Surface Chemistry in the KOSMA-τ PDR Code

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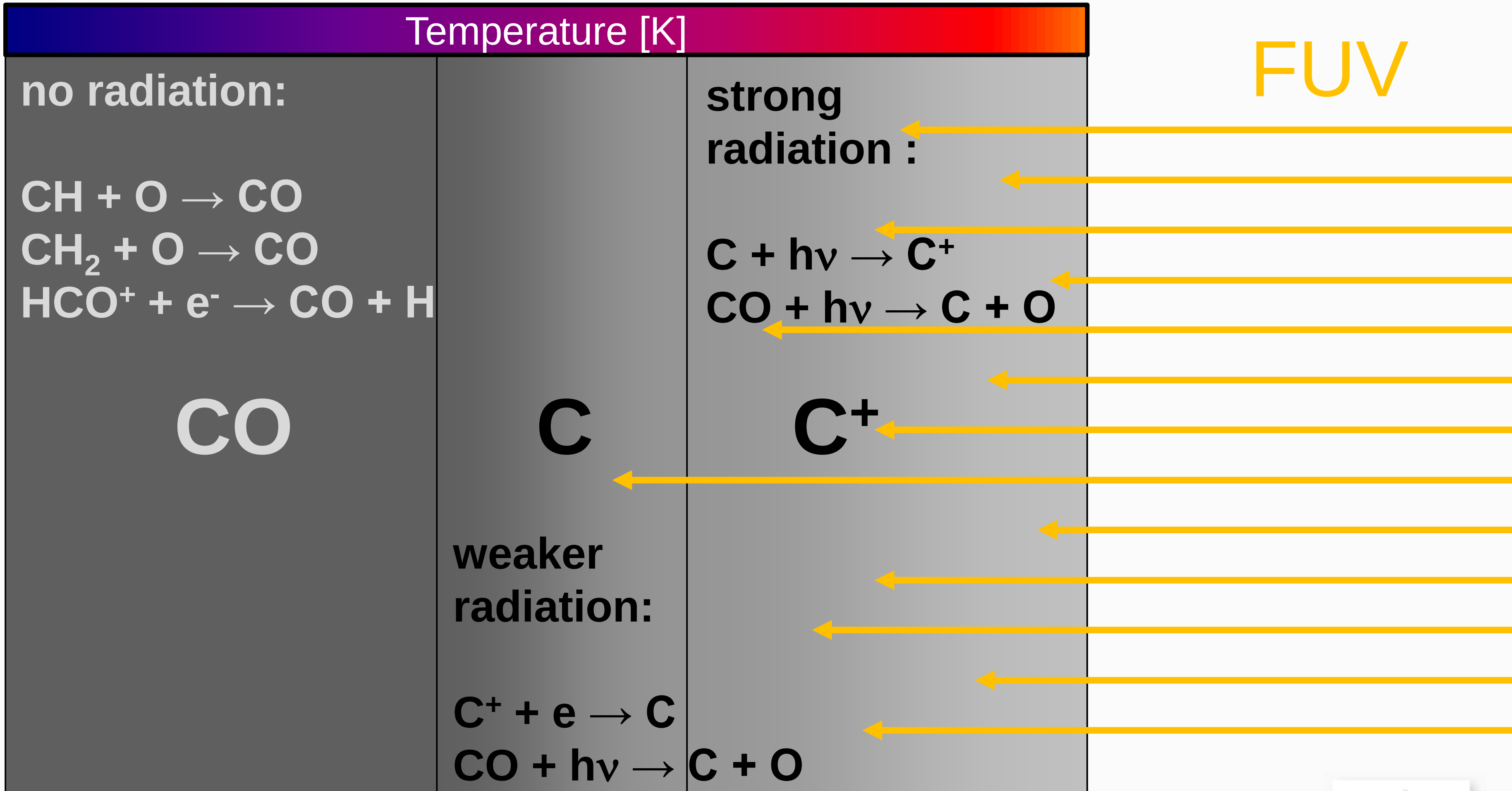
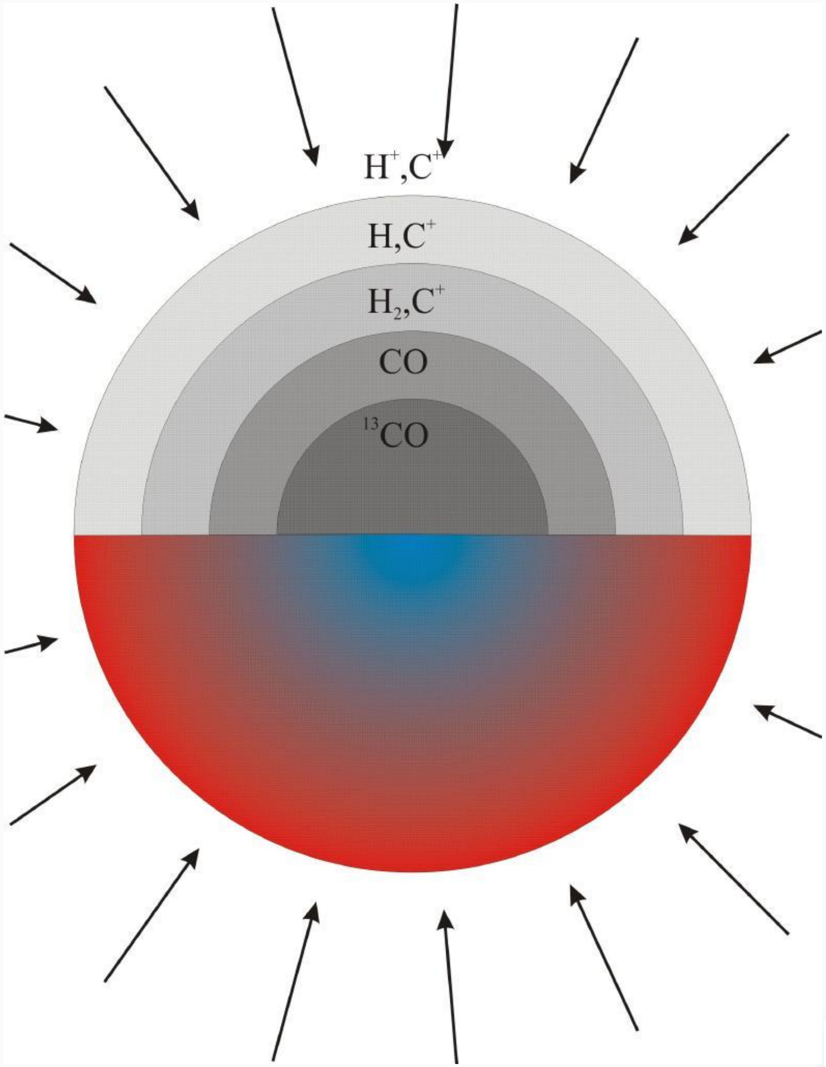
Photodissociation Region



Interstellar cloud surface (cross section)

The KOSMA-τ PDR Code

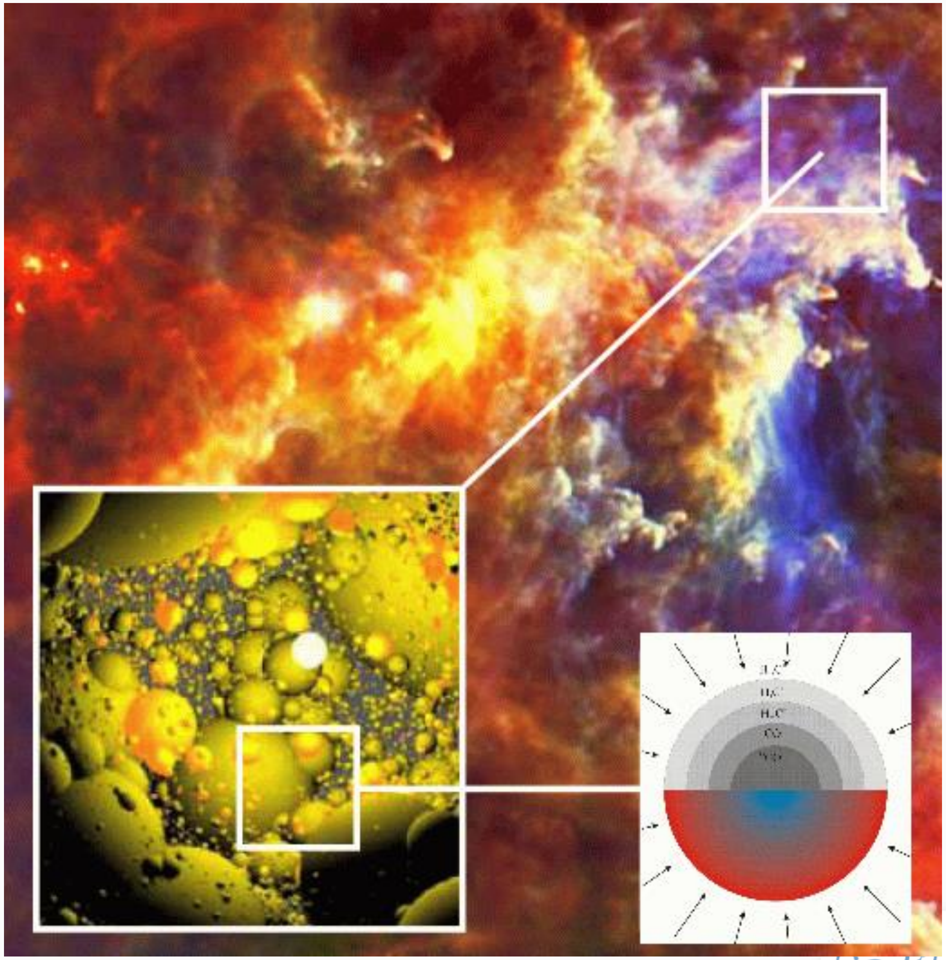
- 1-D, spherical geometry
- isotropic illumination
- self-consistent solution of energy- and chemical balance
- modular chemistry (steady-state)
- ^{13}C and ^{18}O isotopologue chemistry



The KOSMA-τ PDR Code

- 1-D, spherical geometry
- isotropic illumination
- self-consistent solution of energy- and chemical balance
- modular chemistry (steady-state)
- ^{13}C and ^{18}O isotopologue chemistry

