PDR Modelling with KOSMA-τ

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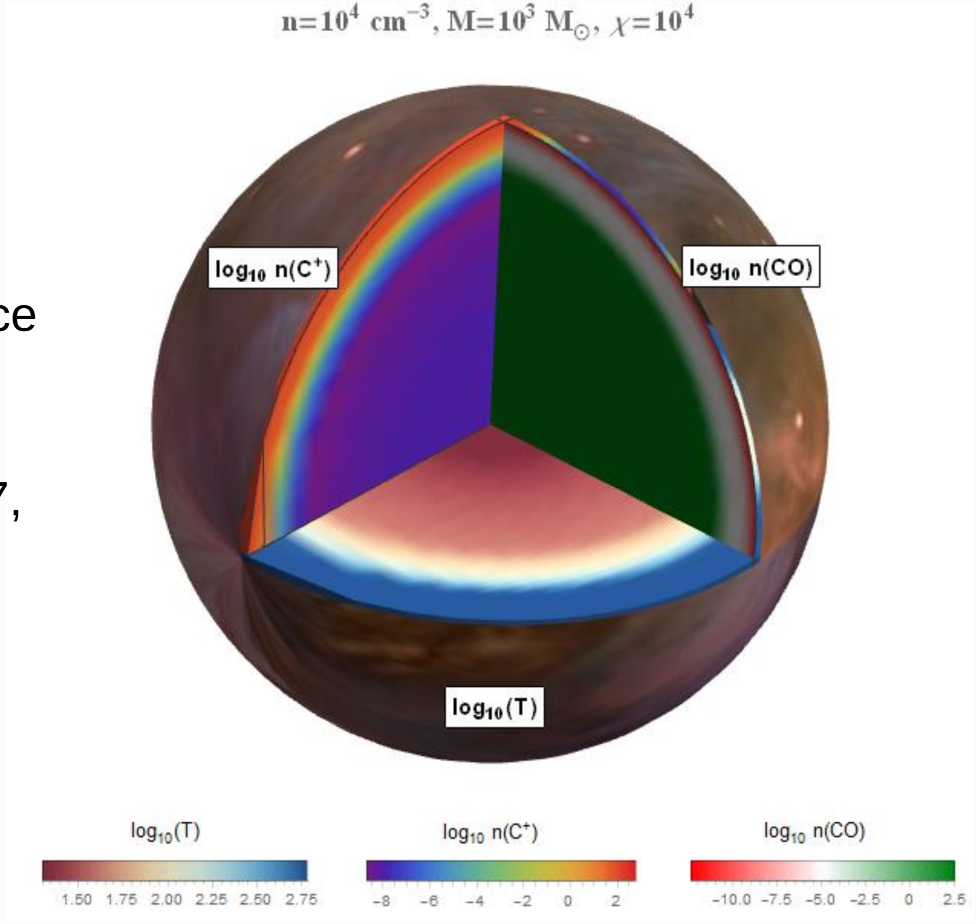
The KOSMA-τ PDR Code

- 1-D, spherical geometry
  - power-law density profile
  - isotropic illumination
- self-consistent solution of energy- and chemical balance and radiative transfer
- self-shielding of H_2, CO (FGK, Draine & Bertoldi 1997, Visser et al. 2009)
- full dust RT and temp. computation for varying dust distribution



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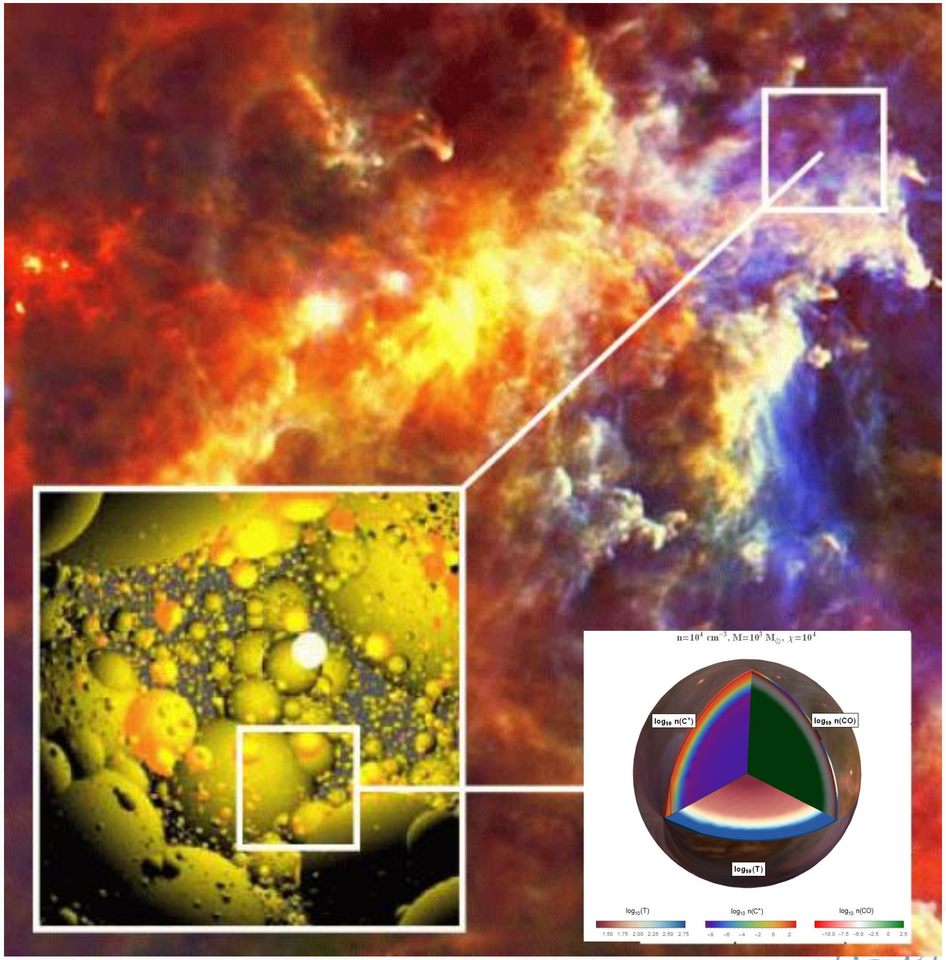
- full dust RT and temp. computation for varying dust distribution
- clumpy cloud composition
  - stochastic clump ensemble
  - **KOSMA-τ 3D** (Andree-Labsch et al. 2017)



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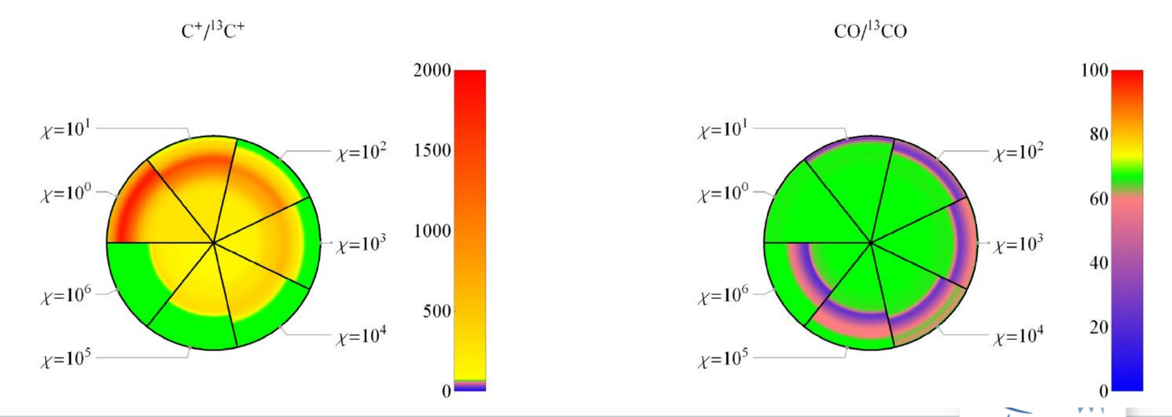
Chemistry in KOSMA-τ

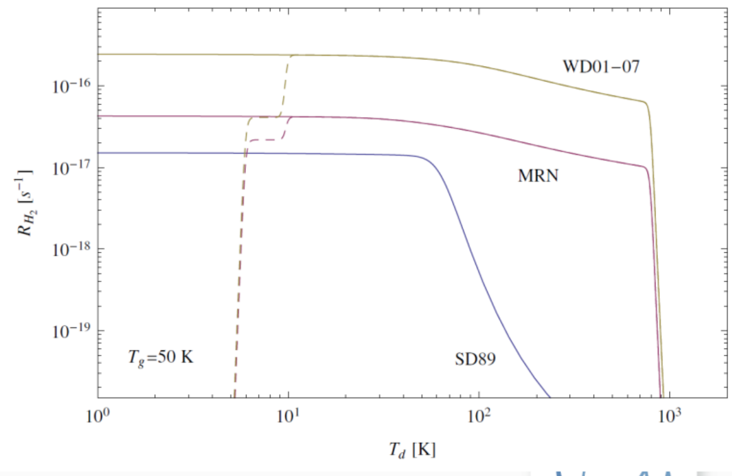
- Rate equation approach
- Steady-state chemistry
  - LAPACK: DGESV, DGELSD (least squares), DGESVX (w. equilibration)
- modular chemistry
  - user selects species, code selects reactions, creates conservation equations and computes Jacobian
- isotopologue chemistry: ^{13}C and ^{18}O
  - update to the fractionation reaction from Langer et al. 84 (Mladenovic & Roueff,2014)
  - isotopic reaction set (Röllig et al. 2013)
- Standard database: UDfA 2012 (McElroy et al. 2013)



