Upgrade of A&M database and CRM for hydrogenic molecules

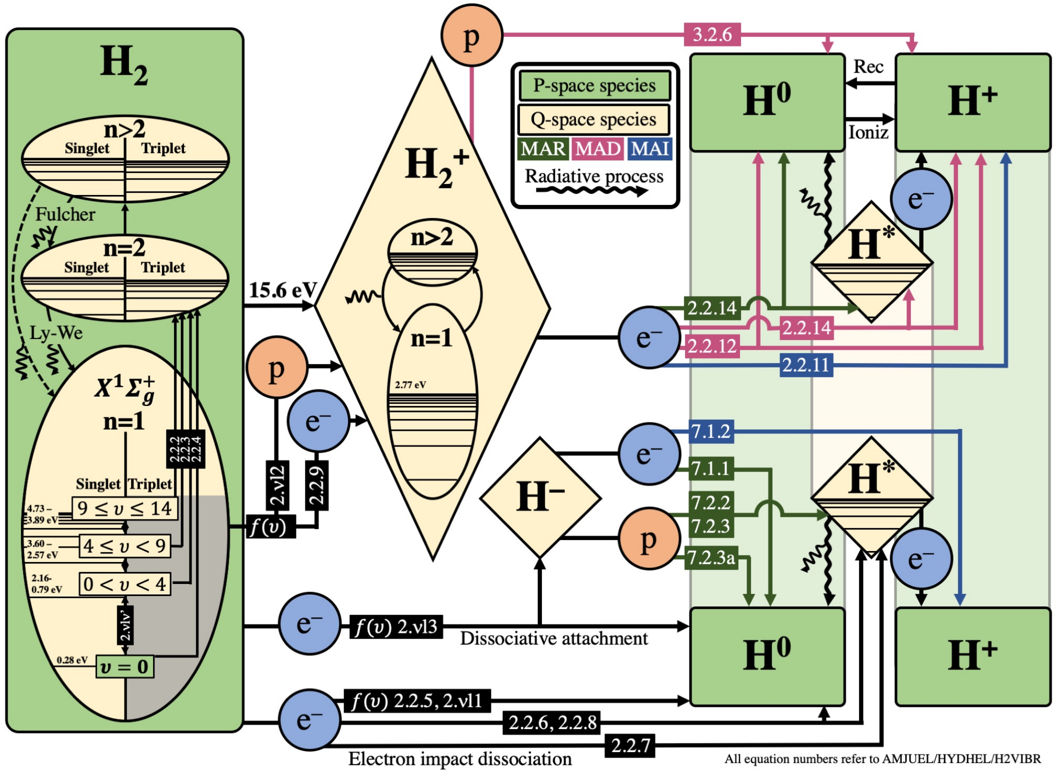
Andreas Holm, Mathias Groth

Aalto University

June 21st 2021

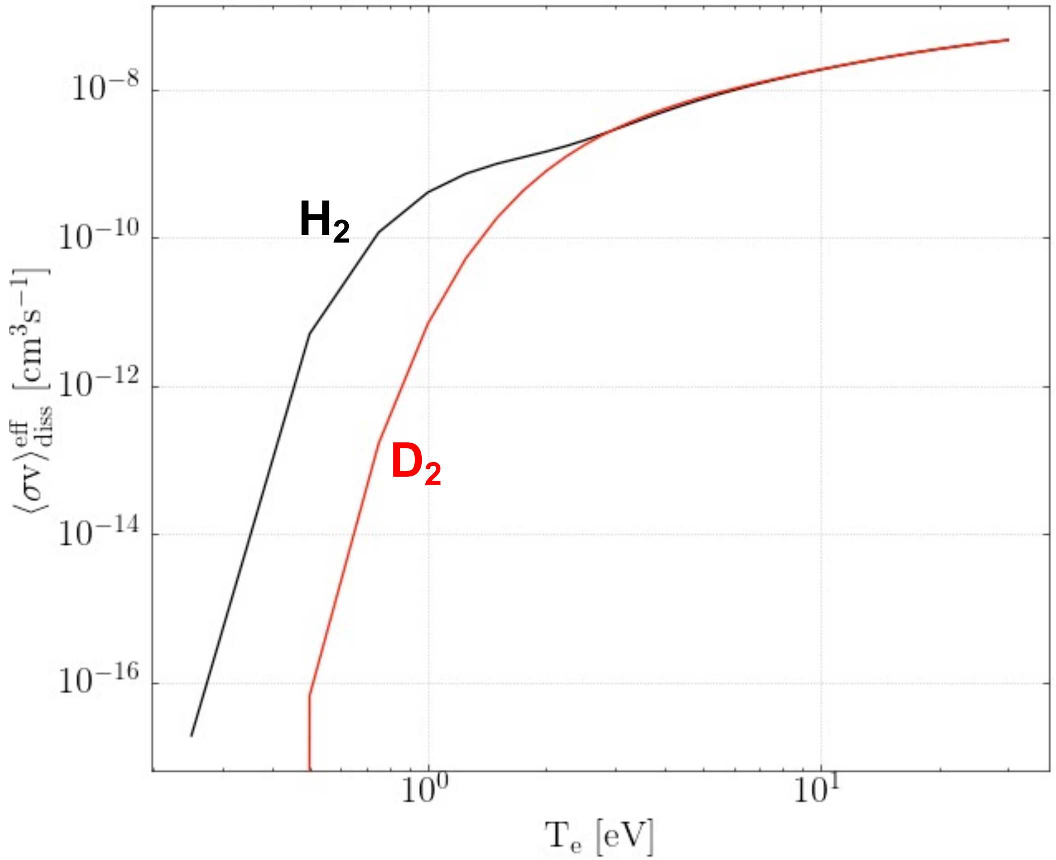
CRMs consider a large set of species, states, and reactions and calculates effective rates for a smaller subset of species