- clumpy cloud composition



Dust in KOSMA-τ

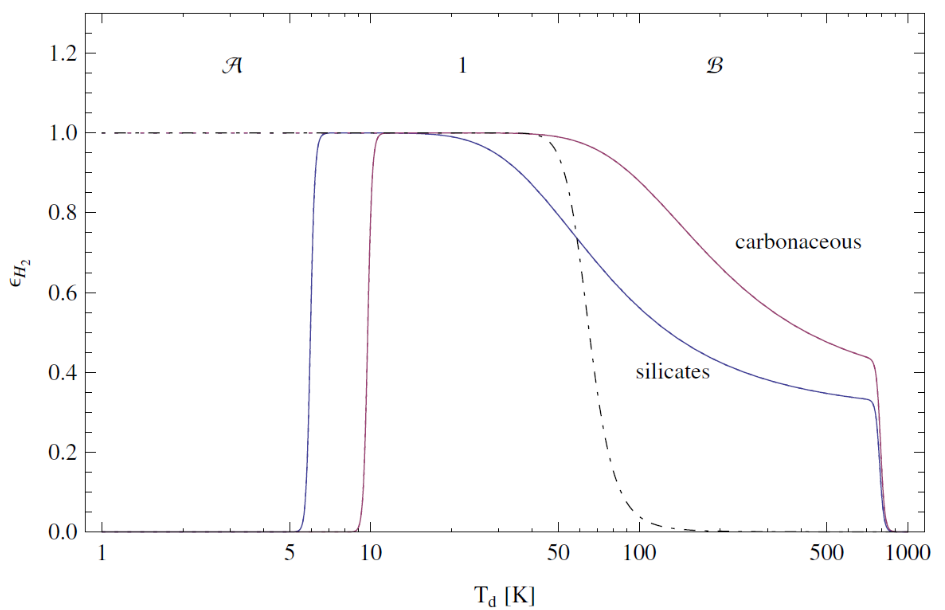
- Recent upgrade of dust treatment in the code. (Röllig et al. 2013)

- Implementation of Weingartner & Draine 2001 dust model
  - multiple dust components
  - dust grain size distribution
  - detailed UV continuum radiative transfer
  - self consistent computation of dust temperature

➢ detailed information on how much available surface at which temperature

H_2 formation heating

formation efficiency



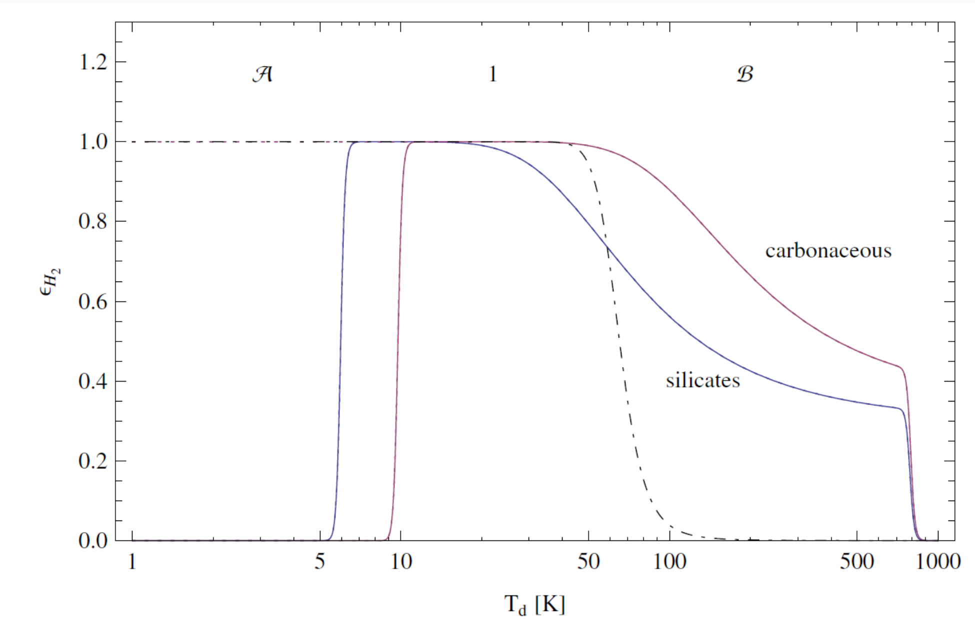
- H-binding to the grain surface determines its mobility and resistance against thermal desorption
  - weak binding (physisorption), T<50-80K
  - strong binding (chemisorption), T<~500-800 K

Chemisorption leads to efficient H_2 formation at high dust temperatures

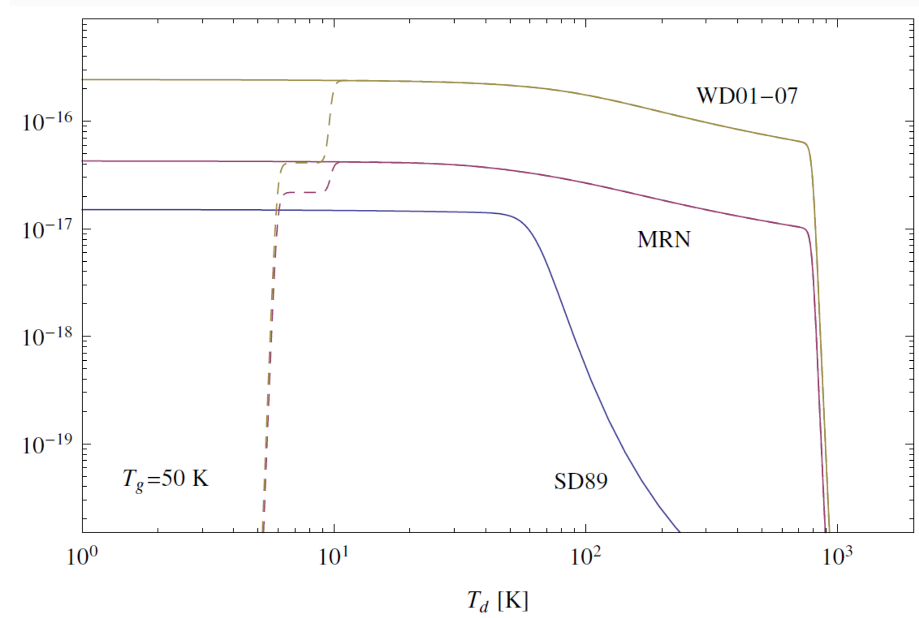
Cazaux & Tielens (2002, 2010)

H_2 formation heating

formation efficiency



formation rate

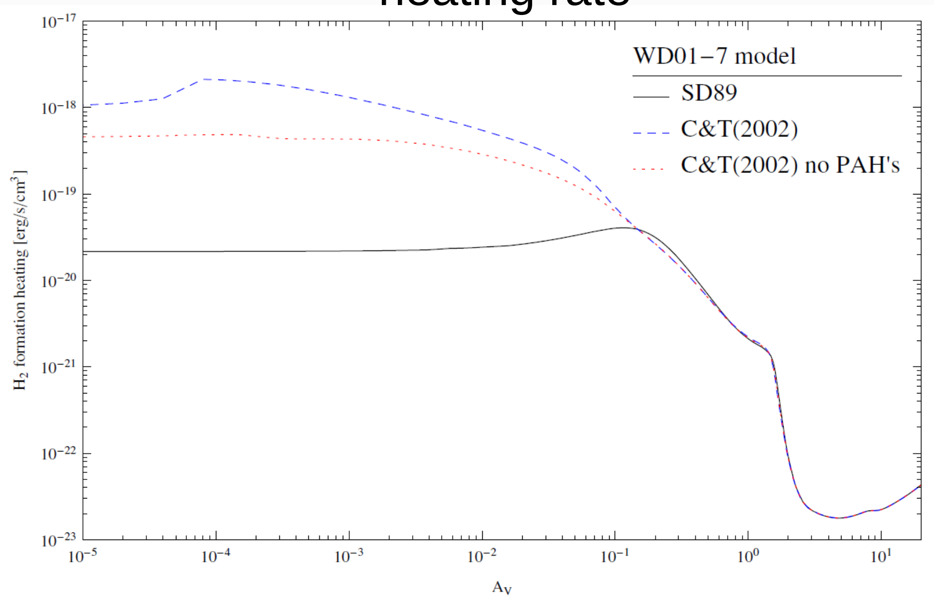


Cazaux & Tielens (2002,2010)

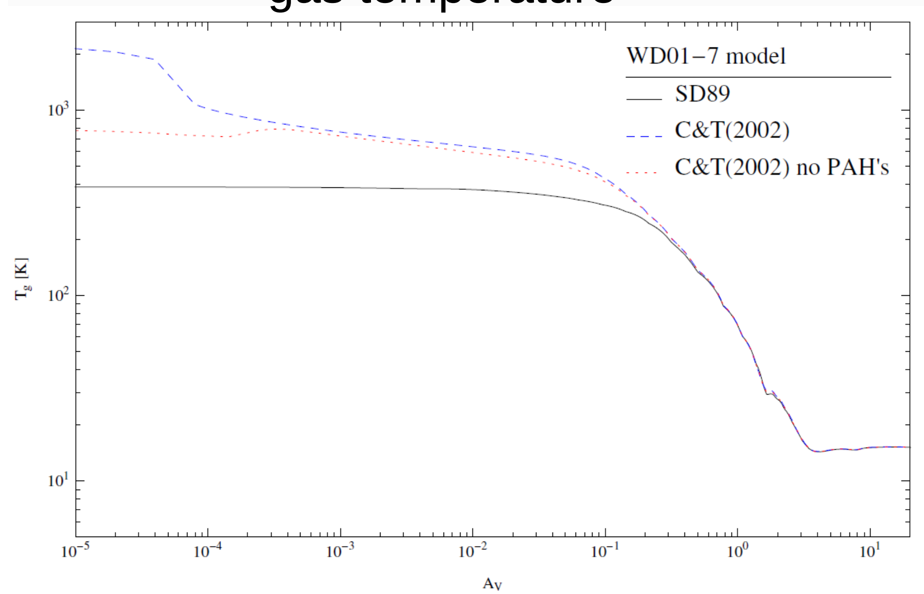
Chemisorption leads to efficient H_2 formation at high dust temperatures