Chemistry in KOSMA-τ

- Standard database: UDfA 2012
  - reactions with H_2^* overcome activation energy
  - CH^+ and SH^+ formation (Agundez et al. 2010, Nagy et al. 2012)
  - cyclic and linear-isomers included (new branching ratios from Chabot et al. 2013) with all isotopologues
    - l-$C_3H_3^+$, l-$C_3H_2^+$, l-C_3H_2, l-C_3H
  - additions
    - Fluorine chemistry (Neufeld et al. 2005)
    - Photodissociation of CS_2, N_2O (van Dishoeck et al.)
  - H_2 formation
    - Chemi- & physisorption (Cazaux & Tielens 2002,04,10)

Röllig et al. 2013

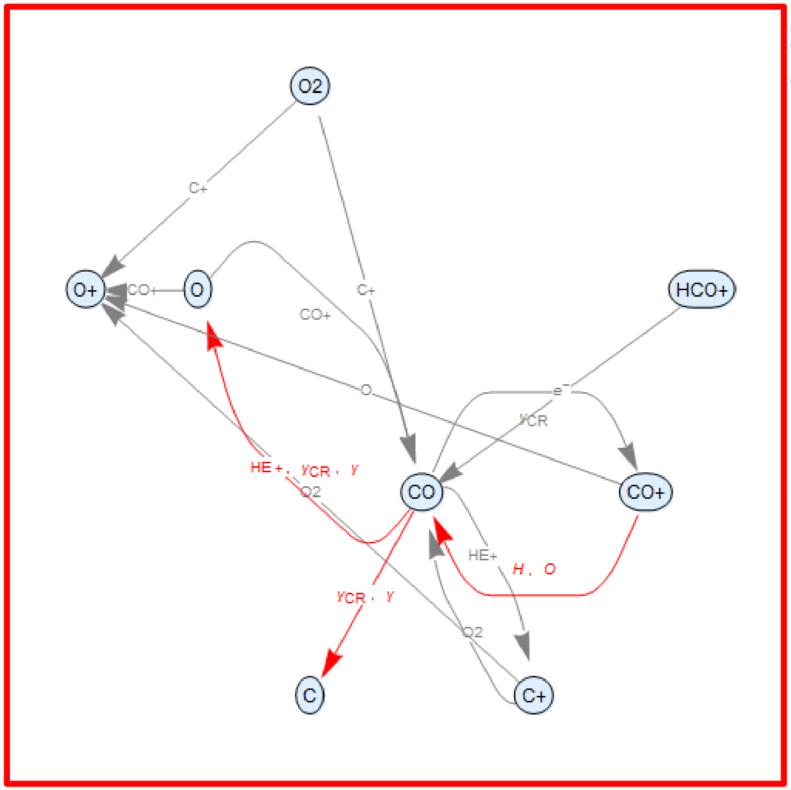


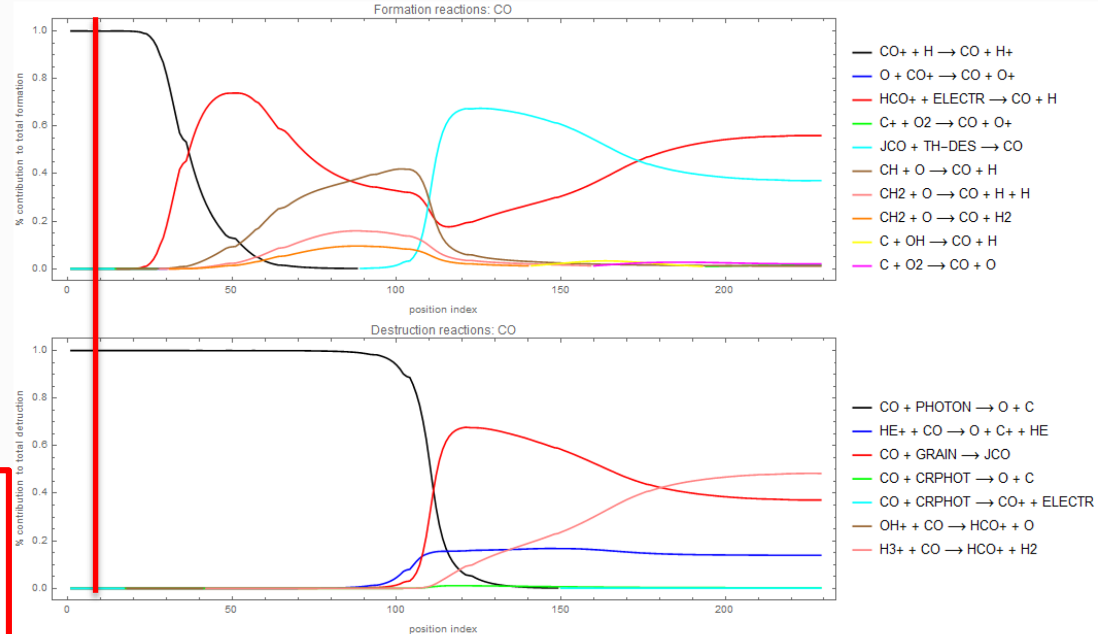
Full Surface Chemistry Upgrade

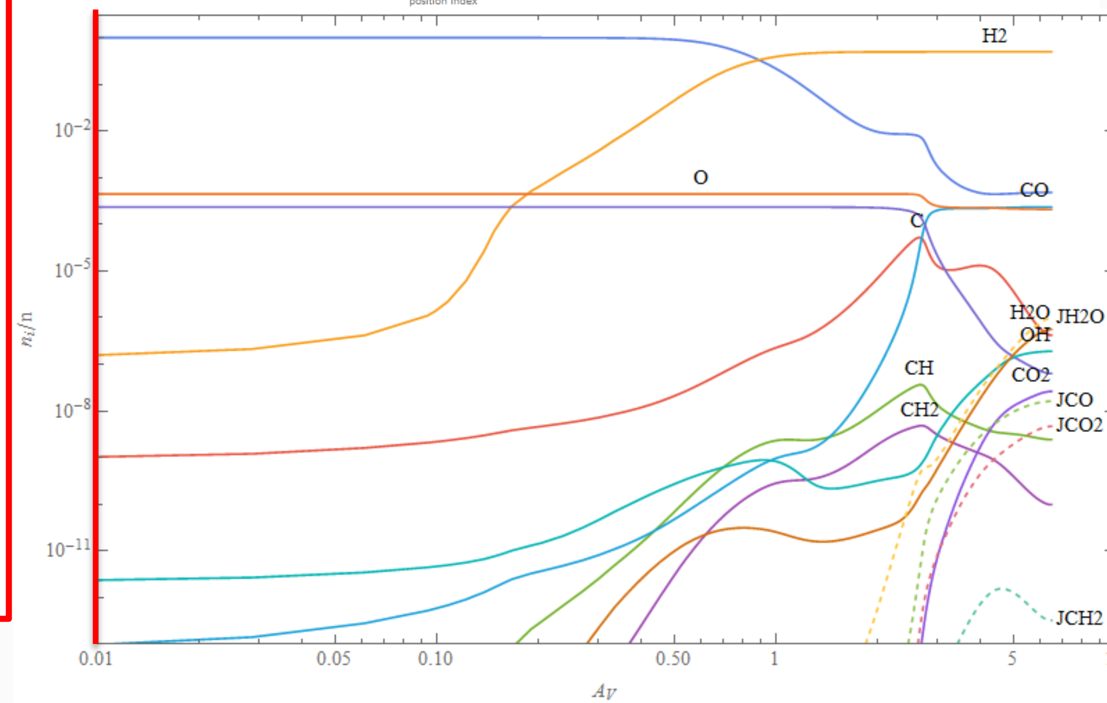
- Coupling of gas-phase and surface chemistry
- Steady-state chemistry
- Rate equation approach (Hasegawa et al. 1992,1993)
- Processes included:
  - adsorption (only neutrals, no sticking of H_2)
  - desorption only from 2 top layers (Aikawa et al. 1996)
    - thermal desorption (binding energies from UDfA + updates)
    - photo-desorption (photo cross-section like gas-phase)
      photo-dissociative desorption (eg.JH_2O +hv → OH + H Andersson+ 08)
    - photo-dissociation on grains (equivalent to gas-phase)
    - CR induced photo-desorption/diss. (Hasegawa & Herbst 1993)
    - H_2-formation induced desorption (Willacy et al. 1994, 2007)
    - chemistry induced desorption (Minissale et al. 2015, Cazaux et al. 2015)
  - surface-surface processes (Langmuir-Hinshelwood)

$$n = 10^4 cm^{-3}$$
$$\chi = 10^4$$

small chemical network







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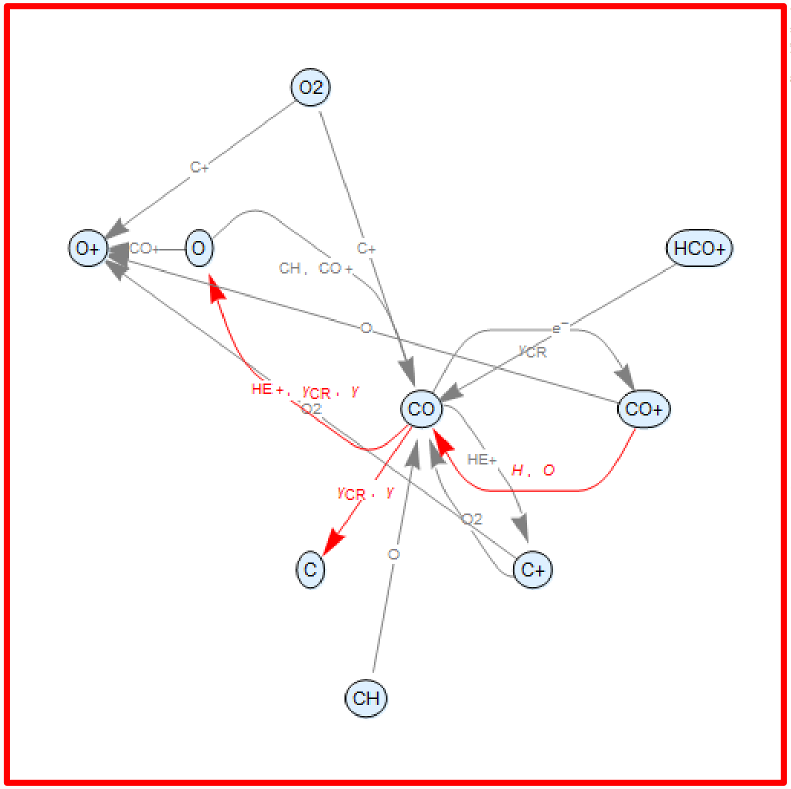

