Impact of vibrationally resolved H_2 on the particle balance in Eirene simulations

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Conventionally, Eirene is run vibrationally-unresolved using effective rates calculated by an external CRM

CRM

(Collisional Radiative Model)

- 1000s of transitions and reactions
  - Vibrational
  - Electronic
  - Reactions
- $n_{H_2}^{tot} \approx n_{H_2(v=0)}$
- Local equilibrium

→ $\langle \sigma v \rangle (T_e, T_i, V_{H2}, n_e)$

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AMJUEL effective rates

- Tabulated data/fits
- $T_e = T_i$ assumed

→ $\langle \sigma v \rangle (T_e, n_e)$

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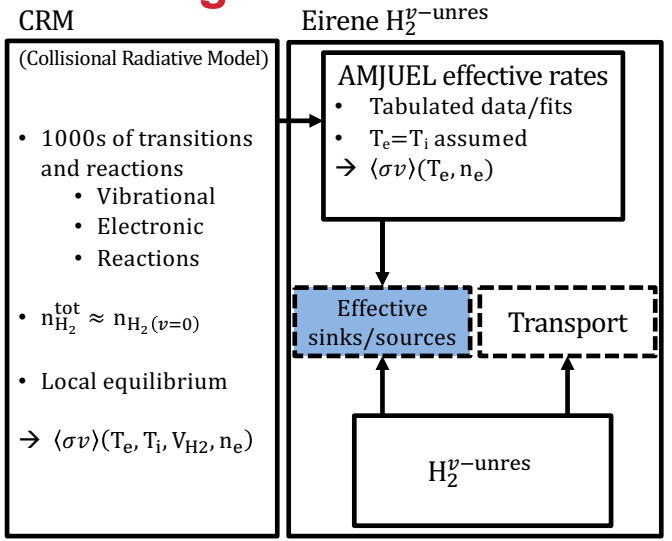

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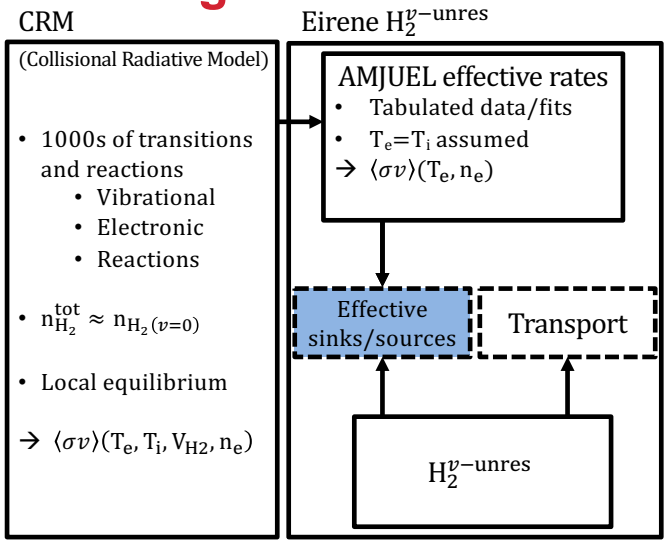

- The CRM used to derive the tabulated AMJUEL data has been phased out

→ The up-to-date CRM Yacora is used for CR calculations throughout this work

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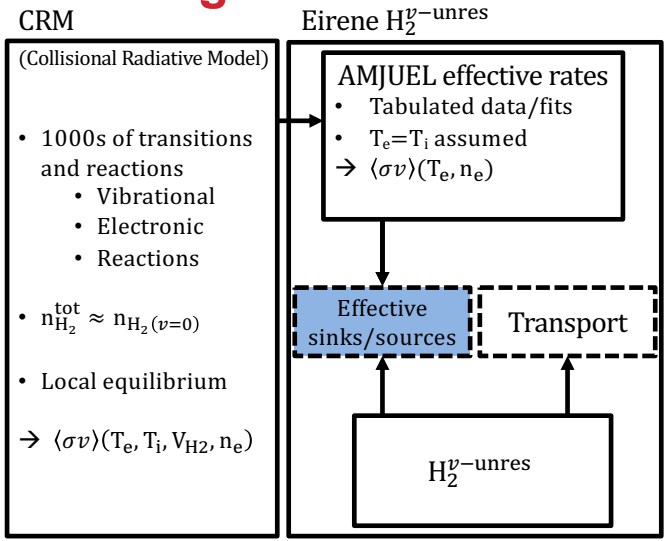

H2VIBR vibrationally resolved rates

- Same H_2 loss processes as the CRM
- Vibrational transitions (ladder-like)
- No re-distribution via electronic states
- Reaction rates assume $H_2(v)$ at rest

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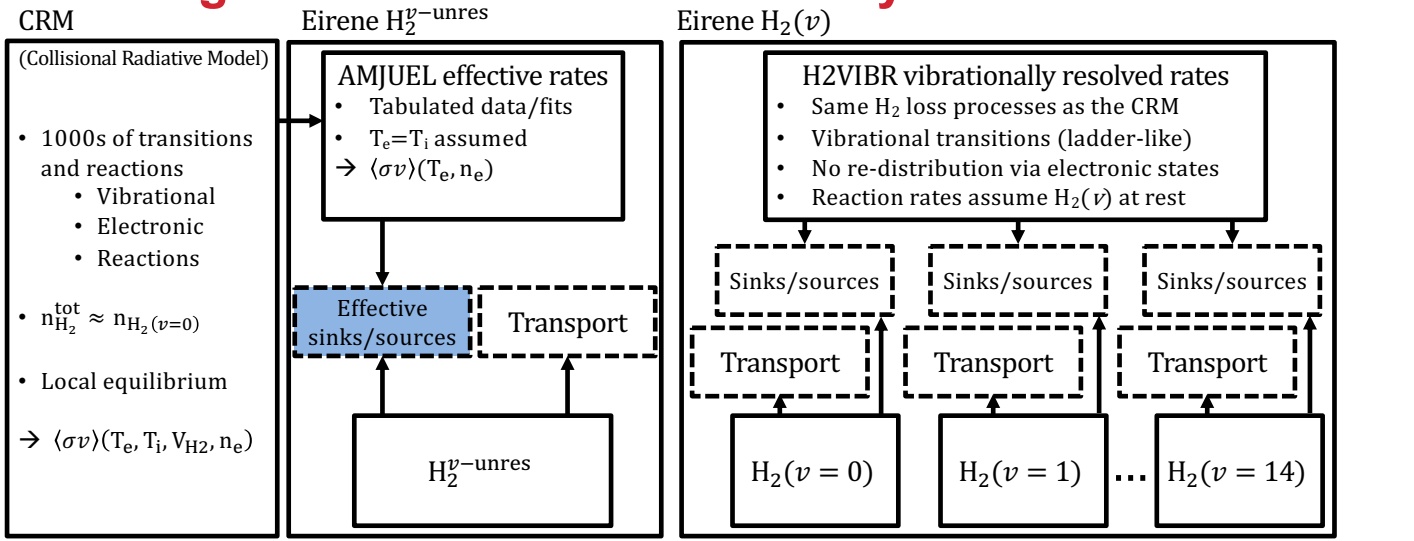

