Sunblock extreme

Astrophysics and astrochemistry in photo-dissociation regions

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Outline

- Introduction
- Modelling
- Observations
- Outlook

Credits: ESA/PACS & SPIRE Consortium/HOBYS Key Programme Consortia

Introduction

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- Modelling
- Observations
- Outlook

- Photo-dissociation Regions

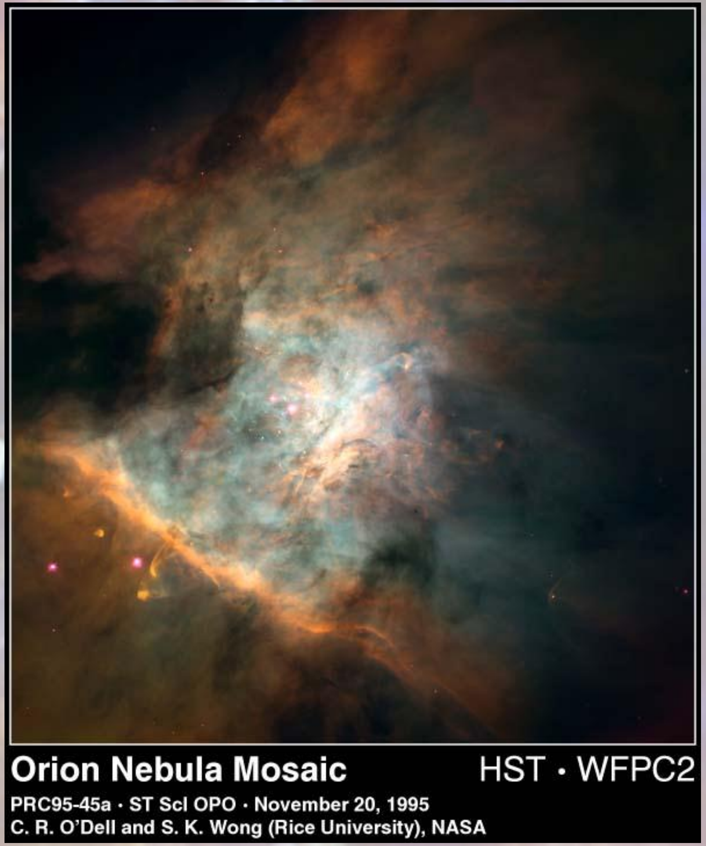
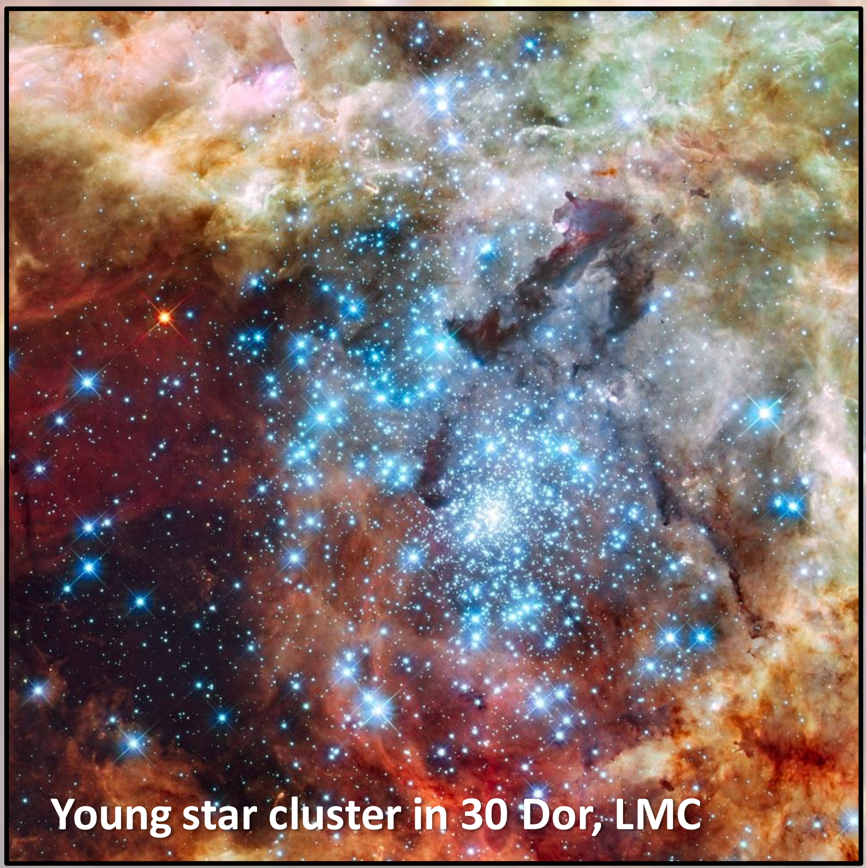


Photo-dissociation regions

- Definition

„A PDR is a region where far-ultraviolett (FUV) photons from young, massive stars dominate the physics and chemistry of the interstellar medium“



Young star cluster in 30 Dor, LMC

Image Credit: NASA, ESA, and E. Sabbi (ESA/STScI)

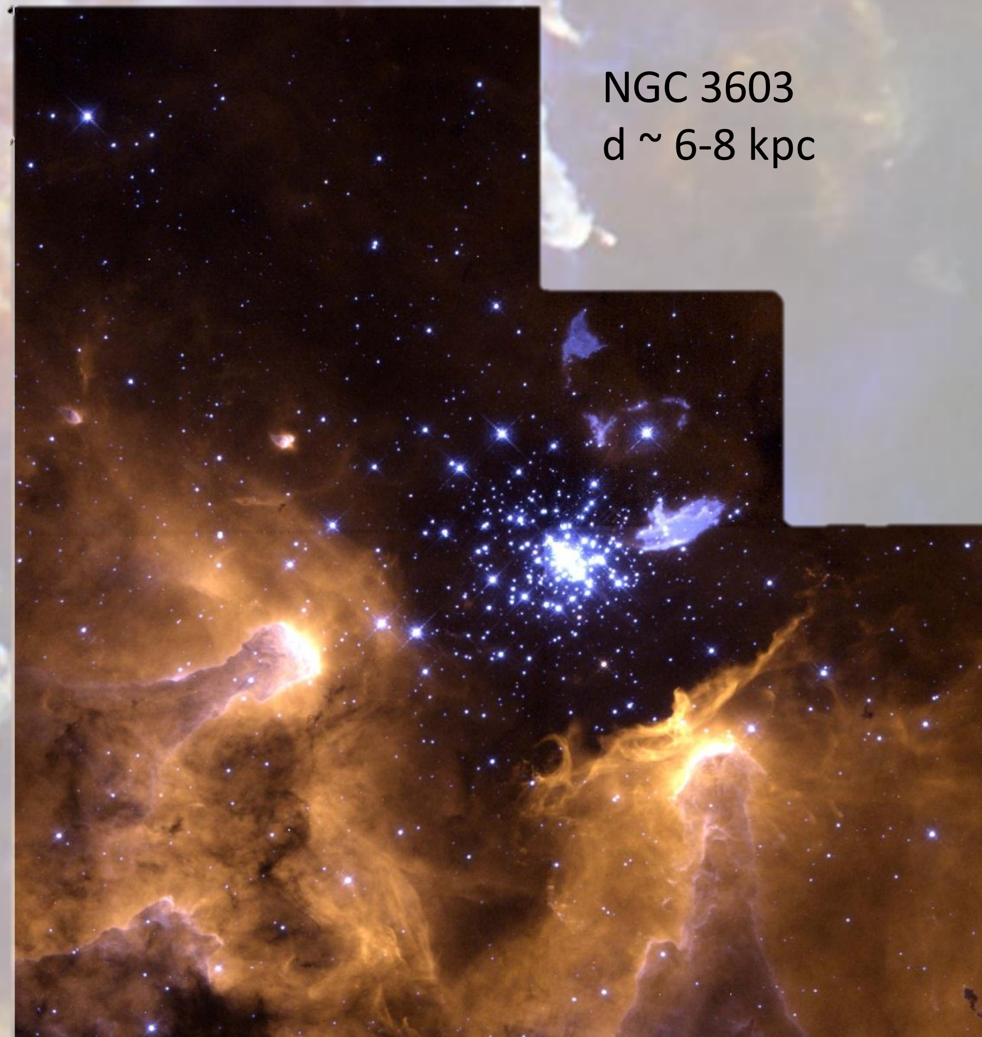
Photo-dissociation regions

- Stars form through grav. collapse in molecular clouds.
- Massive stars form in clusters (massive: $M > 8M_{\odot}$).
- Star formation efficiency ~ few %.
- Life-time of massive stars ~ few Myrs.

→ Massive stars, remain close to their natal cloud

- They emit large fraction of their energy in the UV.

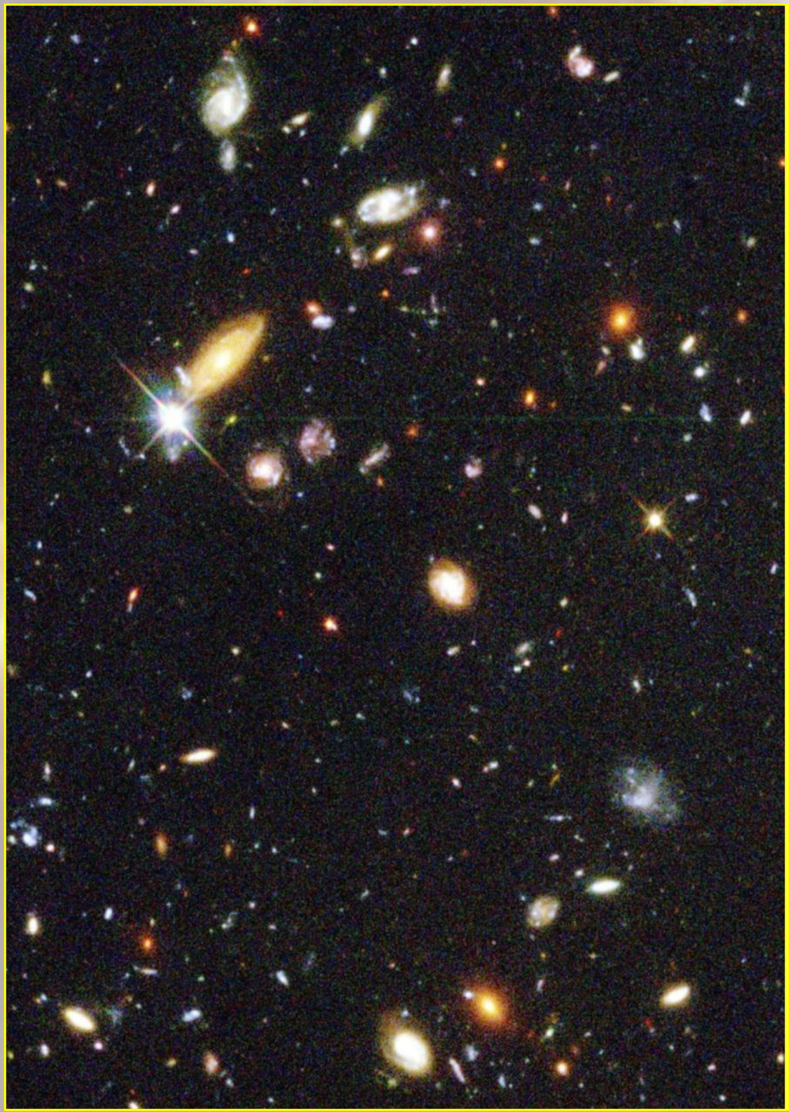
→ **Observing PDRs = observing ongoing massive star formation**



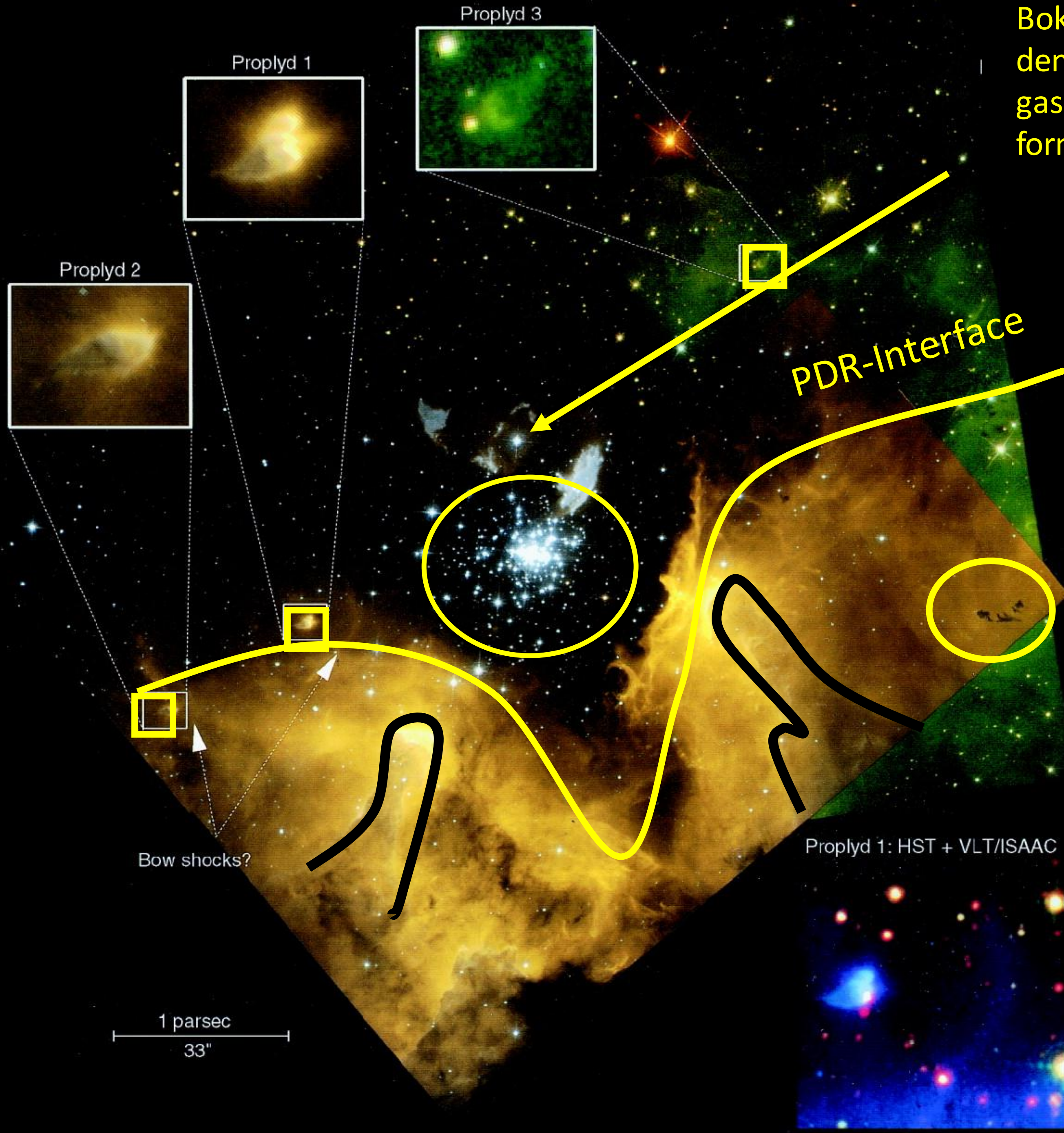
NGC 3603
d ~ 6-8 kpc

Credit: Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (Univ. Washington), You-Hua Chu (Univ. Illinois Urbana-Champaign), and NASA