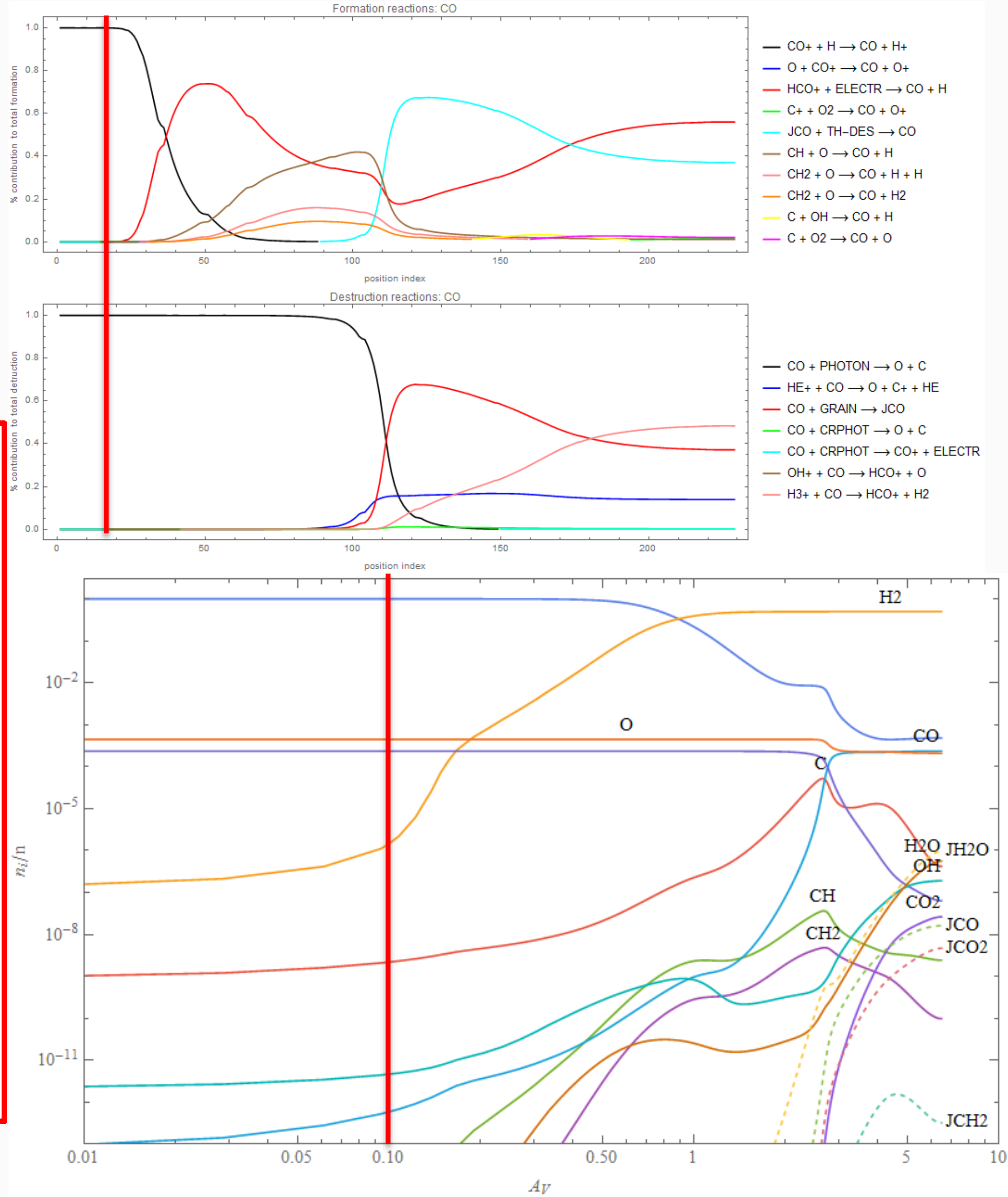

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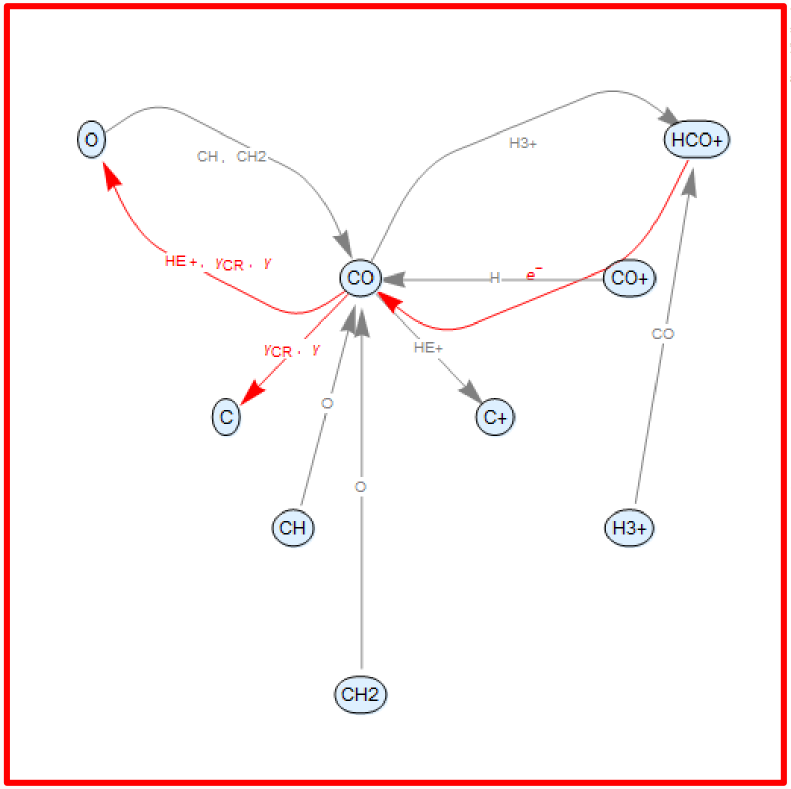

