CRM and photon tracing module in EIRENE

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H colrad or the CRM in Eirene

- Based on the collisional radiative model by Sawada (1995)
- Resolve population coefficients for each Eirene cell
- Derive effective rates such as effective ionization and recombination rates to be used in EIRENE
- Provide population densities of excited species as a bulk ion species for the Photon tracing module

CRM for atomic hydrogen

$$\frac{dn_H(p)}{dt} = -\left[\sum_{p>q}\left(A_{(p,q)} + F_{(p,q)}n_e\right) + S_{(p)}n_e + \sum_{p<q} C_{(p,q)}n_e\right] n_{H(p)} + \sum_{q<p} C_{(q,p)}n_e\, n_{H(q<p)}$$

$$+\sum_{q>p}\left[A_{(q,p)} + F_{(q,p)}\, n_e\right] n_{H(q>p)} + \left[\alpha(p)n_e + \beta(p)\right] n_e\; n_{H^+} + \Gamma_{\mathrm{H(p)}}$$

A = Spontaneous emission rate
F = De-excitation rate coefficient
S = ionization rate coefficient
C = Excitation rate coefficient
α = 3-body recombination rate coefficient
β = radiative recombination rate

CRM in steady-state, matrix form

$$\begin{bmatrix} -(S_{(1)} + \sum C_1)\, n_e & A_{(1,p)} + F_{(1,p)} n_e & A_{(1,q)} + F_{(1,q)} n_e & (\alpha_{(1)} n_e + \beta_{(1)}) n_e \\ C_{(1,p)}\, n_e & -A_{(1,p)} - (S_{(p)} + F_{(1,p)} + C_{(p,q)}) n_e & A_{(p,q)} + F_{(p,q)} n_e & (\alpha_{(p)} n_e + \beta_{(p)}) n_e \\ C_{(1,q)}\, n_e & C_{(p,q)}\, n_e & -\sum A_{(q)} - (S_{(q)} + \sum F_{(q)}) n_e & (\alpha_{(q)} n_e + \beta_{(q)}) n_e \\ S_{(1)} n_e & S_{(p)} n_e & S_{(q)} n_e & -(\sum \alpha n_e + \sum \beta) n_e \end{bmatrix} \begin{bmatrix} n_H \\ n_{H(p)} \\ n_{H(q)} \\ n_{H^+} \end{bmatrix} = \begin{bmatrix} -\Gamma_H \\ -\Gamma_{\mathrm{H(p)}} \\ -\Gamma_{\mathrm{H(q)}} \\ -\Gamma_{\mathrm{H^+}} \end{bmatrix}$$

$$\begin{bmatrix} -A_{(1,p)} - (S_{(p)} + F_{(1,p)} + C_{(p,q)}) n_e & A_{(p,q)} + F_{(p,q)} n_e \\ C_{(p,q)}\, n_e & -\sum A_{(q)} - (S_{(q)} + \sum F_{(q)}) n_e \end{bmatrix} \begin{bmatrix} n_{H(p)} \\ n_{H(q)} \end{bmatrix} = \begin{bmatrix} C_{(1,p)}\, n_e \\ C_{(1,q)}\, n_e \end{bmatrix} n_H + \begin{bmatrix} (\alpha_{(p)} n_e + \beta_{(p)}) n_e \\ (\alpha_{(p)} n_e + \beta_{(p)}) n_e \end{bmatrix} n_{H^+} + \begin{bmatrix} -\Gamma_{\mathrm{H(p)}} \\ -\Gamma_{\mathrm{H(q)}} \end{bmatrix}$$

$$\begin{bmatrix} n_{H(p)} \\ n_{H(q)} \end{bmatrix} = R_1 n_H + R_0 n_{H^+} + \mathrm{R}_{ext}$$

R_1, R_0 and R_{ext} are population coefficients

General EIRENE test case for testing rate coefficients

- EIRENE 2D grid with ne and Te varied along x and y dimensions
- Ne, 20 points, ~1e8 – 1e16 cm3
- Te, 200 points, ~0.5 – 1e4 eV