Cycle of matter

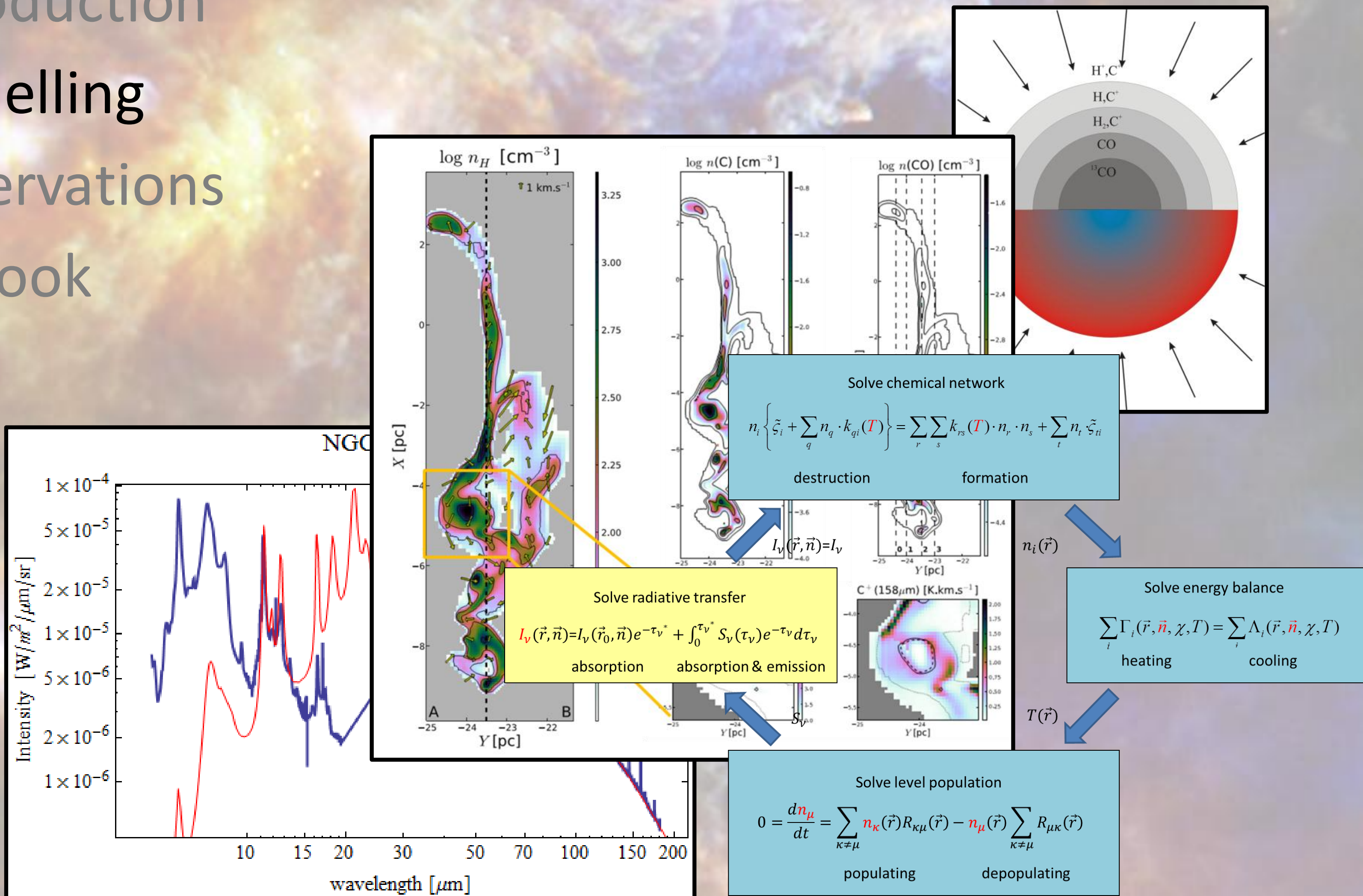


NGC 3603
distance:
6-8 kpc

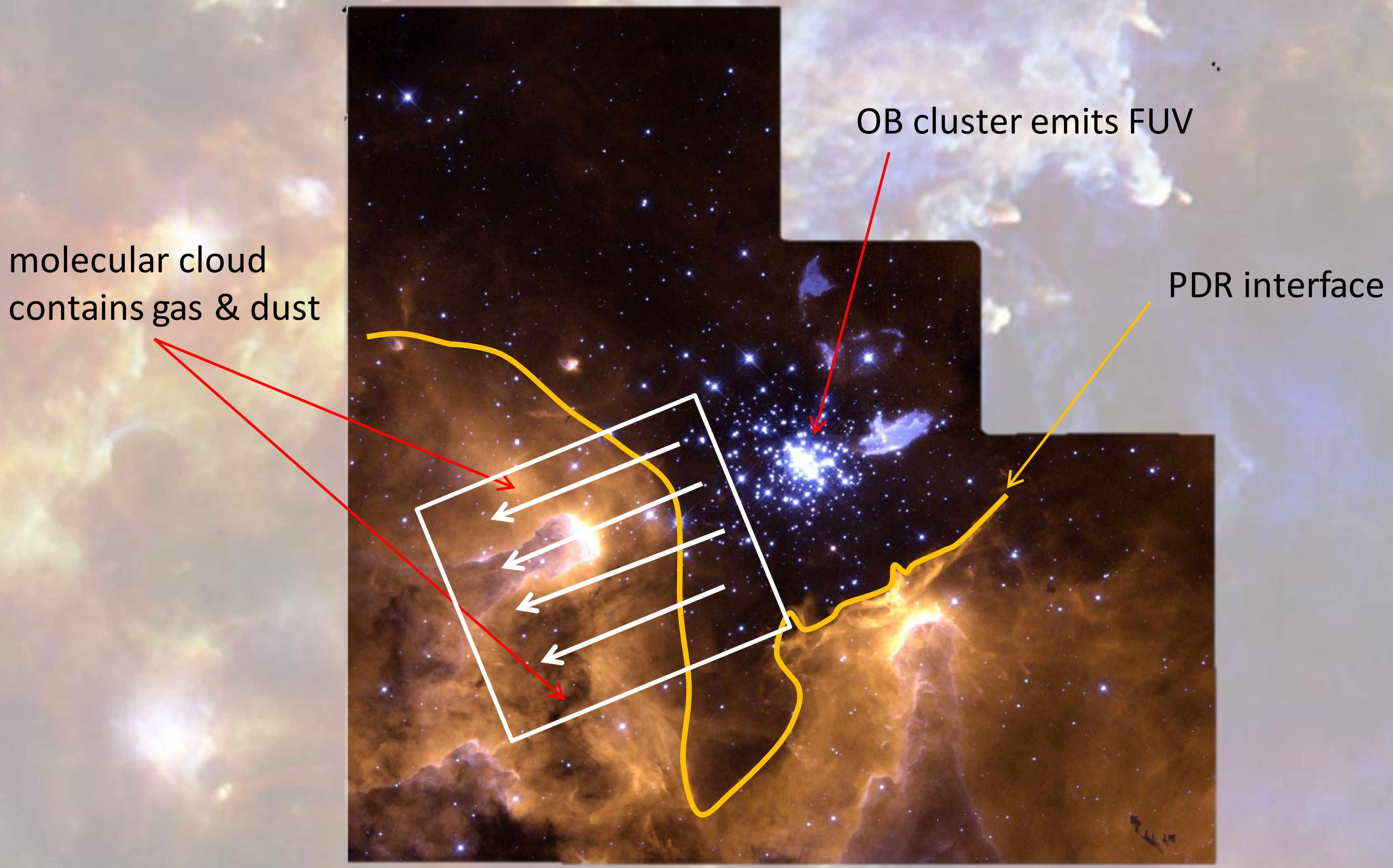


Modelling

- Introduction
- **Modelling**
- Observations
- Outlook



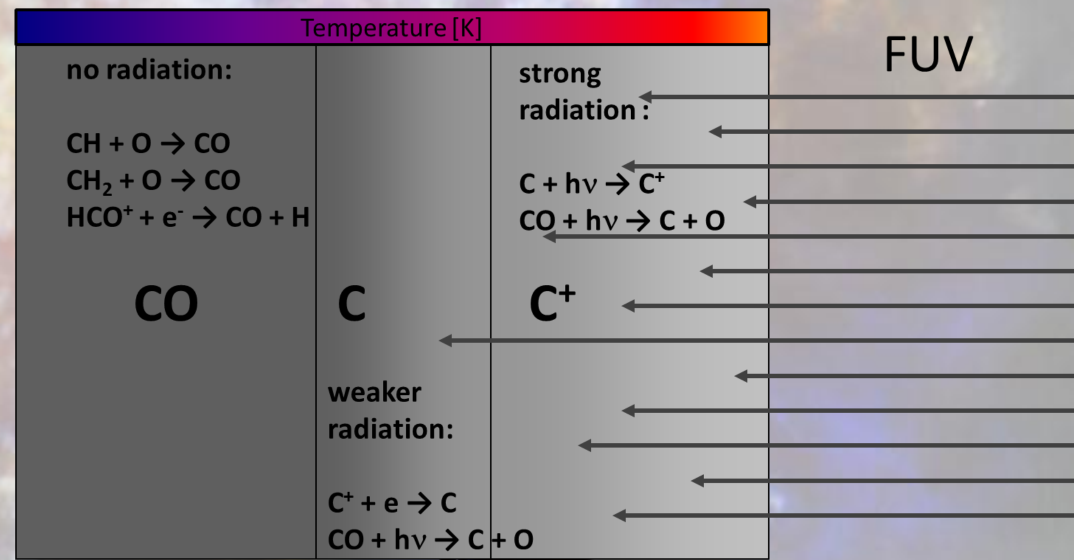
PDR models

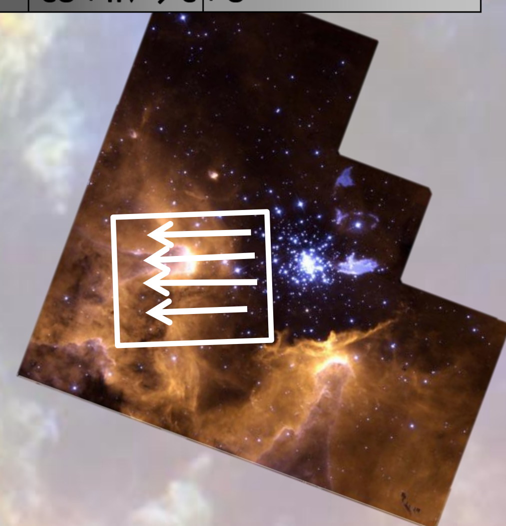


Credit: Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (Univ. Washington), You-Hua Chu (Univ. Illinois Urbana-Champaign), and NASA

PDR models

- calculate the change of physical and chemical conditions when travelling into a molecular cloud.





Model scheme

Solve chemical network

$$n_i\left\{\tilde{\varsigma}_i + \sum_q n_q \cdot k_{qi}(T)\right\} = \sum_r \sum_s k_{rs}(T)\cdot n_r \cdot n_s + \sum_t n_t \cdot \tilde{\varsigma}_{ti}$$

destruction — formation

$n_i(\vec{r})$

Solve energy balance

$$\sum_i \Gamma_i(\vec{r},\vec{n},\chi,T) = \sum_i \Lambda_i(\vec{r},\vec{n},\chi,T)$$

heating — cooling

$T(\vec{r})$

Solve level population

$$0 = \frac{dn_\mu}{dt} = \sum_{\kappa\neq\mu} n_\kappa(\vec{r})R_{\kappa\mu}(\vec{r}) - n_\mu(\vec{r})\sum_{\kappa\neq\mu} R_{\mu\kappa}(\vec{r})$$

populating — depopulating

S_ν

Solve radiative transfer

$$I_\nu(\vec{r},\vec{n}) = I_\nu(\vec{r}_0,\vec{n})e^{-\tau_\nu^*} + \int_0^{\tau_\nu^*} S_\nu(\tau_\nu)e^{-\tau_\nu}d\tau_\nu$$

absorption — absorption & emission

$I_\nu(\vec{r},\vec{n}) = I_\nu$

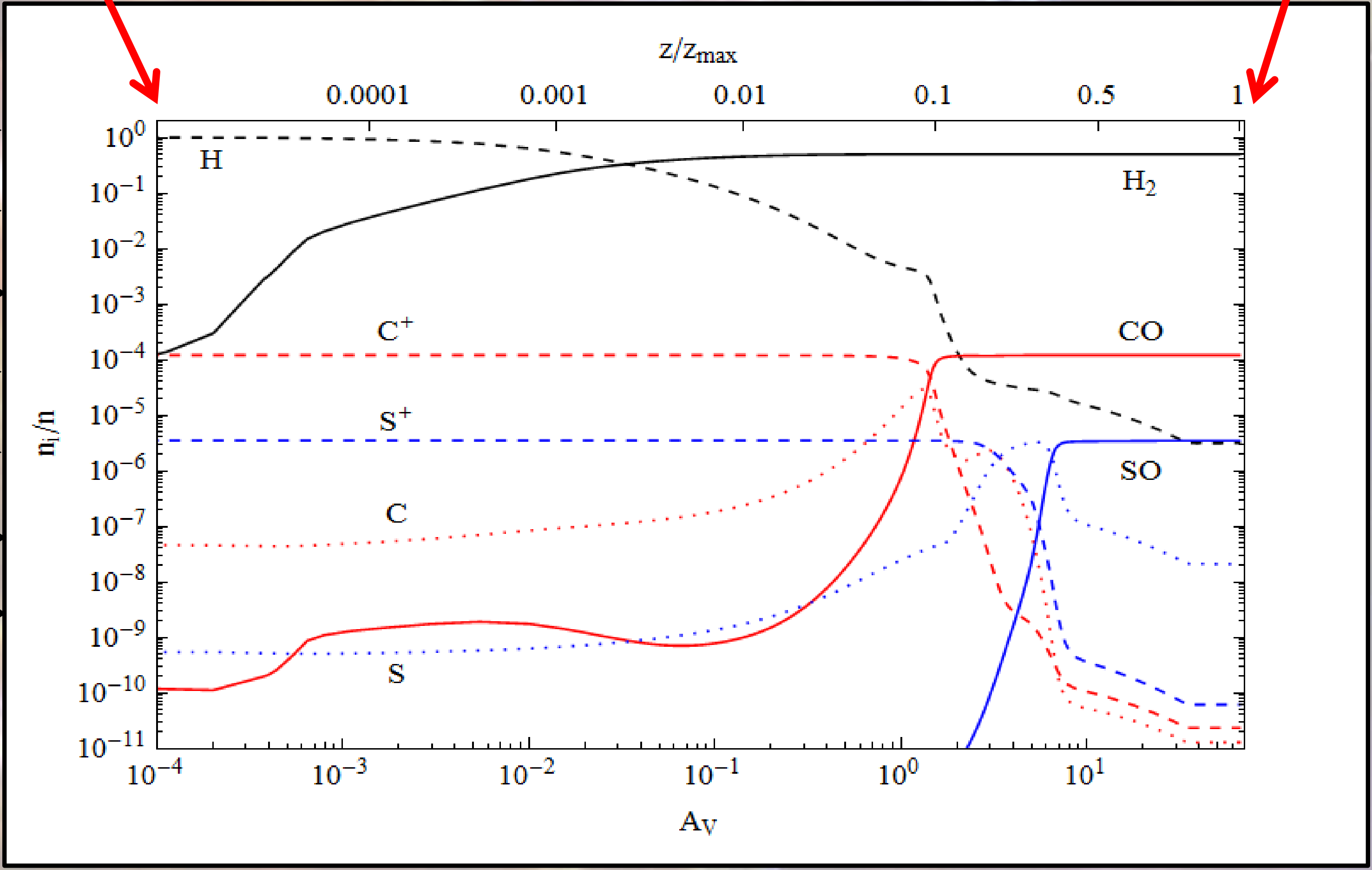
blue: local processes
yellow: non-local processes

Model outcome

cloud edge

cloud center

FUV



plot flipped, AND Log-Log scale!