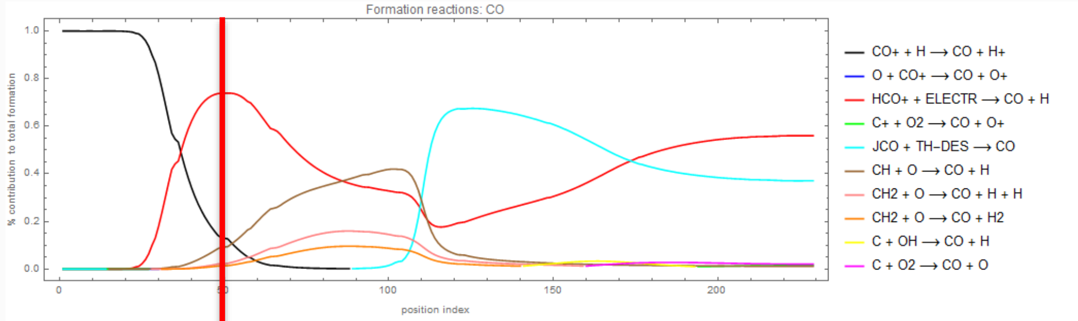

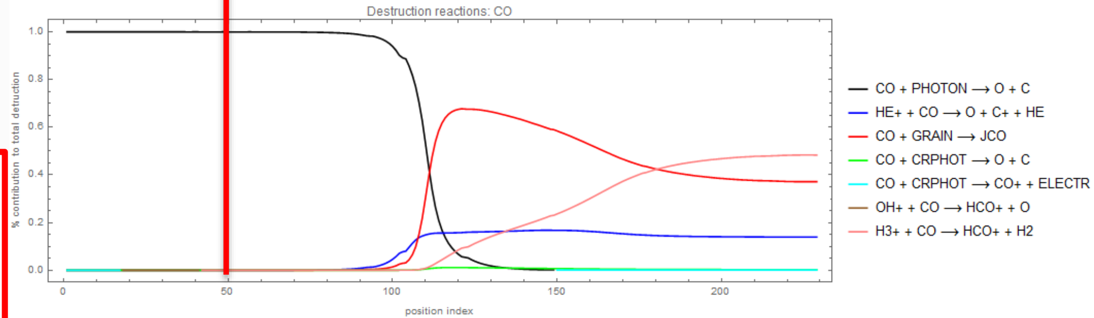

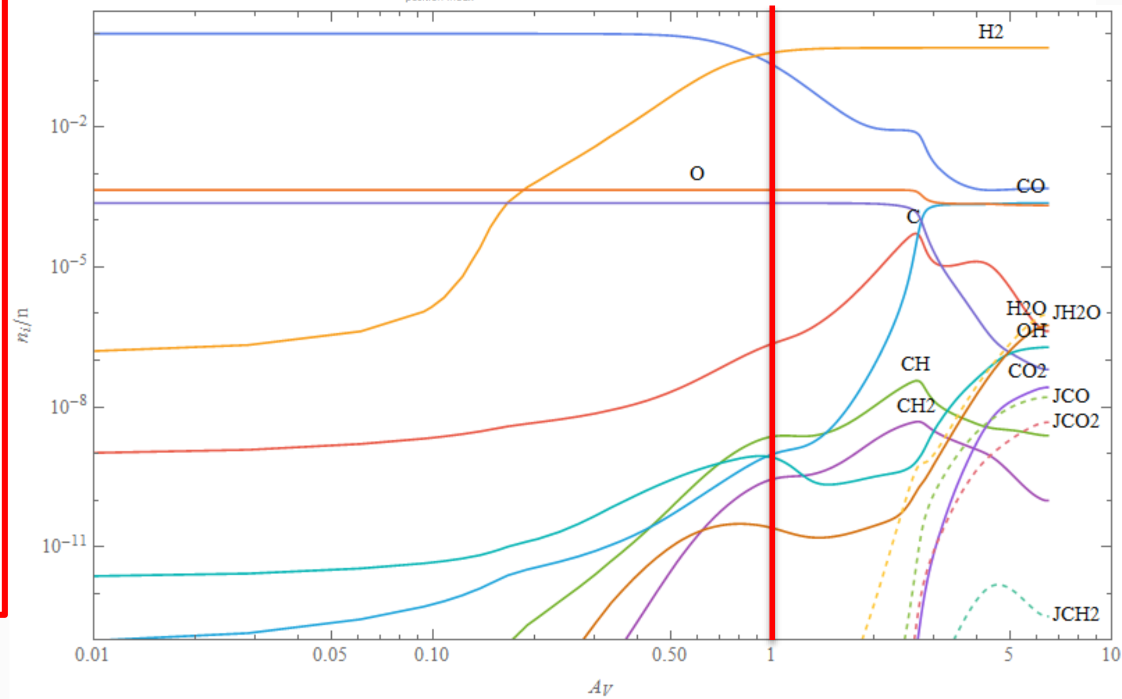

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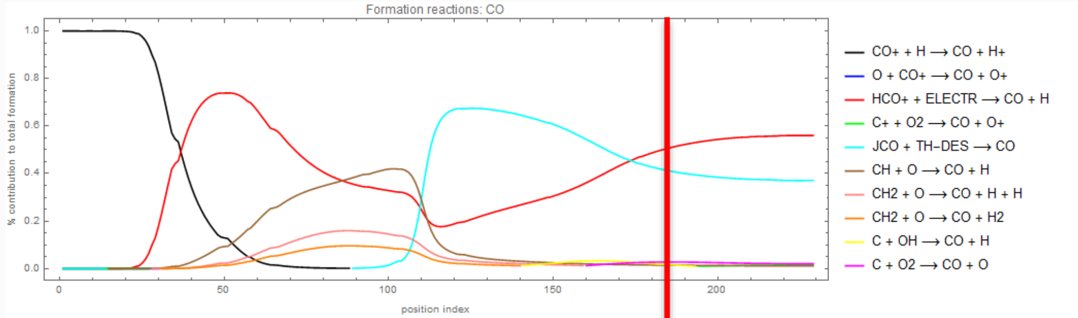