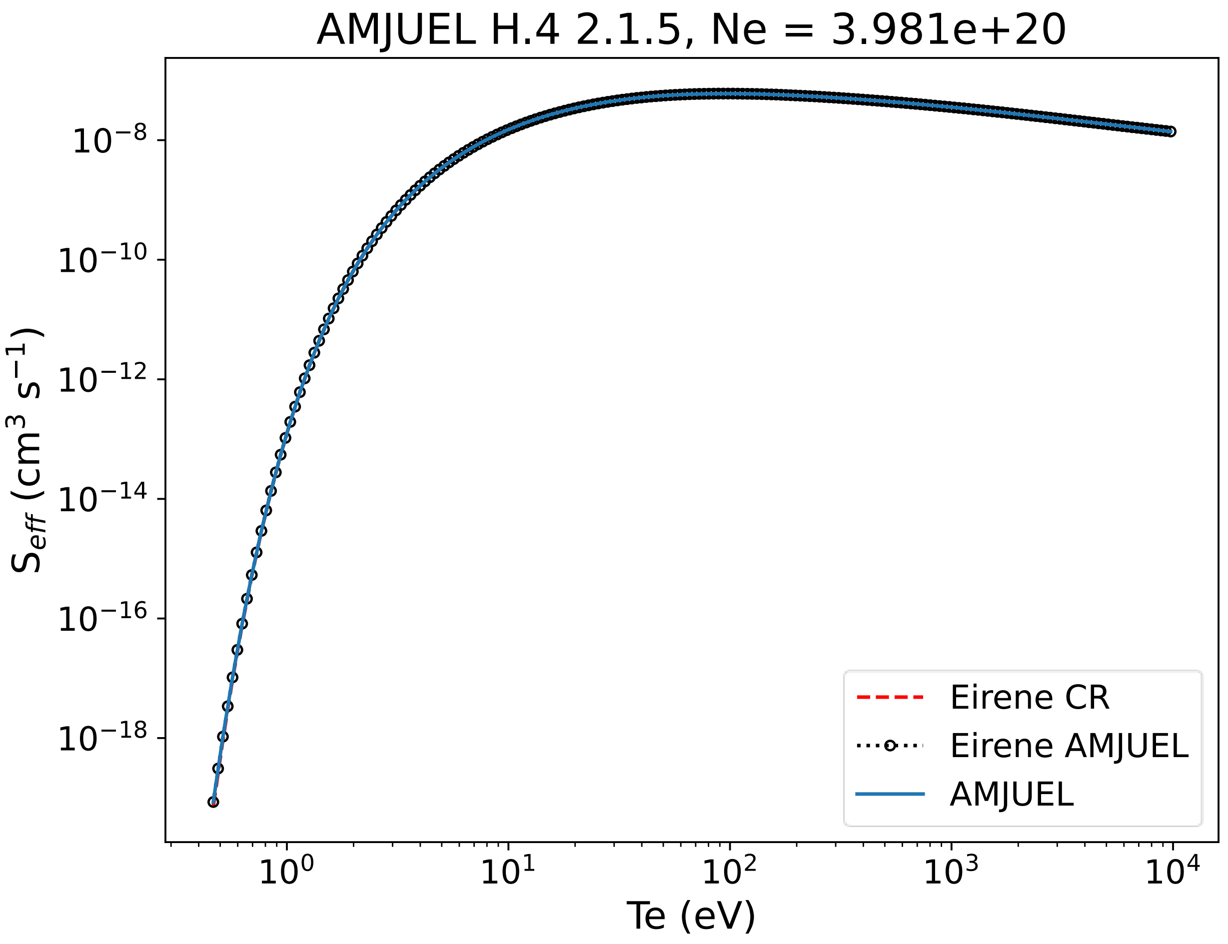
The effective ionization rate of H colrad line perfectly with AMJUEL

Effective ionization rate S_{eff} :

$$S_{eff} = S_{(1)} + \sum_{p} \left(C_{(1,p)} - R_{1(p)} (F_{(p,1)} + \frac{A_1}{n_e}) \right)$$