H_2 formation heating

heating rate



gas temperature

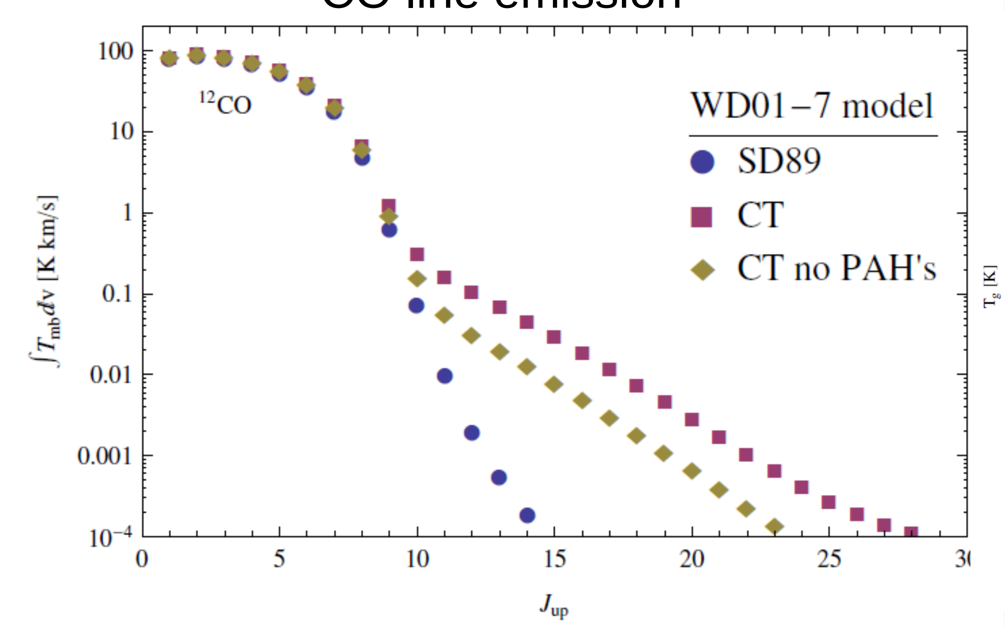


Röllig et al. 2013

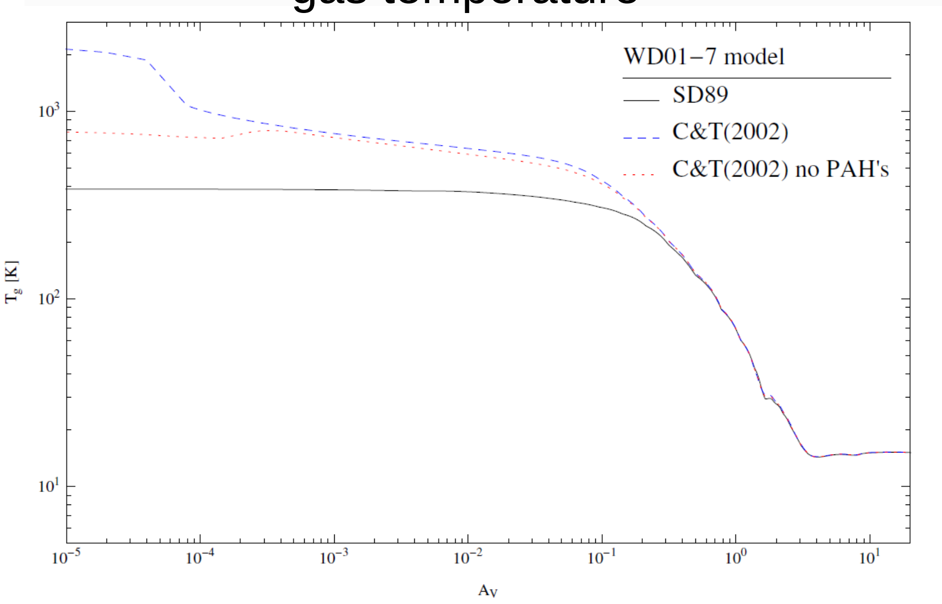
More efficient H_2 formation leads to stronger gas heating.