A_V: visual extinction

Model chemistry

Solve chemical network

$$n_i\left\{\tilde{\varsigma}_i + \sum_q n_q \cdot k_{qi}(T)\right\} = \sum_r \sum_s k_{rs}(T)\cdot n_r \cdot n_s + \sum_t n_t \cdot \tilde{\varsigma}_{ti}$$

destruction — formation

$n_i(\vec{r})$ →

Solve energy balance

$$\sum_i \Gamma_i(\vec{r},\vec{n},\chi,T) = \sum_i \Lambda_i(\vec{r},\vec{n},\chi,T)$$

heating — cooling

$T(\vec{r})$ →

Solve level population

$$0 = \frac{dn_\mu}{dt} = \sum_{\kappa\neq\mu} n_\kappa(\vec{r})R_{\kappa\mu}(\vec{r}) - n_\mu(\vec{r})\sum_{\kappa\neq\mu} R_{\mu\kappa}(\vec{r})$$

populating — depopulating

S_ν →

Solve radiative transfer

$$I_\nu(\vec{r},\vec{n})=I_\nu(\vec{r}_0,\vec{n})e^{-\tau_\nu^*} + \int_0^{\tau_\nu^*} S_\nu(\tau_\nu)e^{-\tau_\nu}d\tau_\nu$$

absorption — absorption & emission

$I_\nu(\vec{r},\vec{n})=I_\nu$ →

blue: local processes
yellow: non-local processes

System of Rate Equations

$$\frac{dn_i}{dt} = n_i \left\{ \tilde{\zeta}_i + \sum_q n_q k_{qi} \right\} - \sum_r \sum_s k_{rs} n_r n_s + \sum_t n_t \tilde{\zeta}_{ti}$$

- Examples of chemical reactions:

$$\mathrm{H + CH \longrightarrow C + H_2}$$
$$\mathrm{CO} + h\nu \longrightarrow \mathrm{C + O}$$

- Described by reaction rates

$$R_{\mathrm{C}} = R_{\mathrm{H_2}} = k \times n_{\mathrm{H}} \times n_{\mathrm{CH}}$$
$$R_{\mathrm{C}} = R_{\mathrm{O}} = \zeta \times n_{\mathrm{CO}}$$

Chemical networks

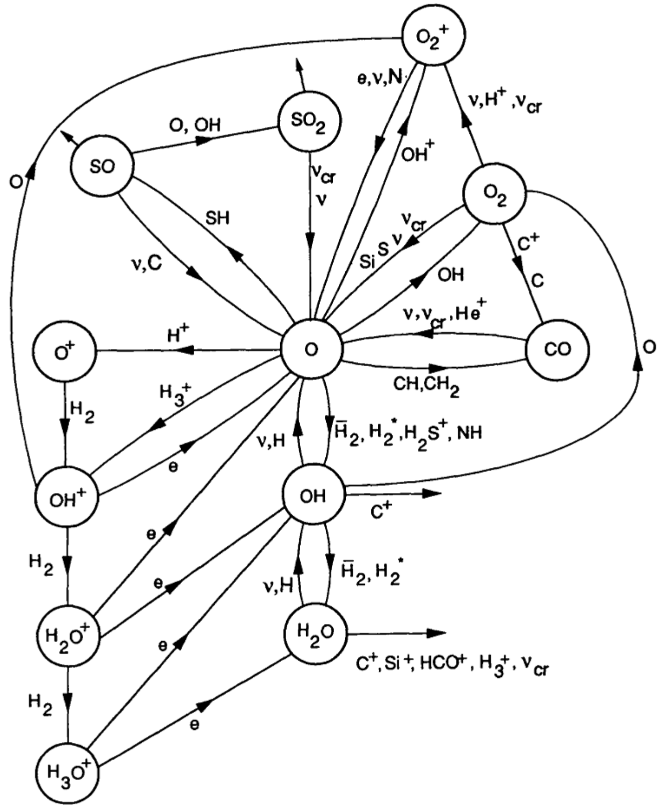


FIG. 2.—Oxygen network

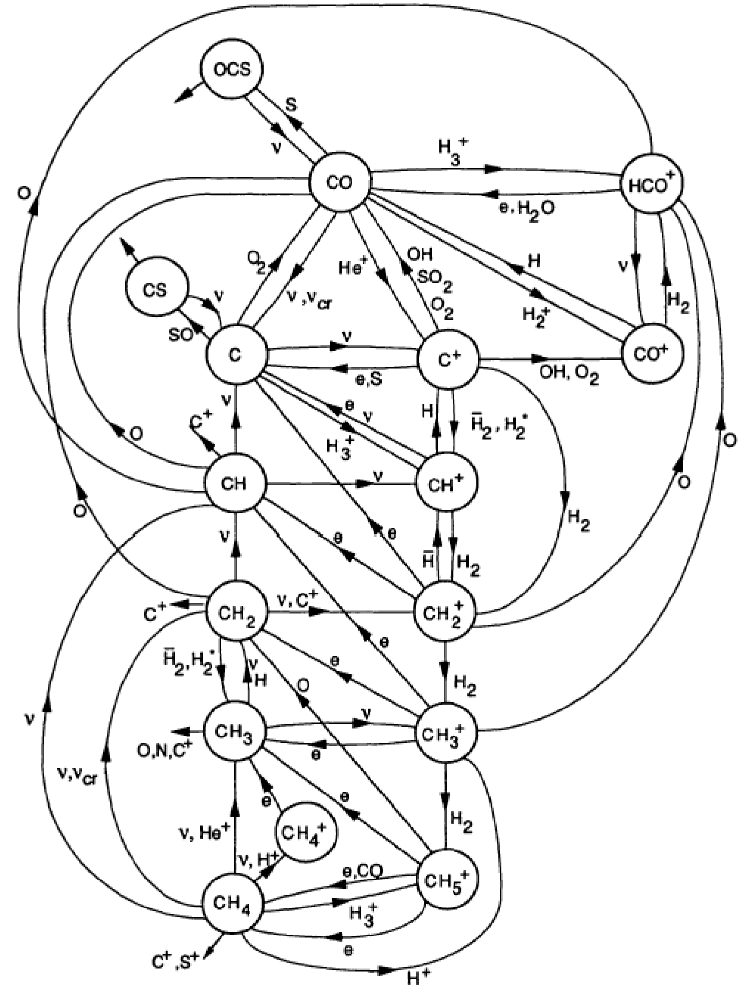


FIG. 3.—Carbon network

Sternberg & Dalgarno, 1995, ApJSS, 99

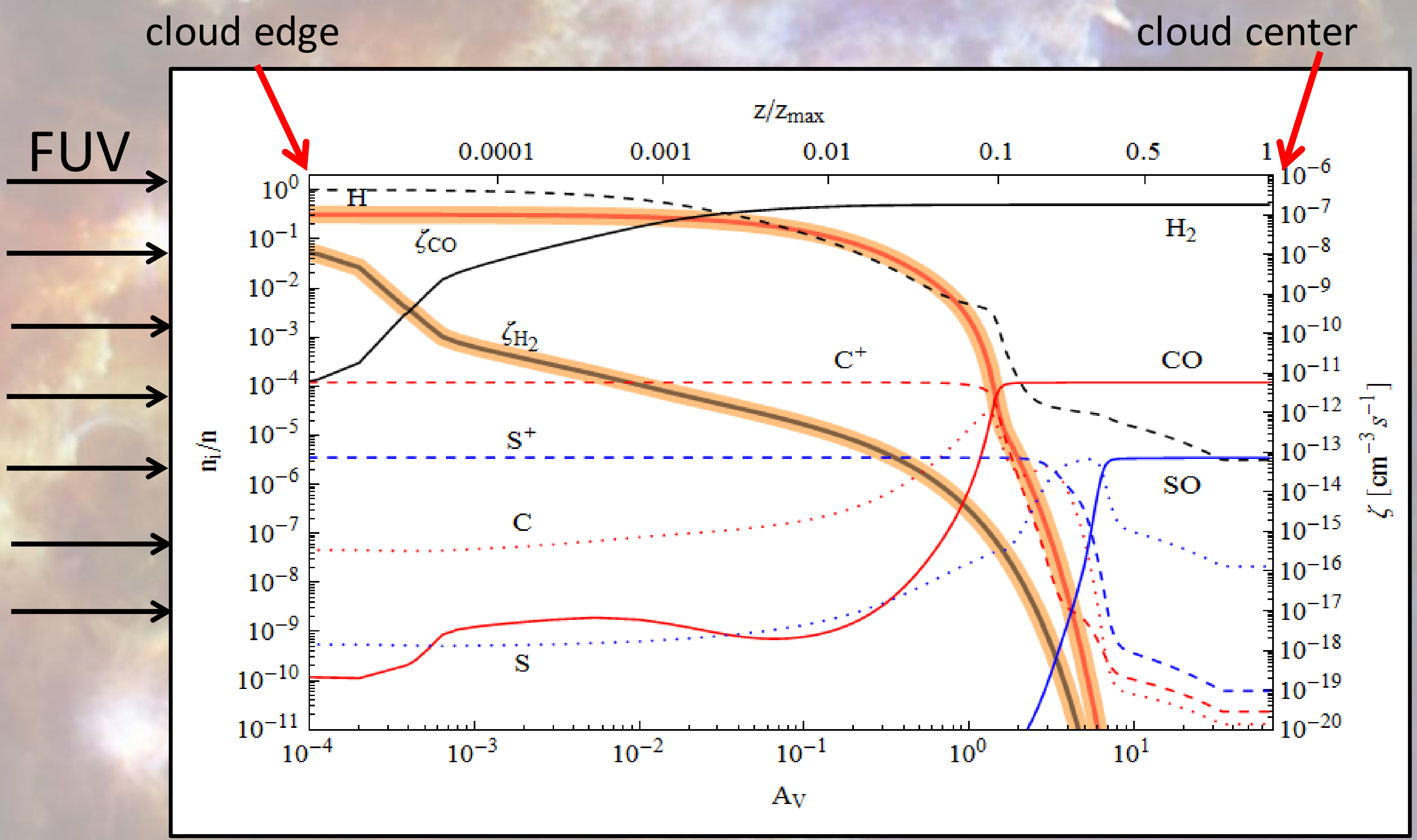
Model chemistry

$$\frac{dn_i}{dt} = n_i \left\{ \tilde{\zeta}_i + \sum_q n_q k_{qi} \right\} - \sum_r \sum_s k_{rs} n_r n_s + \sum_t n_t \tilde{\zeta}_{ti}$$

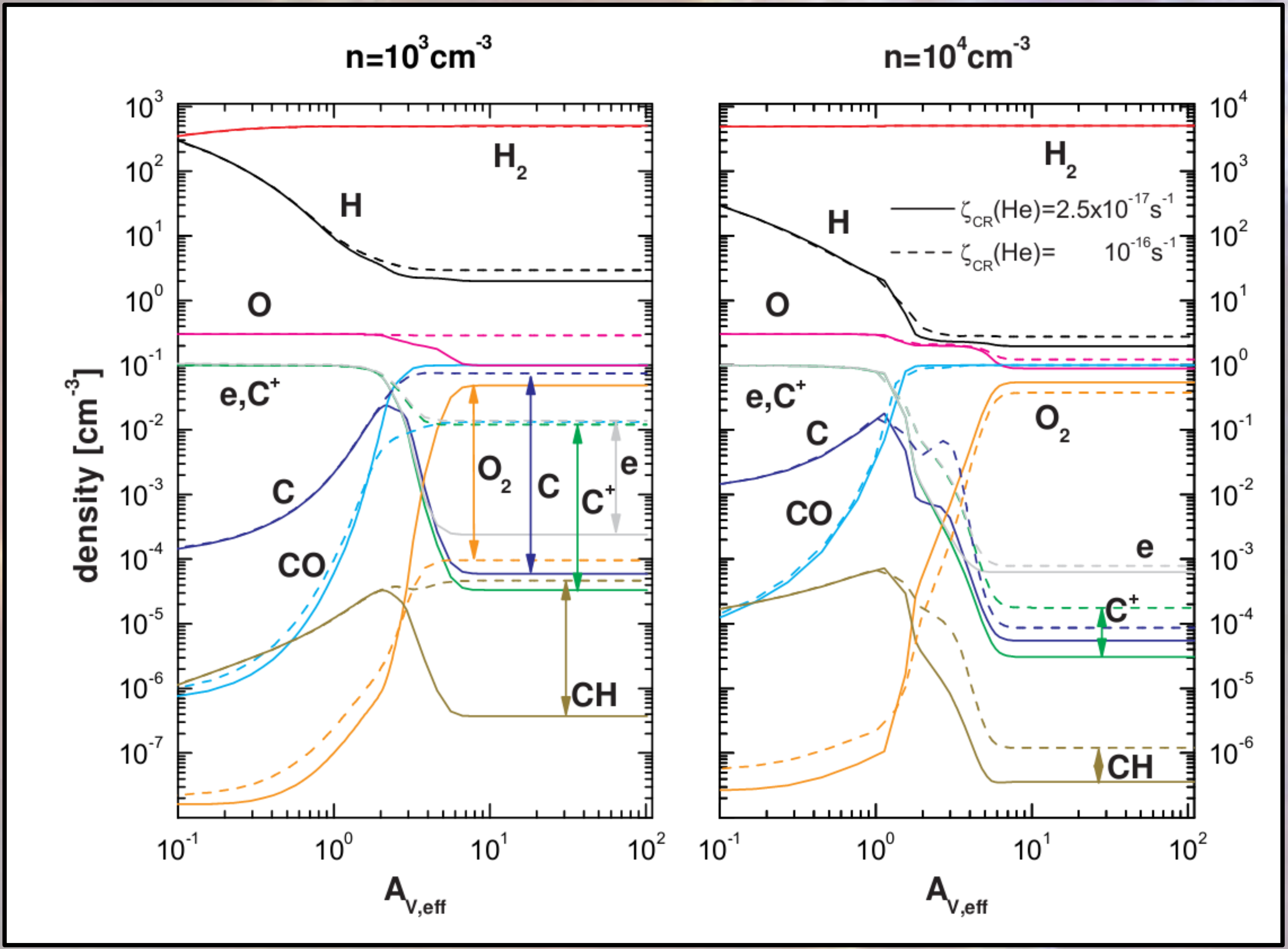
- density n_i (species $i=1,\ldots N$), hundreds of species, thousands of reactions
- reaction rate coefficients: $k_{xy}(T_{gas}$=5-5000 K, T_{dust}=5-500 J), ζ_z(J)
- steady-state, time-dependent
- pure gas-phase (2-body collisions) or surface chemistry (grain surface reactions)
- high dimensional, highly non-linear problem! (with unknown initial conditions)

