Collisional-radiative model with molecular source for Eirene simulations

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Summary

- Reference CRM model (poster at EPS)

- Discussion:
  - Molecular Spectroscopy
  - HYDKIN: data quality assessment

Ref CRM model: motivation

- Detachment control: crucial role of molecular gas injection.
- CRM models do not account for transport (0D).
    - 1D approximation: introduction of velocity to account for beams (STRAHL code, HYDKIN).
- Parametrization of transport through effective source term.

Ref CRM model

- **Stationary Yacora run with:**

Particle species

p, H, H_2^+, H_2, Z

Reactions

$$H_2 + e \rightarrow H_2^+ + e + e$$
$$H_2 + e \rightarrow H_2(b_{triplet}) \rightarrow H + H + e$$
$$H_2 + e \rightarrow H + H^+ + e + e$$
$$H_2 + p \rightarrow H_2^+ + H$$
$$H + e \rightarrow H^+ + e + e$$
$$H_2^+ + e \rightarrow H + H^+ + e$$
$$H_2^+ + e \rightarrow H^+ + H^+ + e + e$$
$$H_2^+ + e \rightarrow H + H$$
$$Z \rightarrow H_2$$

molecular dissociation

induced ionization

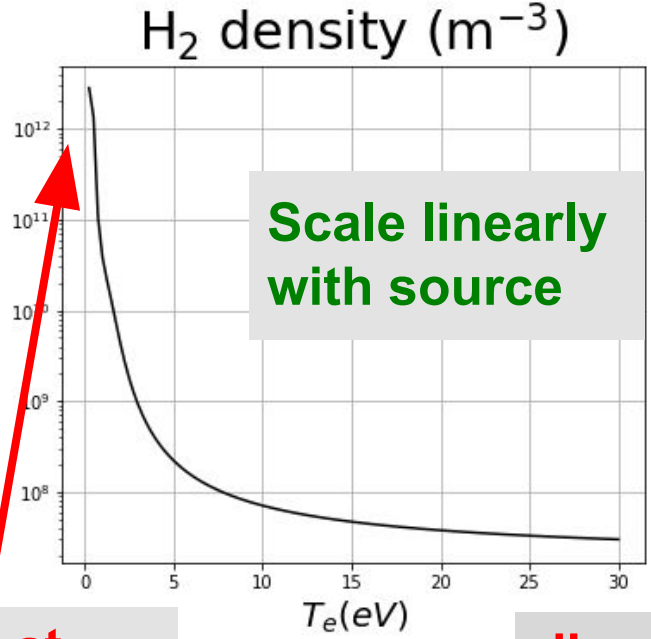
molecular ion dissociation

H_2 source term

source= 10^{21} $m^{-3}s^{-1}$

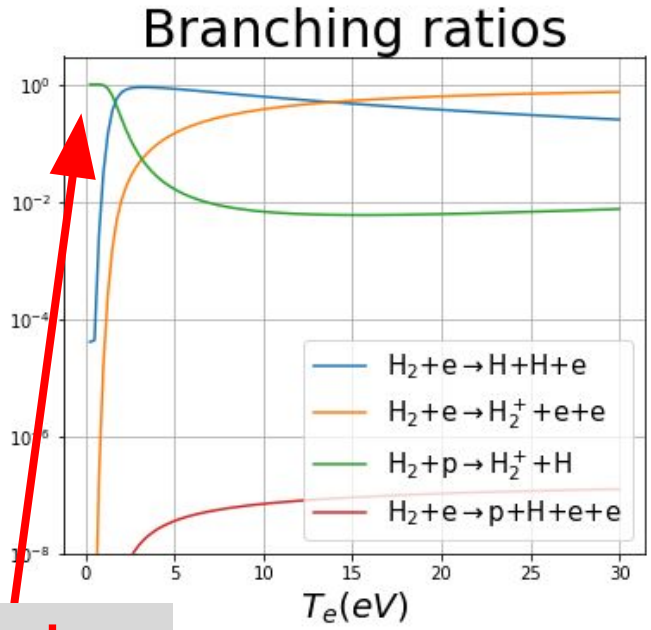
Ref CRM model

- **Stationary Yacora run:**



Scale linearly with source

Density peak at small temperature



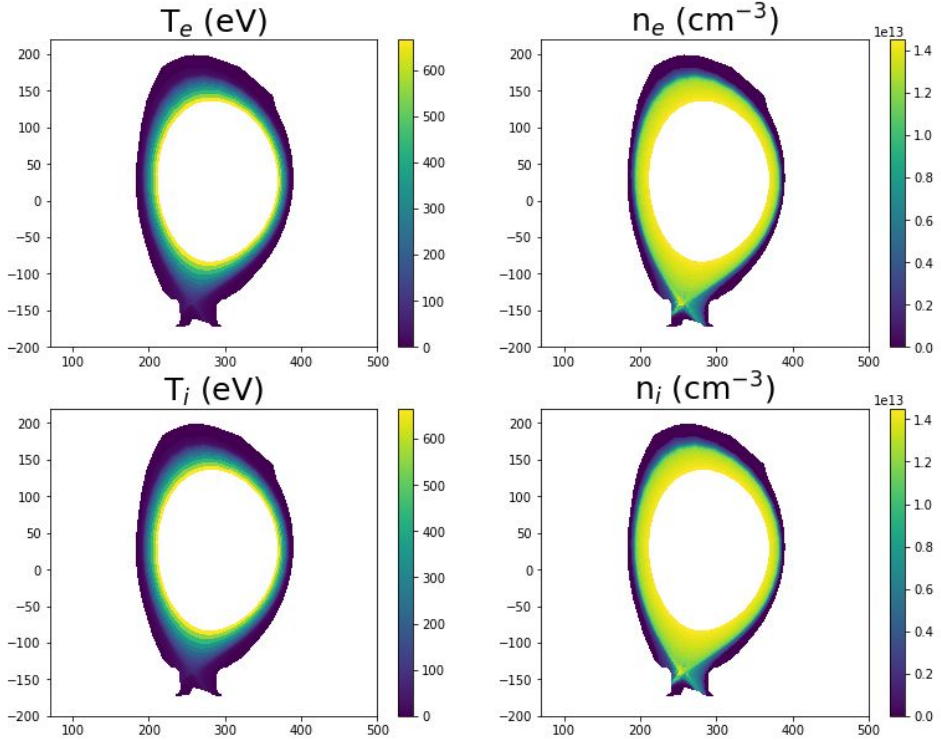
dissociation by proton impact

Ref CRM model: edge2d simulations

- **2D Eirene simulations for JET runs**

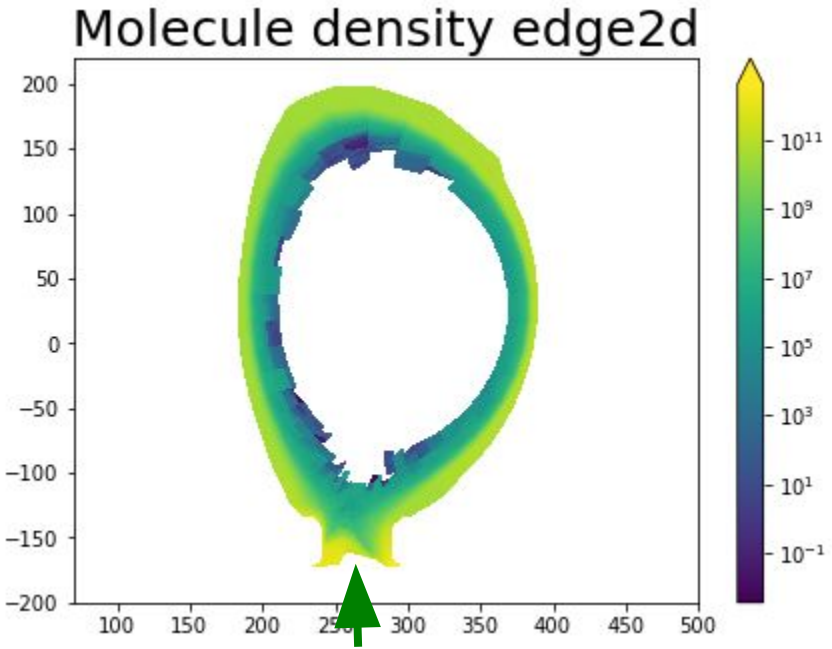
Particle species

$$D^+, D, D_2^+, D_2$$

