CRUMPET, EIRENE A&M data, and CRMs

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YACORA A&M data discussion

Remote connection

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Ongoing work with the multi-fluid neutral code UEDGE initialized the work with the EIRENE neutral model

- CRUMPET was developed in order to implement a CR model into the multi-fluid code UEDGE

- CRUMPET/UEDGE predictions were compared to standalone EIRENE simulations for verification purposes

- The role of vibrational molecules was investigated → outstanding questions regarding vibrationally resolved rates, processes, isotopologues, etc.

- L-mode deuterium experiments in DIII–D with HR-VUV of the molecular Fulcher band

CRUMPET is a Python tool for evaluating neutral processes and creating CRMs

- Reads A&M data from various databases (AMJUEL/ADAS/HYDHEL/H2VIBR etc)

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```
** SETTINGS
# Define the most central parameters to the simulations

# Maximum number of molecular vibrational levels to be considered
* vmax       14
# Maximum number of atomic excited levels to be considered
* nmax        8
# P-space size: P-space is built on the NW corner of the rate matrix..
# Thus, the first Np entries of species are considered to belong to the P-space.
# The Q-space is taken as the inverse intersect of N and P spaces
* Np          2
* Isotope   H
* Mass        1

# Initial densities
# Species without specified densities are assumed to be zero at t=0
* n0
H(n=1)        0e12
H2(v=0)       1e10
* verbose    0    # Show verbose output
```

```
** SPECIES
* H(n=1)
      V 2.375
* H2(v=0)
      V 0.27504
* H2+
      V 15.56
* H2(v=1)
      V 0.79104
* H2(v=2)
      V 1.27809
* H2(v=3)
      V 1.73664
* H2(v=4)
      V 2.16685
* H2(v=5)
      V 2.56873
* H2(v=6)
      V 2.94214
* H2(v=7)
      V 3.28667
* H2(v=8)
      V 3.60148
* H2(v=9)
      V 3.88512
* H2(v=10)
      V 4.13553
* H2(v=11)
      V 4.34985
* H2(v=12)
      V 4.52401
* H2(v=13)
      V 4.65343
```

```
** RATES
# Define the files for the standard inputs
AMJUEL   rates/amjuel.tex
HYDHEL   rates/hydhel.tex
H2VIBR   rates/h2vibr.tex
```

```
** BACKGROUND
* e
* p
      V 15.975

** REACTIONS

* HYDHEL_2.2.4
e + H2(v=0) > e + H2(n=EF)

* HYDHEL_2.2.5
e + H2(v=0) > e + H2(n=a)