} very stiff system

Photodissociation of H_2 and CO



Model non-linearity



Rölliget al. 2007, A&A, 467

Non-linear system:

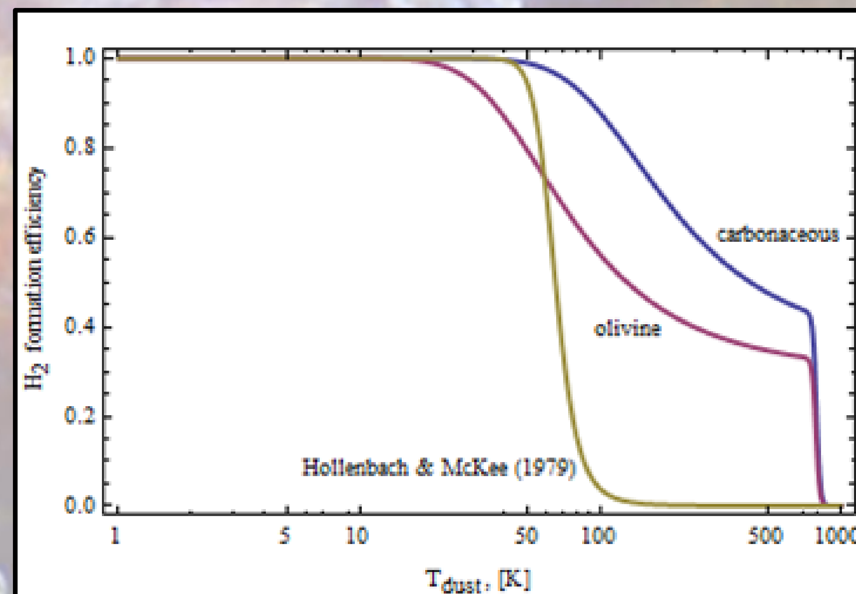
Slight input changes may affect the outcome significantly

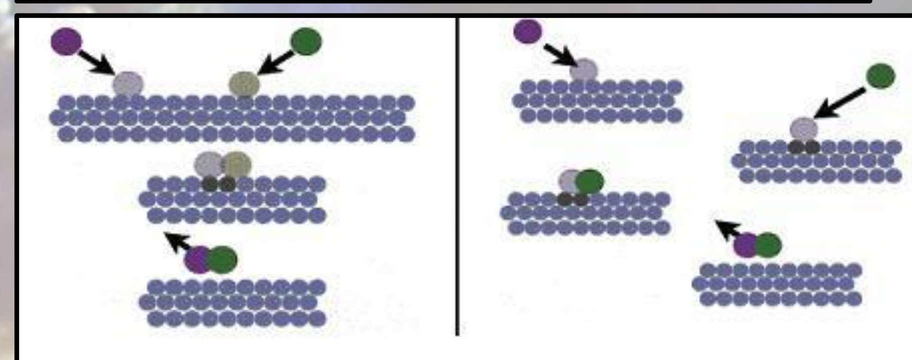
Changing only one process:
ζ_{CR}(He) by factor 4 changes density by factor **1000**

H_2 formation

- most important astrochemical reaction
- inefficient in the gas phase – requires dust surface
- quenched by high T_{dust}
- still not fully understood

Röllig et al. 2012, A&A, in press



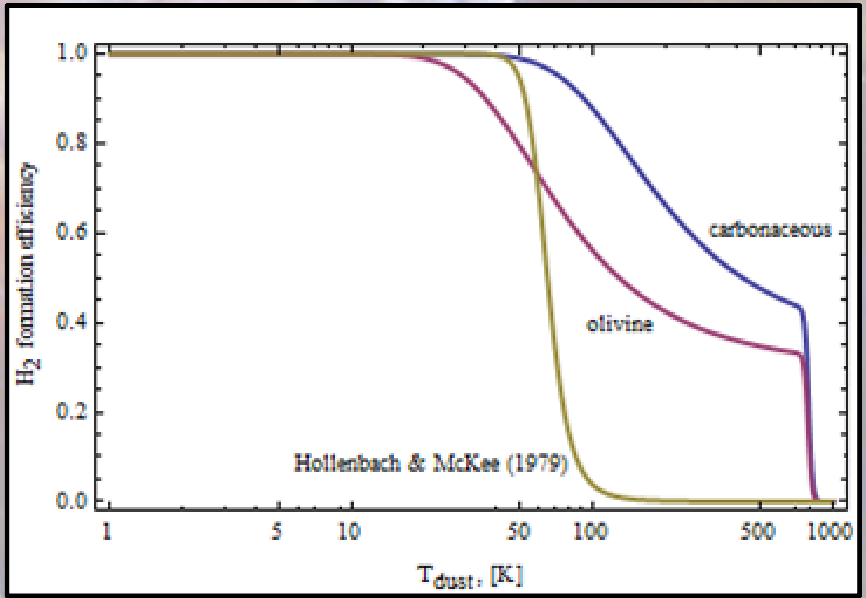


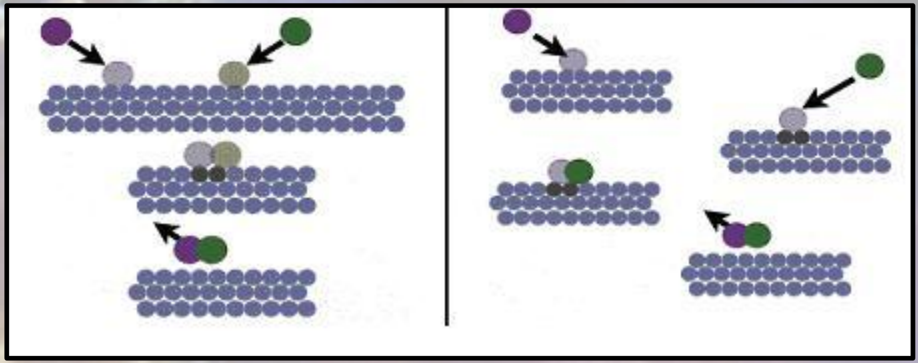
Langmuir-Hinshelwood Elay-Rideal

H_2 formation

- depends on grain surface temperature
- depends on available grain surface area (PAHs, VSGs, …)
- depends on grain material

Rölllig et al. 2012, A&A, in press





Langmuir-Hinshelwood Elay-Rideal

$$R_{\mathrm{H}_2} = \frac{1}{2} n_{\mathrm{H}} v_{\mathrm{H}} n_d \sigma_d \epsilon_{\mathrm{H}_2} S_{\mathrm{H}}$$

H_2 formation

- depends on grain surface temperature
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  (PAHs, VSGs, …)
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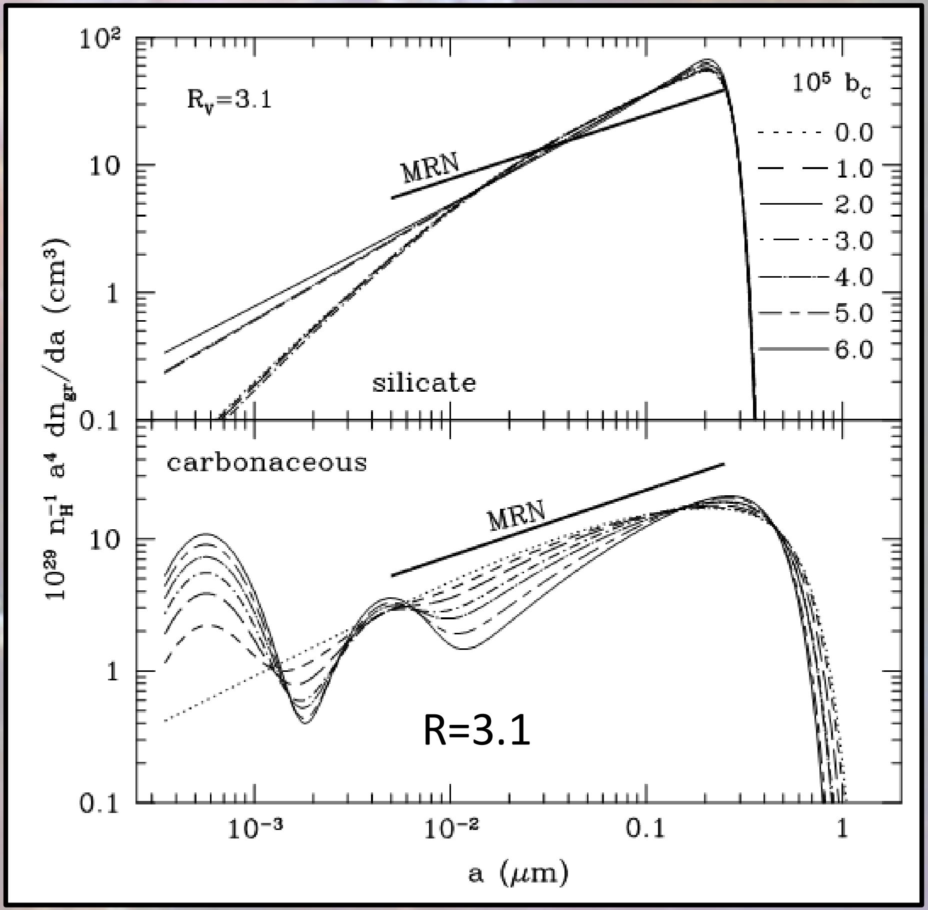
Weingartner & Draine 2001, ApJ, 548

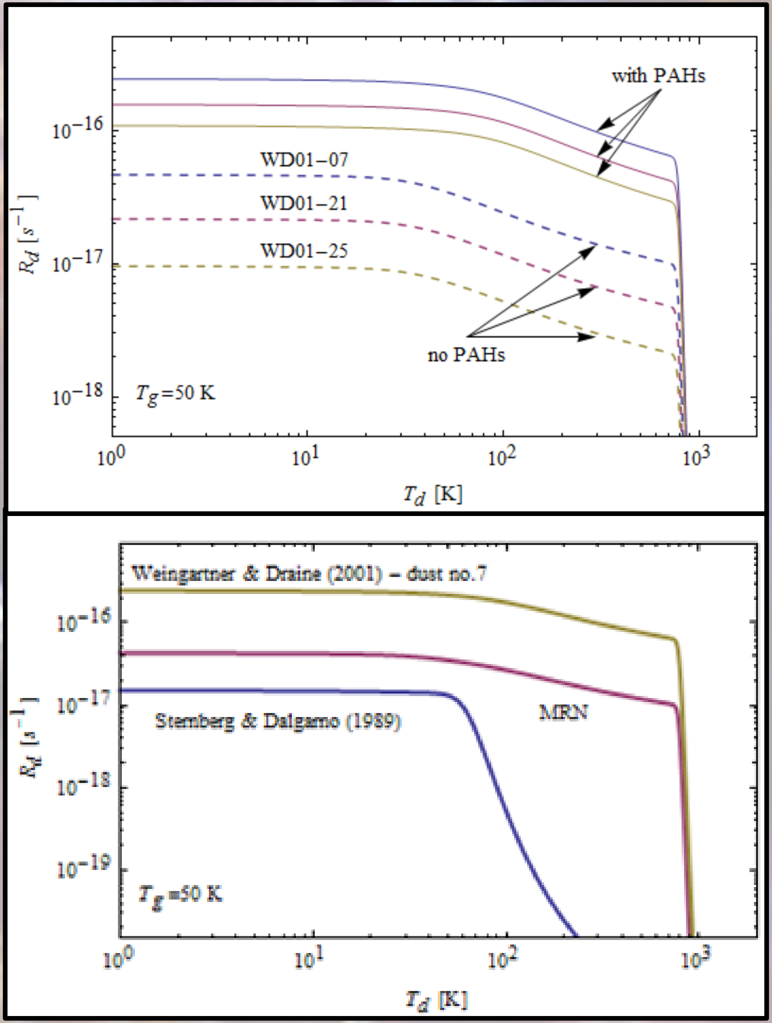


H_2 formation

- depends on grain surface temperature
- depends on available grain surface area (PAHs, VSGs, …)
- depends on grain material

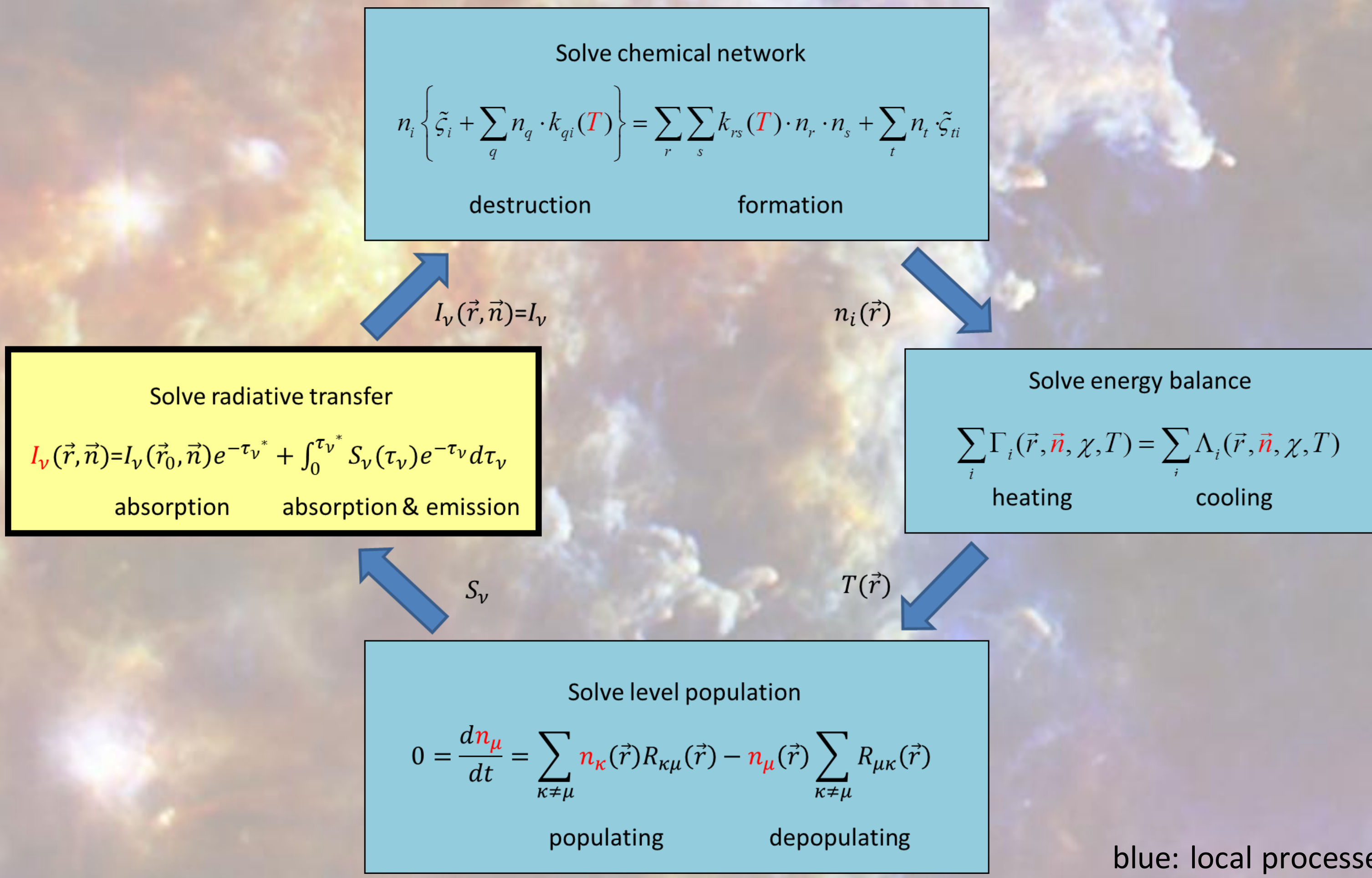
Real properties of interstellar dust grains are unknown !

$$R_{H_2} = \frac{1}{2} n_H v_H n_d \sigma_d \epsilon_{H_2} S_H$$



Röllig et al. 2012, A&A, in press

Radiative Transfer



blue: local processes
yellow: non-local processes

Radiative Transfer

- Radiative transfer describes the propagation of photons through a medium along a line of sight.