Eirene CR -> H colrad
Eirene AMJUEL -> using AMJUEL rates within Eirene

AMJUEL – last update entry: May 18

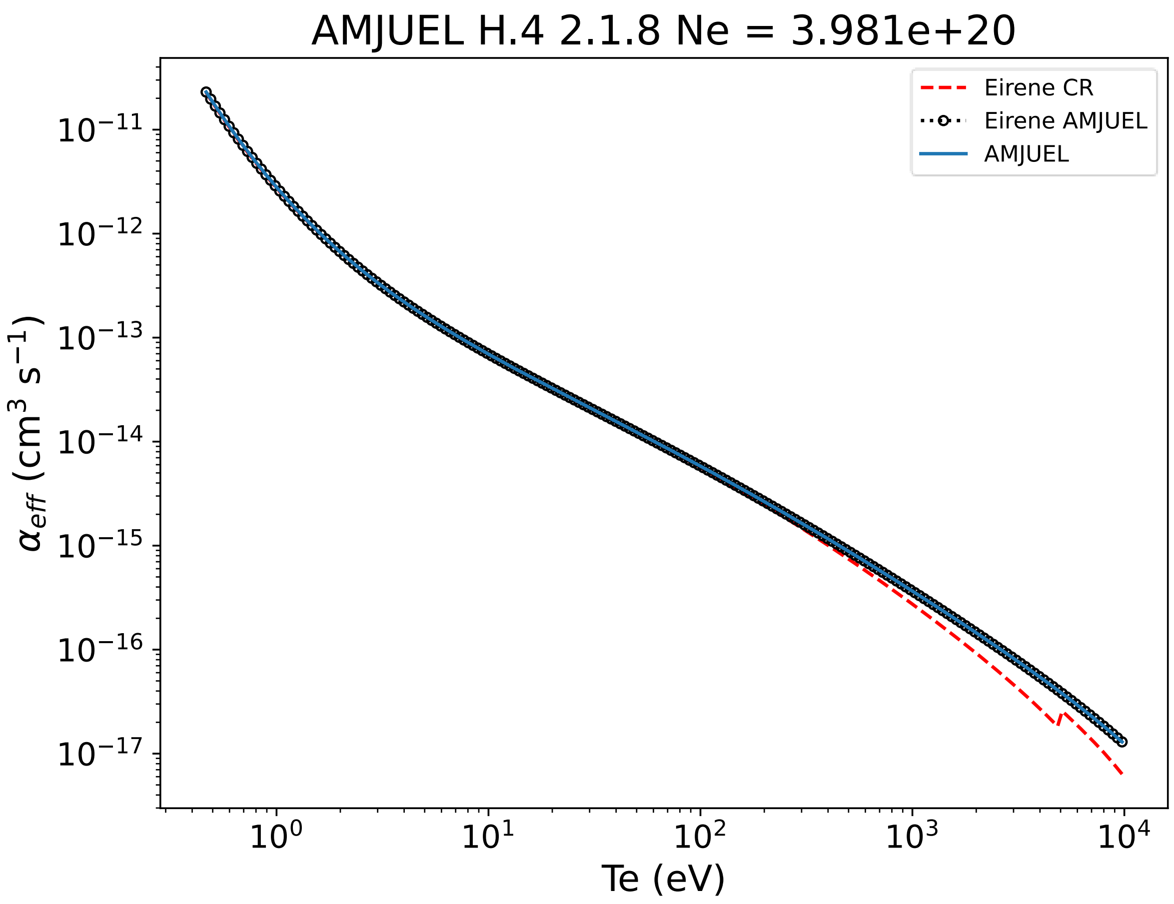


The H colrad recombination rate starts to diverge at Te > 400 eV

Effective recombination rate α_{eff} :

$$\alpha_{eff} = \alpha_1 n_e + \beta_1 + \sum_p R_{0(p)}(F_{(p,1)} + \frac{A_1}{n_e})$$

- Discrepancy can be due to the different expressions of the recombination rate coefficient



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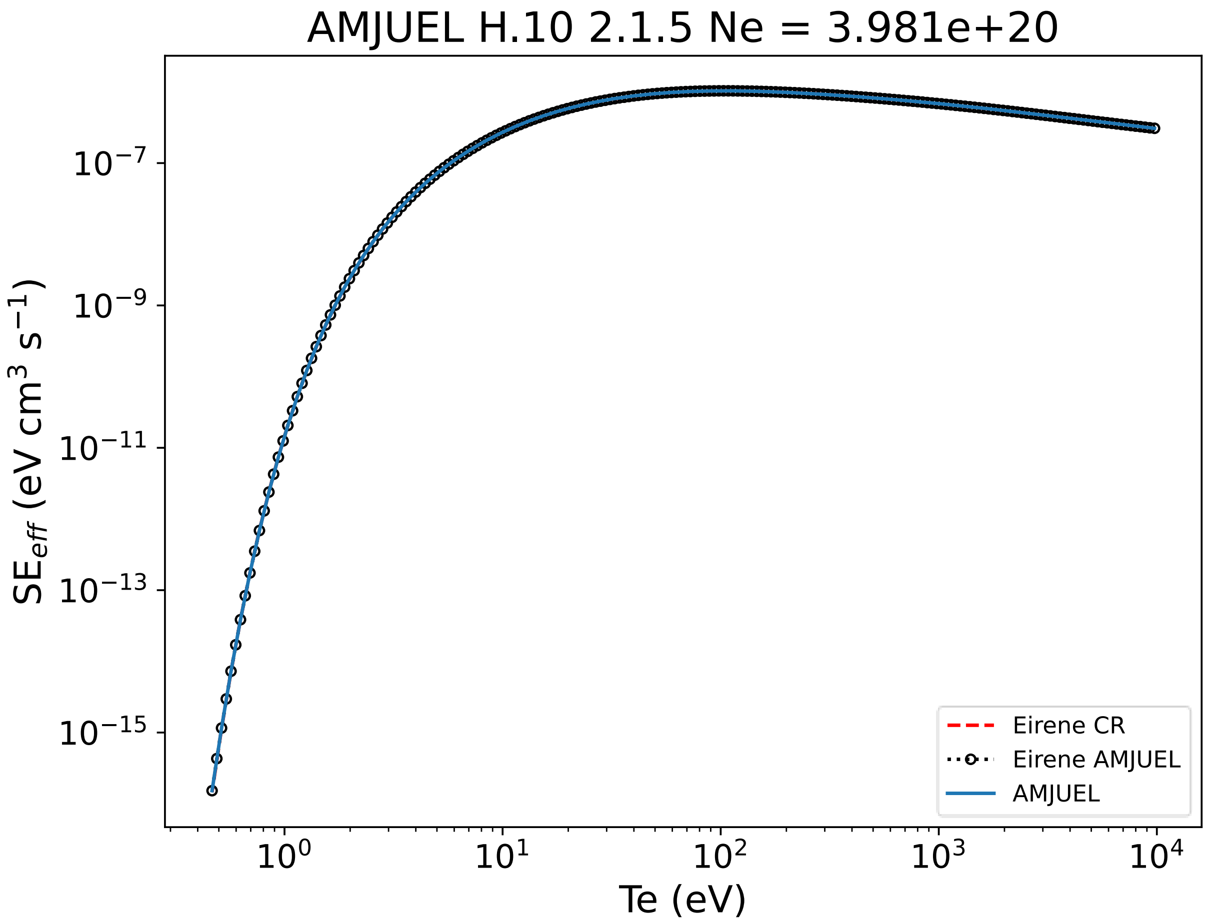
The effective ionization cooling rate of H colrad line perfectly with AMJUEL