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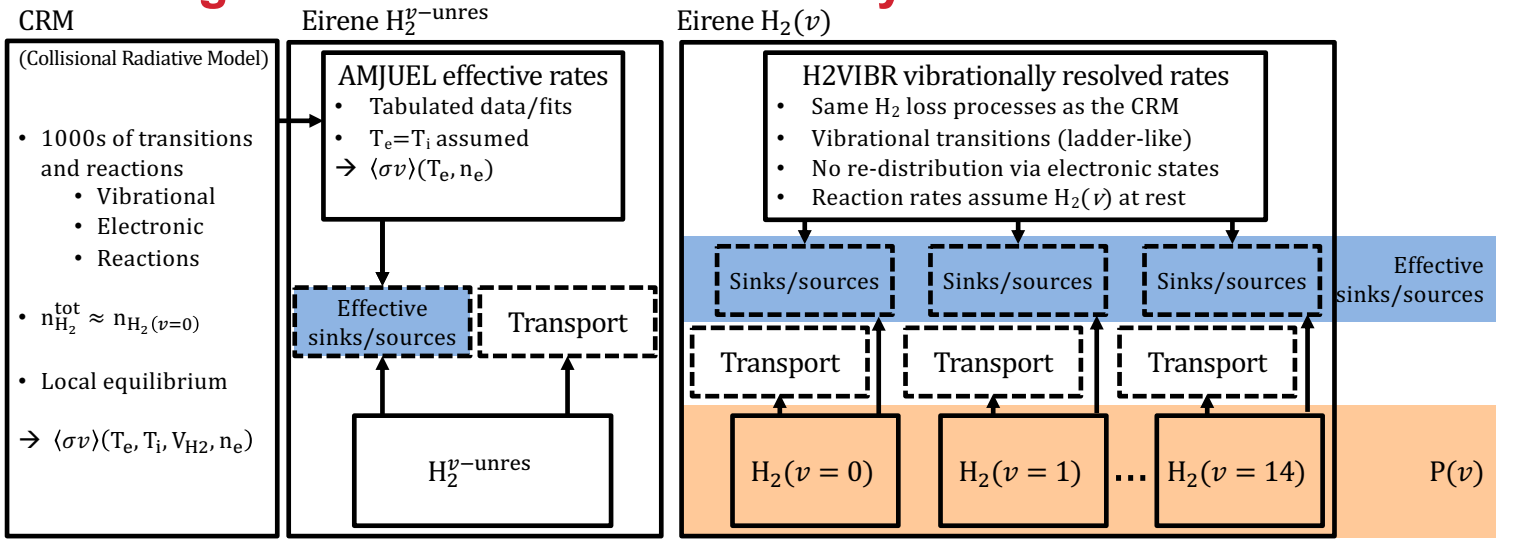


Inclusion of vibrationally resolved H_2 in B2.5-Eirene simulations was observed to re-attach SOL plasmas*

- An >50% increase in the upstream density was required to recover detachment

→ Vibrationally resolving hydrogen molecules ($H_2(v)$) may affect the upstream density threshold for detachment

- This work will investigate and explain the observed effect in order to advance future code developments

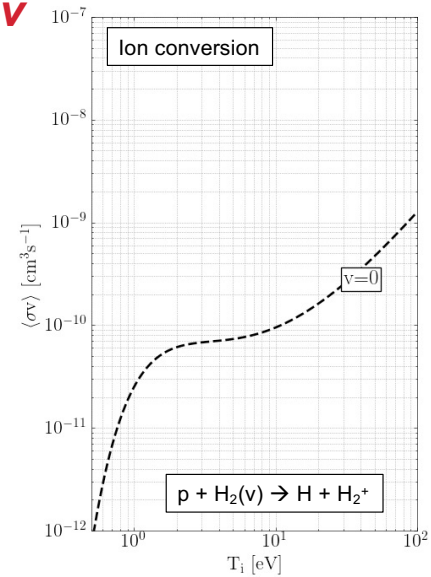
Vibrationally resolved standalone Eirene simulations predict lower effective sinks due to:

→ vibrationally resolved Eirene setup does not capture all CR effect

→ transport of vibrational states

* U. Fantz, NME (2001)

Molecular reaction rates increase by 2 orders of magnitude with increasing vibrational quantum number *v*



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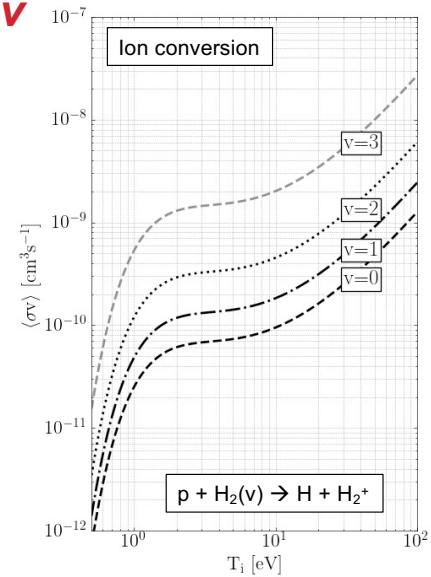

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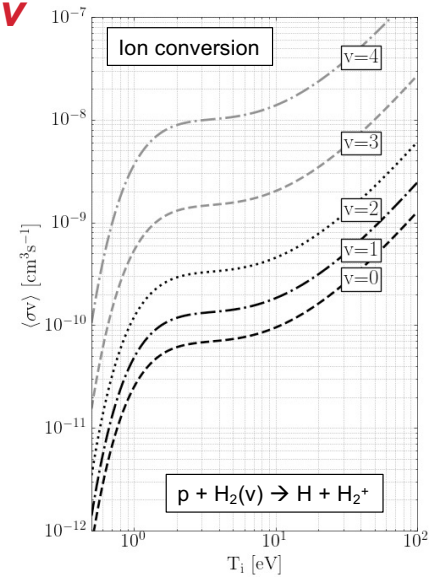