* HYDHEL_2.2.6
e + H2(v=0) > e + H(n=1) + H(n=2)
      K=2*0.3

* H2VIBR_2.$l1
e + H2(v=$) > e + 2*H(n=1)
      K=2*3
```

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- Creates a set of coupled ODE's based on a user input file

- Time-dependent simulations and analytic equilibrium solutions

$$\frac{d}{dt}n_k = \sum_{i,j} \mathcal{R}_{i,j}^k(T)n_i n_j + \sum_j A_j^k n_j - n_k \sum_{i,j} \mathcal{R}_{i,k}^j(T)n_i - n_k \sum_j A_k^j + \Gamma_{i,l}^k$$

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

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CRUMPET is a Python tool for evaluating neutral processes and creating CRMs

- Reads A&M data from various databases (AMJUEL/ADAS/HYDHEL/H2VIBR etc.)
- Creates a set of coupled ODE's based on a user input file
- Time-dependent simulations and analytic equilibrium solutions
- Used to generate and evaluate Greenland-style CRMs
  - P.T. Greenland, Proc. R. Soc. A **457** (2001) 1821

$$\begin{bmatrix} \dot{\mathbf{n}}_P \\ \dot{\mathbf{n}}_Q \end{bmatrix} = \begin{bmatrix} \mathbf{M}_P & \mathbf{H} \\ \mathbf{V} & \mathbf{M}_Q \end{bmatrix} \begin{bmatrix} \mathbf{n}_P \\ \mathbf{n}_Q \end{bmatrix} + \begin{bmatrix} \mathbf{\Gamma}_P \\ \mathbf{\Gamma}_Q \end{bmatrix}$$

$$\Downarrow$$

$$\dot{\mathbf{n}}_P = \mathbf{M}_{\text{eff}} \mathbf{n}_P + \mathbf{\Gamma}'_P,$$

where

$$\mathbf{M}_{\text{eff}} = \mathbf{M}_P - \mathbf{H} \mathbf{M}_Q^{-1} \mathbf{V}$$

and

$$\mathbf{\Gamma}'_P = \mathbf{\Gamma}_P - \mathbf{\Delta} \mathbf{T}_Q^{-1} \mathbf{\Gamma}_Q.$$
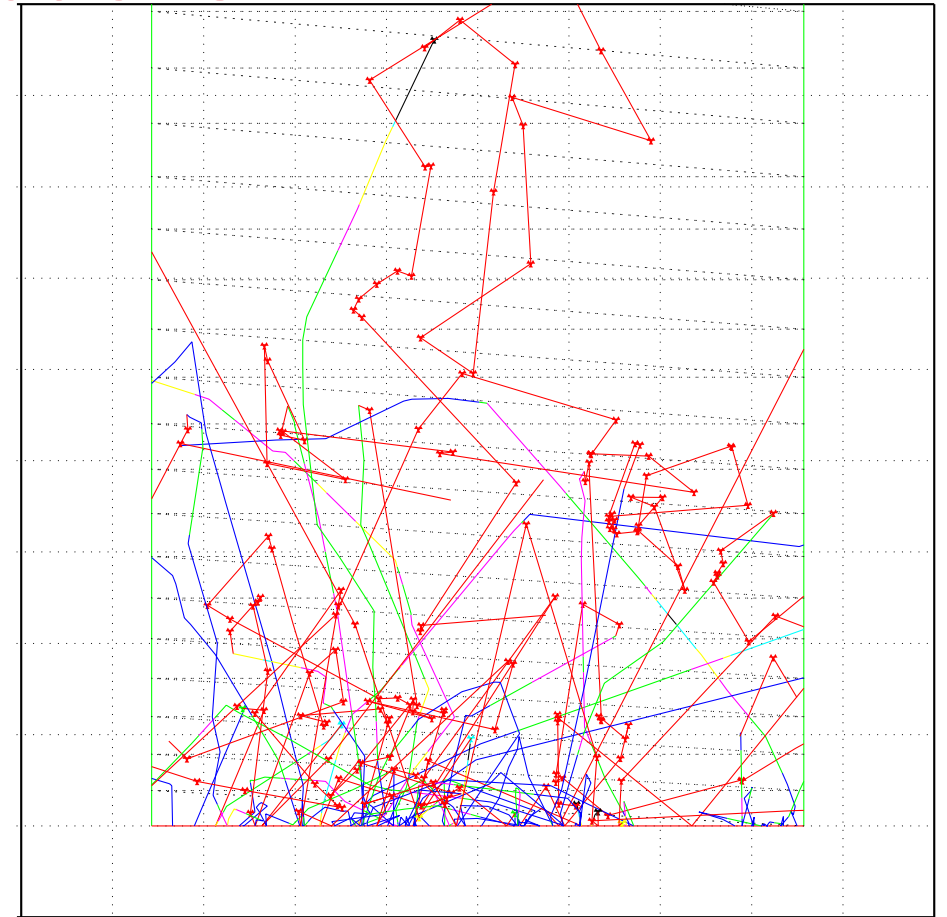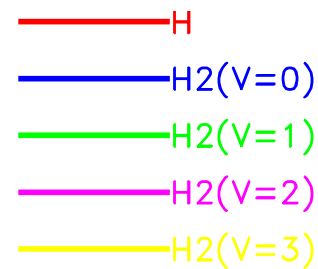
Here,

$$\mathbf{MT} = \mathbf{TD} = \begin{bmatrix} \mathbf{T}_P & \mathbf{\Delta} \\ \mathbf{\delta} & \mathbf{T}_Q \end{bmatrix} \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$$