Effective ionization cooling rate SE_{eff} :

$$SE_{eff} = S_{(1)}E_{\alpha} + \sum_{p}\left(R_{1(p)}\left(S_p E_{p-\alpha} + C_{(1,p)}\, E_p\right)\right) + \sum_{q>p}\left(R_{1(p)}C_{p,q}E_{p-q} - R_{1(q)}F_{(p,q)}E_{p-q}\right)$$

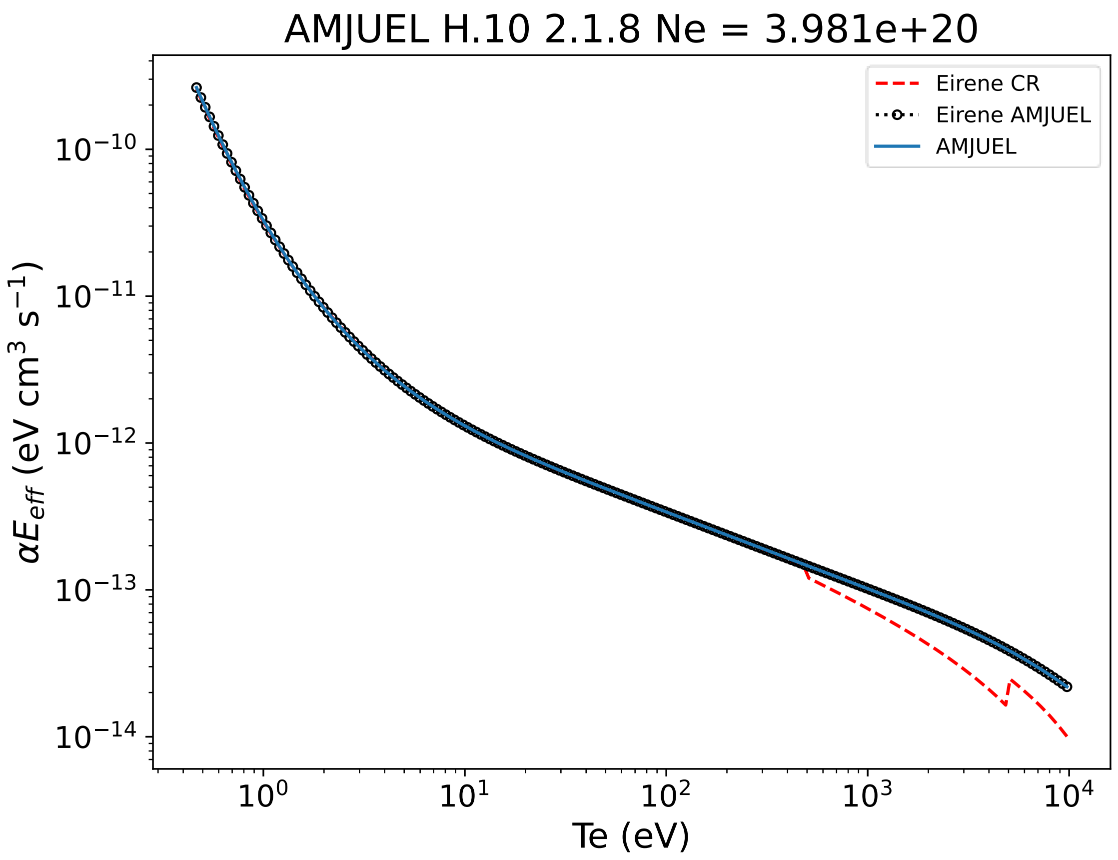


The H colrad recombination cooling rate starts to diverge at Te > 400 eV

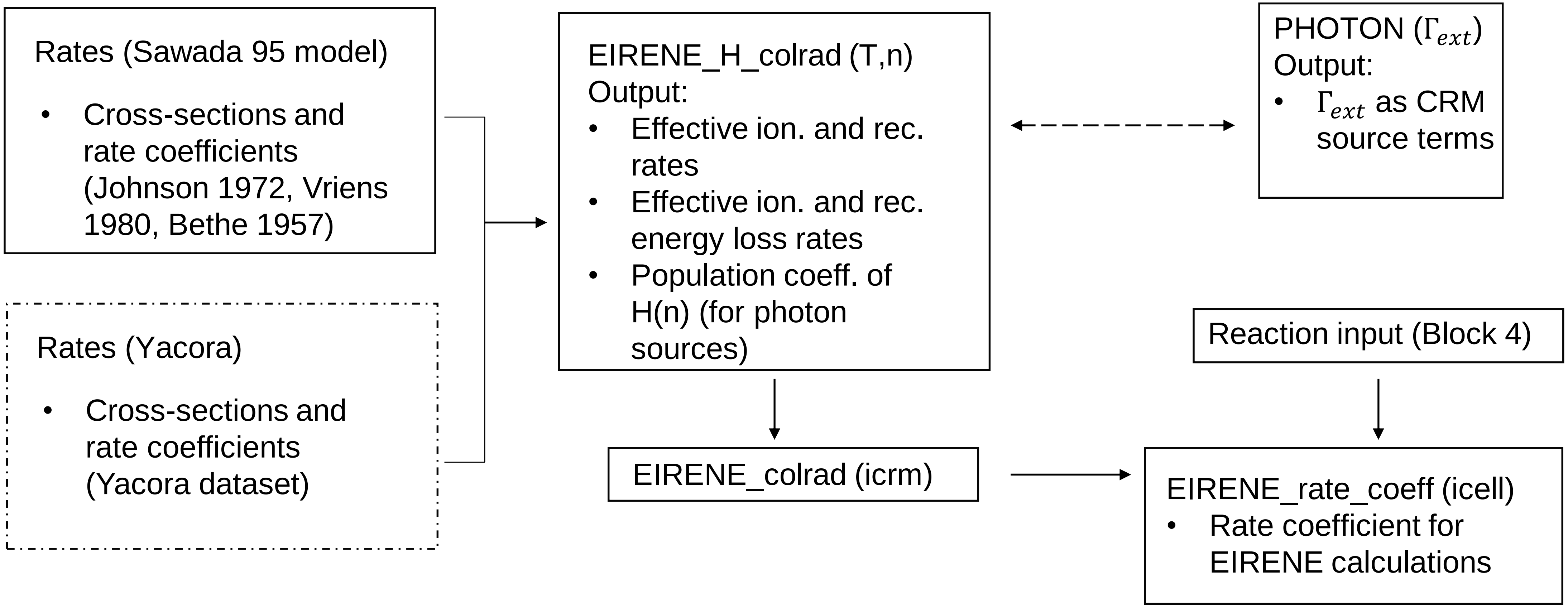
Effective recombination cooling rate αE_{ef}

$$\alpha E_{eff} = \beta_1 \bar{E}_1 - \alpha_{(1)} n_e E_\alpha + \sum_p R_{0(p)} \left(S_p E_{p-\alpha} + \beta_p \bar{E}_p - \alpha_p n_e E_{p-\alpha} \right) + \sum_{q>p} \left(R_{0(p)} C_{p,q} E_{p-q} - R_{0(q)} F_{(p,q)} E_{p-q} \right)$$

- Directly derived from recombination rate, so same discrepancy occurs



Proposed CRM structure in Eirene (H Colrad)



Proposed *H2* Colrad structure in Eirene (currently non-existent)

Rates (Sawada 2005 model)

- Cross-sections and rate coefficients (Janev 2003, Miles 72, Celiberto, etc)

Rates (Yacora)

- Cross-sections and rate coefficients (Yacora dataset)

Tabulated data?

EIRENE_H2_colrad (T,n,Ti?)

Output:
- Effective ion. and rec. rates