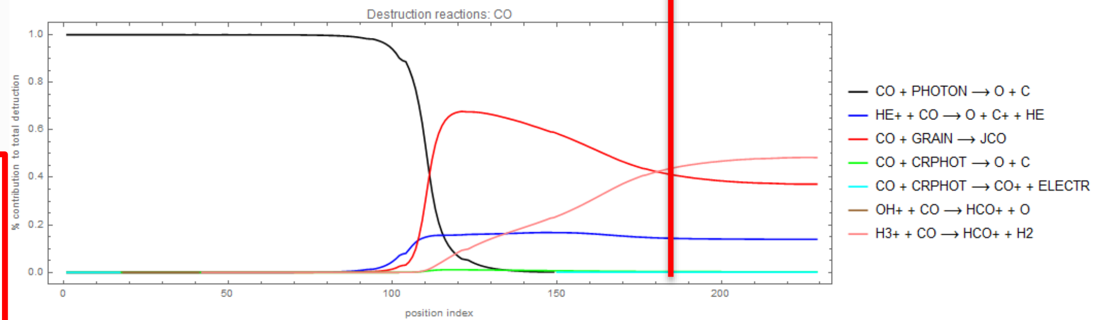

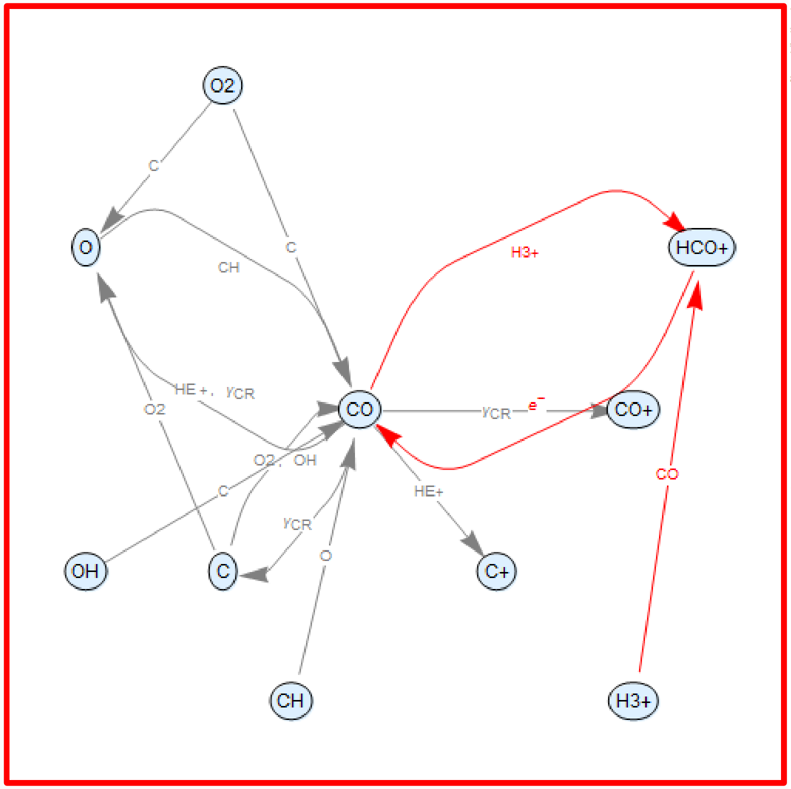

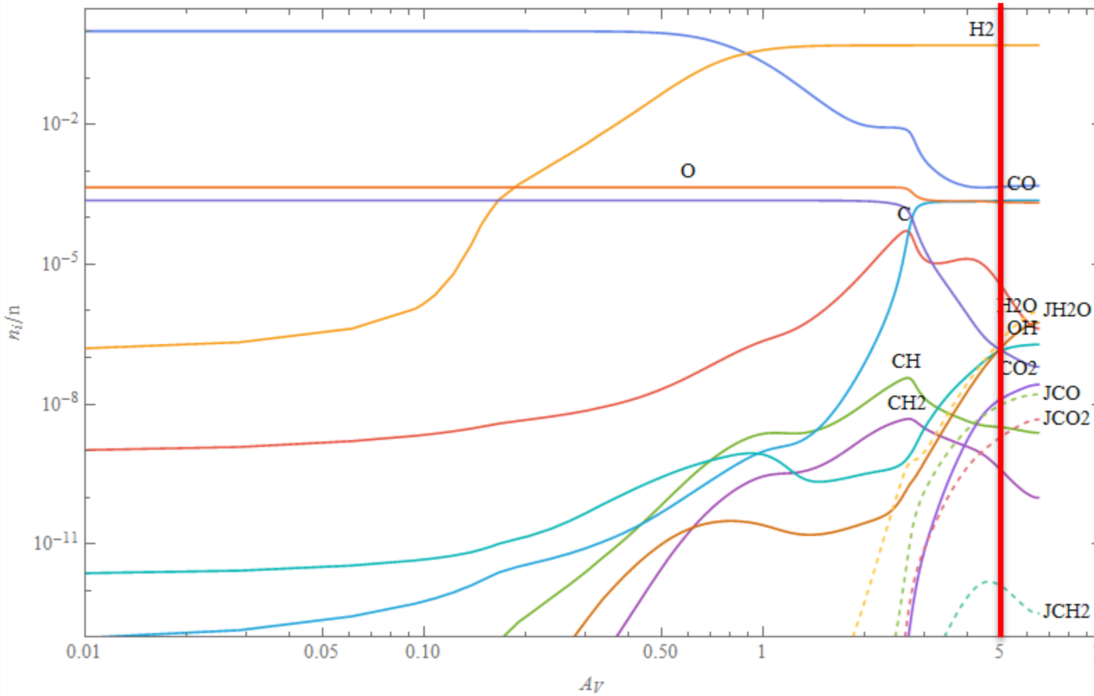

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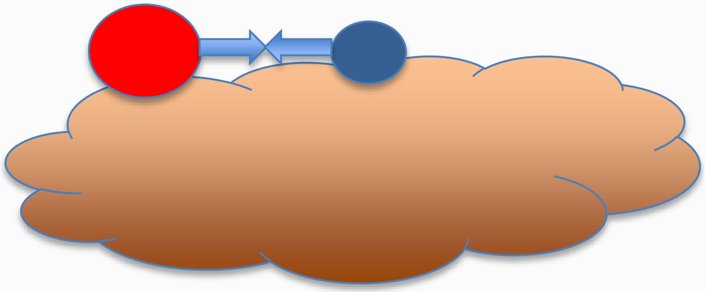
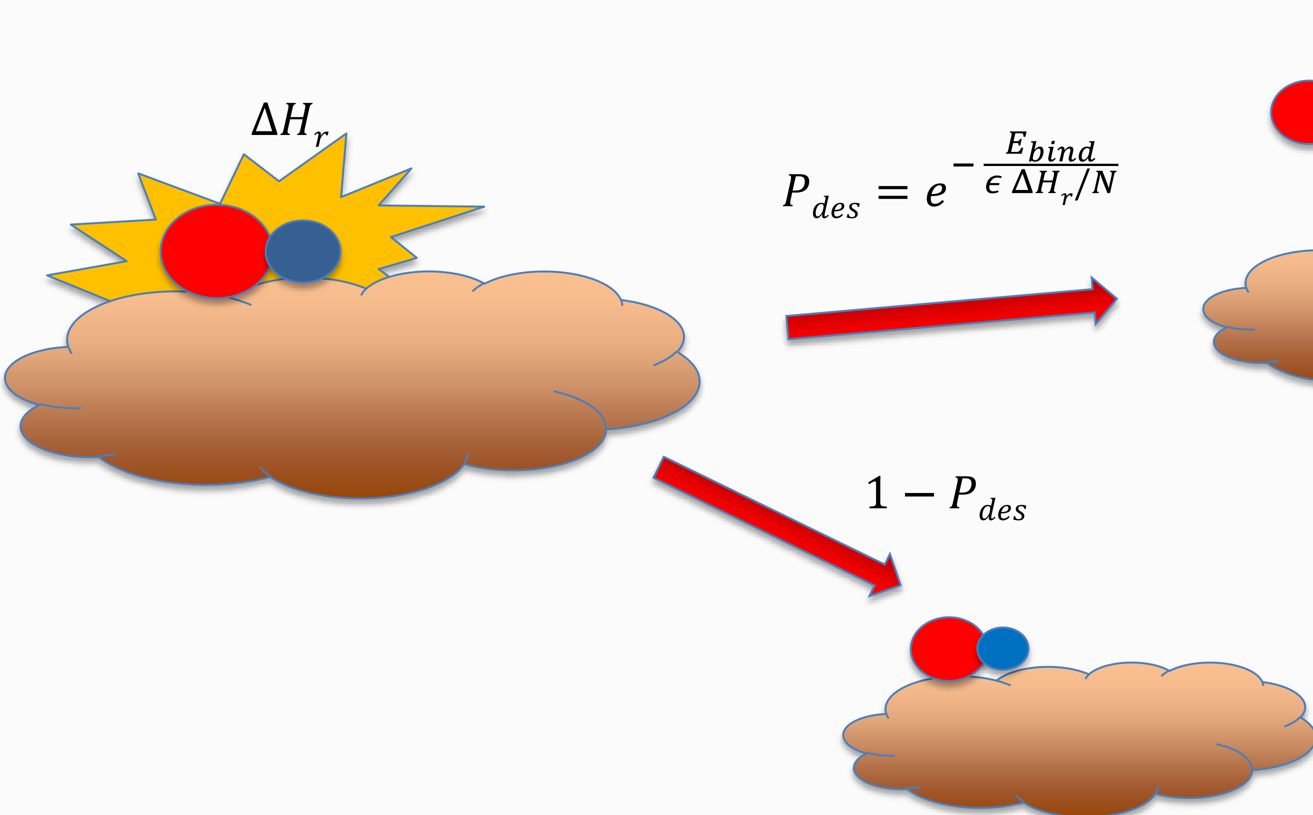
Full Surface Chemistry Upgrade

- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption (Minissale et al. 2015, Cazaux et al. 2016)



Full Surface Chemistry Upgrade

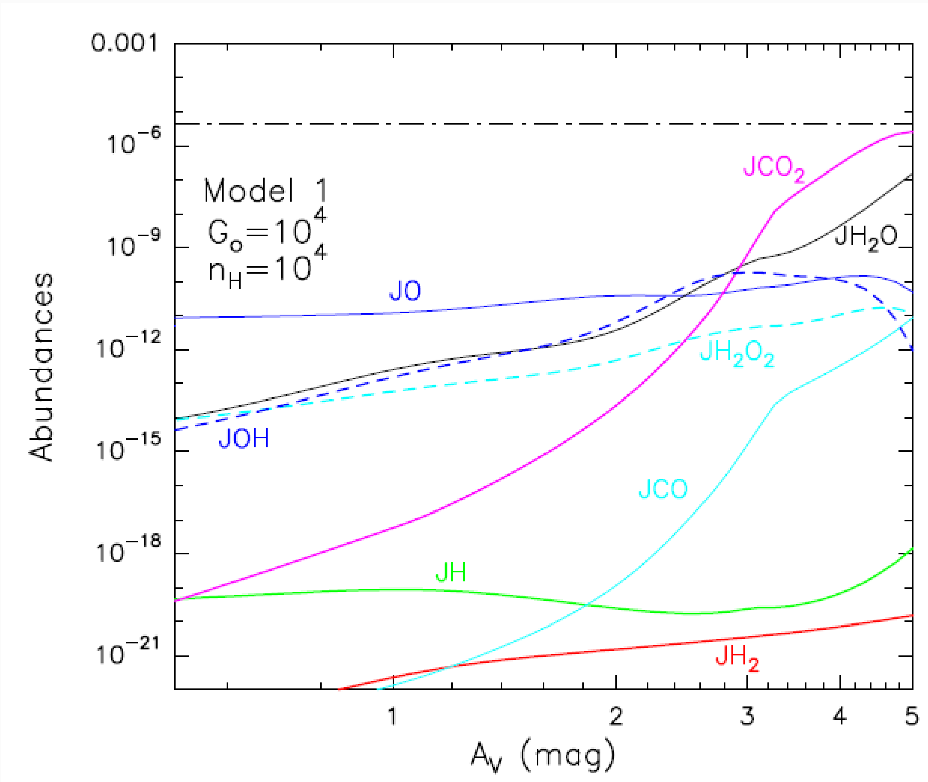
– surface-surface processes (Langmuir-Hinshelwood)
– exoenergetic reactions may lead to desorption of the product (Minissale et al. 2015, Cazaux et al. 2016)