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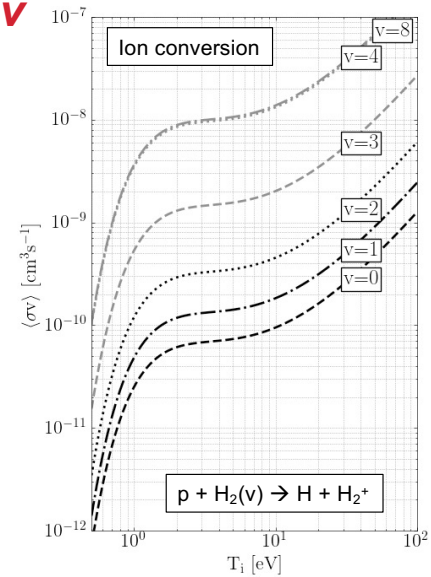
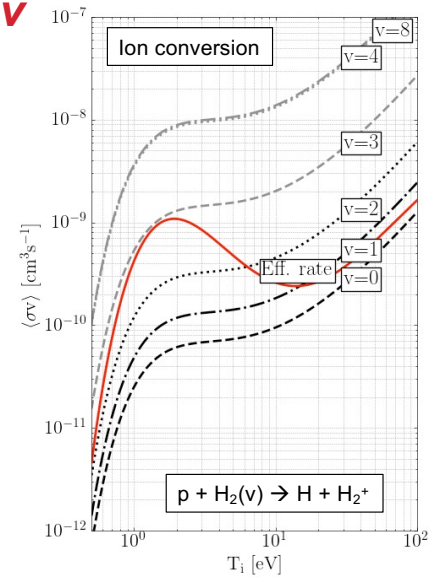
- Excitation over *v*>4 have negligible effect



Molecular reaction rates increase by 2 orders of magnitude with increasing vibrational quantum number *v*

- Excitation over *v*>4 have negligible effect
- CRMs derive the effective reaction rates
- 0D models, local equilibrium assumed

→ The equilibrium vibrational distribution $P_{eq}(v)$ is calculated



CR modeling necessary when the system is in neither coronal or local thermodynamic equilibrium (LTE)

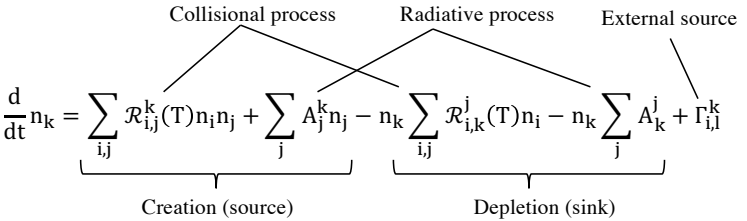
- Coronal equilibrium: excitation an ionization from ground state only, radiation-dominated
  - High temperature, low density

- LTE: each process balanced by its inverse reaction, collision dominated
  - Electron densities in excess of 10^{23} m^{-3}

- Collisional and radiative process in competition for excited states

→ Multi-step processes

CR models linearizes large multi-species systems with density and temperature-dependent reaction



Linearization of the ODEs for suitable $n_{B1} \in B$:

$$\dot{\mathbf{n}}_A = \mathbf{M}(n_{B1}, \dots, n_{BN})\mathbf{n}_A + \mathbf{\Gamma}_A(n_{B1}, \dots, n_{BN})$$

Rate matrix – dependent on the atomic and molecular physics included

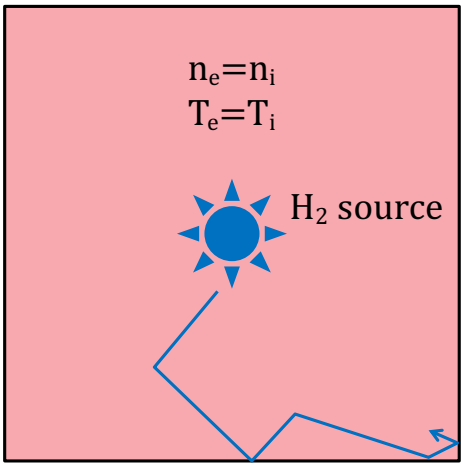
CRM densities

External source

- The CRM model consists of a plasma background $B = \{e^-, p, \dots\}$ and the collisionally-radiatively modeled species $A = \{H^0, H_2, H^*, \dots\}$
- $k, j \in A$ and $i, l \in B$
- $\mathcal{R}^k_{i,j}(T)$ is the reaction rate of collisions between i and j yielding k
- A^k_j is the Einstein coefficient describing radiative decay from j to k
- Γ_k describes production of k from reaction of species $\in B$

Vibrational distributions $P(v)$ calculated using transport-free Eirene $H_2(v)$ simulations match those predicted by Yacora

- The H2VIBR reactions were supplied to Yacora



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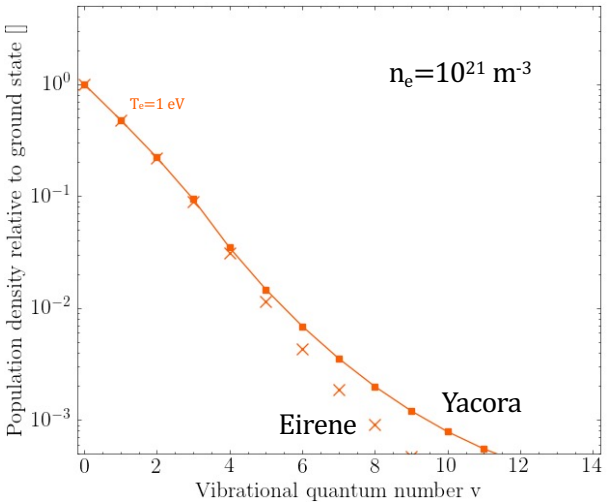