- Effective ion. and rec. energy loss rates
- Effective dissociation rates
- Pop. Coefficients of $H_2(n)$
- Pop. Coefficients of $H_2(v)$
- ?

PHOTON (Γ_{ext})
- ?

Reaction input (Block 4)

EIRENE_colrad (icrm)

EIRENE_rate_coeff (icell)
- res

The previous (2002) photon tracing model (Reiter et al., PPCF 2002) was revisted

The photon tracing routine in EIRENE is analogous to neutral particle tracing, with v=c and E=hv, differences:

- Bulk ions are now excited species (photon sources)
- Rate coefficients for sources and photon-background interaction must take into account line shapes (natural, Doppler, Zeeman, etc)

Determine opacity with local population escape factors

Determining the population escape factor

$$\Theta_p = \frac{E - G}{E} = 1 - \frac{\mathrm{G}}{\mathrm{E}}$$

G → absorption

E → emission

$$\Theta_p = 1 - \frac{\int_\Omega \int_{line} \alpha(x,\lambda)\, L_\lambda(x,\lambda,\Omega)\, d\lambda\, d\Omega}{\int_\Omega \int_{line} \epsilon(x,\lambda)\, d\lambda\, d\Omega}$$

Behringer K 1998 Escape factors for line emission and population calculations MPI-Garching Report, IPP 10/11