H_2 formation heating

CO line emission



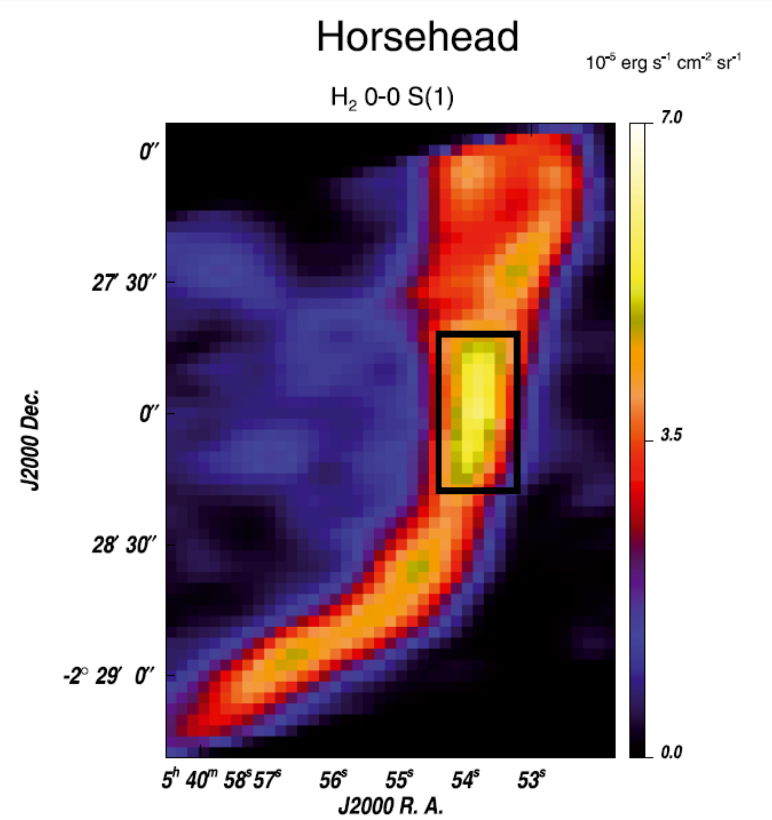
gas temperature

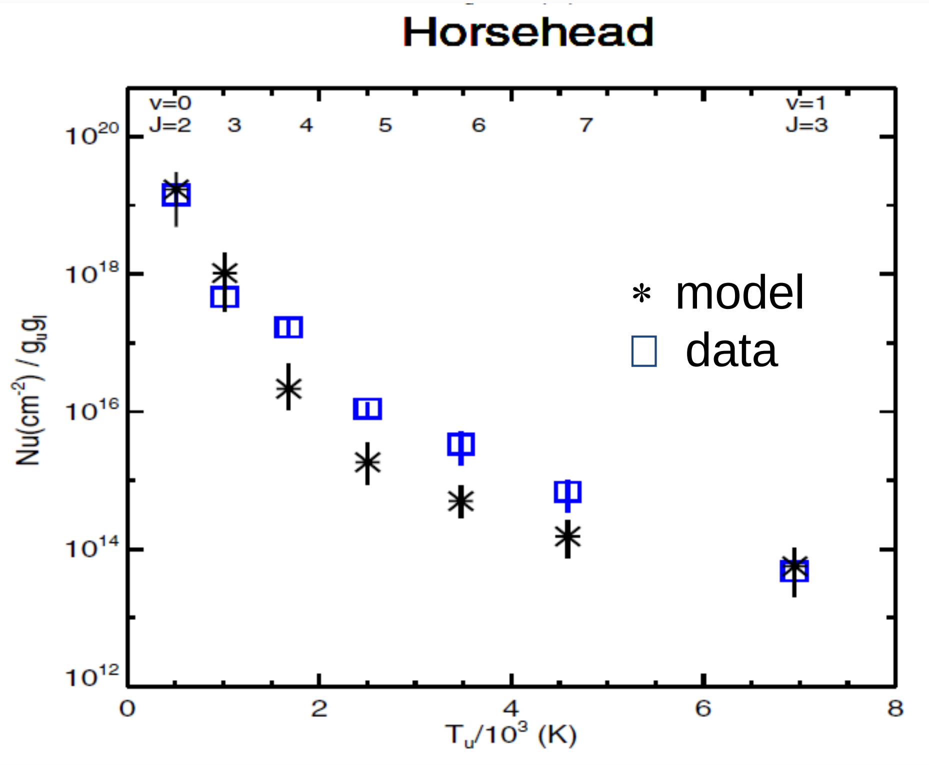


Röllig et al. 2013

Dust content & physics influence high-J CO emission

H_2 excitation



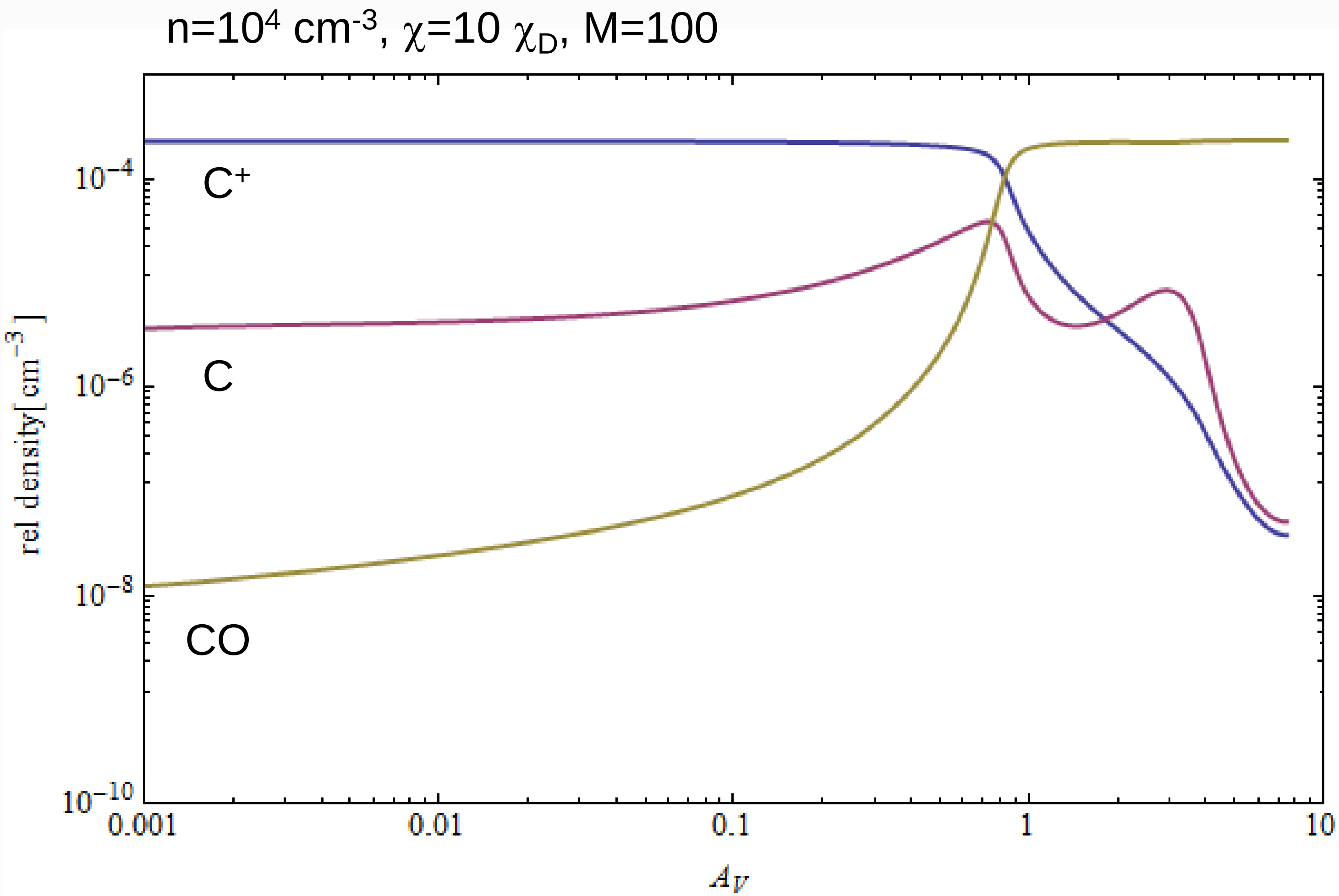


Habart et al. 2011

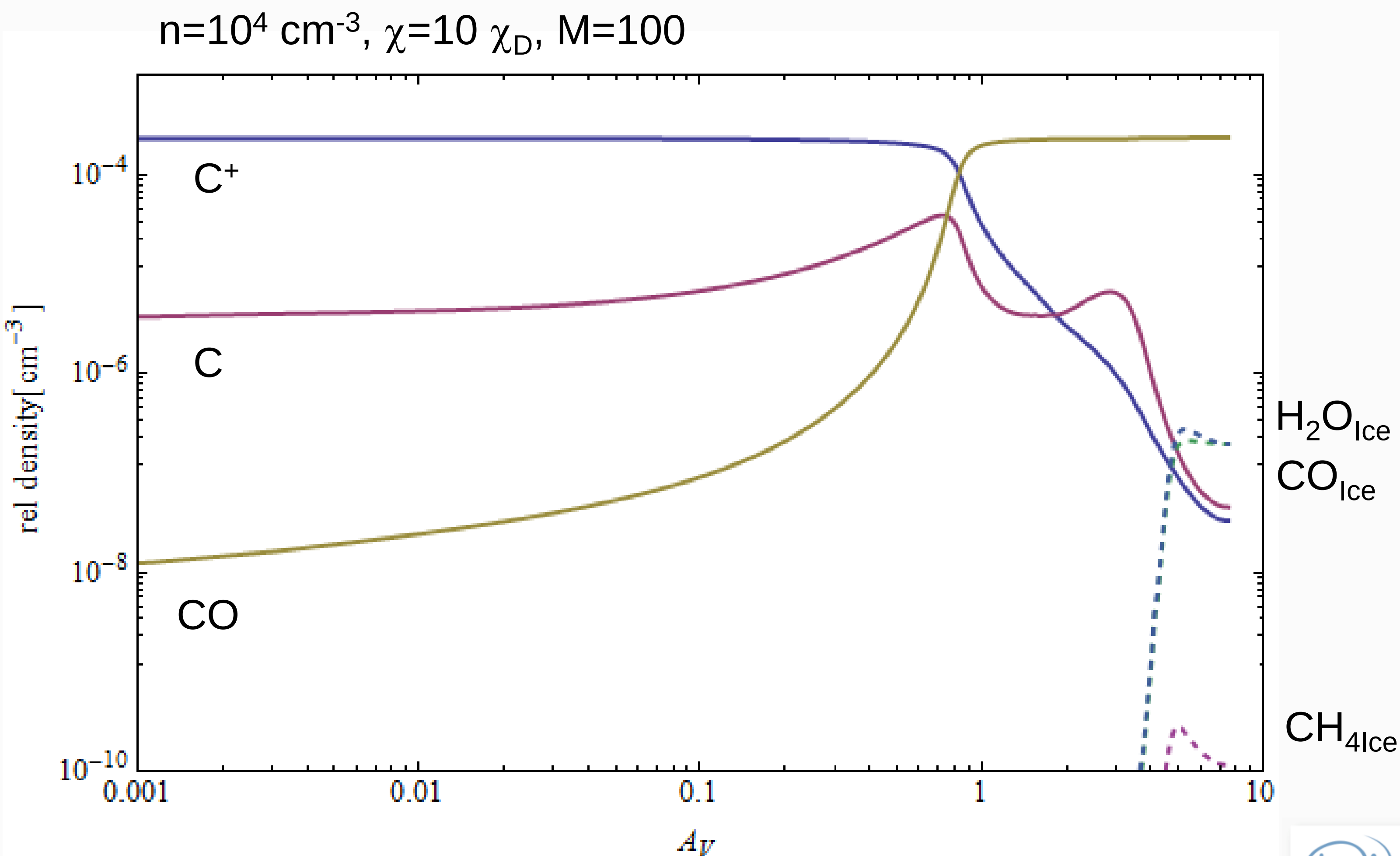
Full Surface Chemistry Upgrade

- Coupling of gas-phase and surface chemistry
- Steady-state chemistry
- Rate equation approach following Hasegawa et al. 1992,1993
- Processes included:
  - adsorption
  - desorption
    - thermal desorption
    - photo-desorption
    - direct CR heating
    - CR induced photo-desorption
    - H_2-formation induced desorption
  - surface-surface processes (Langmuir-Hinshelwood)