- RT accounts for absorption and emission processes.

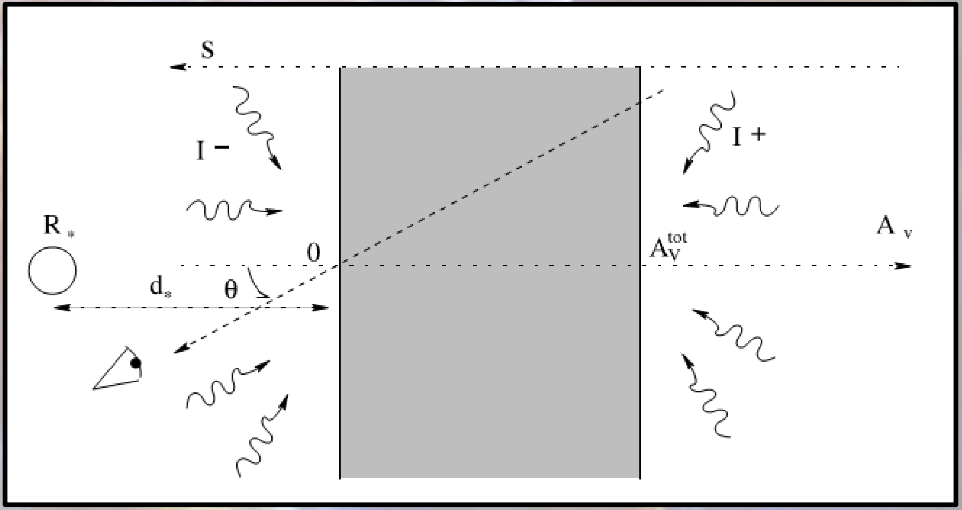
- RT couples physical & chemical conditions of different volume elements along line of sights

  → **non-local problem**

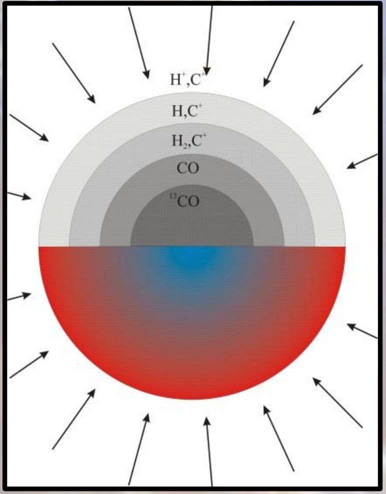
- model geometry becomes important

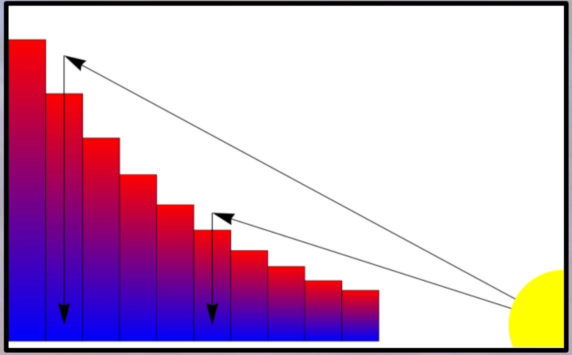
Model geometry

- Numerous configurations
  - Cloud geometry
    - plane-parallel (1D)
    - spherical (1D)
    - disk (1D+1D)
    - full 3-D
  - Illumination
    - isotropic
    - uni-directional



Le Petit et l. 2006, ApJSS 164





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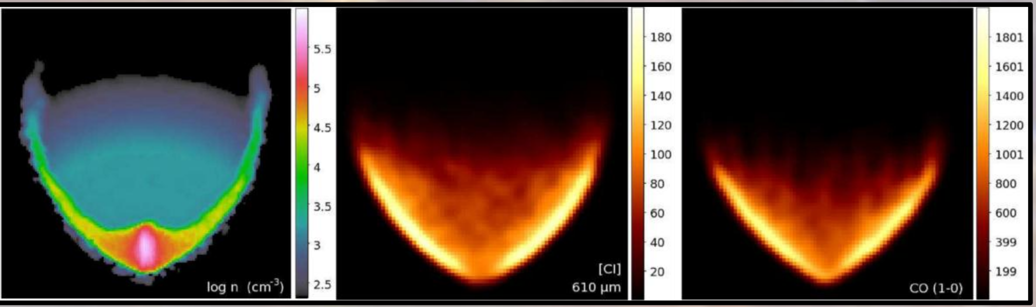
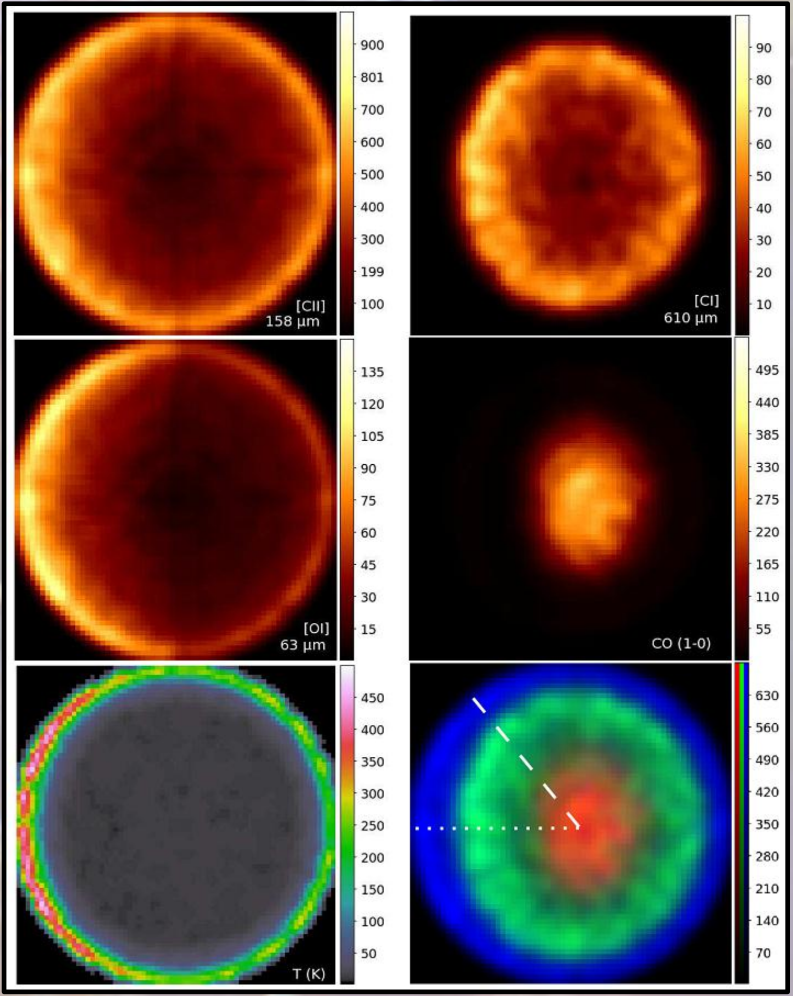




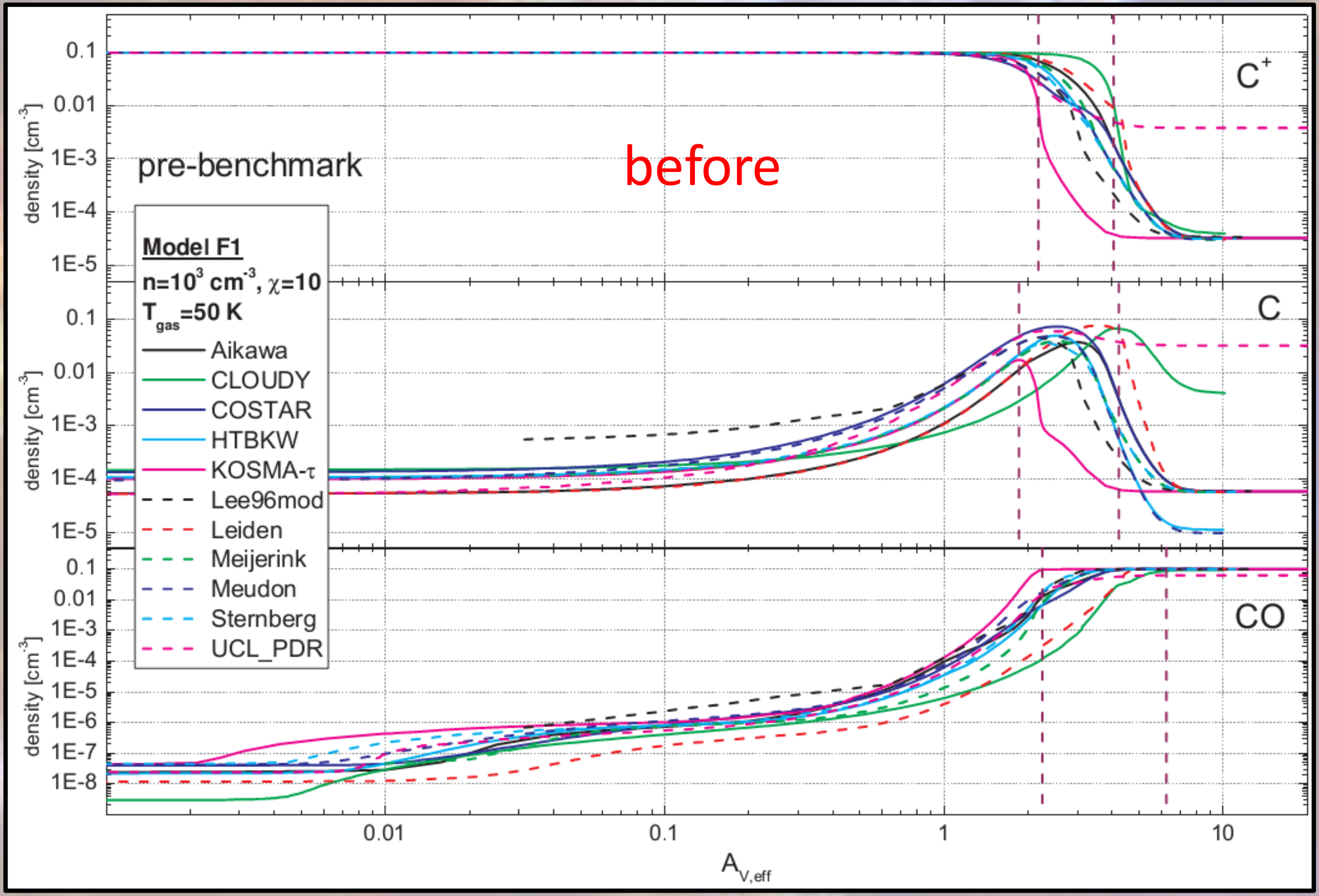
Bisbas et al., 2012, MNRAS, accepted

PDR model benchmark

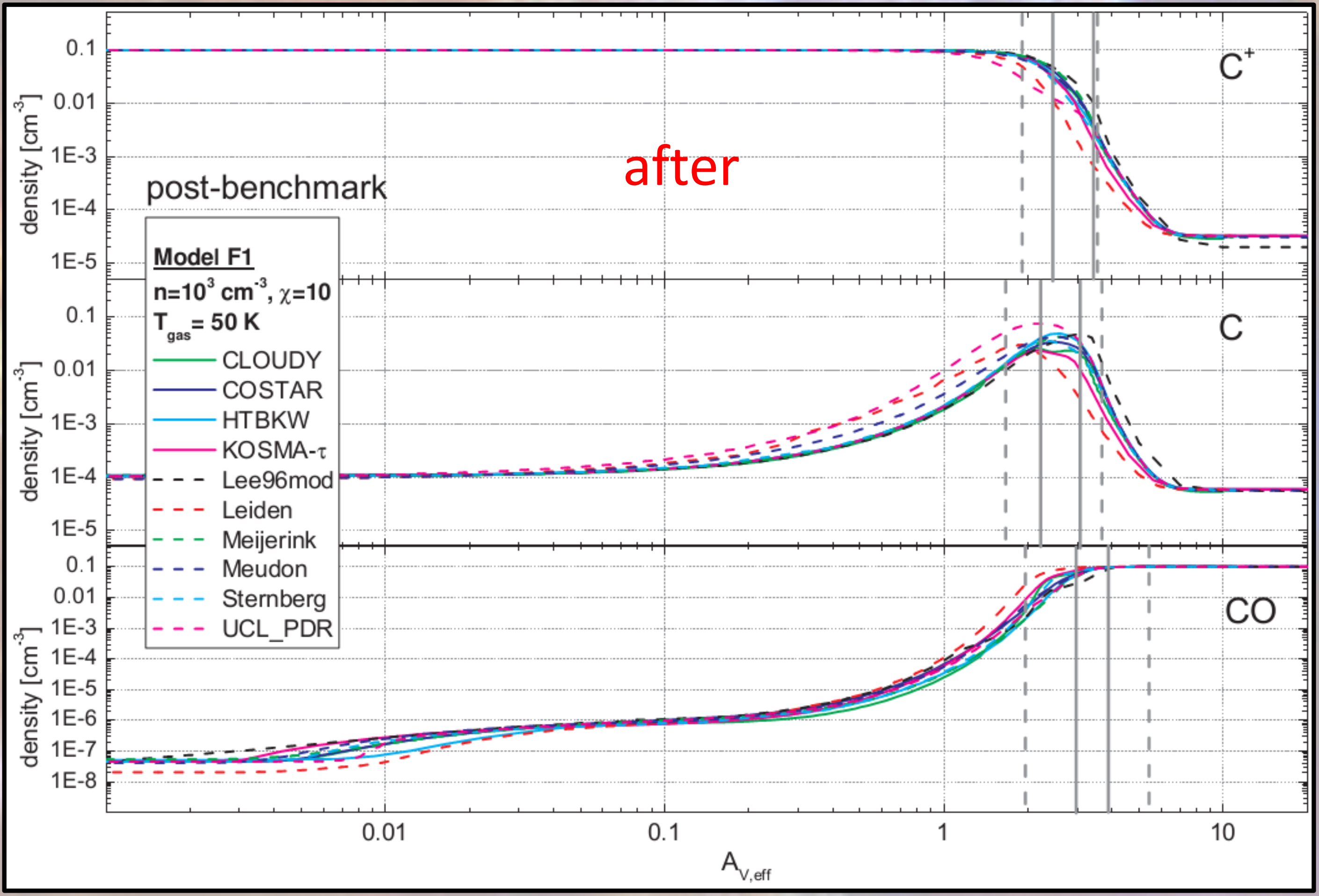
- Large international effort to compare model results from 10 different numerical PDR codes.
- All codes restricted to a minimum common functionality.
- 8 (very) simplified toy-models were calculated
- first and only database of reference PDR model results