- No (reasonable) one-size-fits-all “universal CRM” available
  → Dependent on the local plasma conditions
- CRMs are 0D → transport effects must be evaluated using transport codes
- The model accuracy and applicability is dependent on data availability
  → Isotopologue dependence (H_2, D_2, T_2 ,D-T)



EIRENE uses one- and two-dimensional polynomial fits compiled in the AMJUEL database

- Effective rate coefficients calculated for H_2
  - A&M data from Janev/Sawada
  - Vibrationally resolved rates (H2VIBR) calculated by internally rescaling ground-state rates
- Rates calculated using Sawada's CRM
  - Assumes thermally and vibrationally equilibrated plasmas
  - Electronic excitations omitted to reduce dimensionality
- EIRENE internally applies an isotopologue scaling based on mass
  - Different vibrational distributions not considered



The existing, well-established CR model YACORA will be compared and verified against EIRENE A&M data

- Utilizes a state-of-the-art database of reaction rates, including some vibrationally resolved H_2 rates

- Allows for evaluation of CR models considering additional reactions (electronic transitions, quenching of triplet states, etc)

→ Compare AMJUEL rates vs YACORA CR rates to assess the quality of the reaction rates and CR model

→ Investigate the impact of isotopologue (H_2, D_2, eventually, T_2, D-T) on the CR resolved reaction rates

Step 1: better understand EIRENE A&M data and CR rates to evaluate the data accuracy and its applicability

- Compare AMJUEL H_2 rates to YACORA rates
- Compare EIRENE internally rescaled D_2 rates to YACORA rates
- Evaluate the role of transport of vibrationally excited states on molecular rates

Backups

Status of YACORA A&M data May 2021 (courtesy of D. Wünderlich)

Input data for the different coupling channels.

IPP

Excitation channel…		Initial model (improved Sawada)	Yacora now
H	Direct excitation	Johnson formula & Vriens 1980	Wünderlich 2009
H^+	Recombination	Inverse ionization / Based on Gaunt factor	Inverse ionization / Based on Gaunt factor
H_2	Dissociative excitation	Measured emissivties, scaled	Measured emissivties, scaled
H_2^+	Dissociative recombination	Janev 1987, scaled.	Janev 2003
H_3^+	Dissociative recombination	Not included	Janev 2003
H^- with H^+	Mutual neutralization	Janev 1987	Stenrup 2009
H^- with H_2^+	Mutual neutralization	Not included	Janev 2003, Eerden 1995

Status of YACORA A&M data May 2021 (courtesy of D. Wünderlich)

Input data used for H_2.

Excitation channel…		Initial model (improved Sawada)	Yacora now
$H_2(X^1) \rightarrow H_2^*$	Direct excitation	Miles 1971	Fursa / Scarlett (MCCC)
$H_2^* \rightarrow H_2^+$	Ionization	scaled results for H	Wünderlich 2011
$H_2(n=2) \rightarrow H_2(n=2)$	Excitation of excited states	Zygelman (for hydrogen-like ions)	Fursa / Scarlett (MCCC)
$H_2(n=2) \rightarrow H_2(n=3)$	Excitation of excited states	scaled results for H	Fursa / Scarlett (MCCC)
$H_2(n>1) \rightarrow H_2(n>3)$	Excitation of excited states	scaled results for H	scaled results for H
$H_2(a^3 \text{ or } c^3)+H_2 \rightarrow 2H_2$	Quenching of triplet states	Not included	Wedding 1988
$H_2^*+H^+ \rightarrow H_2^++H$	Charge exchange with H^+	Not included	Janev 2004
$H_2^*+e^- \rightarrow H^-+H$	Dissociative attachment	Not included	Hiskes 1996, Datskos 1997

Additionally:

- Available are ro-vibrationally resolved Corona models for Fulcher, Lyman, Werner, $a^3 \rightarrow b^3$ continuum. Partially for D_2 also.
- Planned next steps: use MCCC cross sections for fully vibrationally resolved model. H_2 and D_2.