Θ_p in Eirene

$$\Theta_p = \frac{E - G}{E} = 1 - \frac{G}{E}$$

G → absorption

E → emission

G is simply the number of absorbed photons i.e volume photon sink tallies

E is the volume photon source

Thus Θ_p can be evaluated per cell of Eirene

Photon tracing test case

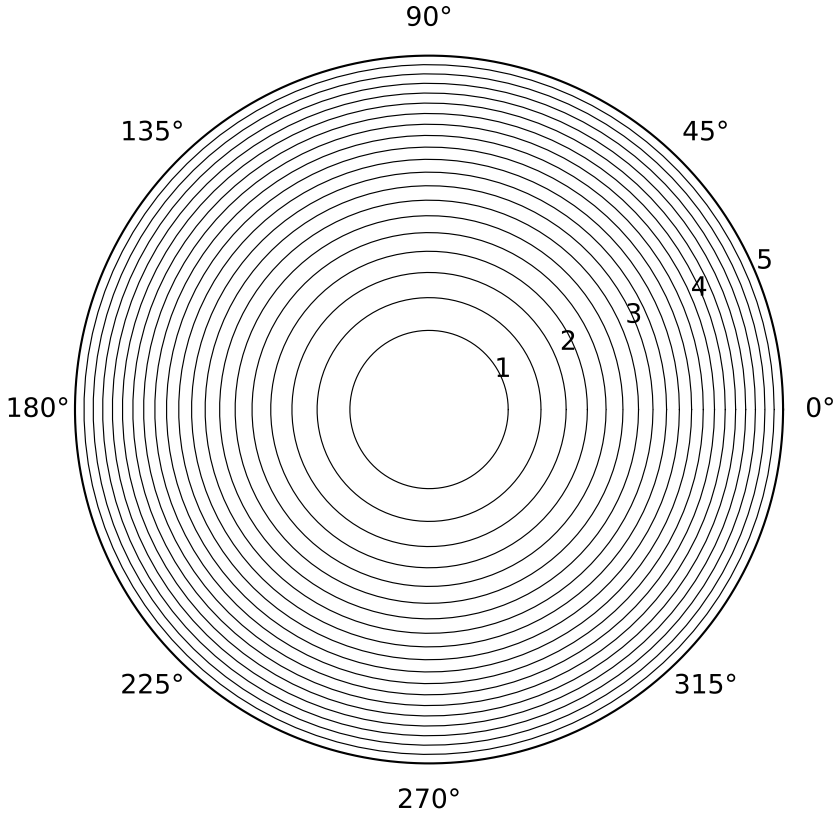
Cylindrical test case, 20 radial points

Homogeneous plasma and atomic density

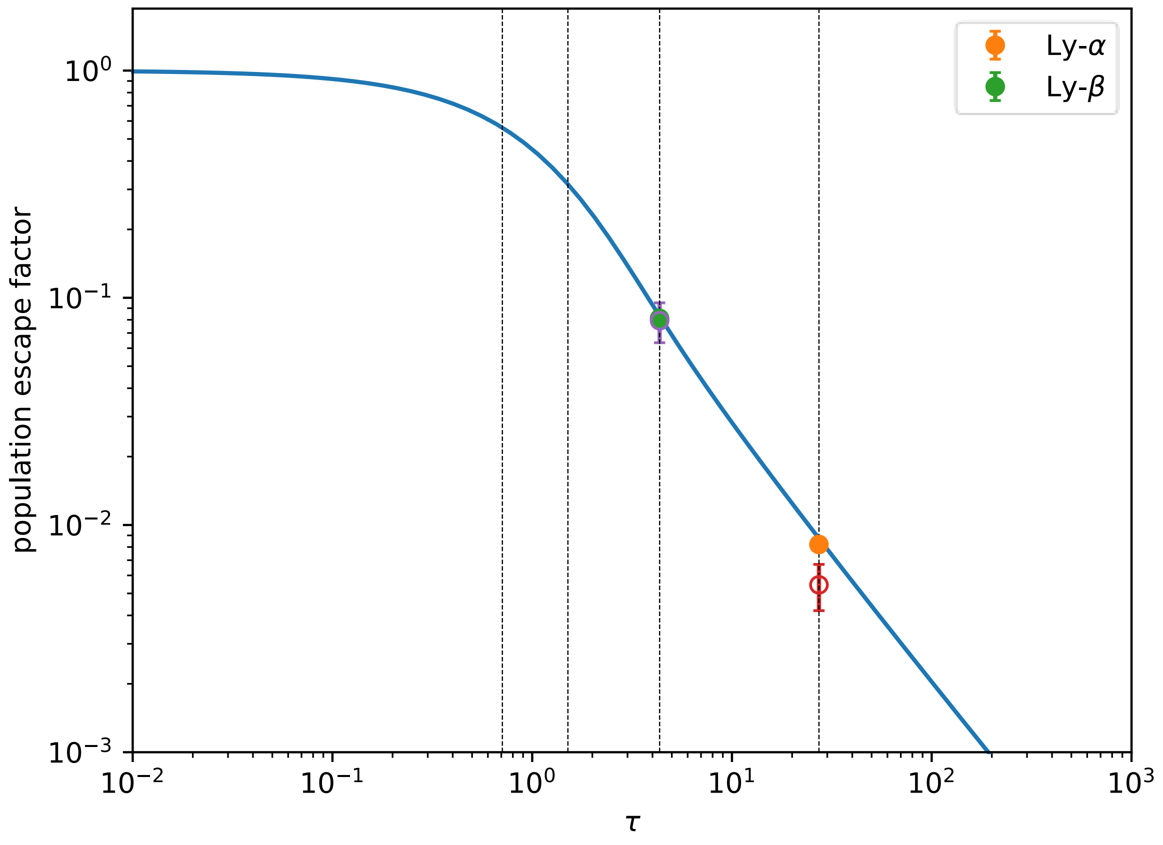
T_H = 1 eV, $n_H = 10^{14}$ cm^{-3} , b = 5 cm