F1 T=50 K $n = 10^3$ cm^{-3}, $\chi = 10$	F2 T=50 K $n = 10^3$ cm^{-3}, $\chi = 10^5$
F3 T=50 K $n = 10^{5.5}$ cm^{-3}, $\chi = 10$	F4 T=50 K $n = 10^{5.5}$ cm^{-3}, $\chi = 10^5$
V1 T=variable $n = 10^3$ cm^{-3}, $\chi = 10$	V2 T=variable $n = 10^3$ cm^{-3}, $\chi = 10^5$
V3 T=variable $n = 10^{5.5}$ cm^{-3}, $\chi = 10$	V4 T=variable $n = 10^{5.5}$ cm^{-3}, $\chi = 10^5$

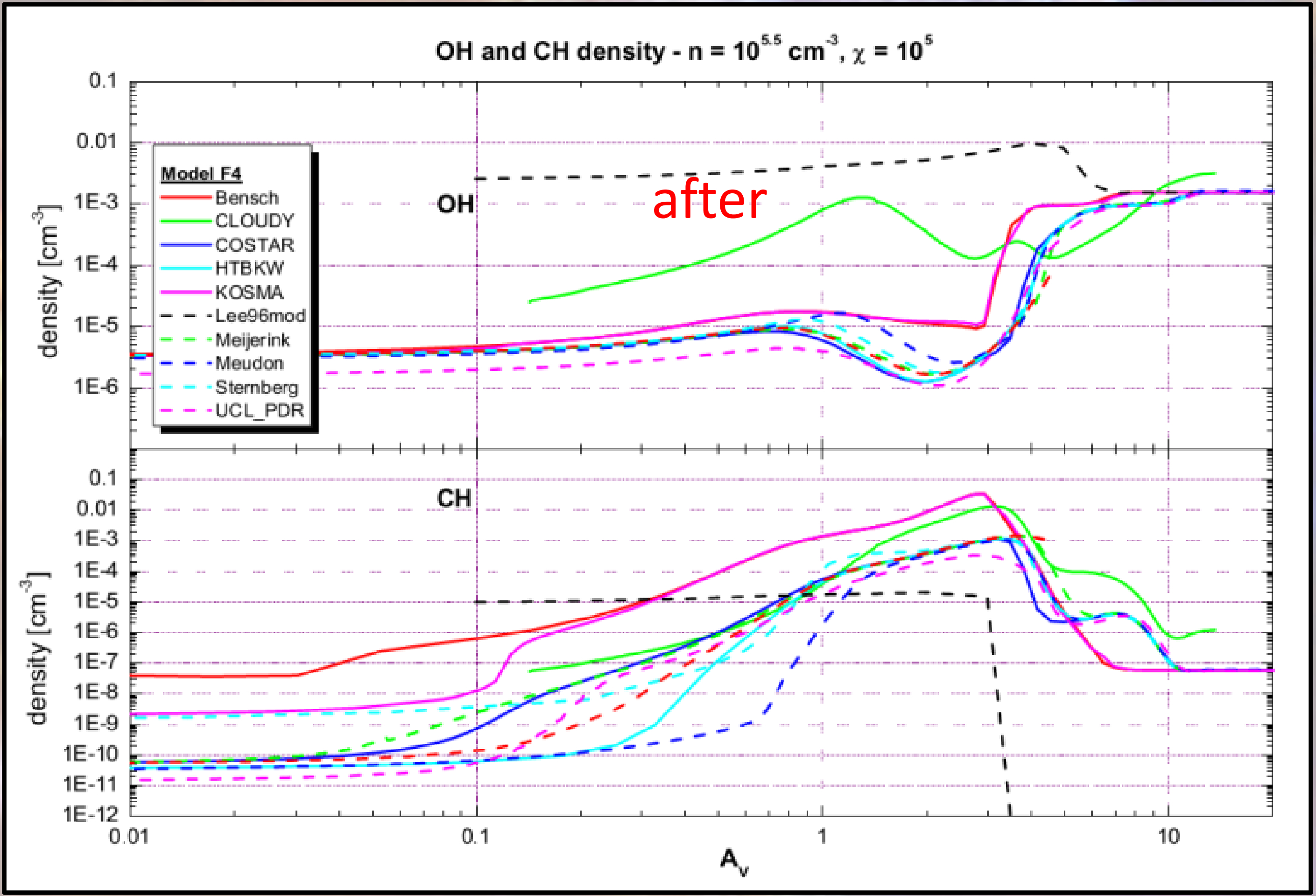
PDR model benchmark



PDR model benchmark



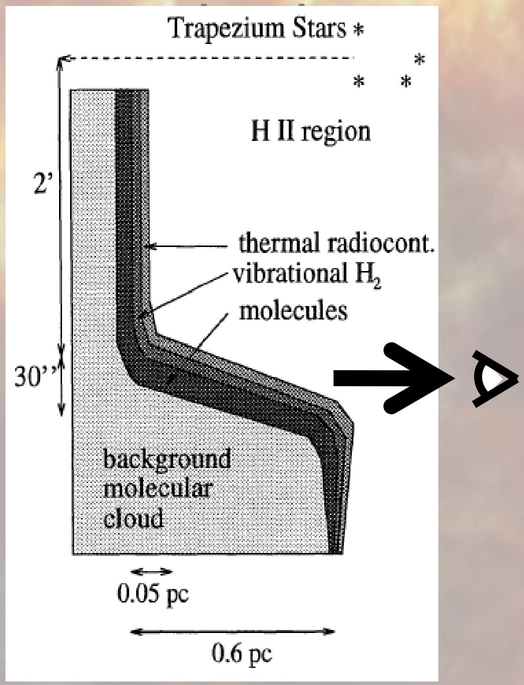
PDR model benchmark



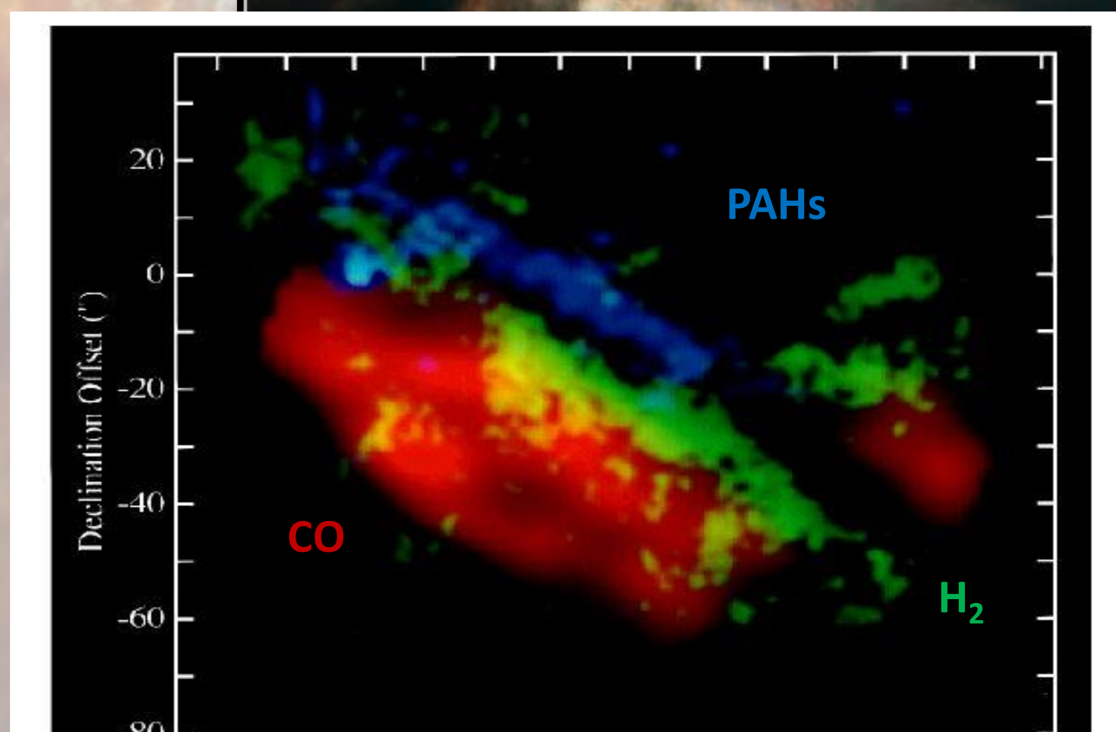
Light hydride chemistry largely unknown, but a lot of progress since then.

Orion bar

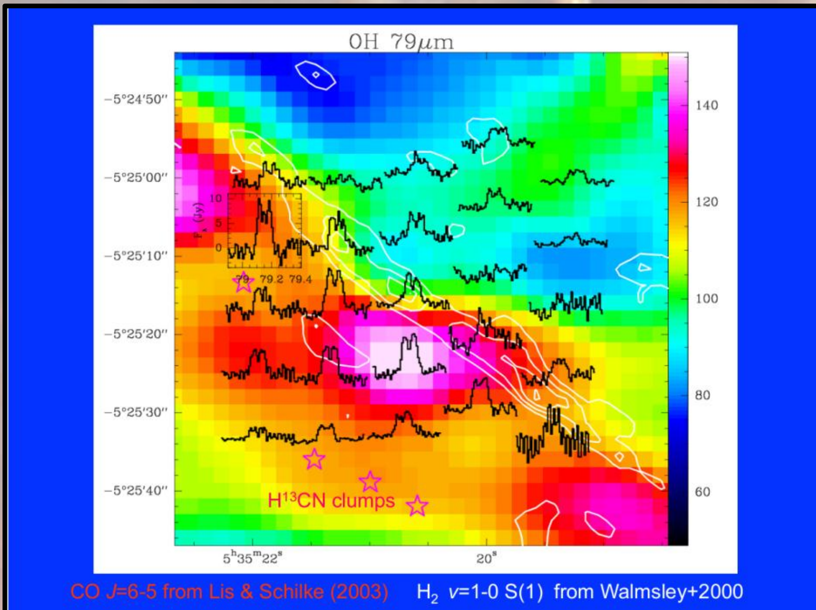
- Introduction
- Modelling
- Observations

