Determination of beam parameter

- Divergence
- Homogeneity
- Intensity
- Stripping losses in accelerator

![Beam Emission Spectroscopy setup](image)

½ size ITER source: ELISE test facility (IPP)

Beam size: 1 × 1 m²

640 apertures, 8 beamlet groups

BES in 2 m distance with 16 horizontal and 4 vertical LOS

Relevance of molecules in ionizing and recombing plasmas

Hydrogen plasmas in fusion with molecules (H₂, H₂⁺, H₃⁺)

Excitation reactions: data for the high energy range

Molecular Assisted Recombination

Collisional Radiative model

![Molecular emission in hydrogen plasmas](image)

Open issue: W surface, Ne seeding