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The CRUMPET/UEDGE simulations were compared to vibrationally unresolved EIRENE simulations

- Vibrationally "unresolved" rates "implicitly" assumes a vibrational distribution
  - → P(v) evaluated by Sawada/Fujimoto's CRM

- EIRENE applies effective CR rates "piecewise" (e.g. postprocessing, etc.) in a manner that might not be self-consistent when run vibrationally unresoved
  - → Propagation and stacking of errors due to approximations/simplifications

- Discrepancies observed between vibrationally resolved and unresolved EIRENE simulations for simple geometries
  - → Differences in P(v) predicted by EIRENE and the CRM (transport effects)
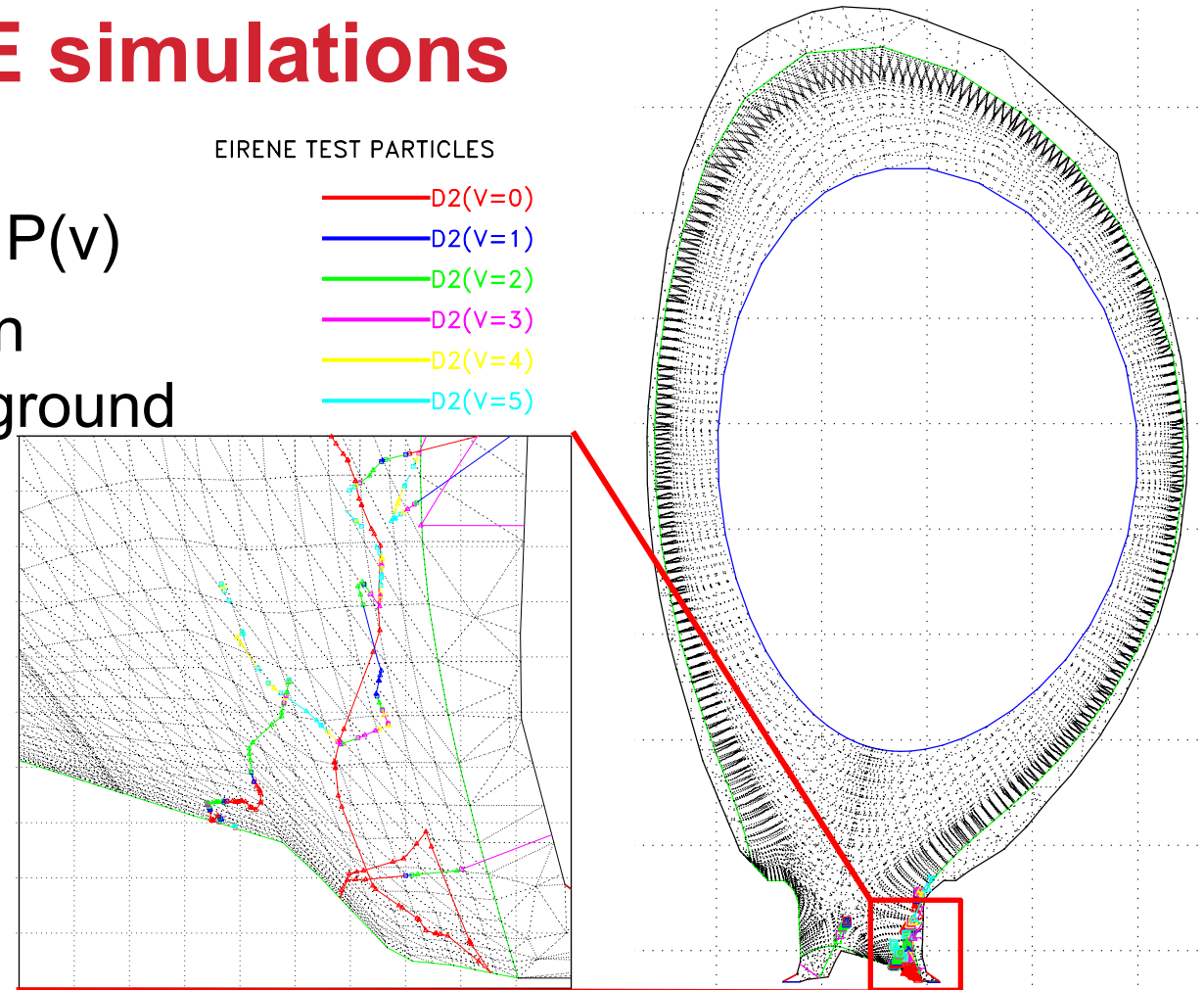
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The role of vibrational excitation was investigated using standalone EIRENE simulations

- Simulations of a single flux-tube highlights the role of transport on P(v)

Legend:
- H (red)
- H2(V=0) (blue)
- H2(V=1) (green)
- H2(V=2) (magenta)
- H2(V=3) (yellow)

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The role of vibrational excitation was investigated using standalone EIRENE simulations

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- Standalone JET simulations on an EDGE2D-predicted plasma background

EIRENE TEST PARTICLES

- D2(V=0)
- D2(V=1)
- D2(V=2)
- D2(V=3)
- D2(V=4)
- D2(V=5)

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The role of vibrational excitation was investigated using standalone EIRENE simulations

- Simulations of a single flux-tube highlights the role of transport on P(v)

- Standalone JET simulations on an EDGE2D-predicted plasma background

→ Coupled SOLPS-ITER runs of a slab to evaluate the impact on the plasma: JET L-mode cases generated, to be run

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A better grasp on the atomic and molecular physics of EIRENE is required