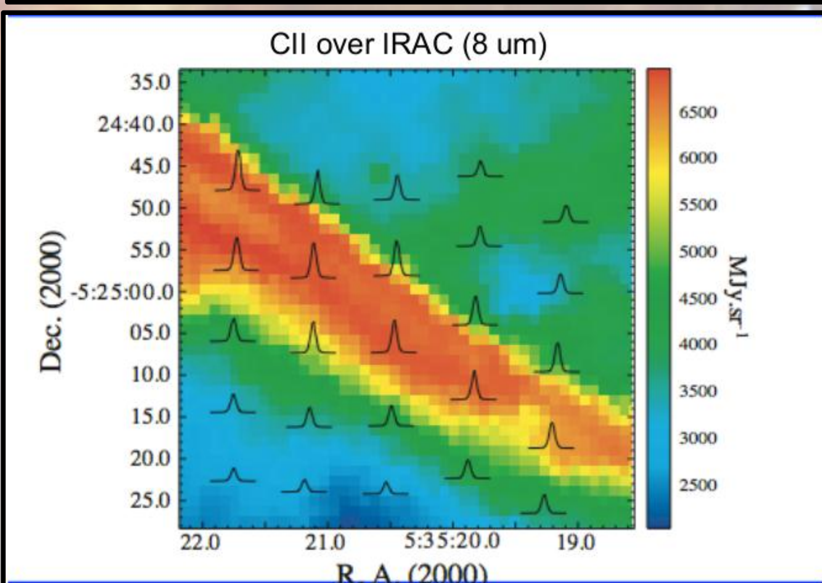


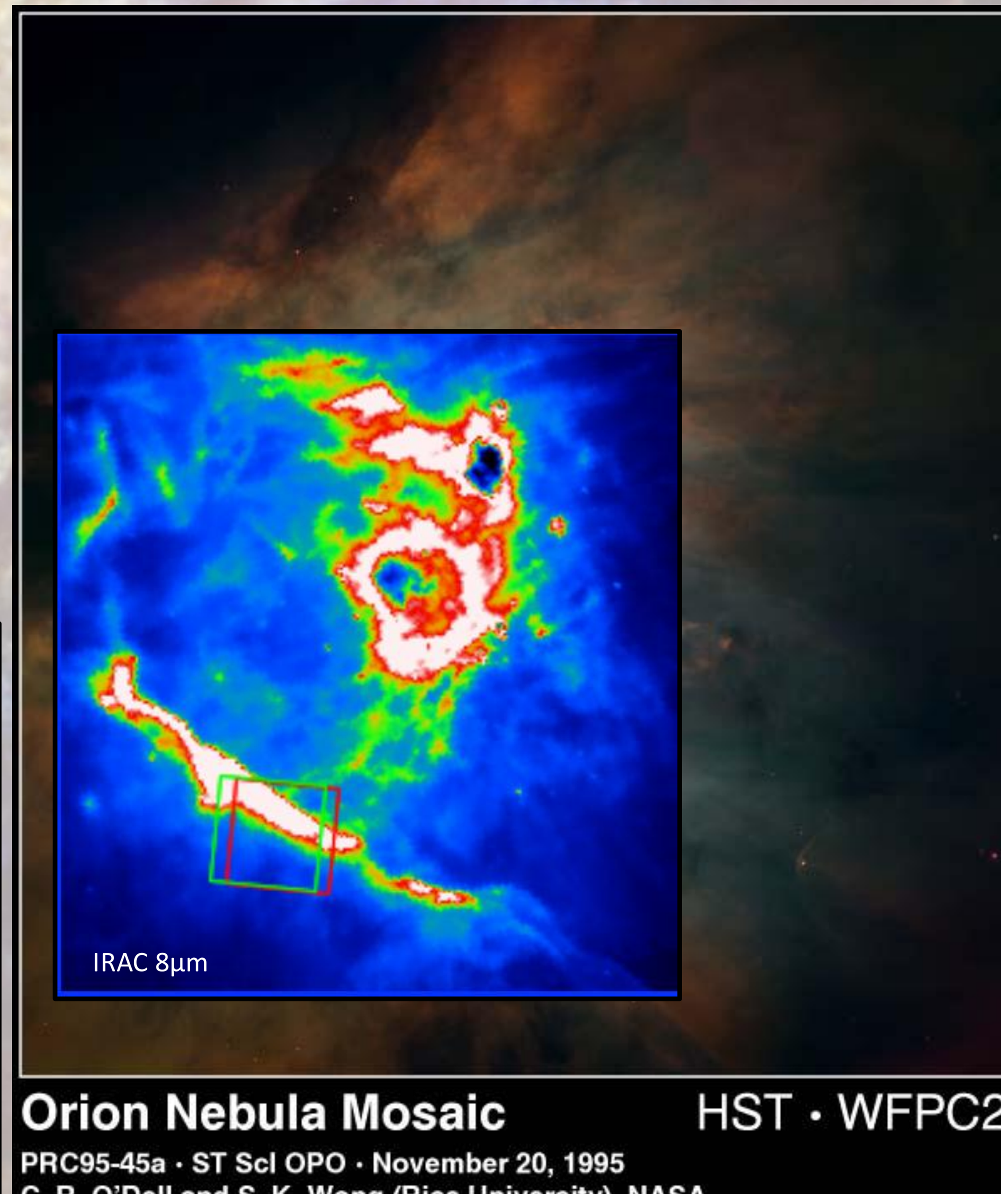
Orion bar PDR



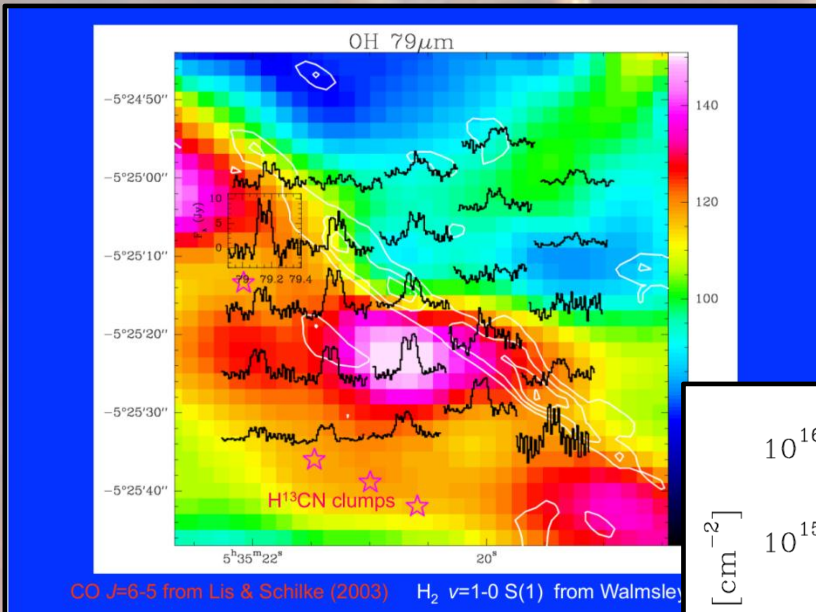
Orion bar


OH 79μm
−5°24'50''
−5°25'00''
−5°25'10''
−5°25'20''
−5°25'30''
−5°25'40''
5h35m22s
20s
140
120
100
80
60
79.2 79.4
H13CN clumps
CO J=6-5 from Lis & Schilke (2003)
H2 v=1-0 S(1) from Walmsley+2000

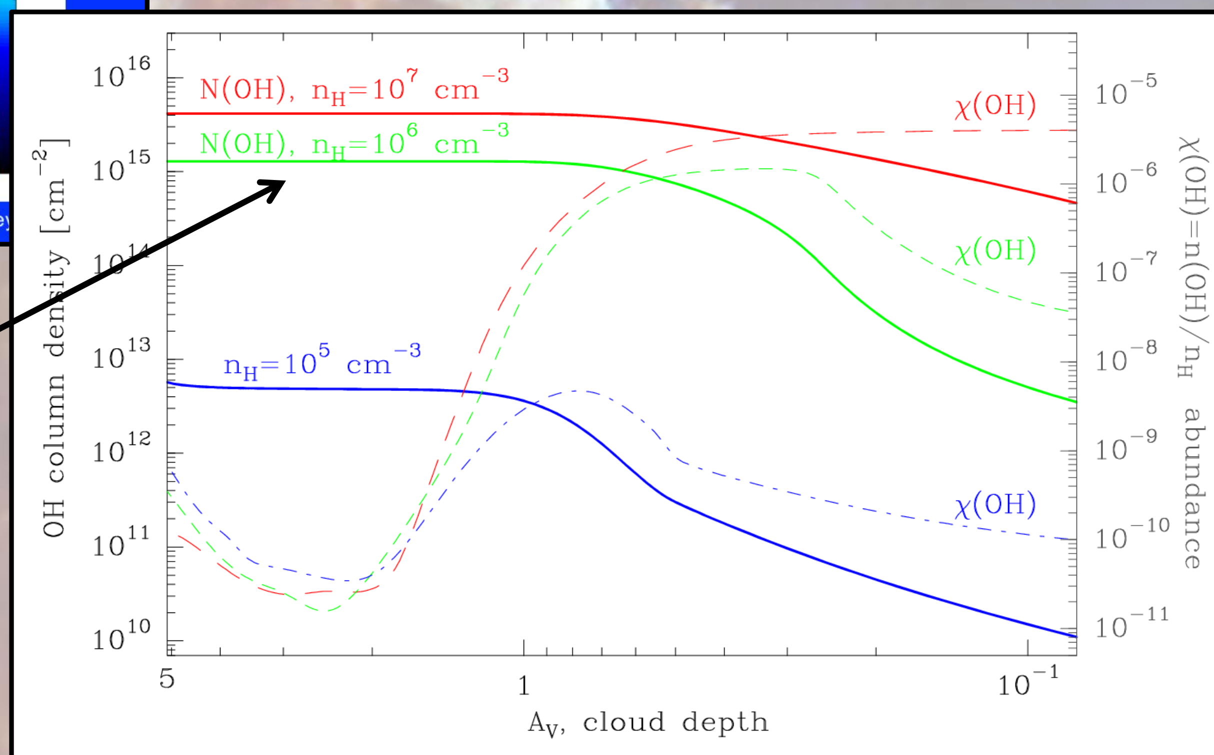

CII over IRAC (8 um)
Dec. (2000)
35.0
24:40.0
45.0
50.0
55.0
-5:25:00.0
05.0
10.0
15.0
20.0
25.0
22.0
21.0
5:35:20.0
19.0
R.A. (2000)
6500
6000
5500
5000
4500
4000
3500
3000
2500
MJy.sr-1


IRAC 8μm
Orion Nebula Mosaic
HST · WFPC2
PRC95-45a · ST ScI OPO · November 20, 1995

Orion bar: OH measurements



The spatial distribution of OH and ist total column density is difficult to reproduce in PDR models and is a strong model constraint.

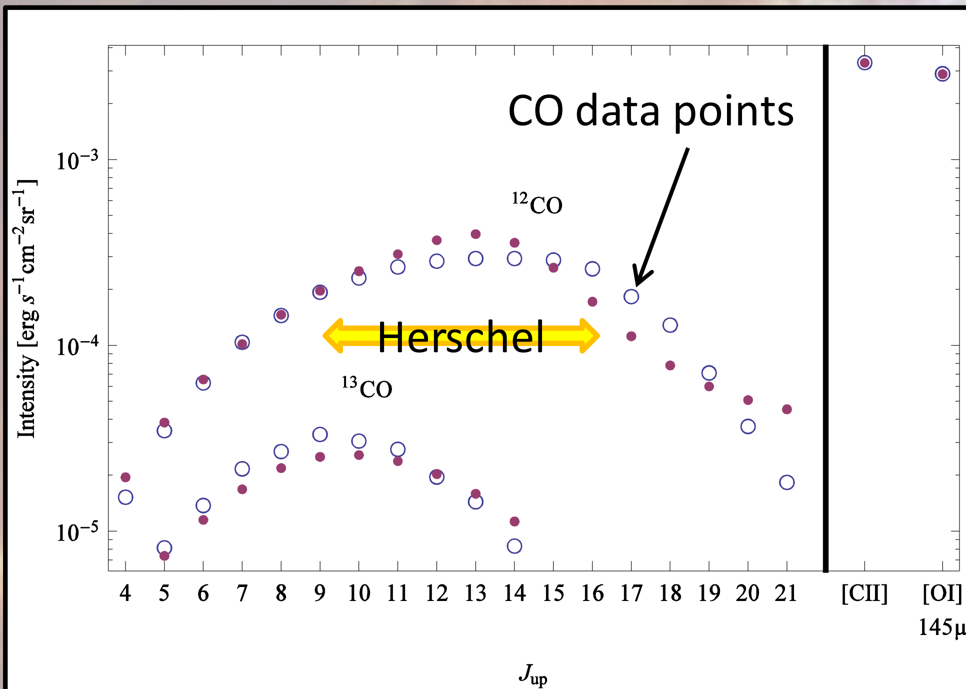


very high gas density required to reproduce the observed amount of OH in PDR models

Le Bourlot et al. 2011

Orion bar model results

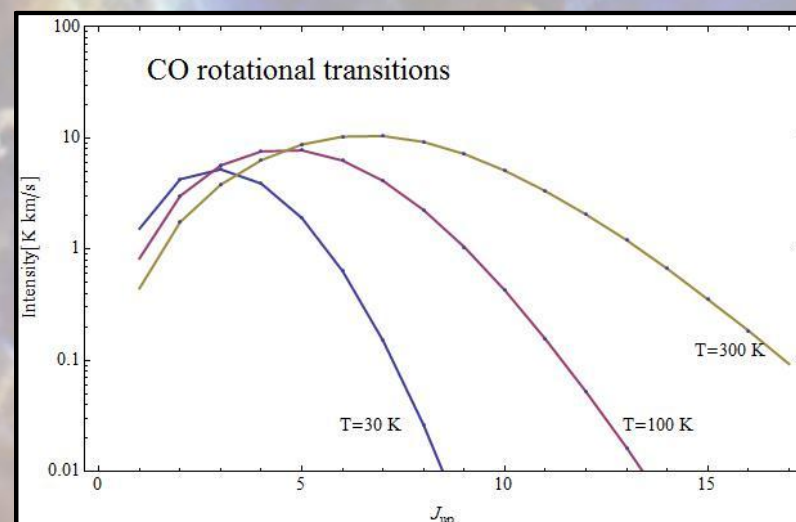
For the first time full J-ladder up to J=21 available.



Spectral line energy distribution SLED

Population of rotational quantum states of CO depends on the local excitation conditions (T, n_{CO}, τ, …).

The CO-SLED is a measure of the local CO excitation conditions.