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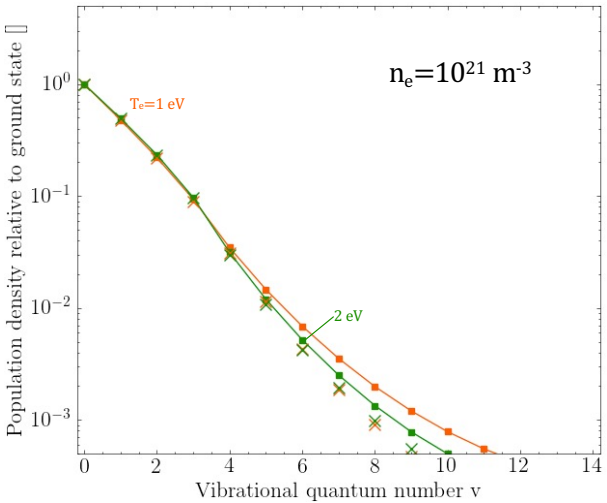

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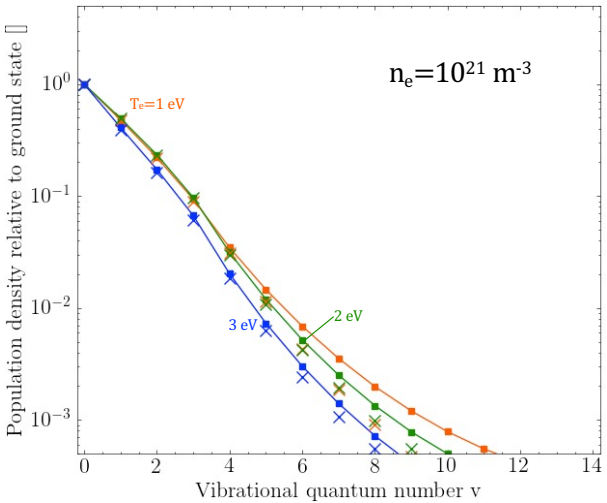

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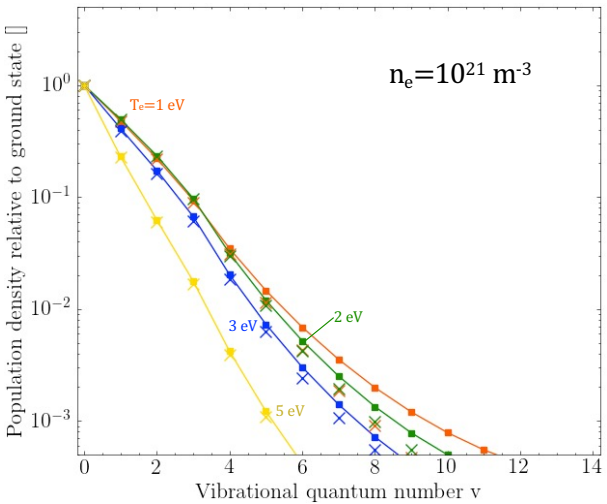

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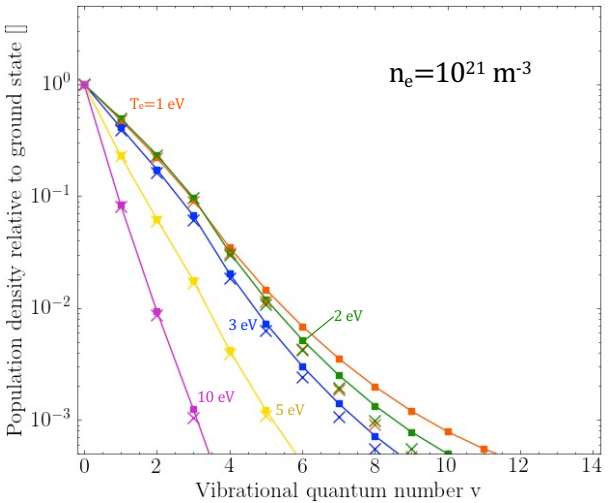
- $\mathrm{T_e} \gtrsim 5$ eV: $\mathrm{n_{H2}} \rightarrow 0\ \mathrm{m^{-3}}$ and ionization-dominated plasmas



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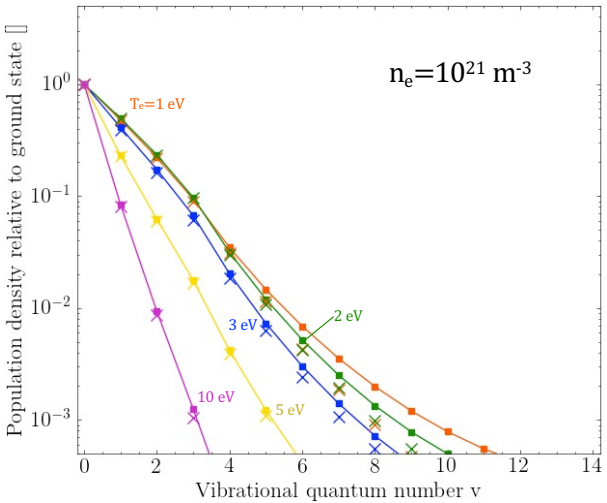
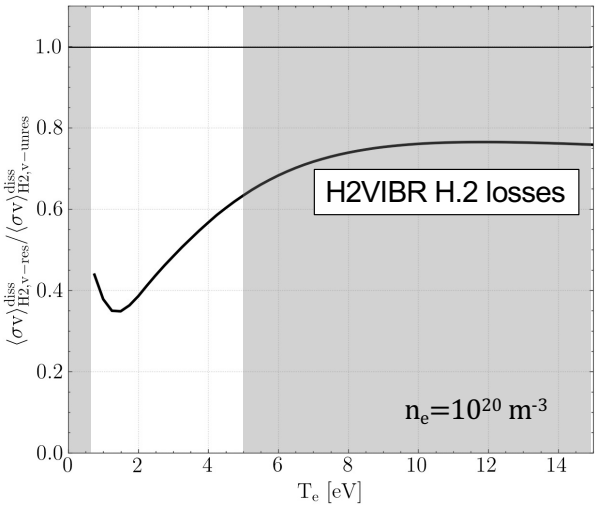
- No electronic transitions considered in the Eirene $\mathrm{H}_2(v)$ setup → P(v) density-independent



The effective dissociation rate is 20-60% lower for vibrationally resolved vs. unresolved H_2 in Eirene

- Effective rates are compared for the two setups, as P(v) not available
- The same H_2 loss processes are considered by both vibrationally resolved and unresolved setup