- What are the underlying assumptions and validity range of the EIRENE A&M data?

- How large is the effects of these assumptions compared to a full/on-the-fly CRM?

- Are the AMJUEL and H2VIBR rates used by EIRENE replicable?

- How to update and maintain the EIRENE A&M data?
  - Pick up Reiter's version of the Sawada/Fujimoto code or switch to something else (YACORA)

YACORA is a well-developed, established CRM with a comprehensive, up-to-data molecular database

- The accuracy of CRM predictions is subject to the accuracy and availability of the A&M data
  - Electronically resolved
  - Vibrationally resolved (also for n>1)
  - Rotationally resolved (also for n>1)
  - First-order data for isotopologues

- Web version provides access to output of CRM $\Rightarrow$ CRM setup, rates, and other "switches" desired for making a comparative investigation

The full capabilities of YACORA would enable comparison to the EIRENE A&M data

- Comparison of effective AMJUEL and vibrationally resolved H2VIBR rates
- Comparison of molecular radiation (Fulcher, Ly-We, H_α/D_α)
- Role and impact of resolving isotopologues (if D rates available in YACORA)
- Impact of "piecewise" post-processing vs full CR evaluation
- Assessment of P(v)
- Assessment of the assumption/simplification validity and impact
  - $T_e = T_i$, $n_e = n_i$, E=0.1 eV, no $H_2(n)$ excitation, etc.
- Momentum losses due to resonant CX from H(n>1)
- Evaluating molecular processes from experimental spectra with local n_e, T_e measurements

EIRENE A&M data must be better understood: YACORA could be used to verify, understand, and extend the A&M data

- Comparison and verification of reaction cross-sections/rates and simulations
- Inclusion of additional effects via post-processing and extension of A&M data

- Accessing, learning and using "full" YACORA

  vs

- Using CRUMPET with YACORA data, after YACORA-CRUMPET verification