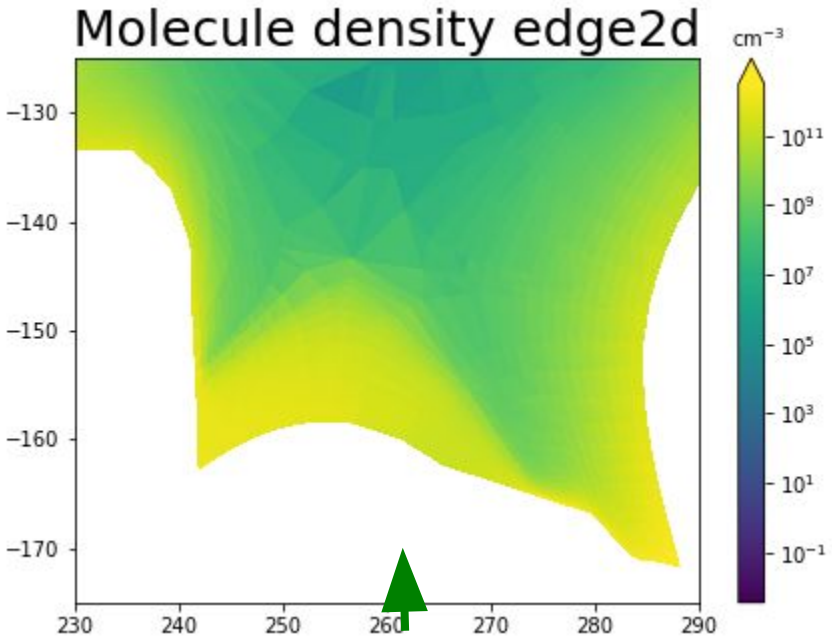


Ref CRM model: edge2d simulations

- 2D Eirene simulations for JET runs



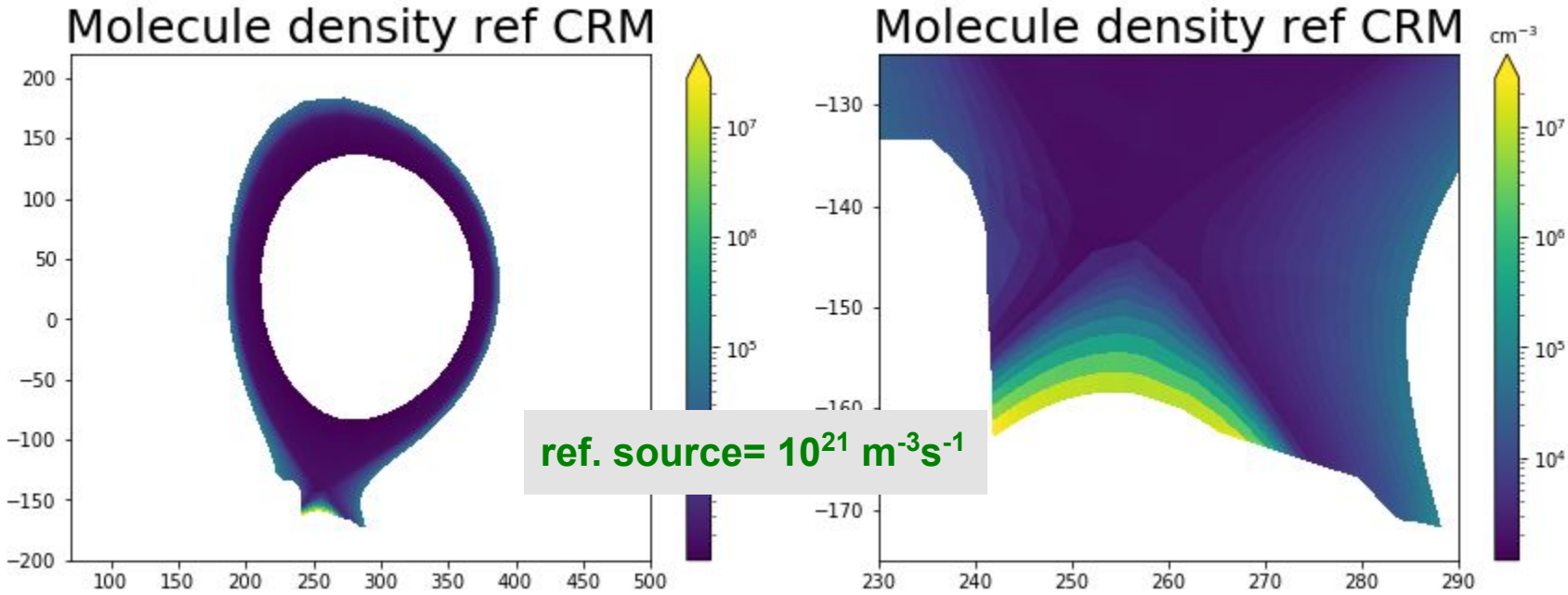
Gas puffing



Gas puffing

Ref CRM model: edge2d simulations

- **Ref CRM model with plasma parameters from edge2d simulations:**



Ref CRM model: effective source

- **Ratio of molecule density for edge2d and ref CRM:**

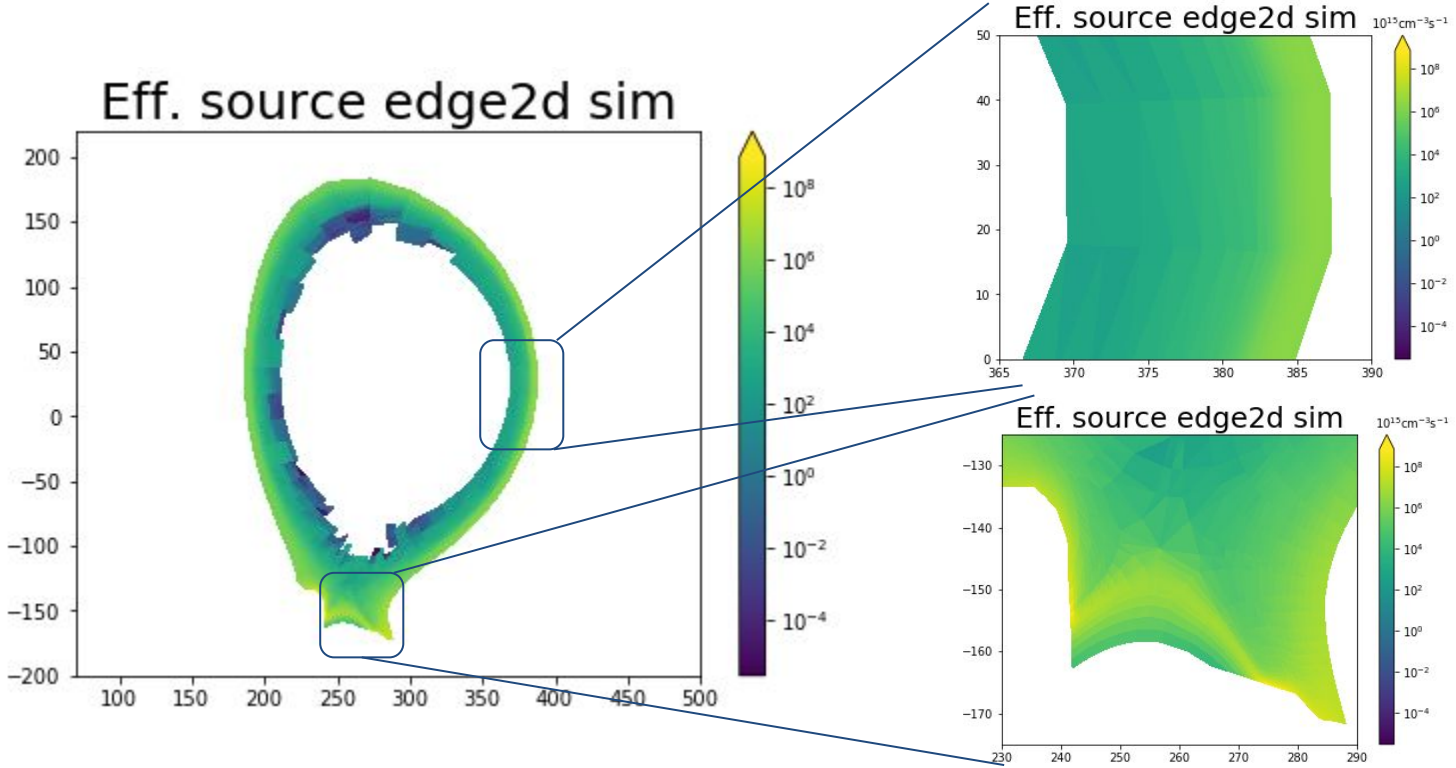
$$\frac{density(edge2D)}{density(CRM)} = \frac{\boldsymbol{effective\ source(edge2D)}}{reference\ source(CRM)}$$