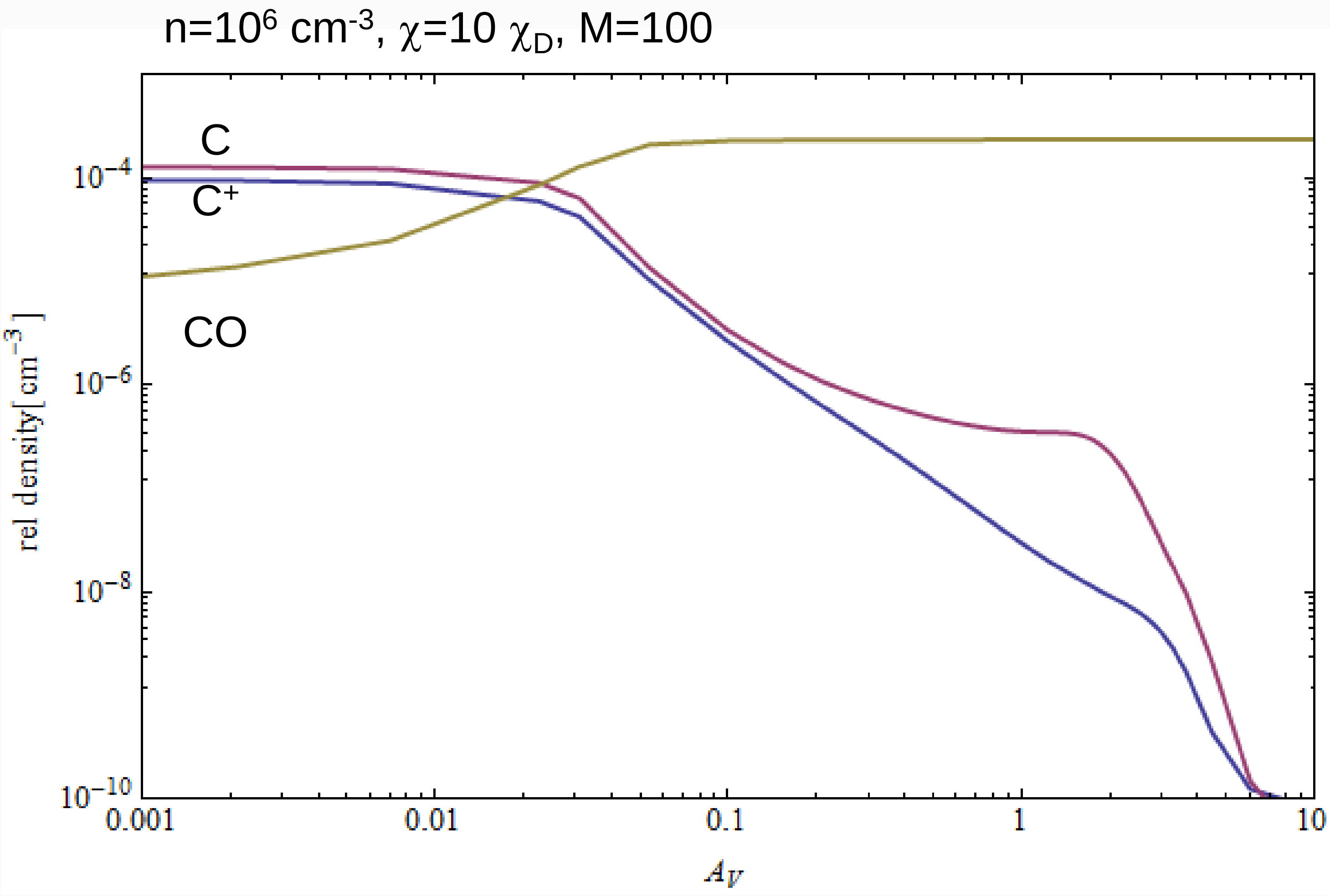
Full Surface Chemistry Upgrade



Full Surface Chemistry Upgrade

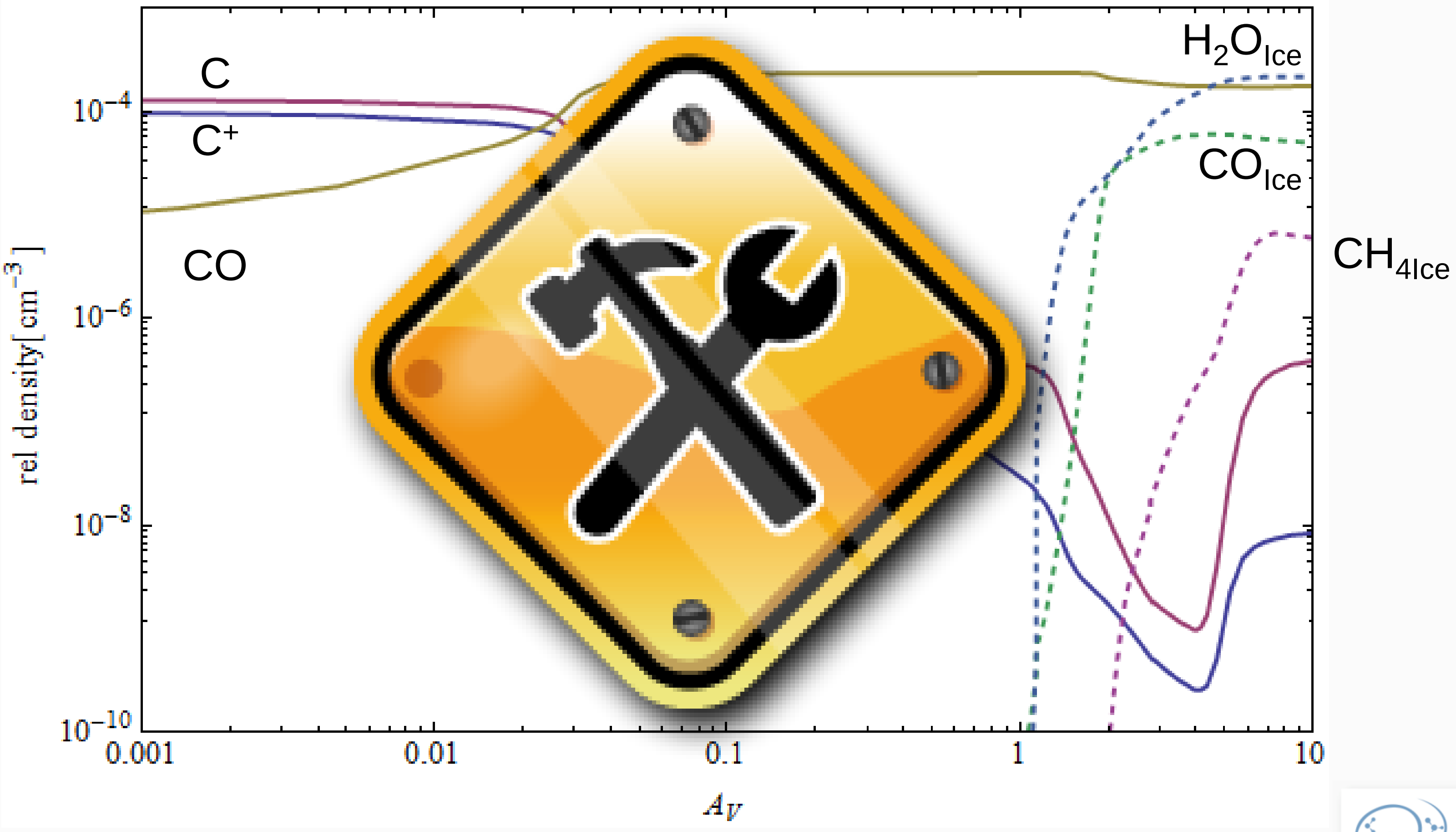


Full Surface Chemistry Upgrade



Full Surface Chemistry Upgrade

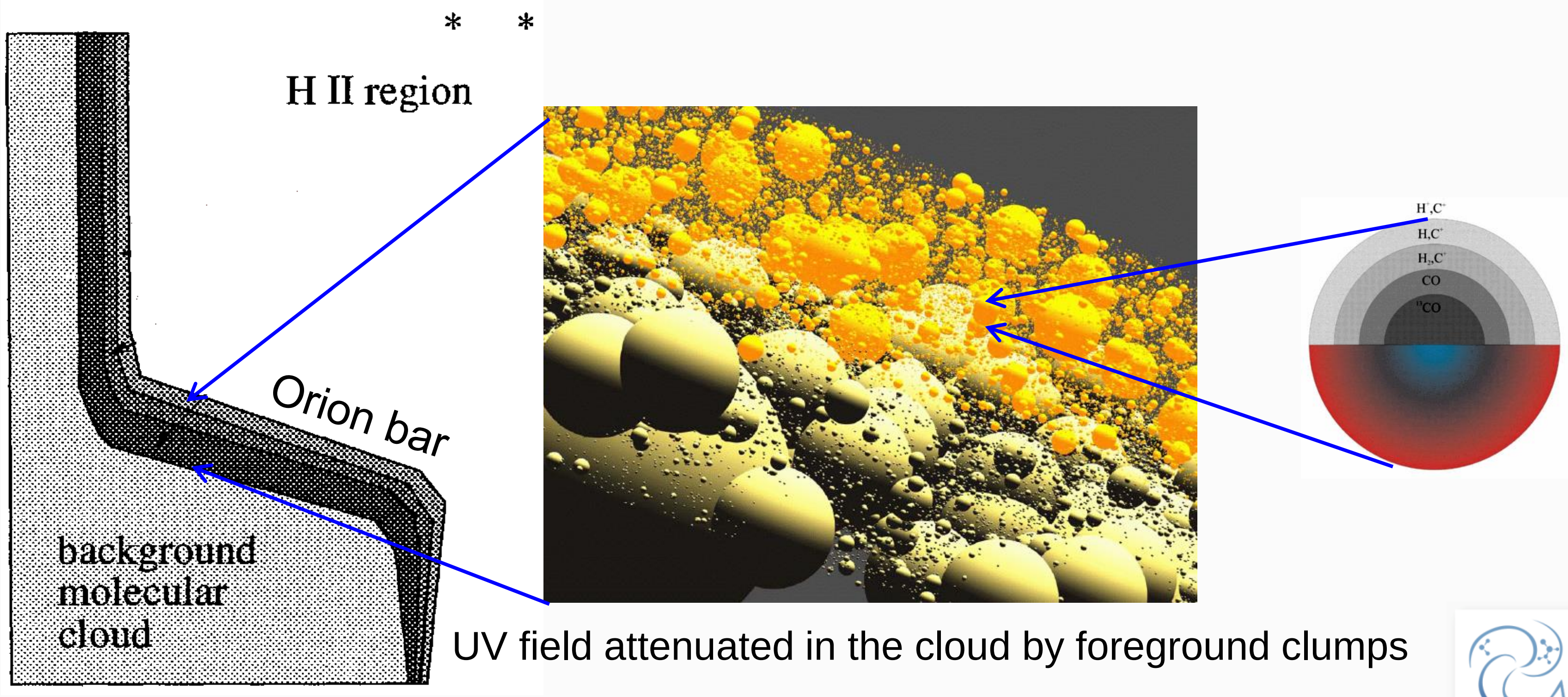
$n=10^6$ cm^{-3}, $\chi=10\ \chi_D$, M=100



The Orion Bar model

KOSMA-τ-3D

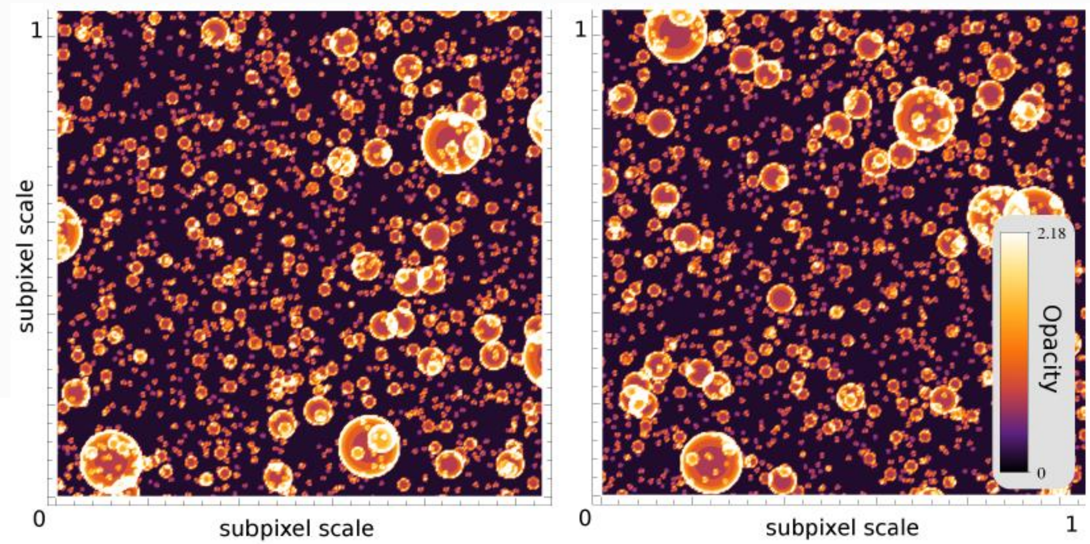
- Simulate PDR by clump ensembles with full size distribution (embedded in interclump medium)
- Individual clumps computed by KOSMA-τ



KOSMA-τ-3D

Radiative transfer

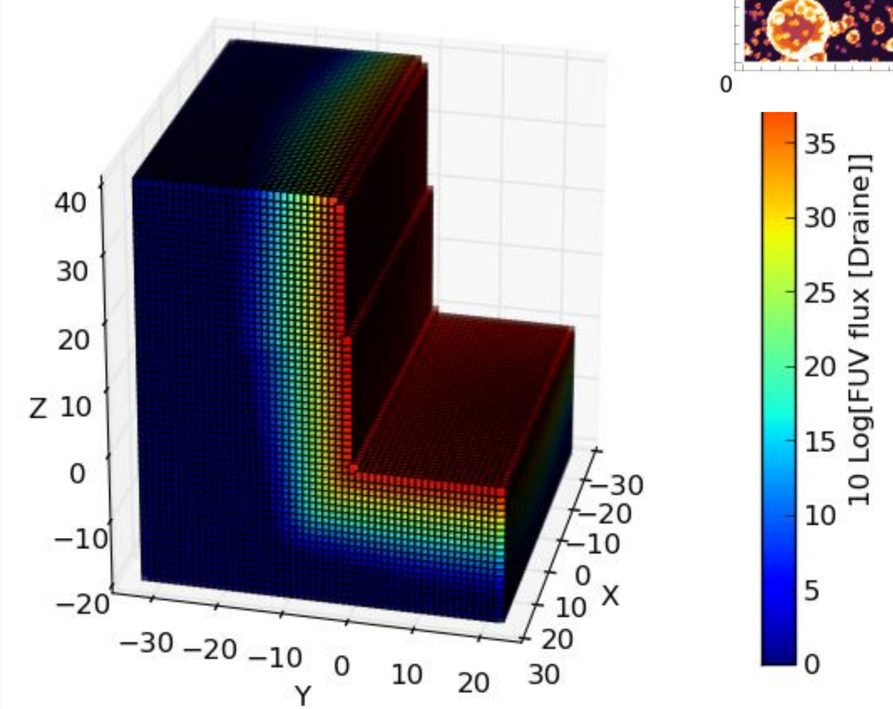
- Probabilistic approach for optical depths
- Common approach for UV extinction and line emission



Random maps of [CII] line peak opacities in scaled voxels.

Probability distribution for line-of-sight optical depths: $p\left(e^{-\tau}\right)$

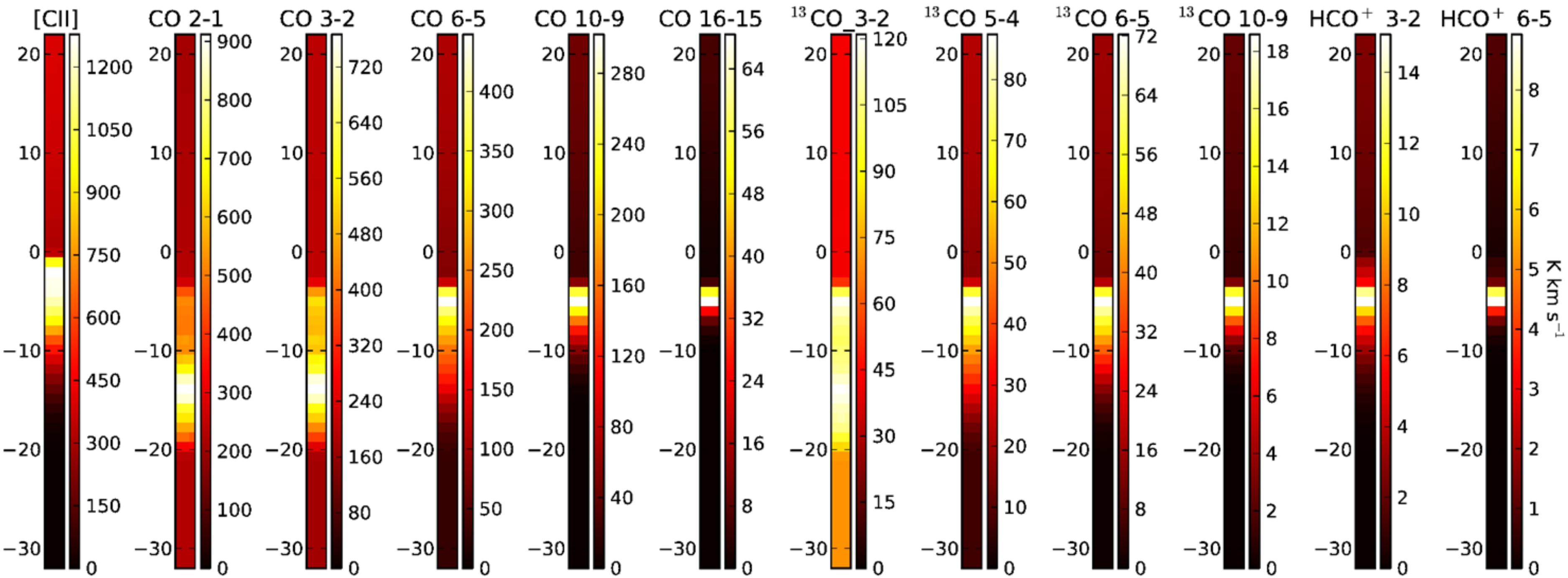
for each pixel



Resulting FUV flux distribution in the best fitting Orion Bar model.