Divertor plasmas span a wide range of temperatures and densities, necessitating collisional-radiative modeling (CRM)

Coronal equilibrium

- Collisional rates << radiative rates
- Low density, high temprature
- Excitations occur from the ground state only: limited by collisions

Hot, tenuous plasmas — Divertor plasmas — Cold, dense plasmas

Divertor plasmas span a wide range of temperatures and densities, necessitating collisional-radiative modeling (CRM)

Coronal equilibrium

- Collisional rates << radiative rates
- Low density, high temprature
- Excitations occur from the ground state only: limited by collisions

Local thermal equilibrium (LTE)

- Collisional rates >> Radiative rates
→ High densities
- Populations can be determined from energies and statistical weights
- Radiative rates negligible

Hot, tenuous plasmas ⟷ Divertor plasmas ⟷ Cold, dense plasmas

Divertor plasmas span a wide range of temperatures and densities, necessitating collisional-radiative modeling (CRM)

Coronal equilibrium

- Collisional rates << radiative rates
- Low density, high temprature
- Excitations occur from the ground state only: limited by collisions

Collisional-radiative regime

- Competing radiative and collisional processes
- Populations calculated from rate equations
  - Collisional rates
  - Radiative rates
  - Plasma effects
- Excited states substantially populated → ladder-like processes

Local thermal equilibrium (LTE)

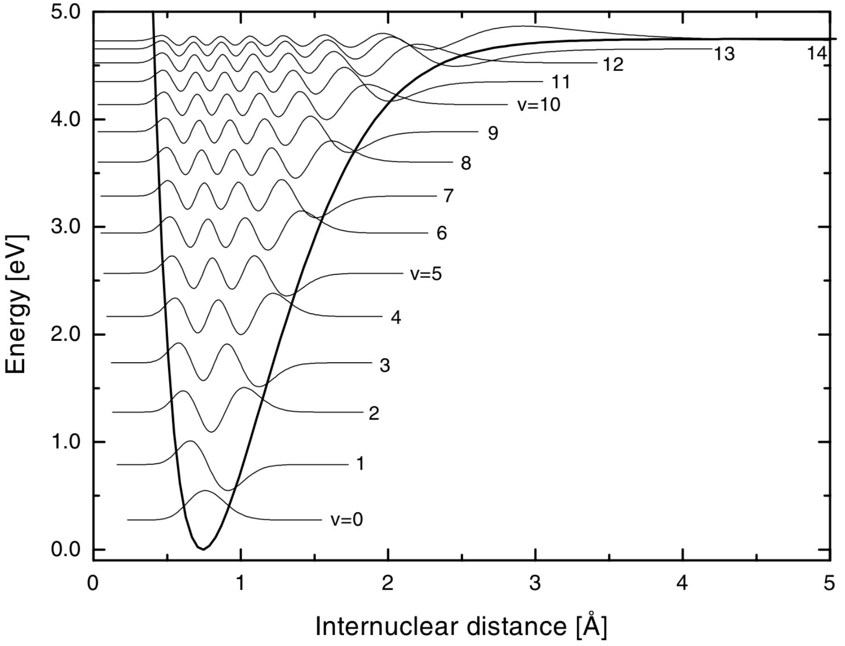
- Collisional rates >> Radiative rates
  → High densities
- Populations can be determined from energies and statistical weights
- Radiative rates negligible

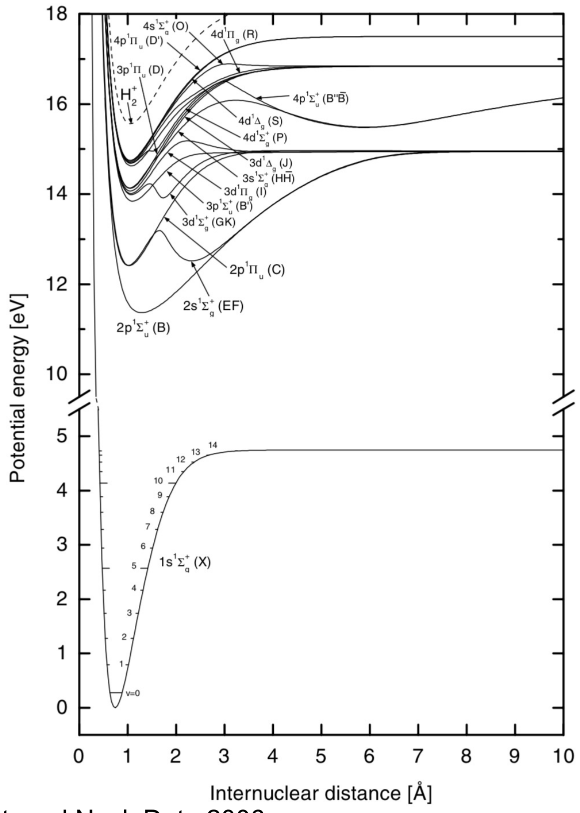
Hot, tenuous plasmas — **Divertor plasmas** — **Cold, dense plasmas**

The different vibrational level distribution of H_2 and D_2 results in fundamentally different reaction rates for the isotopologues

- Internuclear distance a function of mass

- Transition probabilities dependent on the overlap of the vibrational wave function





Fantz & Wünderlich, At. and Nucl. Data 2006