$\boldsymbol{effective\ source(edge2D)}$ **:**

- ❖ **does not depend on plasma parameters**
- ❖ **accounts for transport.**

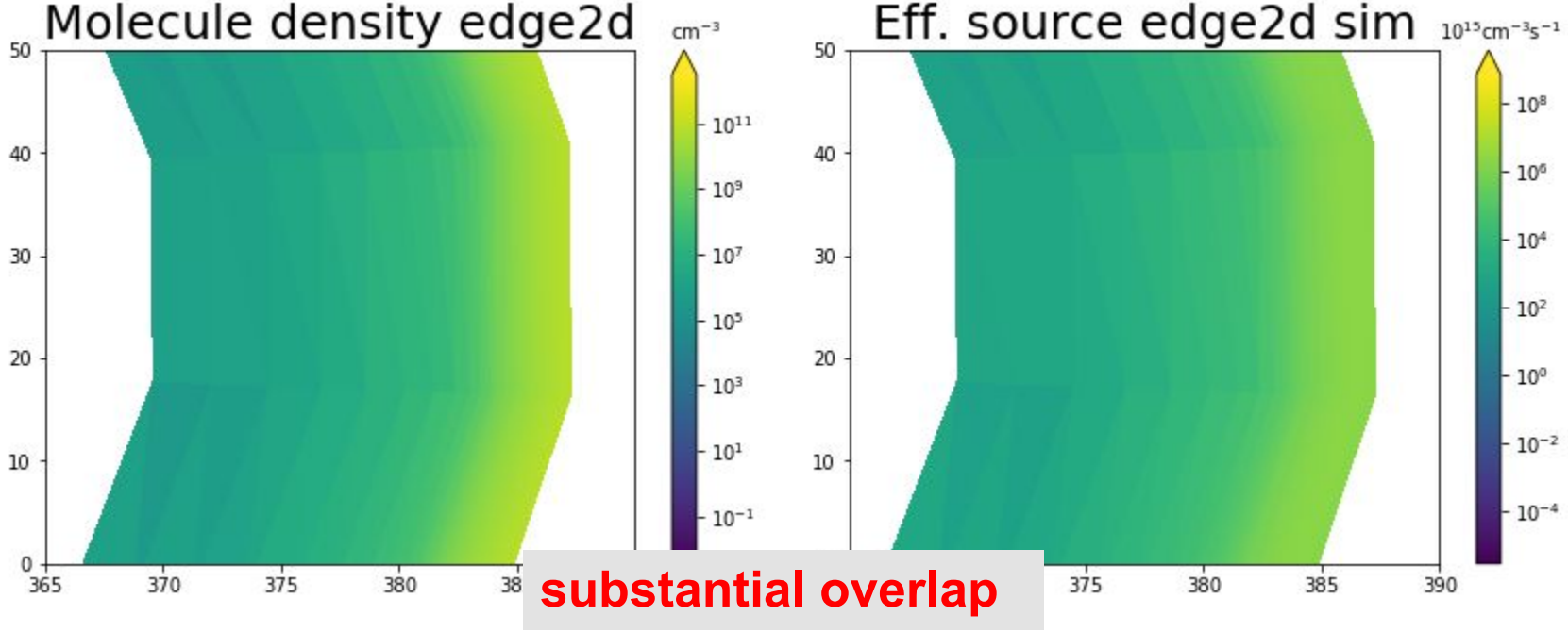
Ref CRM model: effective source

- **Ratio of molecule density for edge2d and ref CRM:**