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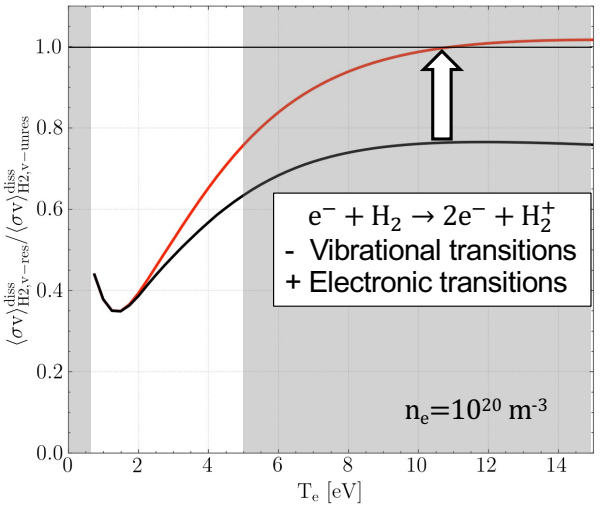

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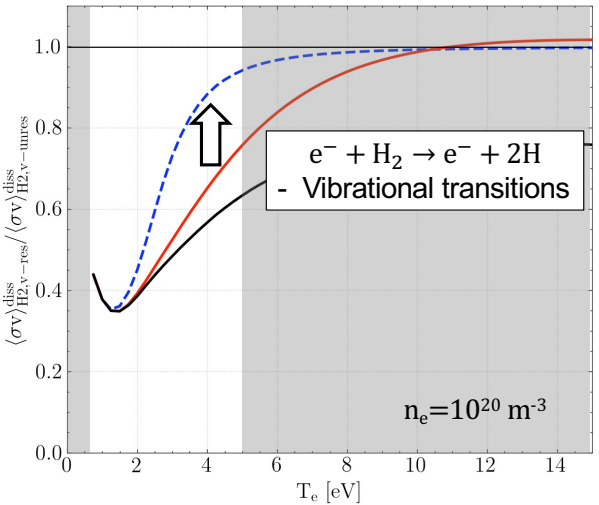

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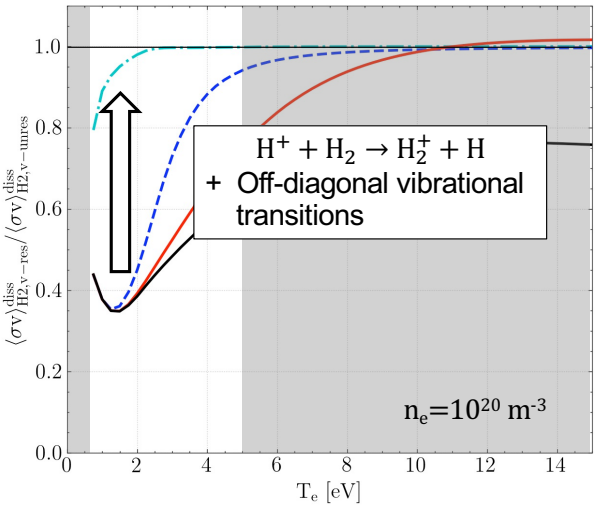

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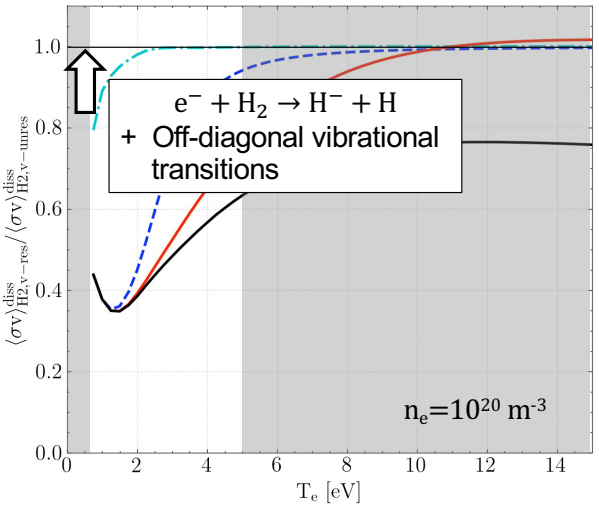
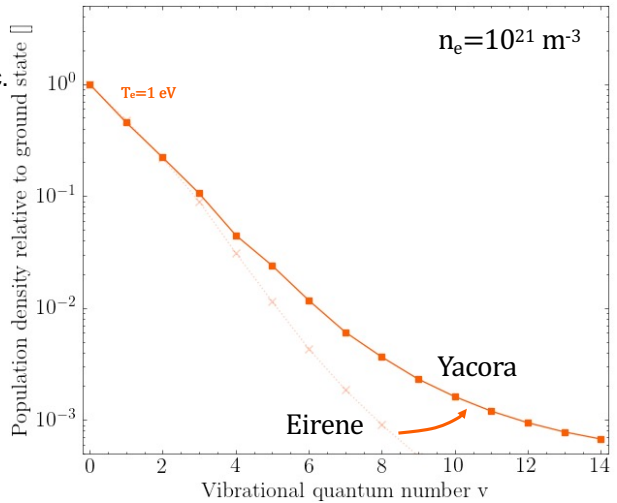
- Differences caused by omission of some CR processes in the H2VIBR data



Re-distribution via electronically excited states shifts $\mathrm{P}(v)$ to higher v, increasing the effective dissociation rate

- Full set of Yacora CR data used
  - Electronic transitions, full vibrational transition matrix, etc.



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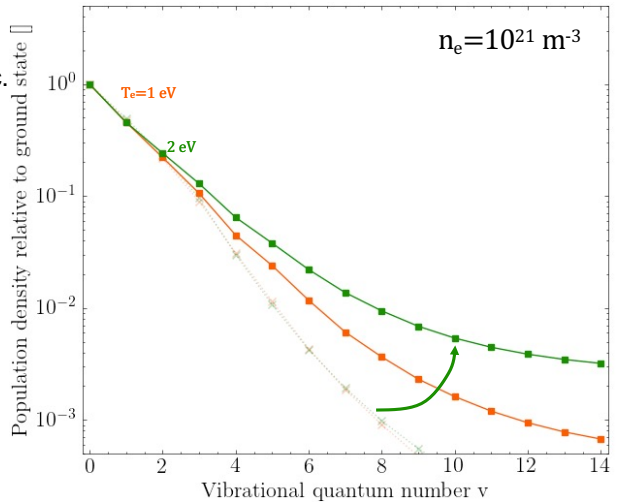