→ Replacement of Reiter's version of the Sawada/Fujimoto CRM with YACORA?

Backups

CRUMPET creates a set of coupled ODEs

Collisional process   Radiative process   External source

$$\frac{d}{dt}n_k = \underbrace{\sum_{i,j} \mathcal{R}_{i,j}^k(T)n_i n_j + \sum_j A_j^k n_j}_{\text{Creation (source)}} - \underbrace{n_k \sum_{i,j} \mathcal{R}_{i,k}^j(T)n_i - n_k \sum_j A_k^j}_{\text{Depletion (sink)}} + \Gamma_{i,l}^k$$

The CRM model consists of a plasma background $B = \{e^-, p, ...\}$ and the collisionally-radiatively modeled species $A = \{H^0, H_2, H^*, ...\}$

$k, j \in A$ and $i, l \in B$

$\mathcal{R}_{i,j}^k(T)$ is the reaction rate of collisions between i and j yielding k

A_j^k is the Einstein coefficient describing radiative decay from j to k

Γ_k describes production of k from reaction of species $\in B$

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

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

Rate matrix   CRM densities   External source

Dependent on the atomic and molecular physics included

CRUMPET evaluates the CRM according to Greenland

- Divide the states into two subsets **P** and $\mathbf{Q} = \mathbf{A} \backslash \mathbf{P}$ with corresponding projection operators P and Q projecting out the subsets, and rearrange the linearized problem

P-species contribution to P-population   Q-species contribution to P-population

$$\begin{bmatrix} \dot{\mathbf{n}}_P \\ \dot{\mathbf{n}}_Q \end{bmatrix} = \begin{bmatrix} \mathbf{M}_P & \mathbf{H} \\ \mathbf{V} & \mathbf{M}_Q \end{bmatrix} \begin{bmatrix} \mathbf{n}_P \\ \mathbf{n}_Q \end{bmatrix} + \begin{bmatrix} \mathbf{\Gamma}_P \\ \mathbf{\Gamma}_Q \end{bmatrix}$$

P-species contribution to Q-population   Q-species contribution to Q-population

- Diagonalizing the matrix, and under the assumption that $\mathbf{T}_Q^{-1}\boldsymbol{\delta} \ll \mathbf{1}$ the P-space population evolution can be solved:

$$\dot{\mathbf{n}}_P = \mathbf{M}_{\mathrm{eff}} \mathbf{n}_P + \mathbf{\Gamma}_P'$$

where

P→Q reactions, redistribution within Q-population, Q→P reactions
"Sinks and sources of the P-species mediated by the Q-species"

$$\mathbf{M}_{\mathrm{eff}} = \mathbf{M}_P - \mathbf{H}\mathbf{M}_Q^{-1}\mathbf{V}$$

External Q-source redistributed to the P-population

$$\mathbf{\Gamma}_P' = \mathbf{\Gamma}_P - \boldsymbol{\Delta}\mathbf{T}_Q^{-1}\mathbf{\Gamma}_Q$$

$$\mathbf{MT} = \mathbf{TD} = \begin{bmatrix} \mathbf{T}_P & \boldsymbol{\Delta} \\ \boldsymbol{\delta} & \mathbf{T}_Q \end{bmatrix} \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$$

The standard CRUMPET input deck contains the following reactions

#	Reaction	Source	#	Reaction	Source
1	$e + H_2(n=1, v=0) \rightarrow e + H_2(n=EF)$	HYDHEL (2.2.4)	18	$e + H^- \rightarrow 3e + p$	HYDHEL (7.1.2)
2	$e + H_2(n=1, v=0) \rightarrow e + H_2(n=a)$	HYDHEL (2.2.5)	19	$p + H^- \rightarrow p + e + H(n=1)$	HYDHEL (7.2.1)
3	$e + H_2(n=1, v=0) \rightarrow e + H(n=1)+H(n=2)$	HYDHEL (2.2.6)	20	$p + H^- \rightarrow p + e + H(n=2)$	HYDHEL (7.2.2)
4	$e + H_2(n=1, v=0-14) \rightarrow e + 2H(n=1)$	H2VIBR (2.XI1)	21	$p + H^- \rightarrow p + e + H(n=3)$	HYDHEL (7.2.3)
5	$e + H_2(n=1, v=0) \rightarrow e + 2H(n=2)$	HYDHEL (2.2.7)	22	$e + H_2(n=1, v=0-14) \rightarrow e + H_2(n=1, v'=v\pm1)$	H2VIBR (2.XvY)
6	$e + H_2(n=1, v=0) \rightarrow e + H(n=1)+H(n=3)$	HYDHEL (2.2.8)	23	$H(n=1) \rightarrow H(n' < n)$	ADAS
7	$e + H_2(n=1, v=0-14) \rightarrow 2e + H_2^+$	H2VIBR (2.XI4)	24	$e + H_2(n=1, v=0-14) \rightarrow e + H_2(n=B)$	JUEL-3858
8	$e + H_2(n=1, v=0) \rightarrow e + p + H(n=1)$	HYDHEL (2.2.10)	25	$e + H_2(n=1, v=0-14) \rightarrow e + H_2(n=C)$	JUEL-3858
9	$e + H_2^+ \rightarrow 2e + 2p$	HYDHEL (2.2.11)	26	$e + H_2(n=EF) \rightarrow e + H_2(n=B)$	SAWADA 19981