Results

Simultaneous fit of line intensities and stratification profile

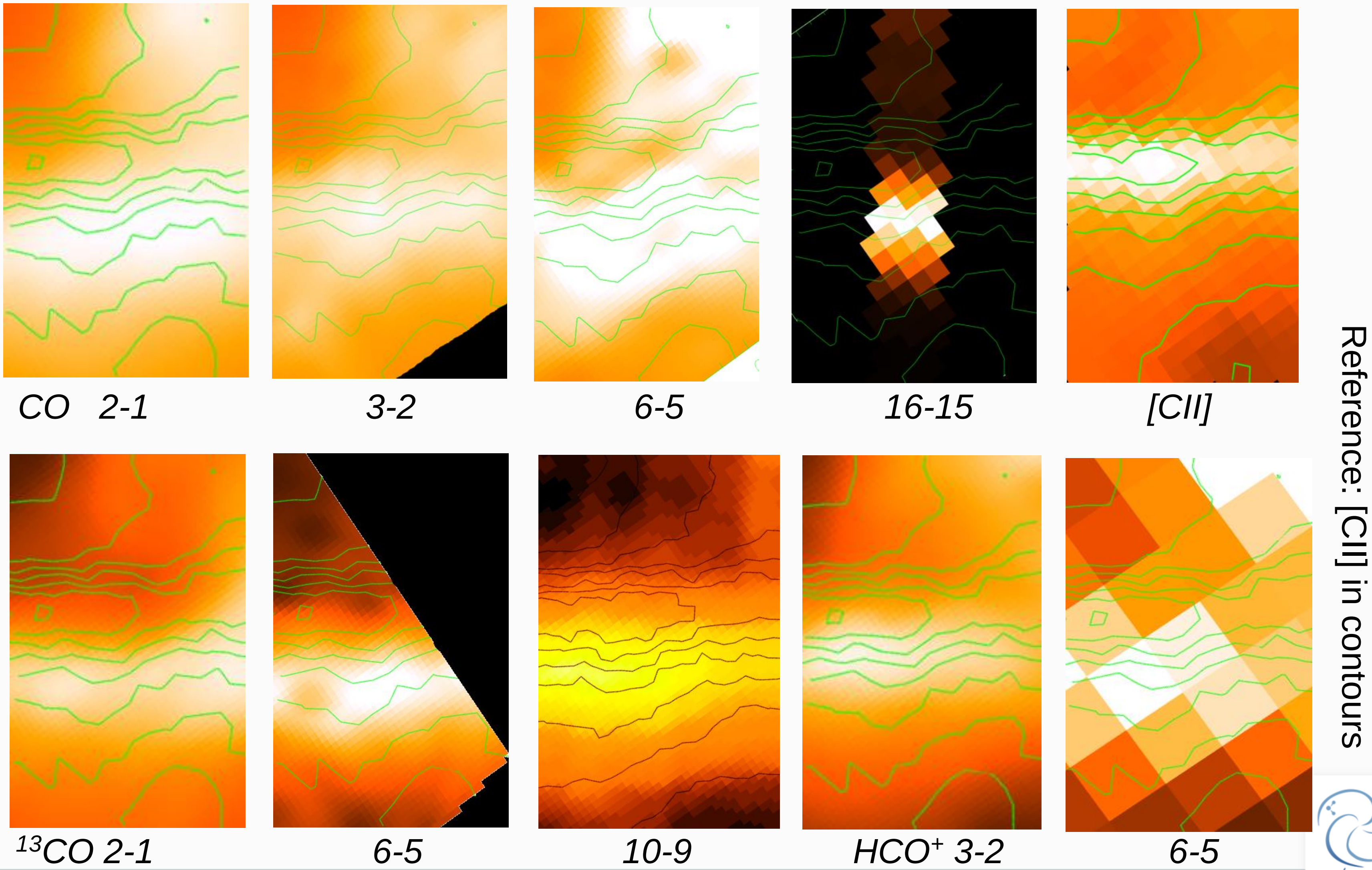


Decent match of the observations

- Large number of free parameters in a 2D model
  - Variation along the Bar ignored here
- No fit in χ^2 sense performed yet, due to huge parameter space

The Orion Bar

New Herschel observations (Combined with ground-based data)



Results

What is the Orion Bar?

Results

What is the Orion Bar?

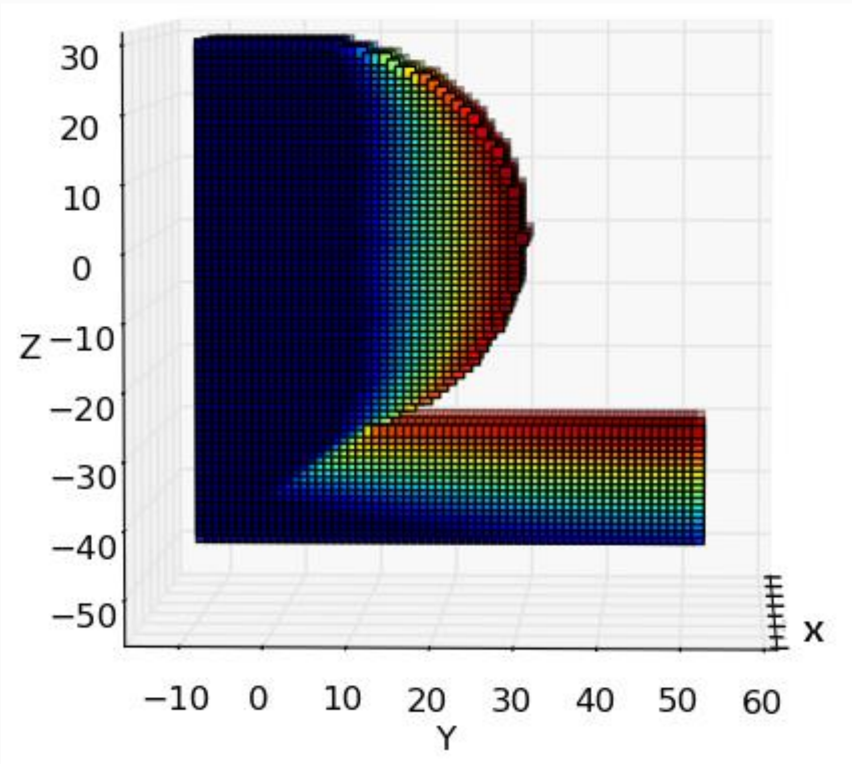
- A successful fit does not prove that we found the true geometry and parameters of the PDR

- **But:**
  - We can exclude scenarios if it turns impossible to reproduce the observed properties in them.

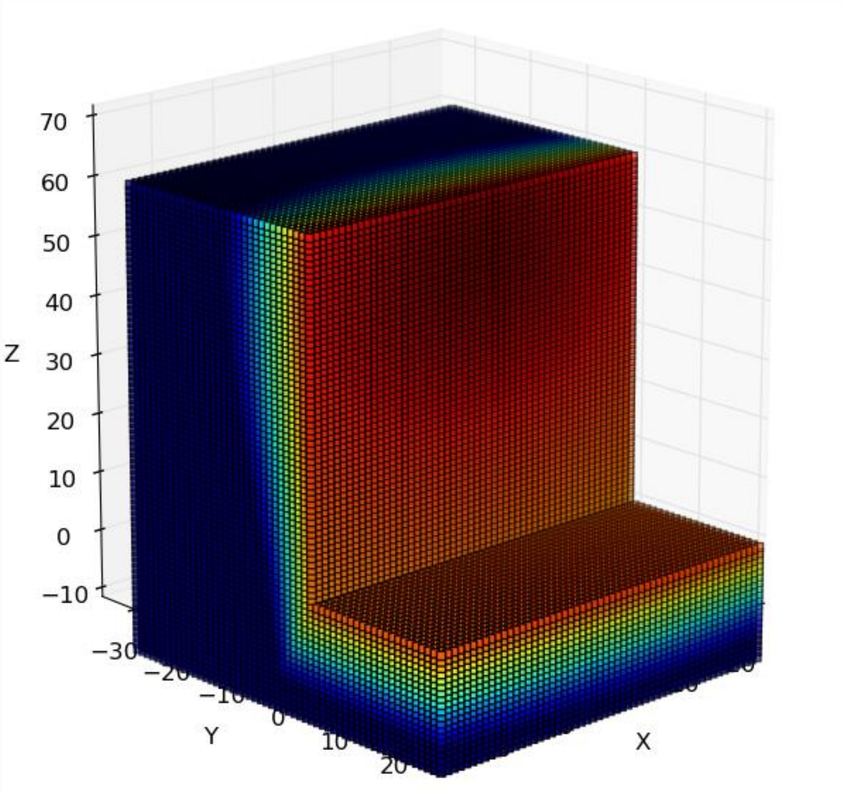
→ We do not know what the Orion Bar is, but we know what it is not:

What is the Orion Bar?