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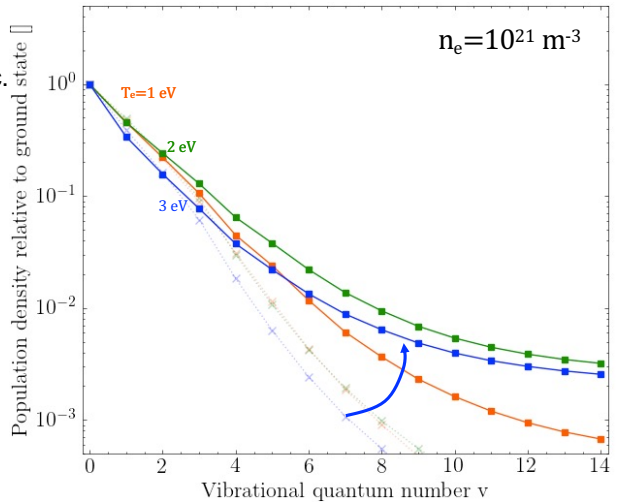

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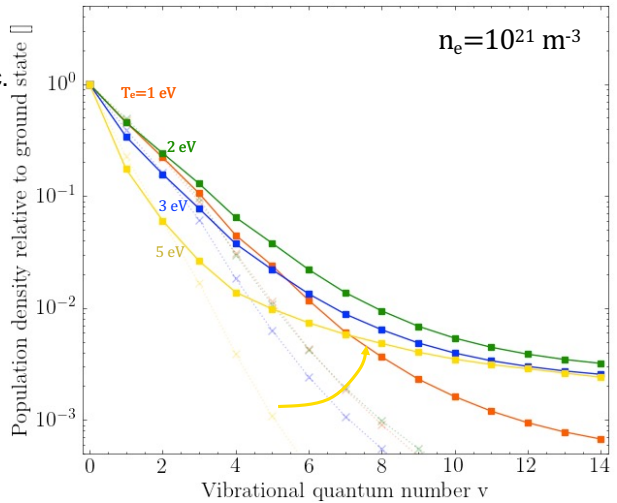

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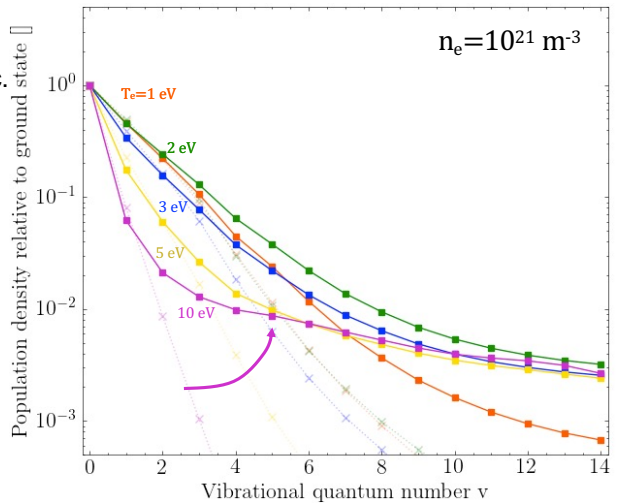

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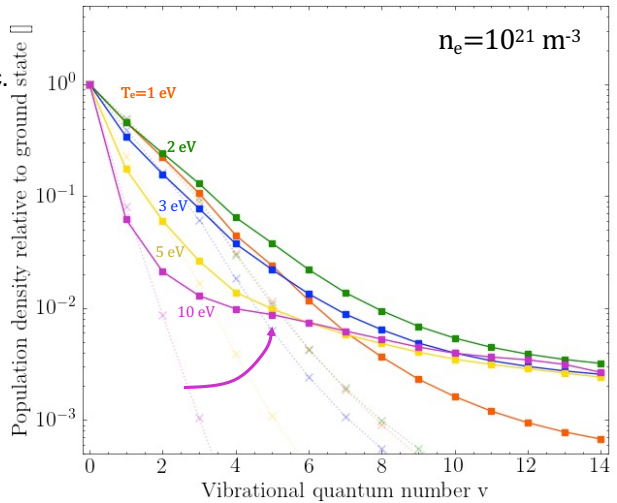
- Strong dependency of reaction rates on *v*

→ Even small shifts of P(*v*) may significantly impact the effective rates



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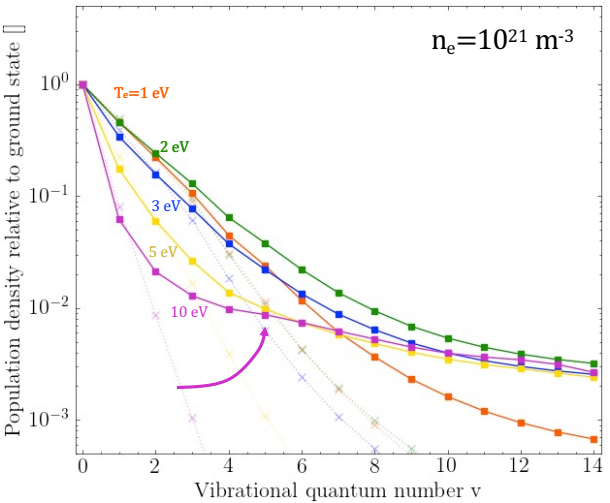

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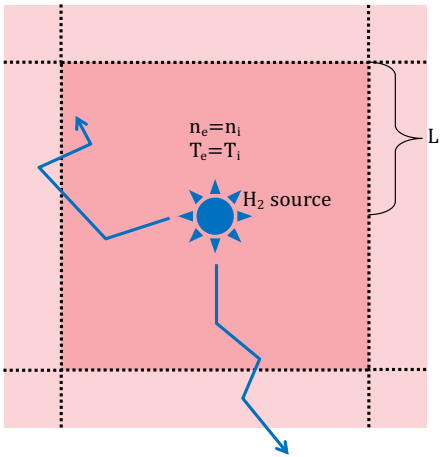
Finite $\lambda_{mfp}^{P_{eq}(v)}$ results in P(v) peaked at lower v for the Eirene $H_2(v)$ simulations compared to Yacora simulations