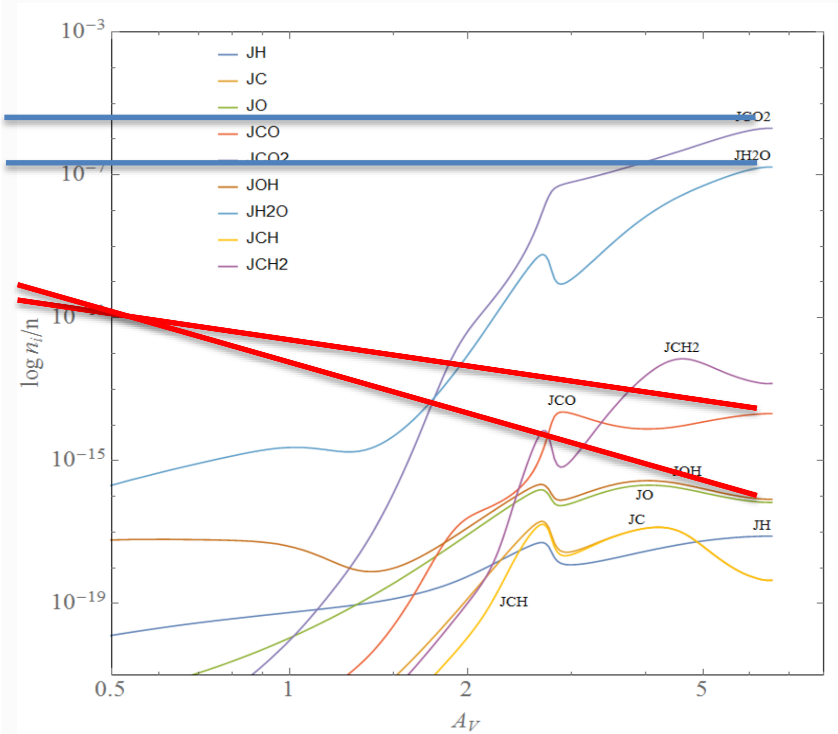
E,p conservation

$$\epsilon = \frac{(M-m)^2}{(M-m)^2}$$

Chemical details with impact

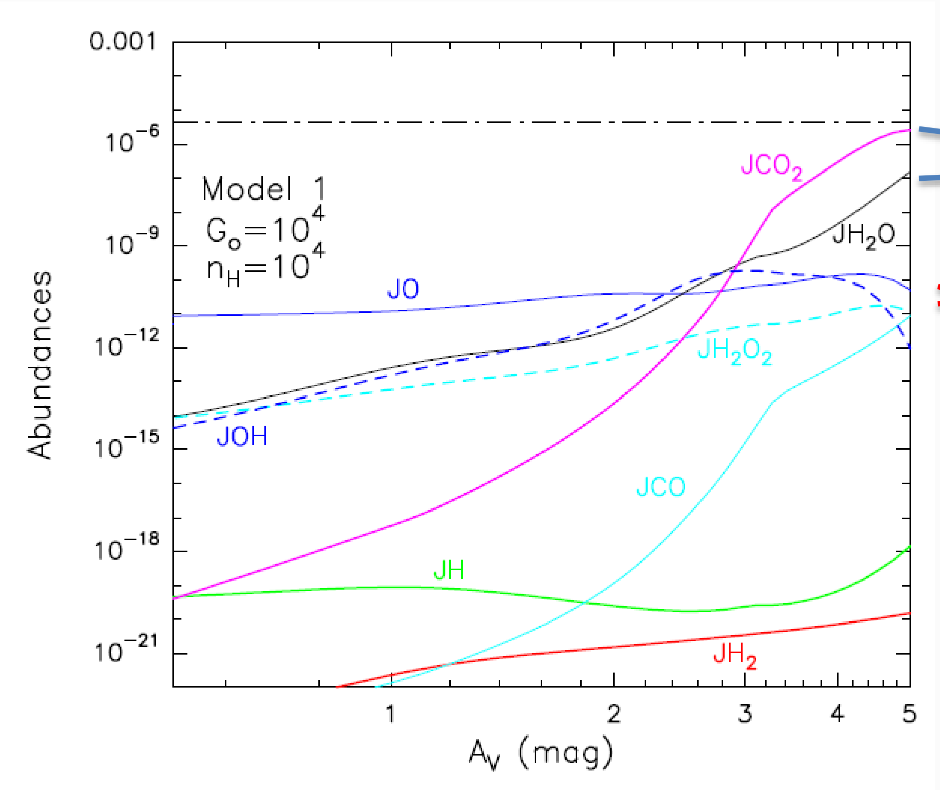


Esplugues et al. 2016



KOSMA-τ with „comparable“ setup

Chemical details with impact



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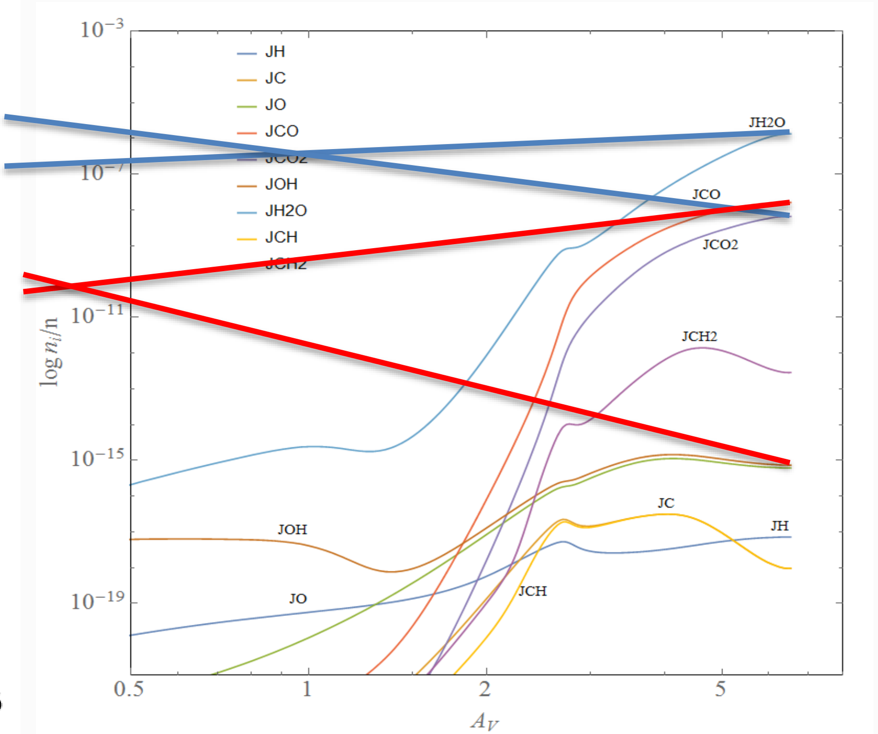


KOSMA-τ with „comparable“ setup

plus

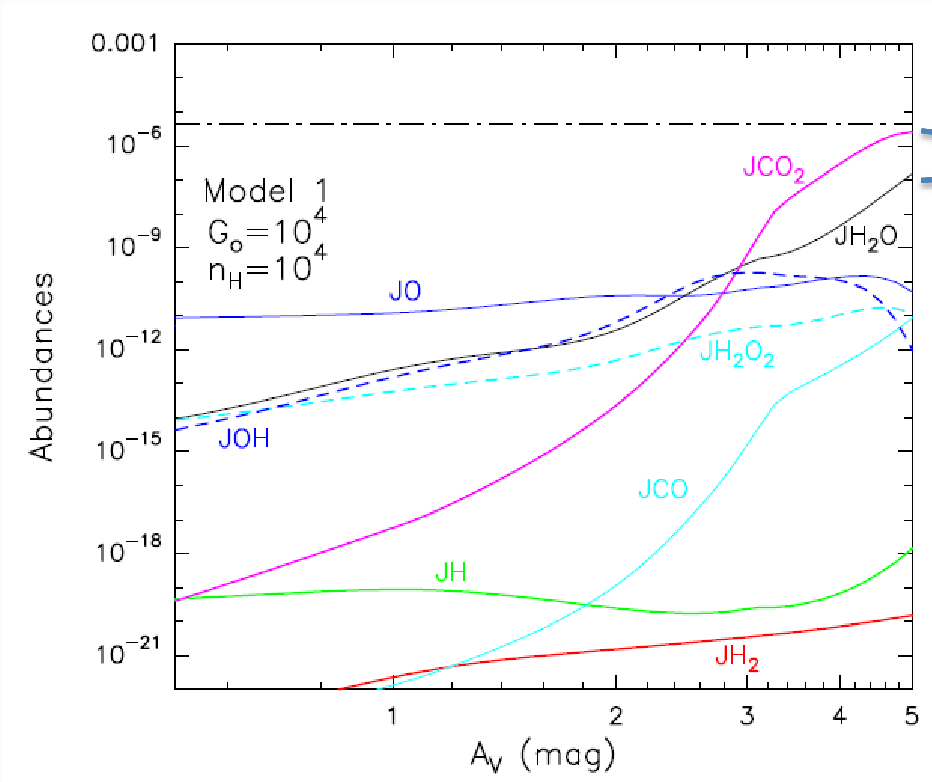
(theoretical BRs)

JCO + JO→ CO_2 (22%)

JCO + JO→ JCO_2 (78%)

→ significantly different ice composition

Chemical details with impact



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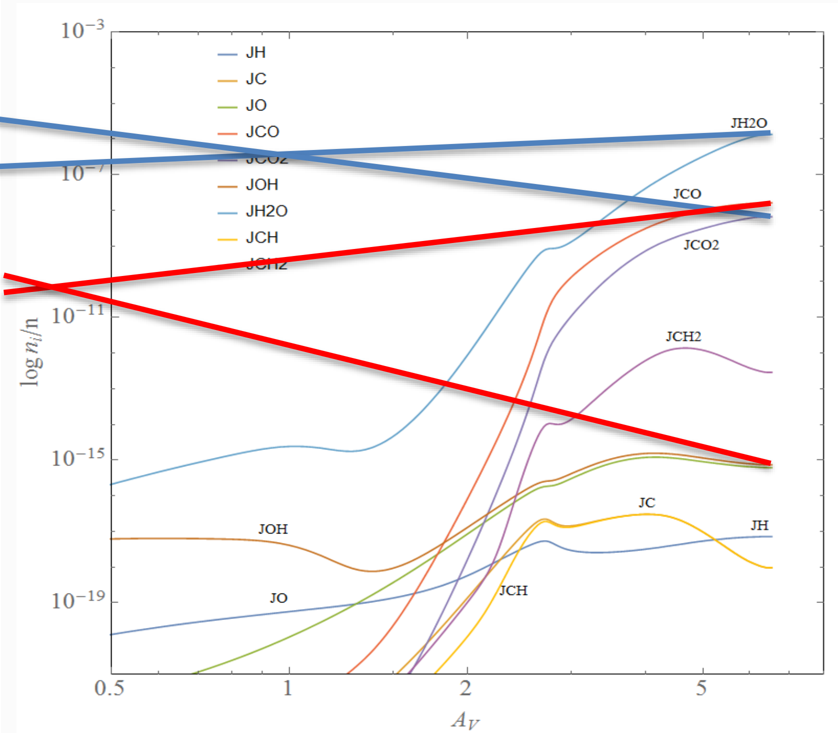


KOSMA-τ with „comparable“ setup

plus

(measured BRs)