Geometry



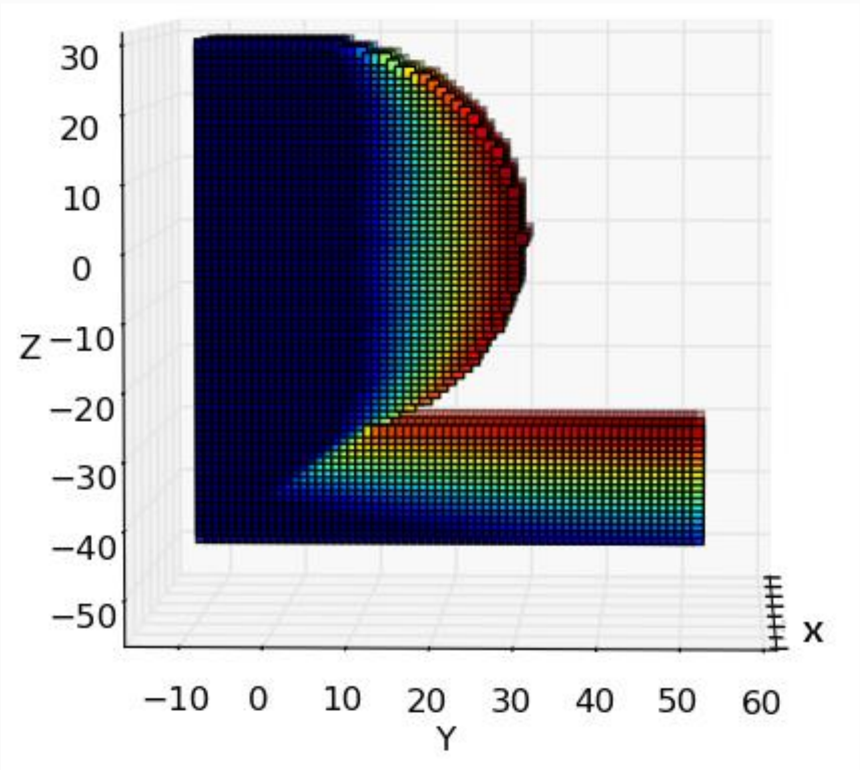
Orion Bar = (cylindrical) filament (Walmsley et al. 2000, Arab et al. 2012)

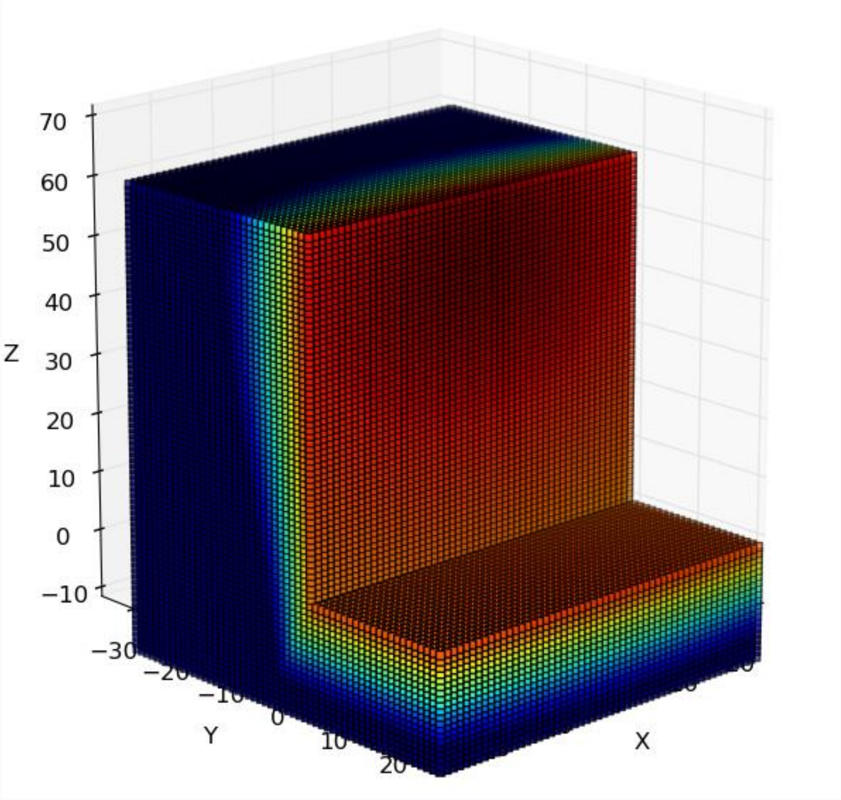


Orion Bar = (straight or concave) cavity wall (Hogerheijde et al. 1995, Pellegrini et al. 2009, Bernard Salas et al. 2012, van der Werf et al. 2013)

What is the Orion Bar?

Geometry

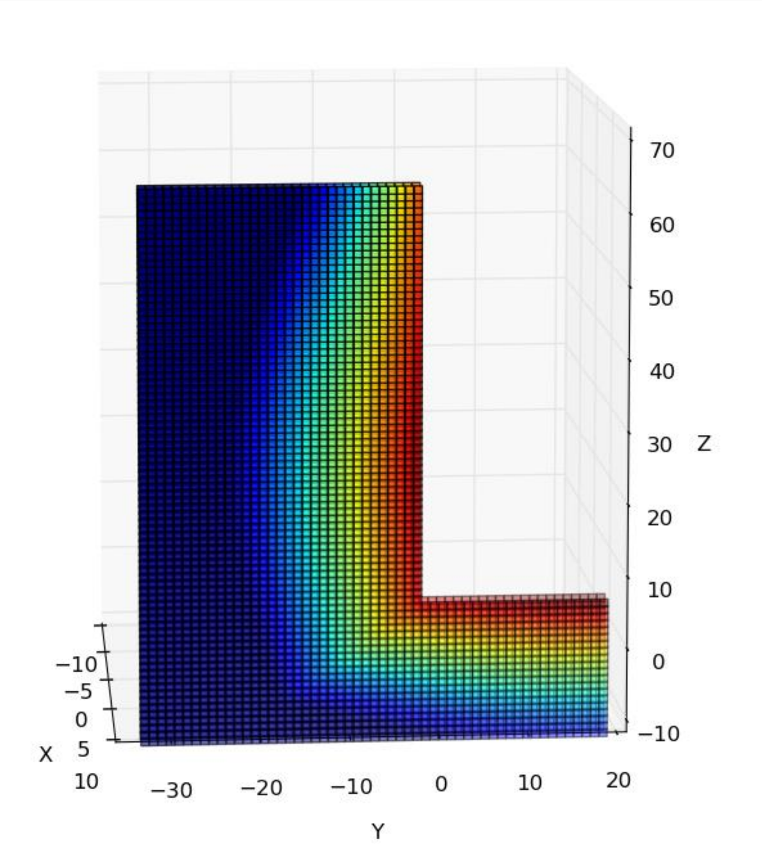




Convex structures provide no layering of high-density tracers

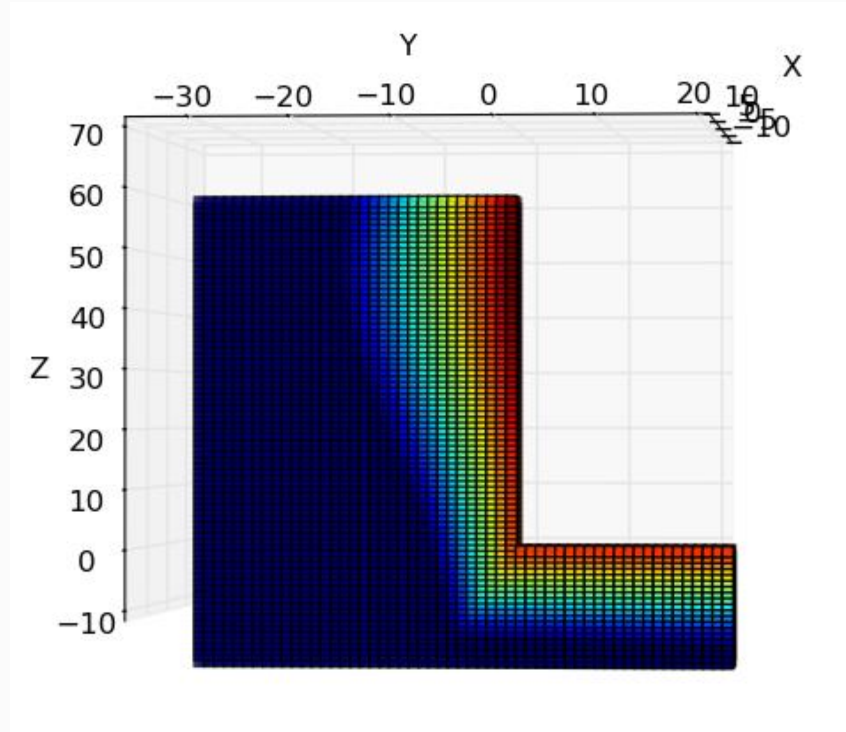
What is the Orion Bar?

Illumination



Θ^1Ori C deep in the cavity

(Jansen et al. 1995, implicite)

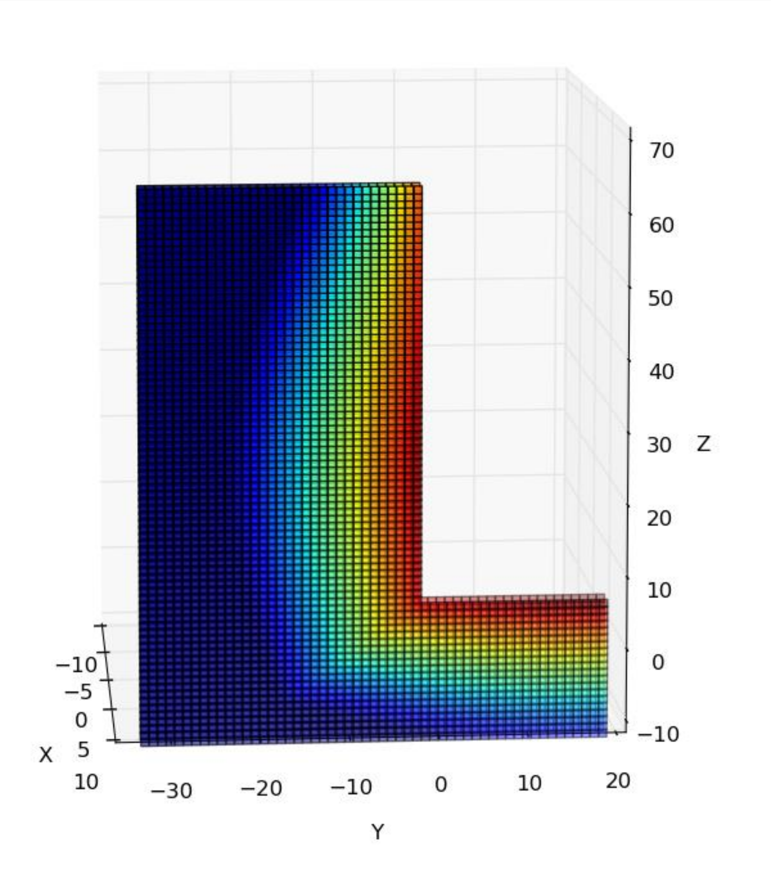


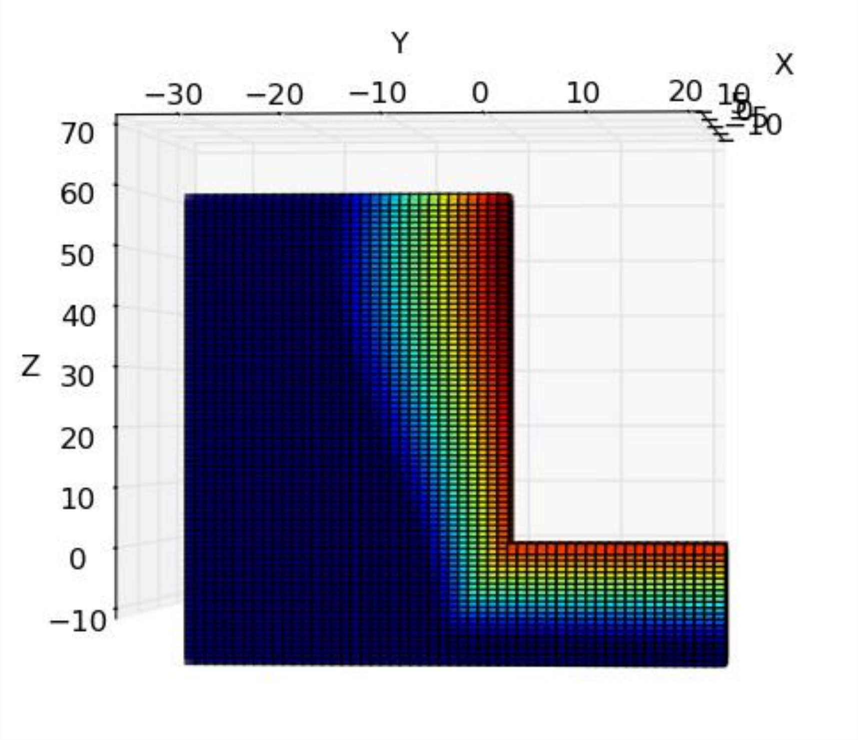
Θ^1Ori C at the cavity upper edge

(Pellegrini et al. 2009, van der Werf et al. 2013)

What is the Orion Bar?