Simulated Ly-a and Ly-b photons (2e6) with volumetric sources (H(n=2,3) as bulk ions)

Line shape only doppler broadening



Population escape factor aligns with analytical function for Ly-α and Ly-β



$\Theta_p = f(\tau)$ (solid blue line)

$\tau = \alpha(\lambda)b$

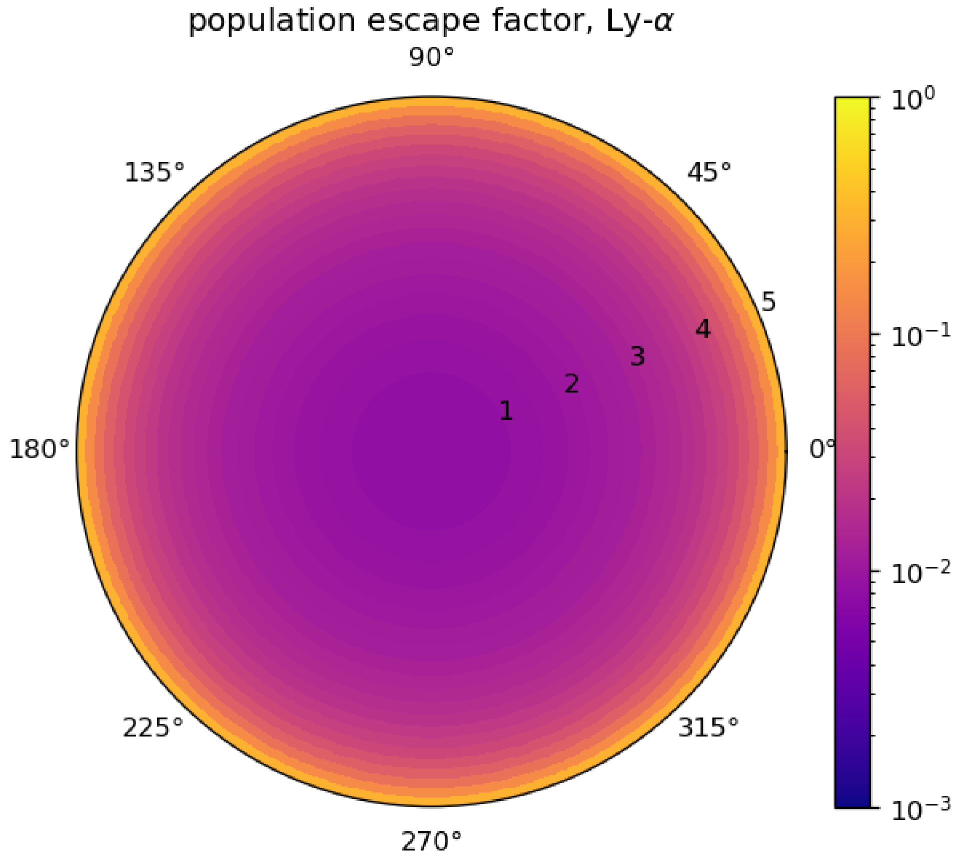
is the optical depth or 'thickness'