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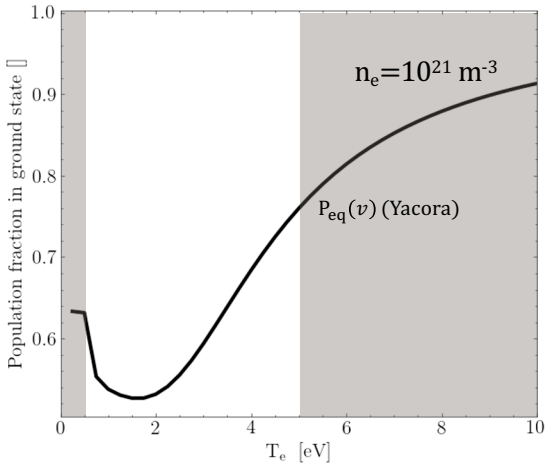

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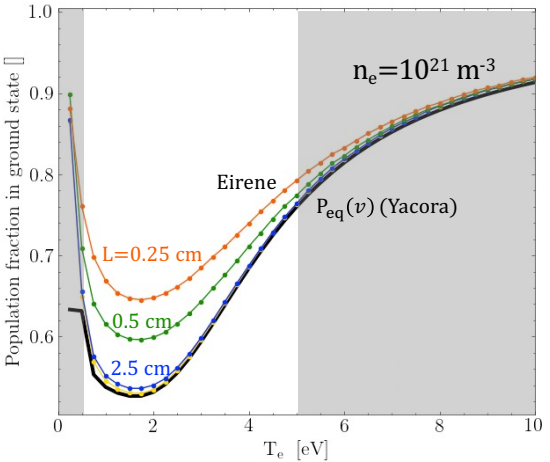

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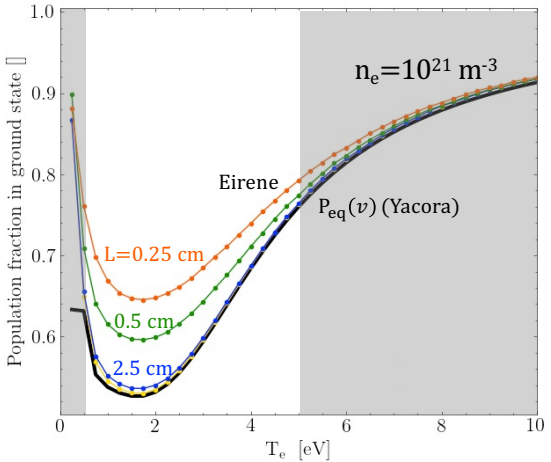
n_e	10^{21} m^{-3}	10^{20} m^{-3}	10^{19} m^{-3}
$\lambda_{mfp}^{P_{eq}(v)}$	~2.5 cm	~10 cm	>10 cm



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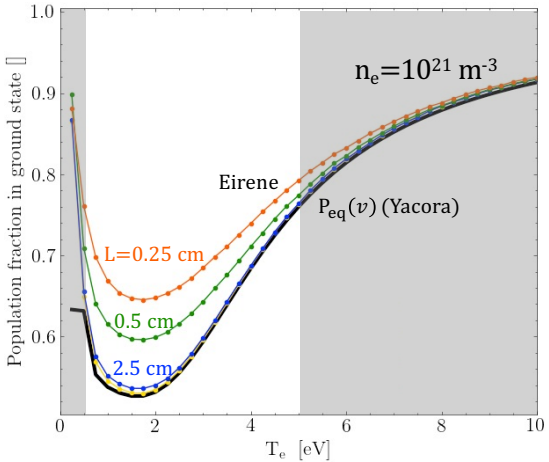
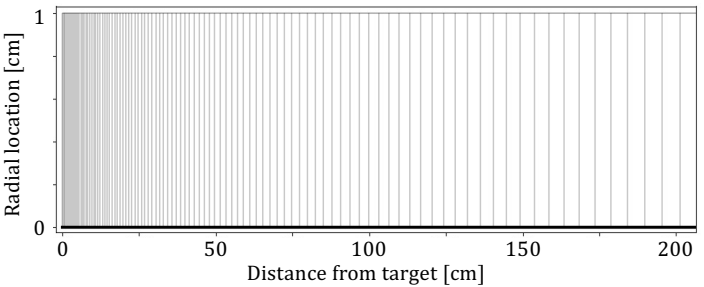
n_e	10^{21} m^{-3}	10^{20} m^{-3}	10^{19} m^{-3}
$\lambda_{mfp}^{P_{eq}(v)}$	~2.5 cm	~10 cm	>10 cm

- If the domain size is shorter than $\lambda_{mfp}^{P_{eq}(v)}$ the molecule escapes before reaching $P_{eq}(v)$

→ Shifts P(v) to lower v



The effect of transport of $H_2(v)$ on particle balance was assessed by 1D simulations for a flux tube were performed



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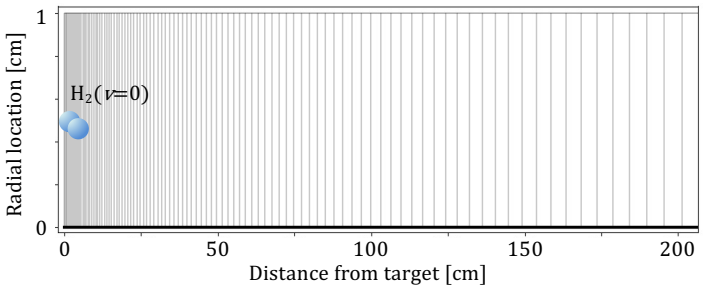

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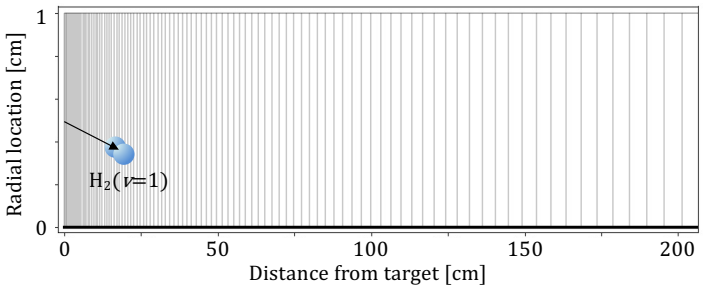
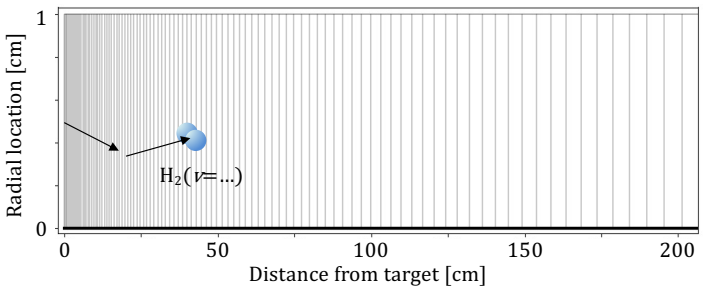
- Fluxes recycled as $H_2(v=0)$ at the target
- $H_2(v=0)$ is transported upstream before becoming vibrationally excited