10	$e + H_2^+ \rightarrow 2e + p + H(n=1)$	HYDHEL (2.2.12)	27	$H_2(n=a) \rightarrow H_2(n=b) \rightarrow 2H(n=1)$	SAWADA 1998
11	$e + H_2^+ \rightarrow 2e + p + H(n=2)$	HYDHEL (2.2.13)	28	$H_2(n=c) \rightarrow 2H(n=1)$	FANTZ 2001
12	$e + H_2^+ \rightarrow H(n=1) + H(n=2-8)$	AMJUEL (2.2.14)	29	$H_2(n=B) \rightarrow H_2(n=1, v=0-14)$	JUEL-3858
13	$e + H_2(n=1, v=0-14) \rightarrow H(n=1) + H^-$	H2VIBR (2.XI3)	30	$H_2(n=C) \rightarrow H_2(n=1, v=0-14)$	JUEL-3858
14	$p + H_2(n=1, v=0-14) \rightarrow H_2^+ + H(n=1)$	H2VIBR (2.XI2)	31	$H_2(n=B) \rightarrow 2H(n=1)$	JUEL-3858
15	$p + H_2(n=1, v=0) \rightarrow p + H_2^+ + e$	HYDHEL (3.2.5)	32	$H_2(n=C) \rightarrow 2H(n=1)$	JUEL-3858
16	$p + H_2^+ \rightarrow 2p + H(n=1)$	HYDHEL (3.2.6)	33	$e + H_2(n=1, v=0-14) \rightarrow e + H_2(n=c)$	SAWADA 1995
17	$e + H^- \rightarrow 2e + H(n=1)$	HYDHEL (7.1.1)			

CRUMPET has the capability to calculate the photon intensity locally – verification undergoing

- The CRUMPET radiation intensities are calculated using

$$\mathbf{I} = \mathbf{R}_\gamma \, \mathrm{diag}(\mathbf{n_{ss}})V,$$

where $\mathbf{R}_\gamma$ is the masked reaction matrix $\mathbf{M}$ containing radiative reactions only ($R_{i,j} = \delta(E_\gamma > 0) \sum_k \mathcal{R}_{i,k}(T) n_k$) and $\mathbf{n_{ss}}$ the steady-state neutral densities

- The calculation requires the steady-state densities of all neutral species
  → Dependent on local plasma conditions, accuracy or CR approximation, etc

The local neutral steady-state densities can be solved from the ODE system but requires knowledge of sinks & sources

- $\dot{\mathbf{n}}_A = \mathbf{M}(n_{B1}, \dots, n_{BN})\mathbf{n}_A + \mathbf{\Gamma}_A(n_{B1}, \dots, n_{BN}) = 0$
  - Solution dependent on $\mathbf{\Gamma}_A$

- Given a steady-state distribution, species lifetimes can be calculated by introducing perturbations to the steady-state