Illumination

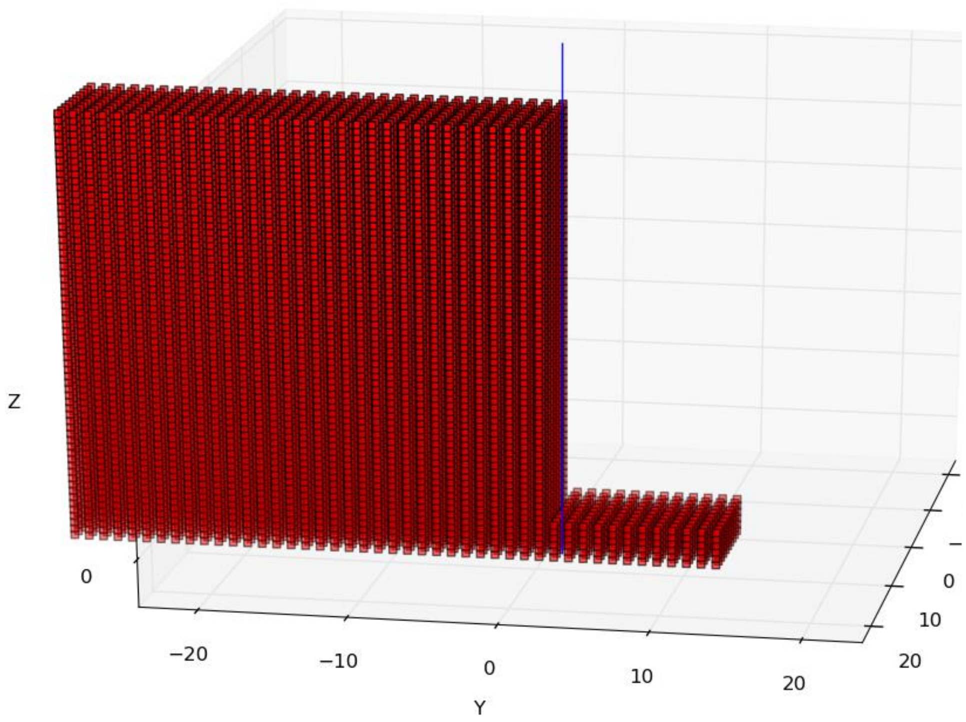


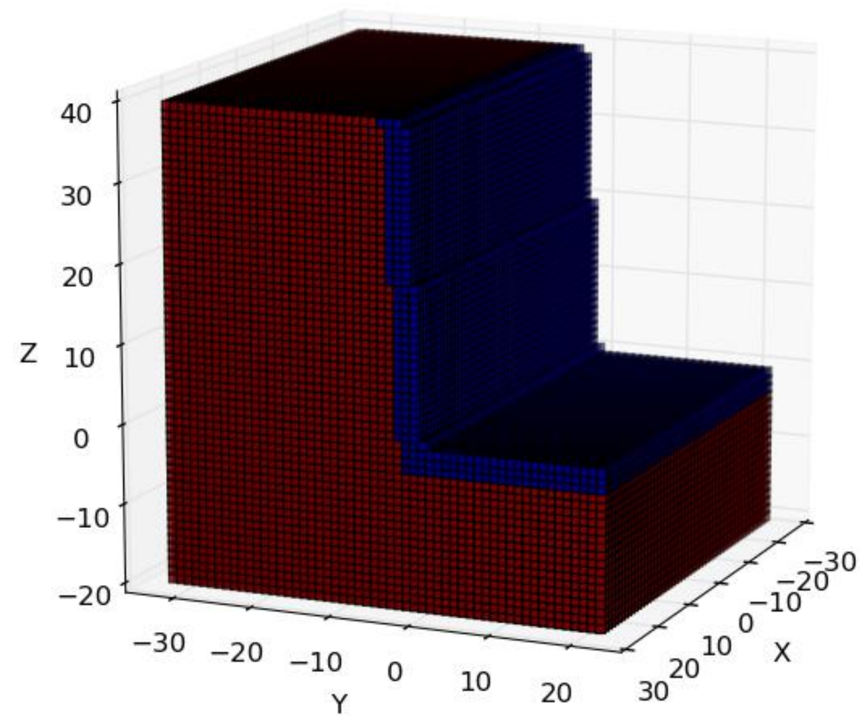


Location deep in the cavity produces foreground self-absorption

What is the Orion Bar?

Density structure



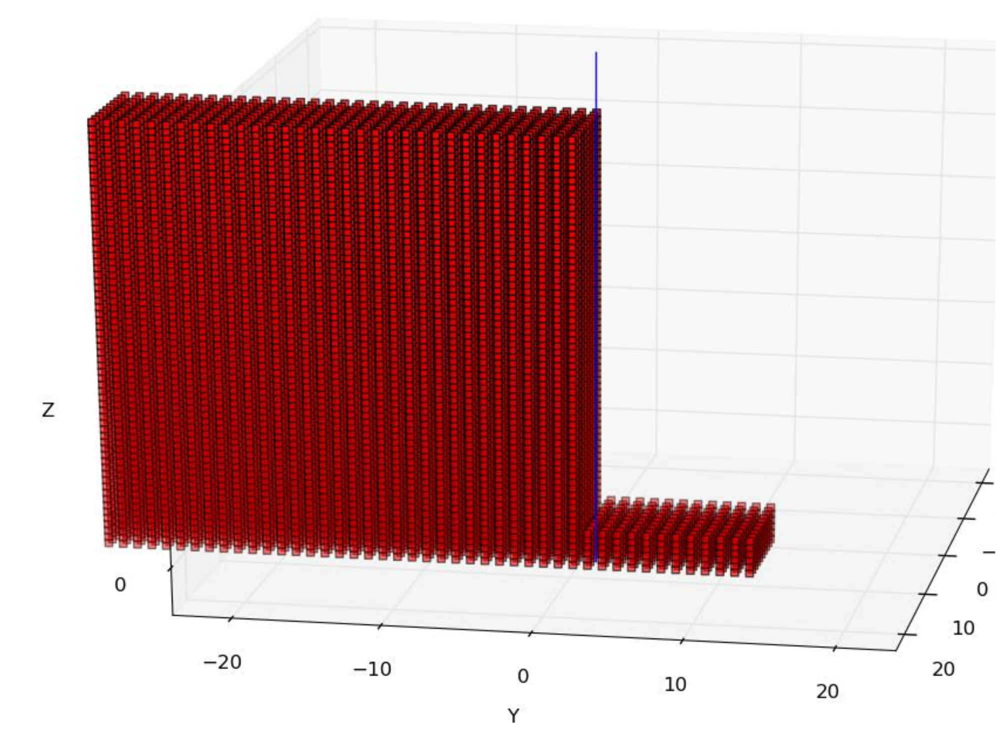


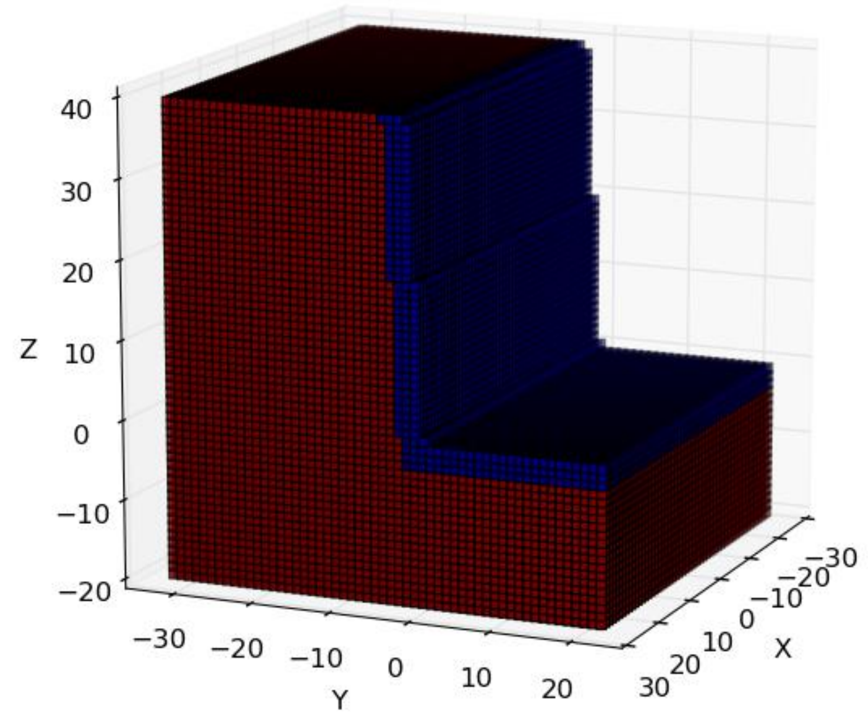
Homogeneous mixture of clumps and interclump medium (simplicity first)

Deficiency of dense clumps at the PDR surface (Parmar et al. 1991, Hogerheijde et al. 1995, Young Owl et al. 2000)

What is the Orion Bar?

Density structure





Stratification between [CII] and HCO^+ requires thin medium in front of dense clumps

What is the Orion Bar?

Other parameters

- **Overall, the scenario proposed by Hogerheijde et al. (1995) matches well**
    - FUV flux $4{\times}10^4\ \chi_0$ confirmed

- **Deviations:**
    - The cavity is only around 0.3pc deep (compared to 0.6pc)
    - Consequently, the mass per voxel is higher by a factor 2.5
    - The clump-to-interclump mass ratio is 4:2 (compared to 1:9)
    - Dense clump and interclump medium densities are slightly higher:
        - $4{\times}10^6$ and $4{\times}10^4$ cm^{-3}