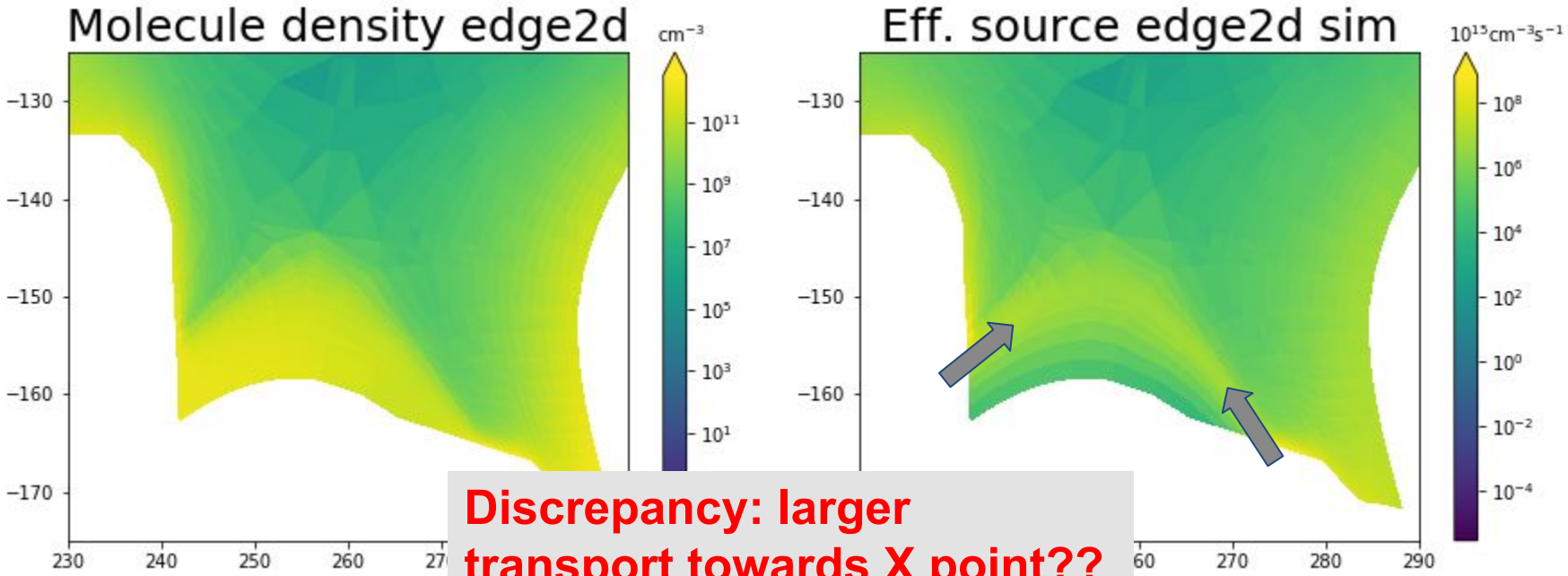
Ref CRM model: effective source

- **Density vs effective source (up-stream region):**



Ref CRM model: effective source

- **Density vs effective source (divertor region):**



Discrepancy: larger transport towards X point??