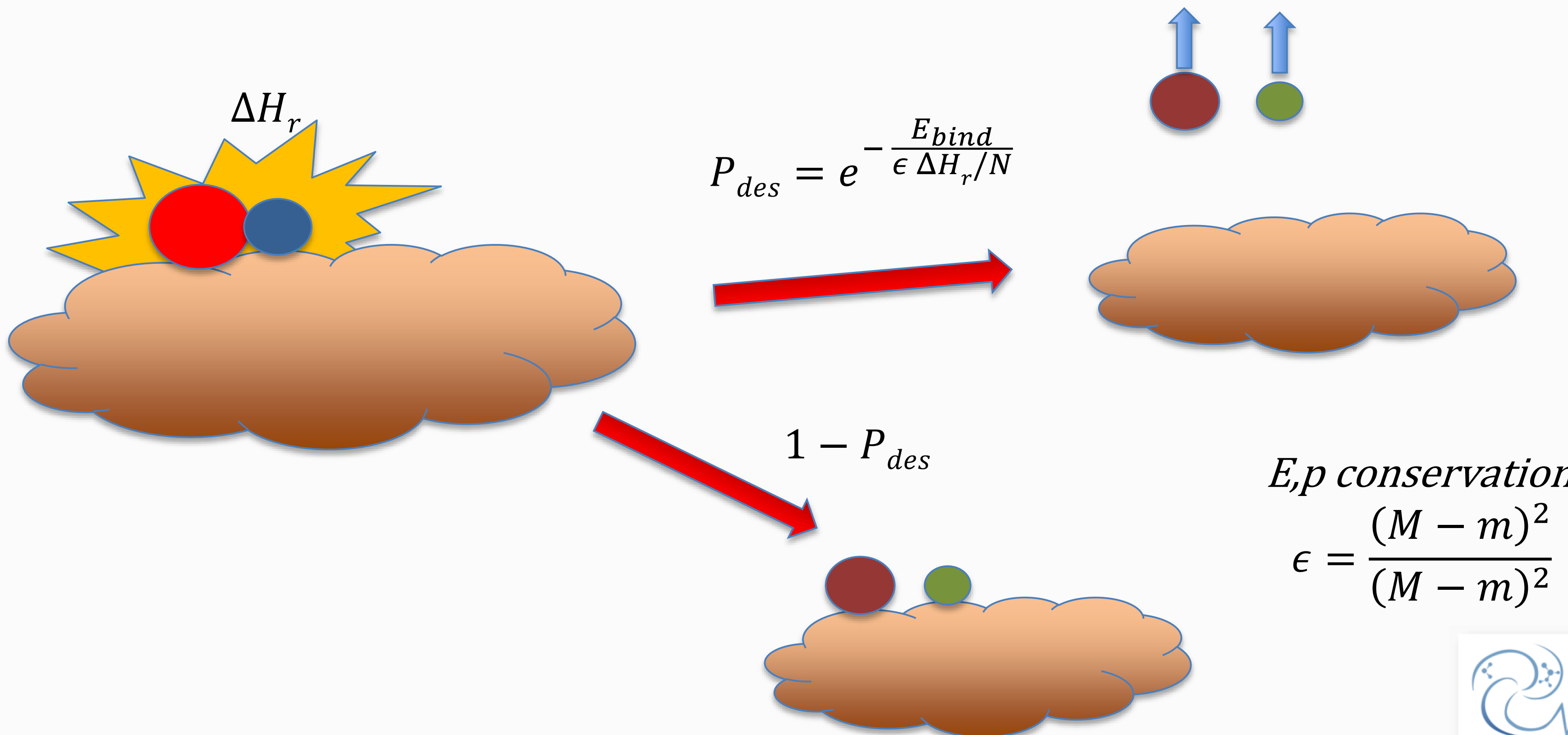
JCO + JO→ CO_2 (4%)

JCO + JO→ JCO_2 (96%)

→ significantly different ice composition

Full Surface Chemistry Upgrade

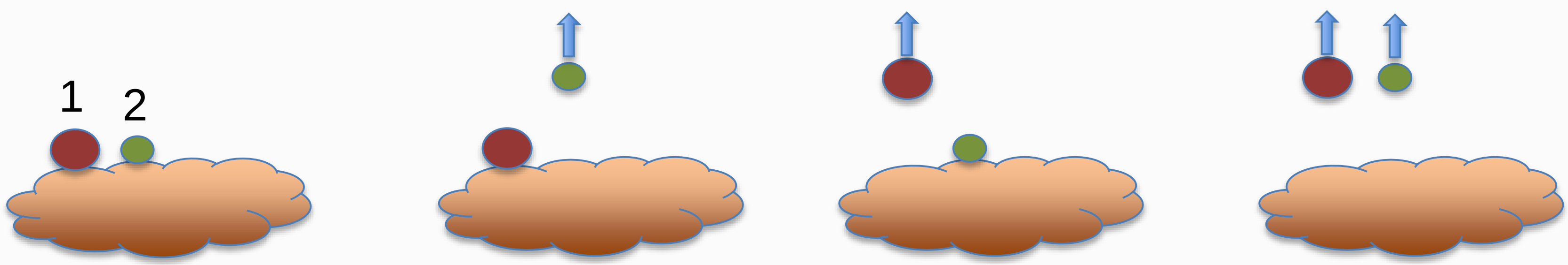
- surface-surface processes (Langmuir-Hinshelwood)
- exoenergetic reactions may lead to desorption of **both products** (Minissale et al. 2015, Cazaux et al. 2016)



Full Surface Chemistry Upgrade

- So far assumed that all products desorb with full reaction enthalpy
- Now, we assume that formation energy is distributed across products
    - analogue to free particle decay: $\frac{E_1}{E_2} = \frac{m_1}{m_2}$, : $\frac{E_1}{E_{tot}} = \eta_1 = \frac{m_1}{m_1+m_2}$
    - $P_{des,i} = e^{-\frac{E_{bind,i}}{\epsilon_i \eta_i \Delta H_r / N_i}}$, $\overline{P_{des,i}} = 1 - P_{des,i}$
    - H_2 always desorbs

$(1\text{-}P_{des,1}) \times (1\text{-} P_{des,2})$ $(1\text{-}P_{des,1}) \times P_{des,2}$ $P_{des,1} \times (1\text{-} P_{des,2})$ $P_{des,1} \times P_{des,2}$



Röllig et al., in prep

Some example branching rates

- $$JOH + JO \longrightarrow \begin{array}{cccc} O_2 & + & H & 7\times 10^{-5}(0.019) \\ JO_2 & + & H & 5.7\times 10^{-4}(-) \\ O_2 & + & JH & 0.11\ (-) \\ JO_2 & + & JH & 0.89(0.981) \end{array}$$
- $$JH_2O_2 + JH \longrightarrow \begin{array}{cccc} H_2O & + & OH & 0.002(0.021) \\ JH_2O & + & OH & 0.16(-) \\ H_2O & + & JOH & 0.01(-) \\ JH_2O & + & JOH & 0.83(0.979) \end{array}$$
- $$JHCO + JH \longrightarrow \begin{array}{cccc} CO & + & H_2 & 0.65(0.47) \\ JCO & + & H_2 & 0.35(-) \\ CO & + & JH_2 & 0(-) \\ JCO & + & JH_2 & 0\ (0.53) \end{array}$$

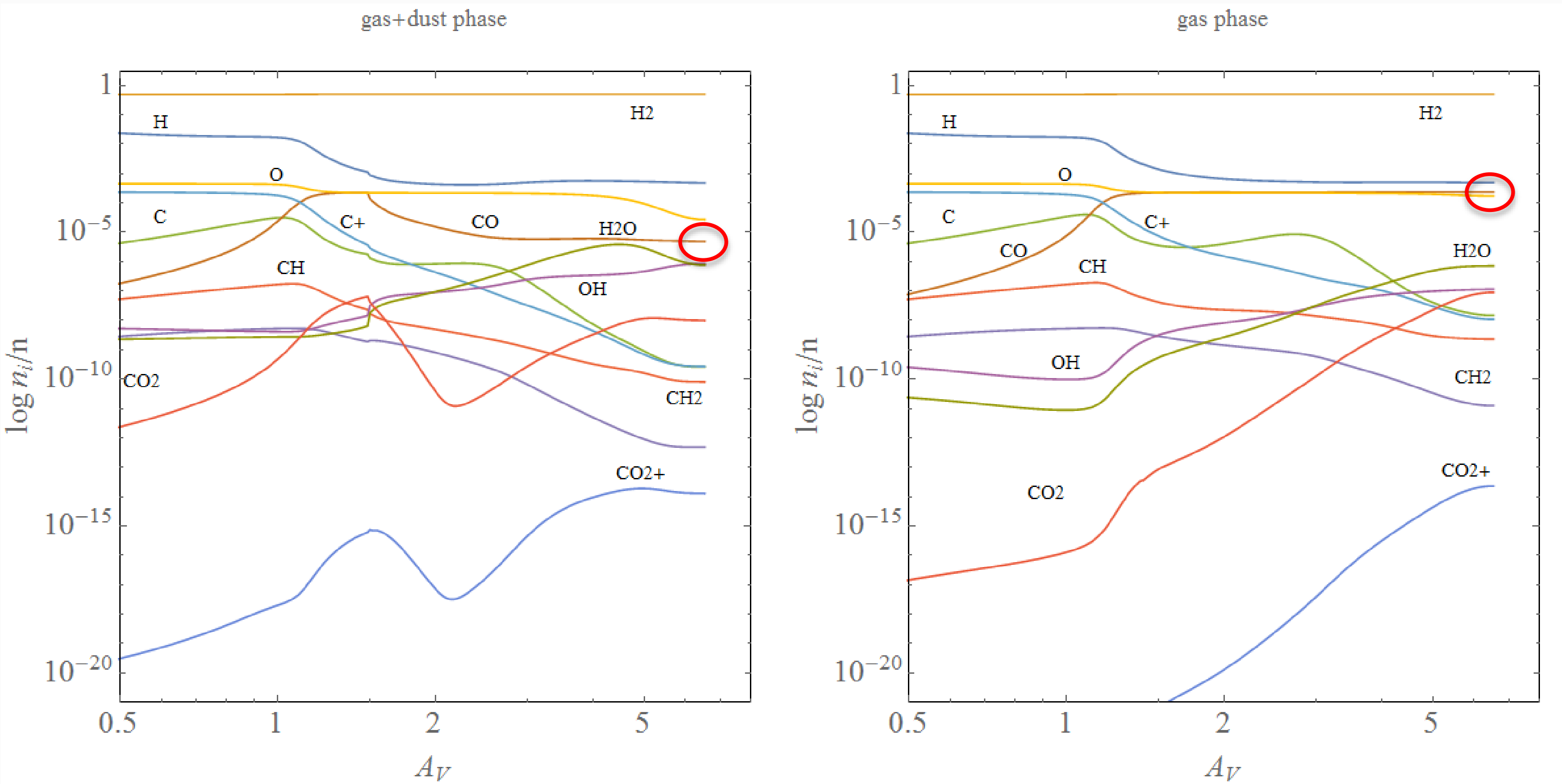
BRs depend on the energy redistribution.