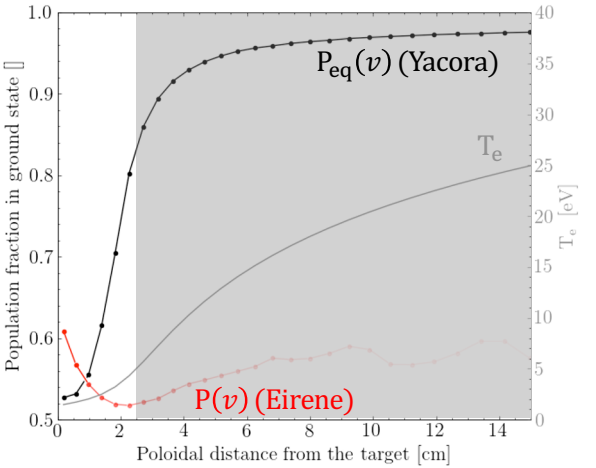
The effect of transport of $H_2(v)$ on particle balance was assessed by 1D simulations for a flux tube were performed

- Fluxes recycled as $H_2(v=0)$ at the target
- $H_2(v=0)$ is transported upstream before becoming vibrationally excited



Eirene simulations on a 1D flux tube do not achieve $P_{eq}(v)$ due to the finite $\lambda_{mfp}^{P_{eq}(v)}$

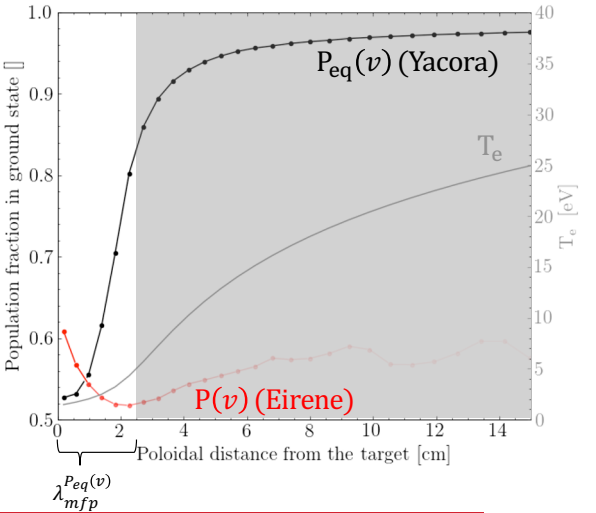
- Temperature and density gradients makes $P_{eq}(v)$ unachievable



Eirene simulations on a 1D flux tube do not achieve $P_{eq}(v)$ due to the finite $\lambda_{mfp}^{P_{eq}(v)}$

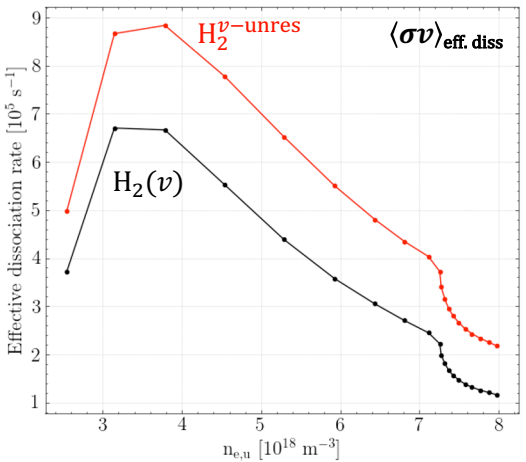
- Temperature and density gradients makes $P_{eq}(v)$ unachievable
- Transport upstream results in increasing temperature and decreasing density

→ H_2 does not achieve $P_{eq}(v)$ before being dissociated



The unequilibrated $\mathrm{P}(v)$ results in a weaker dissociation sink for the vibrationally resolved vs unresolved Eirene results

- The decreased effective dissociation sink results in higher H_2 and lower H density

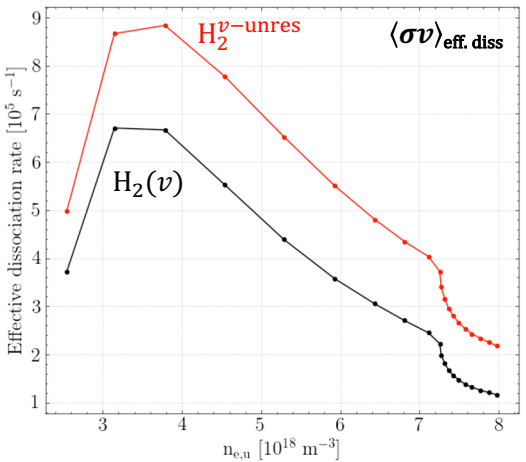


The unequilibrated $\mathrm{P}(v)$ results in a weaker dissociation sink for the vibrationally resolved vs unresolved Eirene results

- The decreased effective dissociation sink results in higher H_2 and lower H density

→ Fewer neutral particles available for momentum exhaust

→ Fewer atoms available for radiative exhaust (stronger radiator than H_2)



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Upstream transport of vibrational states prevents vibrational equilibration, decreasing the effective dissociation rate

- However, the vibrationally resolved setup does not consider significant reactions considered by the CR model, further reducing the effective dissociation rate by 20-60%.

- Both effects contribute to a decrease in dissociation, impacting particle, momentum, and radiation balance: simultaneous evaluation is not presently possible.

→ By coupling Eirene to a CRM, such as Yacora, the full set of reactions, transport of vibrational states, and ion-electron equilibration could be evaluated simultaneously.

Outlook and acknowledgements

- Assess the validity and effect of assumptions ($T_e = T_i$, $n_{H2}^{tot} = n_{H2(v=0)}$, etc)
- Extend work to include isotopologues (D_2, T_2, DT)
- Investigate bundling schemes of vibrational states
- Evaluate impact of the initial vibrational distribution

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