- Lifetimes can also be calculated from the eigenvalues of $\mathbf{M}$
  - $\rightarrow$ Not possible to associate eigenvalues with neutral species

CRUMPET was used to solve a set of ODE's containing the same vibrationally dependent reactions as EIRENE

Database	Rate	Reaction
AMJUEL	2.2.10	$e + H_2 \rightarrow 2e + H + H+$
H2VIBR	2.2.Xv(X-1)	$e + H_2 (v=X) \rightarrow e + H_2 (v=X-1)$
H2VIBR	2.2.Xv(X+1)	$e + H_2 (v=X) \rightarrow e + H_2 (v=X+1)$
H2VIBR	2.2Xl1	$e + H_2 (v=X) \rightarrow e + 2H$
H2VIBR	2.2Xl2	$p + H_2 (v=X) \rightarrow H + H_2^+$
H2VIBR	2.2Xl4	$e + H_2 (v=X) \rightarrow 2e + H_2^+$

- Reaction rates taken from AMJUEL and H2VIBR

- 0-dimensional (transport-free) simulations

- Particle balance conserved by source of $H_2(v=0)$

The distribution predicted by EIRENE differs significantly from CRUMPET predictions with same molecular rates
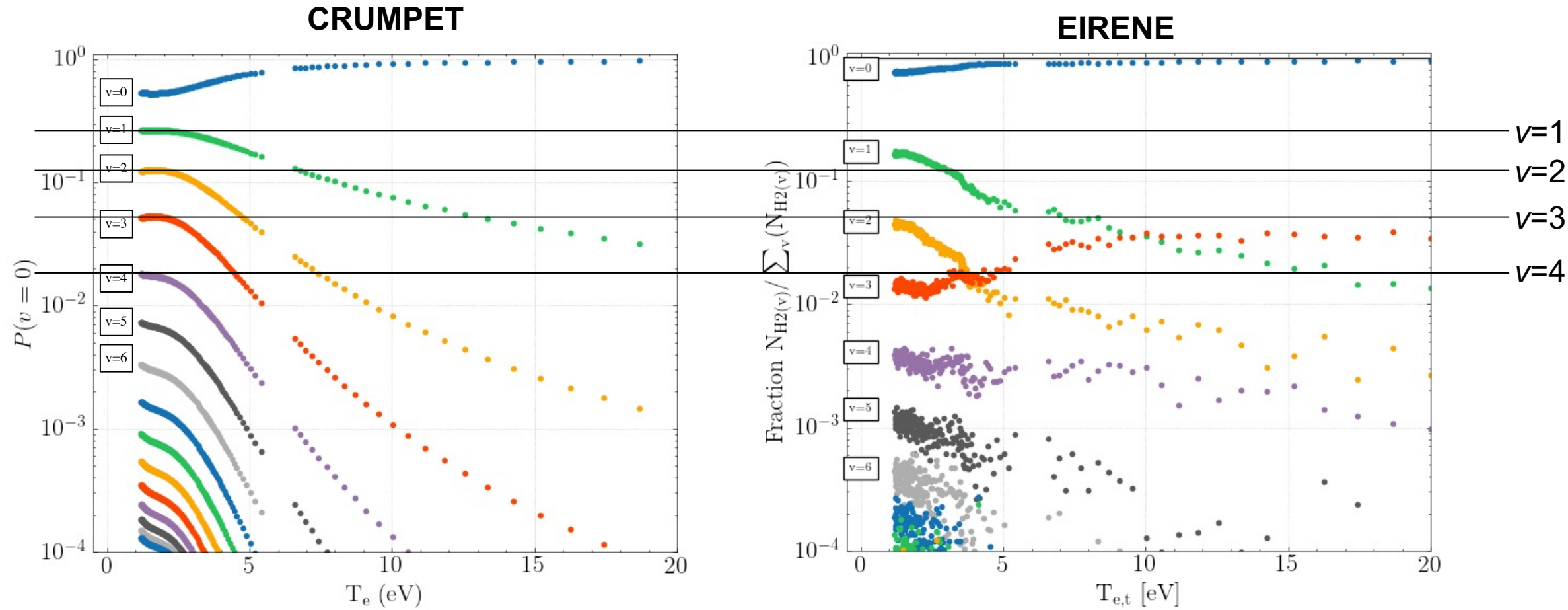
CRUMPET

EIRENE

The effect is significantly reduced when the FT width is increased from 1cm to 10cm: v=3 still shows discrepancy

CRUMPET

EIRENE

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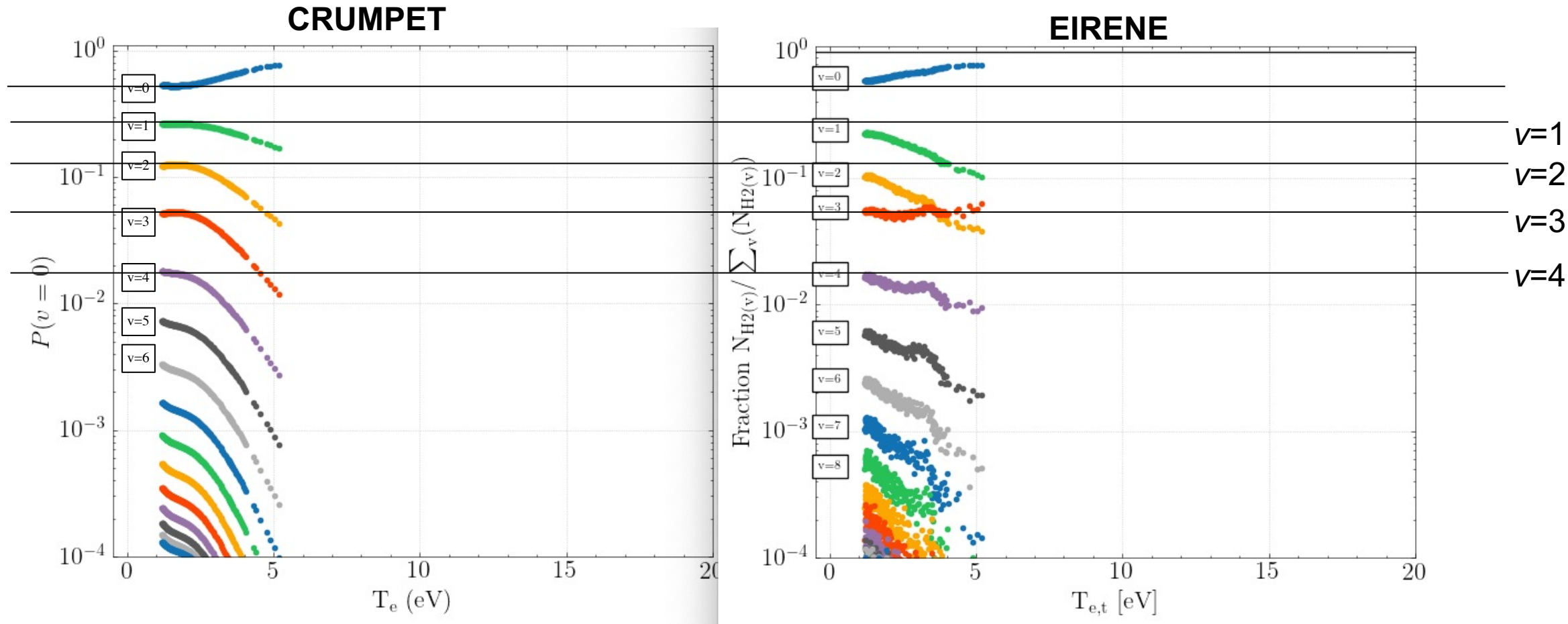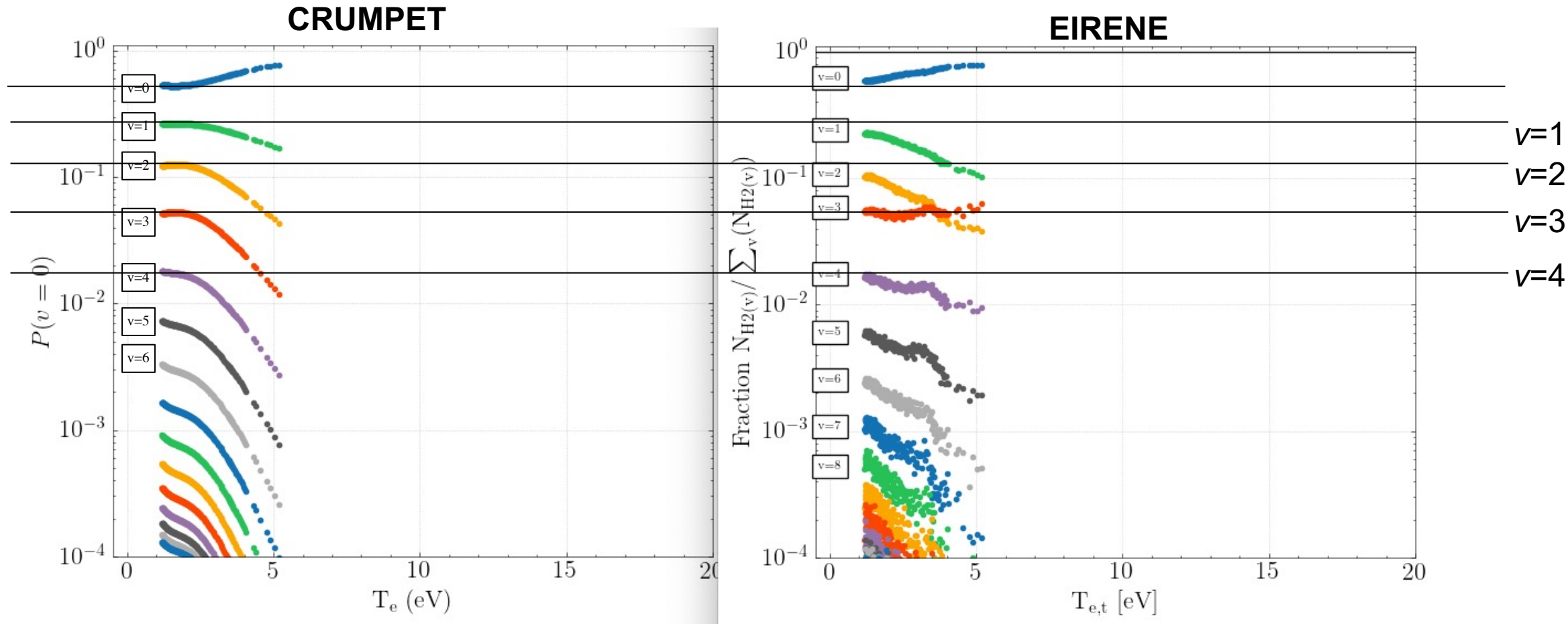
The difference between the effective rates and the vibrationally resolved rates are likely due to P(*v*)

- H2VIBR vibrational rates, including vibrational excitation, derived by rescaling original rates

- Transport of vibrationally excited molecules, which is not considered by CR modelling, likely to be the cause of the difference

H2+ creation rate

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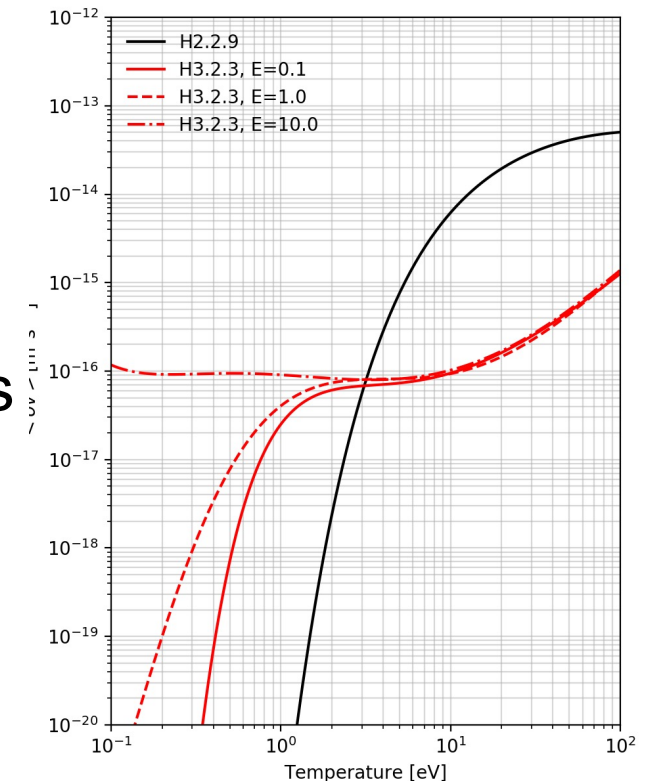
The initial state of the molecules play a significant role for the neutral content: $v=2$ agrees well with vib unresolved H_2

- The behavior supports the theory of the H_2^+ channel being the driver

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