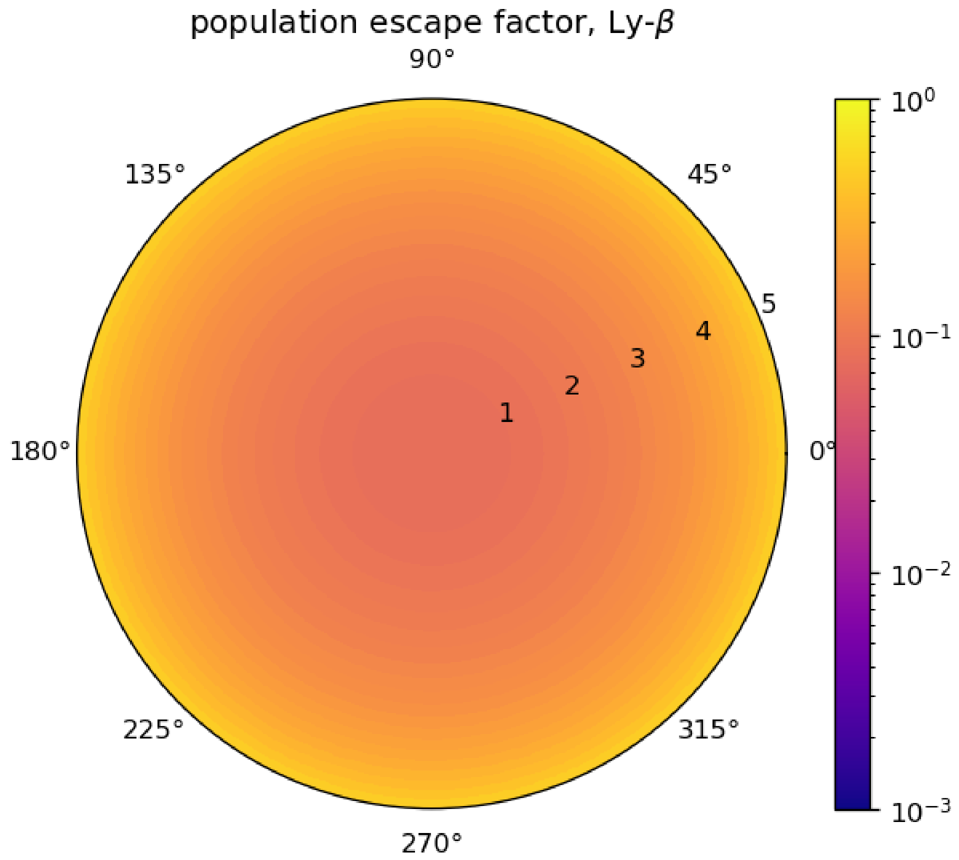
Hollow points with ~10^6 photons

Solid points with ~10^9 photons

Agreement for Ly-α at better statistics

2D (or 1D) profiles of the population escape factor: Ly-α and Ly-β opaque at the center





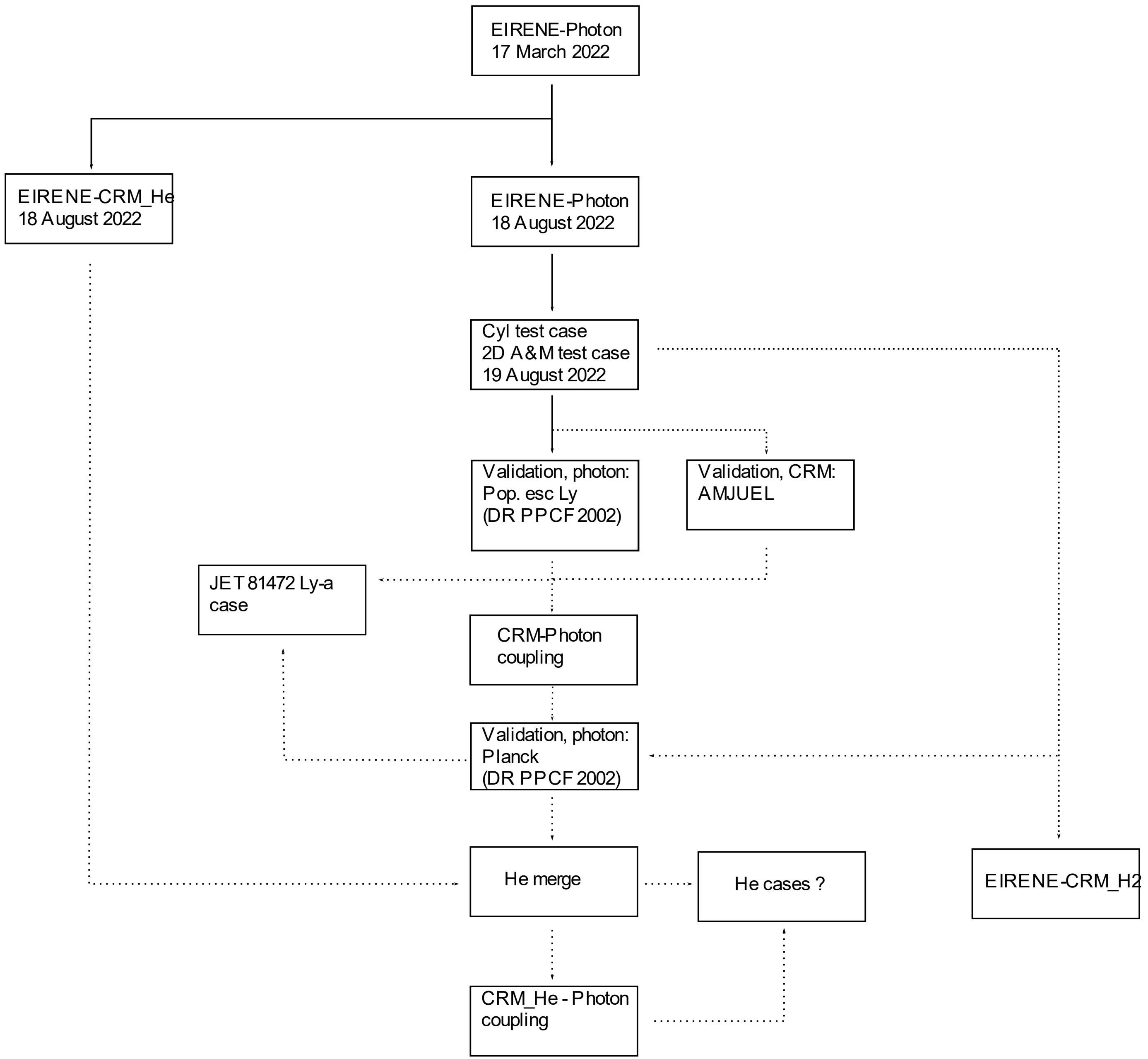
Current project state

Whats on hand:

- H colrad, He colrad
- Photon module
- A&M and photon cylinder test cases

Whats planned:

- CRM-photon coupling (for Planck test)
- Application to JET 81472
- H colrad data update
- He colrad testing
- H_2 colrad creation



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