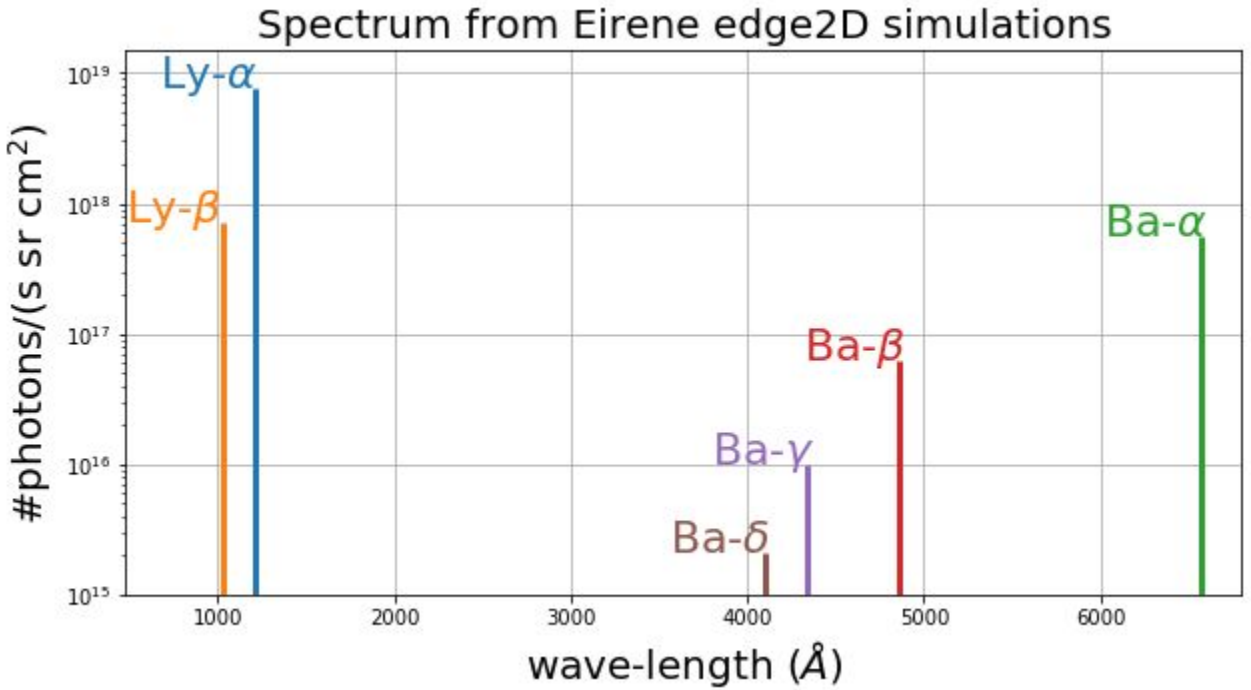
Molecular spectroscopy: Eirene

Looking for signals of molecular transitions from Eirene simulations:

- electronic transitions: Population of excited states from AMJUEL (Reiter/Savada/Fujimoto)
  - ★ atomic transitions up to n=6 (Lyman, Balmer, Paschen ..)
  - ★ molecular transitions:
    - singlet B,C→X (Lyman, Werner)
    - triplet: d → a (Fulcher)