Other distribution schemes?

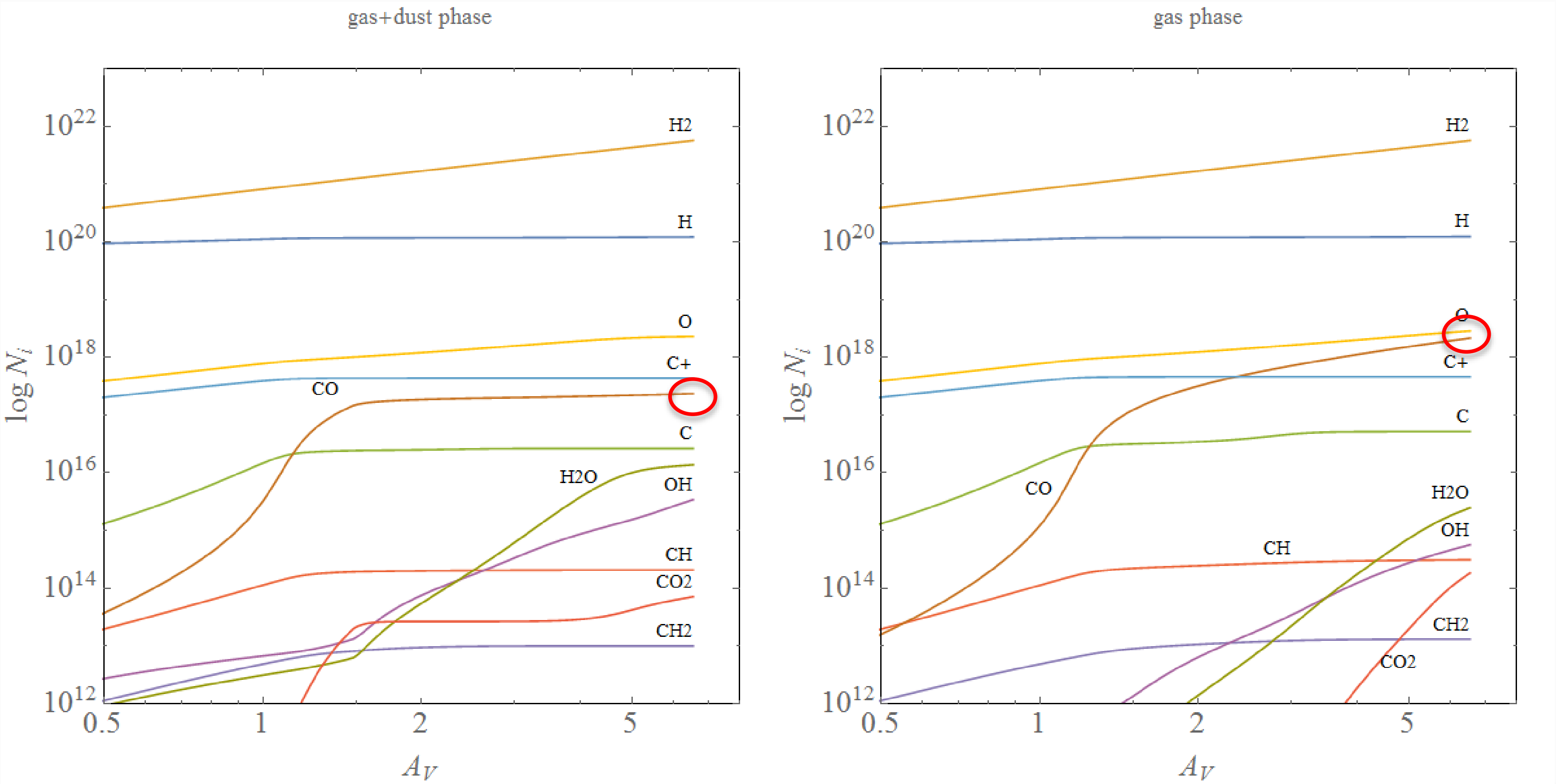
Questions & Concerns

- Binding energies – Yes, but which one? (see Wakelam et al. 2017)
- How about surfaces of very small grains? PAHs?
  - Very important for H_2 formation
  - excitation of small hydrocarbons, H_2, high-J CO
- Cross sections of surface photo-processes
  - Important for PDRs because of FUV attenuation/shielding
  - Photodesorption yields?
- Numerical stability? Convergence/steady-state ?
  - Including/excluding of
    - desorption processes
    - grain + gas phase species
    - initial abundances! PDRs are different from dark cloud models
  - Any technical/numerical comments in your papers are much appreciated.
- (Column) density is no observable.

Density is no observable



Column density is no observable



Line intensities are observed

gas+dust phase

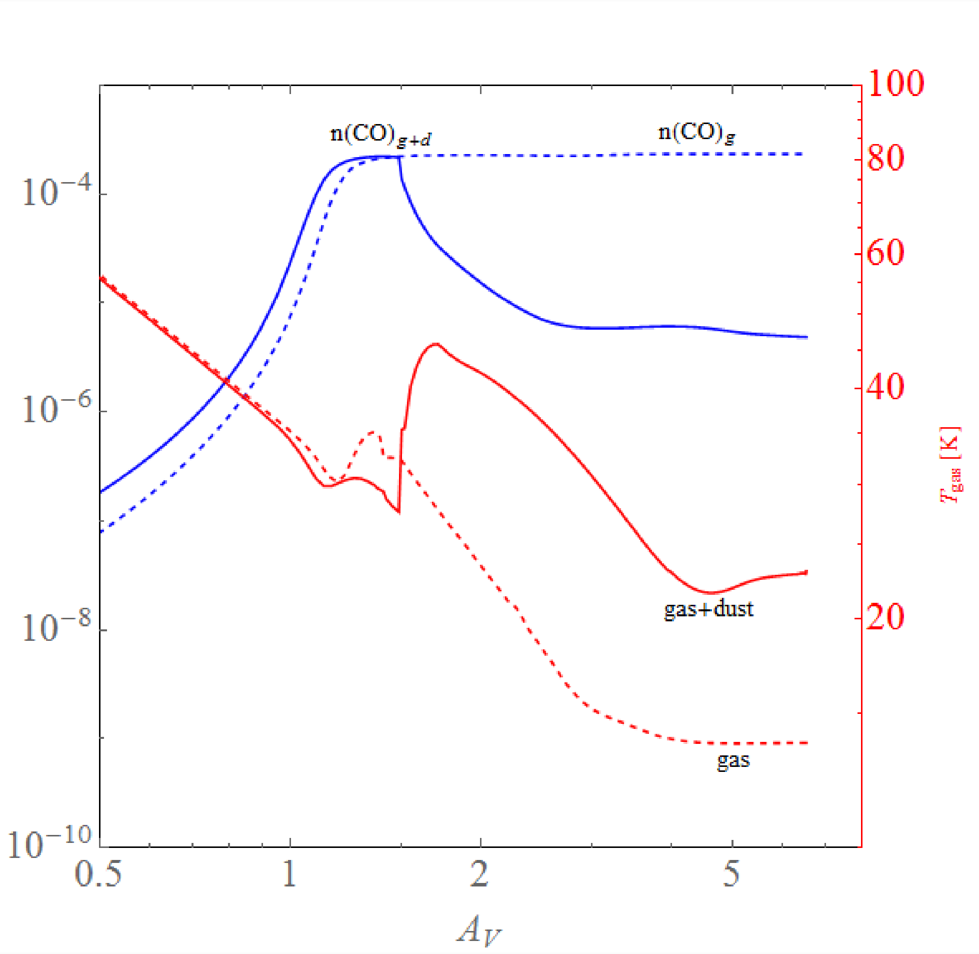
Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	5.8
CO J=2-1	7.3
CO J=3-2	4.3
CO J=4-3	1.4
[CII] 158µm	2.3
[CI] 609 µm	8.7
[CI] 370µm	2.3

lower column densities
higher intensities !

gas phase

Line	$\int T_{mb} dv$ [K km/s]
CO J=1-0	0.66
CO J=2-1	0.55
CO J=3-2	0.14
CO J=4-3	0.016
[CII] 158µm	2.1
[CI] 609 µm	9.5
[CI] 370µm	2.6

Excitation matters



gas cooling is significantly reduced in the absence of CO

→ gas temperatur increases

Questions & Concerns

- Densities and column densities are good for inter-model comparison but are no observables.
- Calibrate model against ‚derived‘ (column) densities? Which ones? Derived under which conditions?
  - We need to make sure that model (column) densities can be compared to ‚observed‘ ones.
- Alternatively one could apply radiative transfer and compare against measured intensities!
  - But then we need to know the density/temperature structure.

It might be time for a follow-up round of the PDR-Benchmark.

Thank you for your attention!