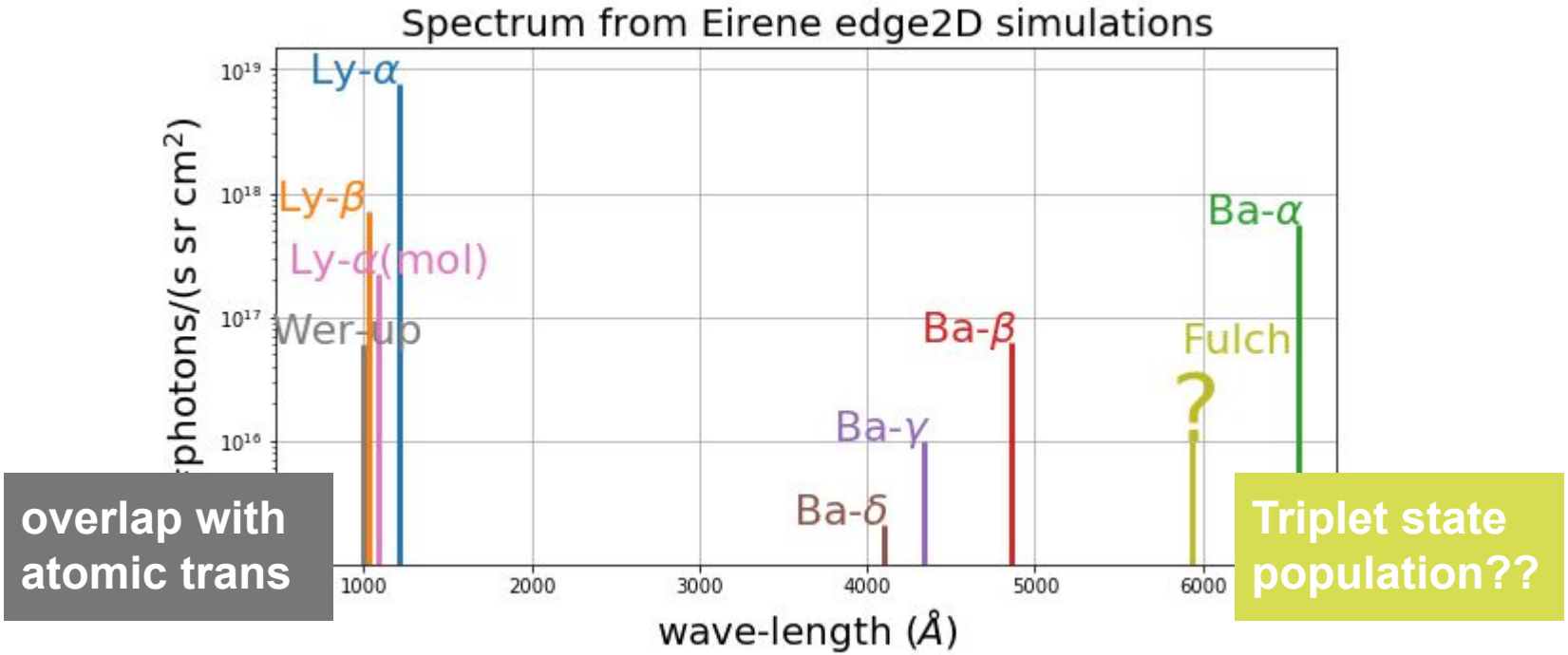
Molecular spectroscopy: Eirene

- Emissivity along a line of sight from the inner divertor (only atomic transitions)



Molecular spectroscopy: Eirene

- Emissivity along a line of sight from the inner divertor (molecule transitions):



overlap with atomic trans

Triplet state population??

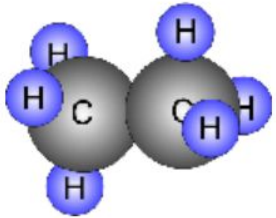
HYDKIN:

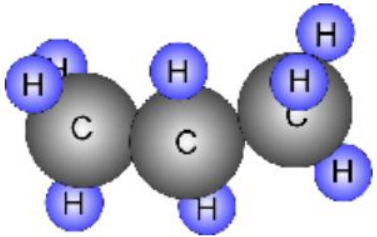
Forschungszentrum Jülich GmbH
Institut für Plasmaphysik

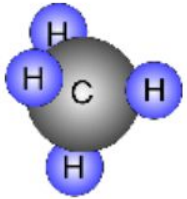
HYDKIN

Reaction kinetics analysis online for Hydrocarbon catabolism in hydrogen plasmas

International Atomic Energy Agency
IAEA Atomic and Molecular Data Unit







Online reaction kinetics analysis, for chemistry in hydrogen plasmas.

HYDKIN: data quality assessment

- Data from different sources (AMJUEL, ADAS, H2VIBR, …)
- Sources based on other sources (AMJUEL refers to Janev(1987), that refers to Takayanagi and Suzuki(1978), …)
- How to assess the quality of data? Are we really using the best (and most recent) available data? Are there documented and accepted data quality tag and criteria?
    - use generations (“A” for ADAS, “L” for literature, ..)
    - use source

HYDKIN: data quality assessment

- Isotope effect in ion-atom collisions:
  - Landau-Zener: just a kinematical effect on relative velocity
  - Shift of ionization potentials.
  - Is there a proper rescaling??

Thanks for the attention!