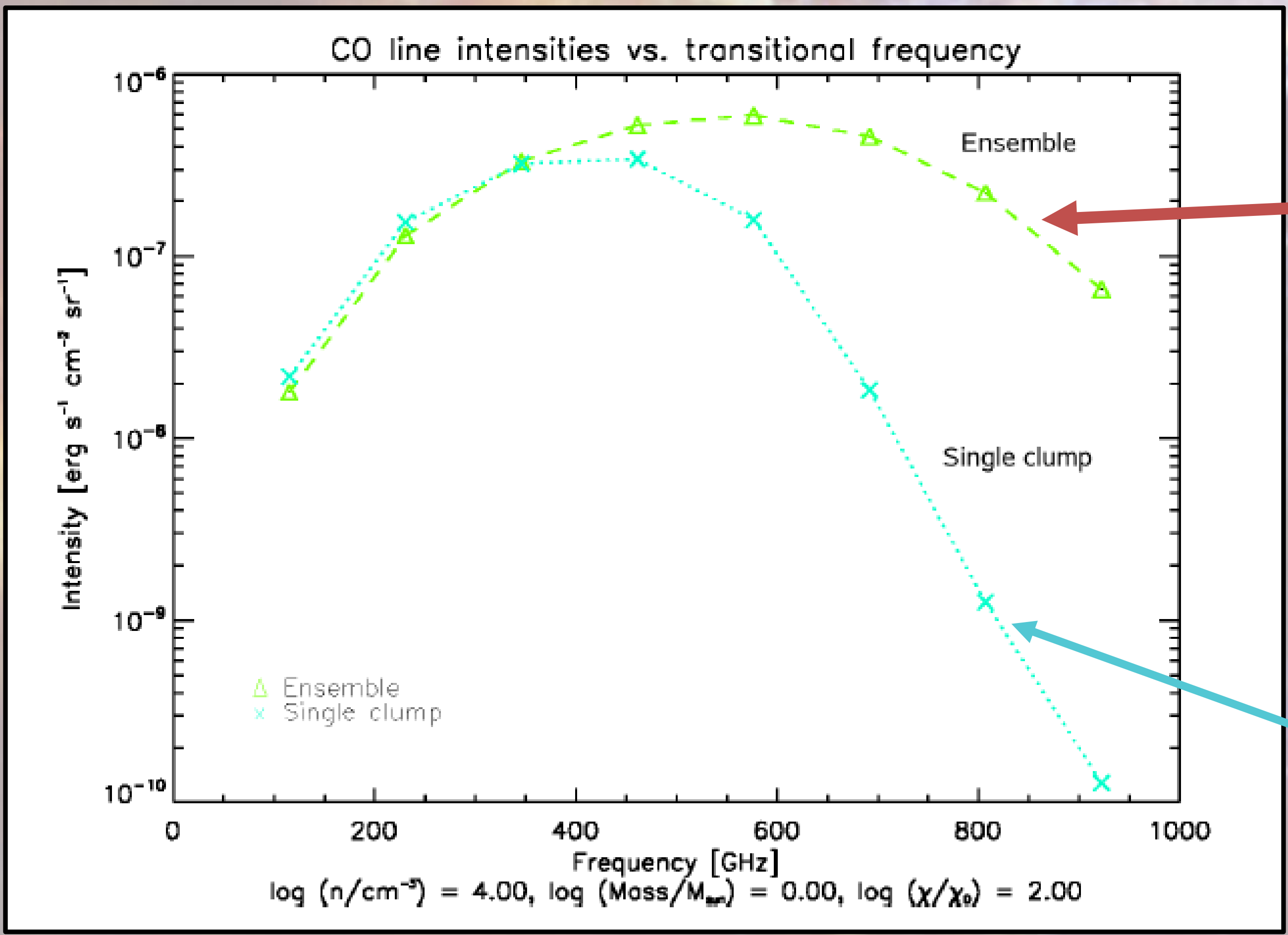


escape prob. simulation: homogeneous slab of gas

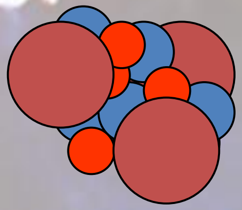
CO: linear rotator

→ allowed transitions ΔJ = ±1

Clumpy Molecular Clouds

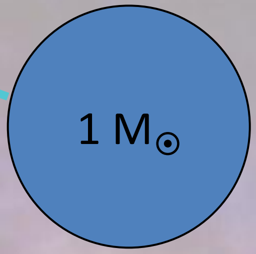


fractal structure
with larger surface to
volume ratio



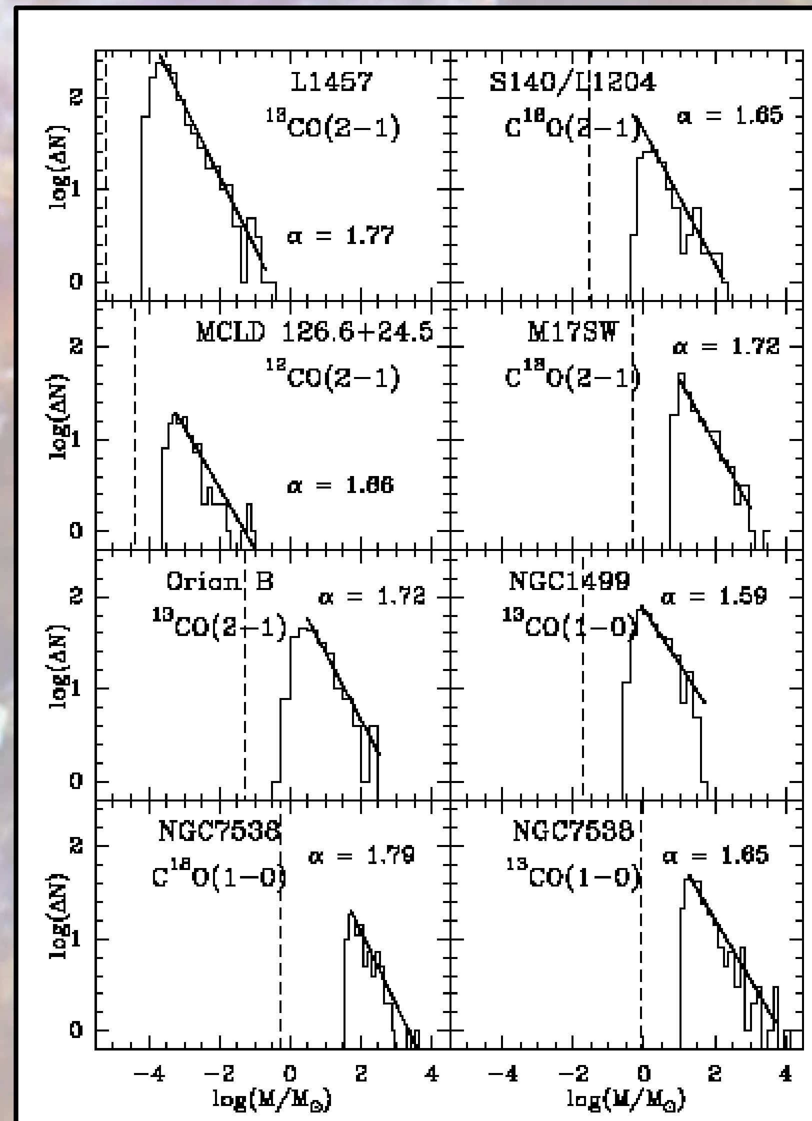
$\Sigma M_i = 1 M_\odot$

monolithic clump



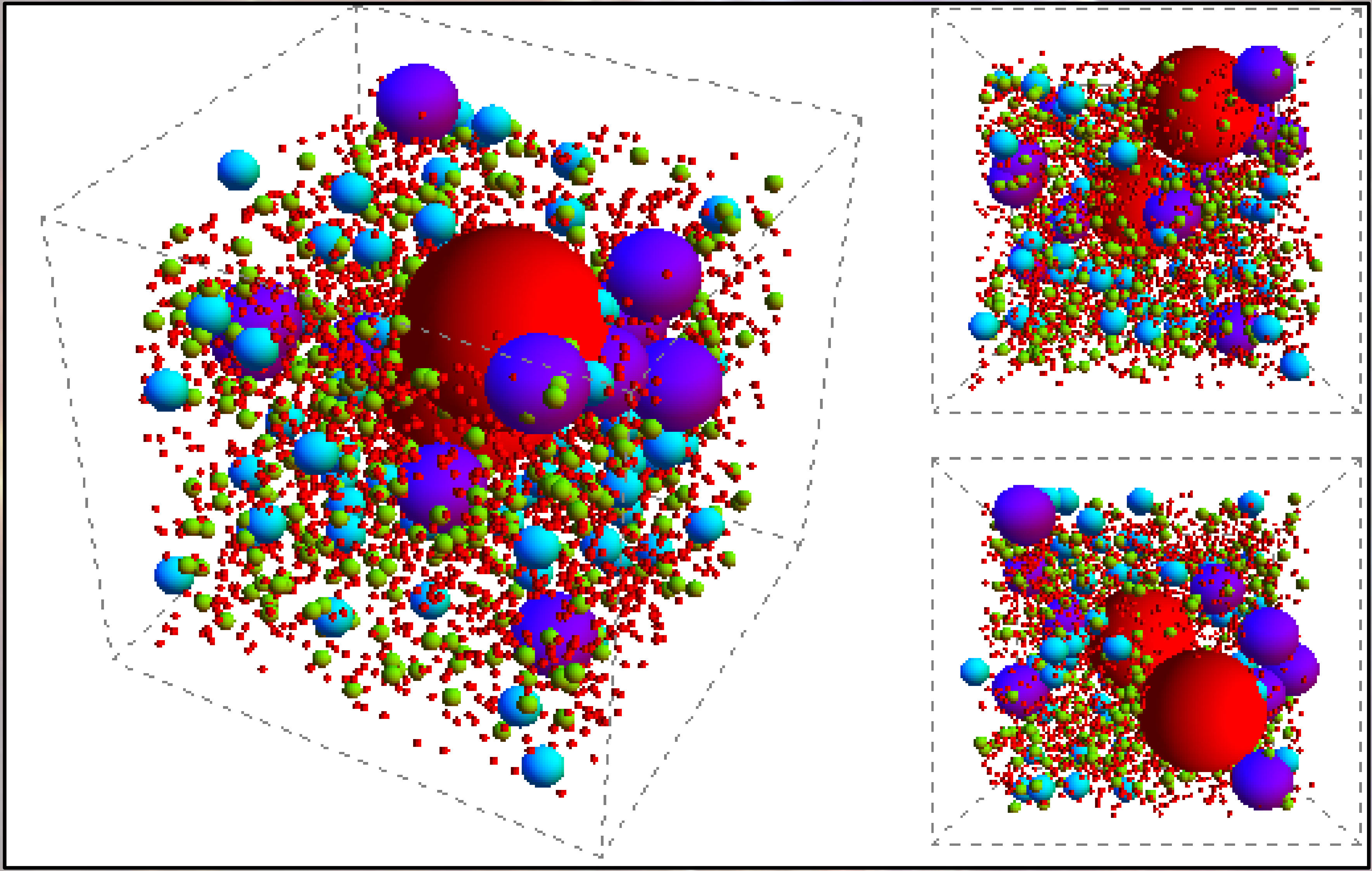
Clumpy Molecular Clouds

- observations show an almost universal clump-mass distribution with $dN/dM \propto M^{-1.6 \ldots 1.8}$ and a mass-size relation of $M \propto R^{2.3}$

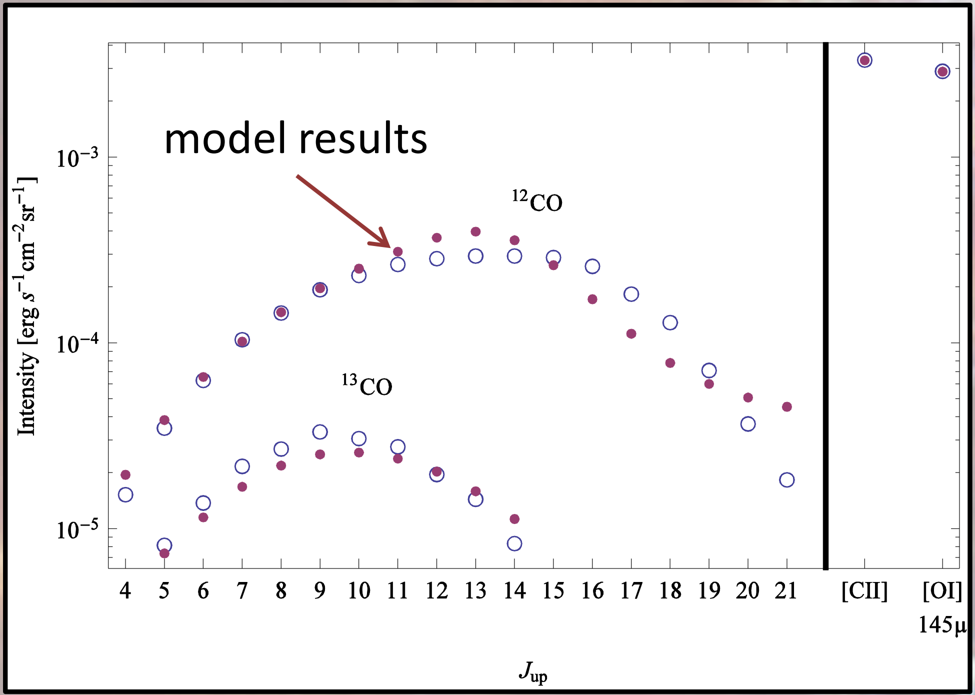


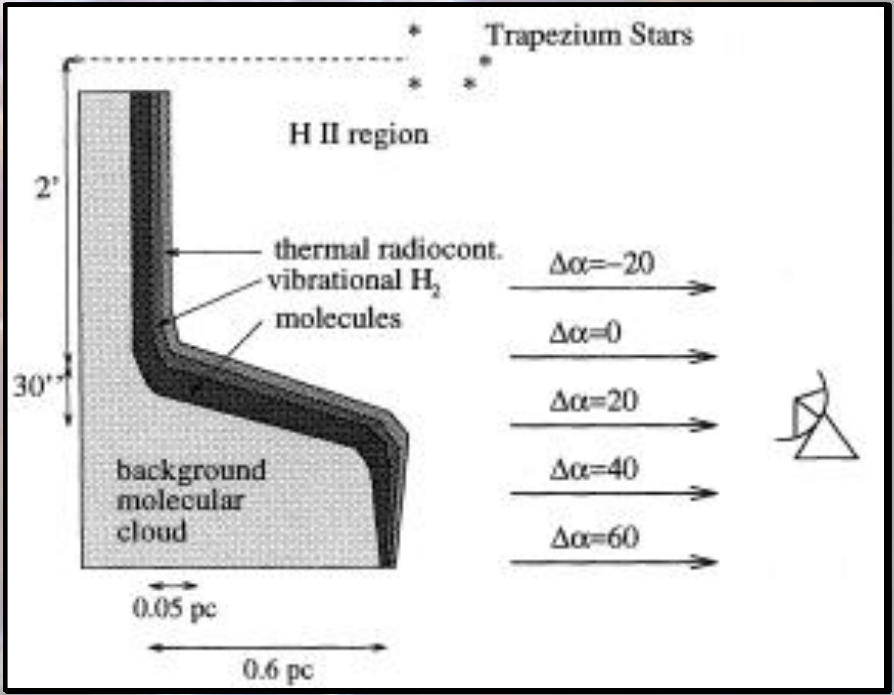
(Kramer et al. 1998)

Clumpy clouds



Orion bar model results





- ^{12}CO lines fitted up to J=15-14 , J>16 require even higher densities (shocks?)
- ^{13}CO well reproduced.
- observed mean col. density of 6.5e22 cm^{-2} and a (9.6“)² pixel implies a mass of 0.2 $M_\odot$ -> model mass ~0.3 $M_\odot$
- reasonable model FUV strength!

DR 21 C

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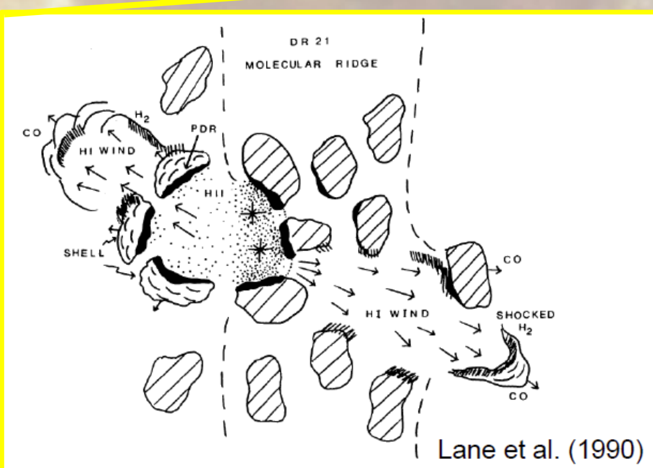
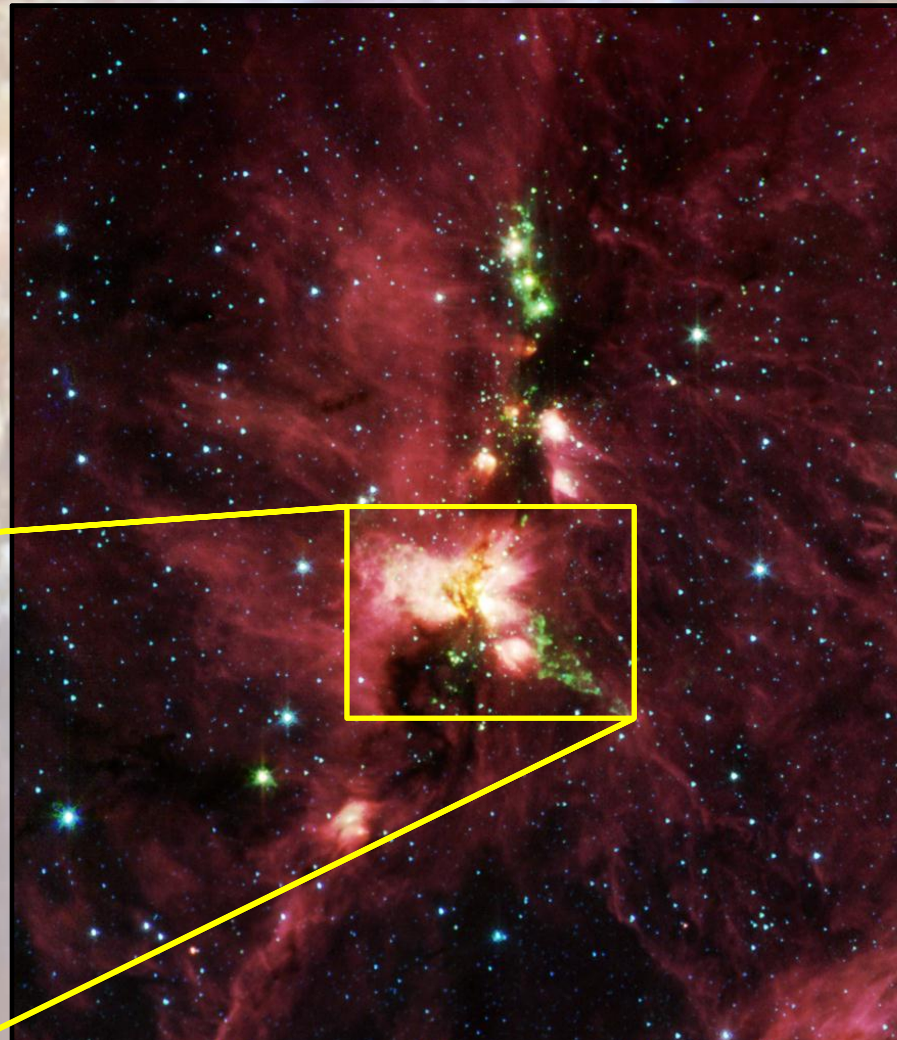
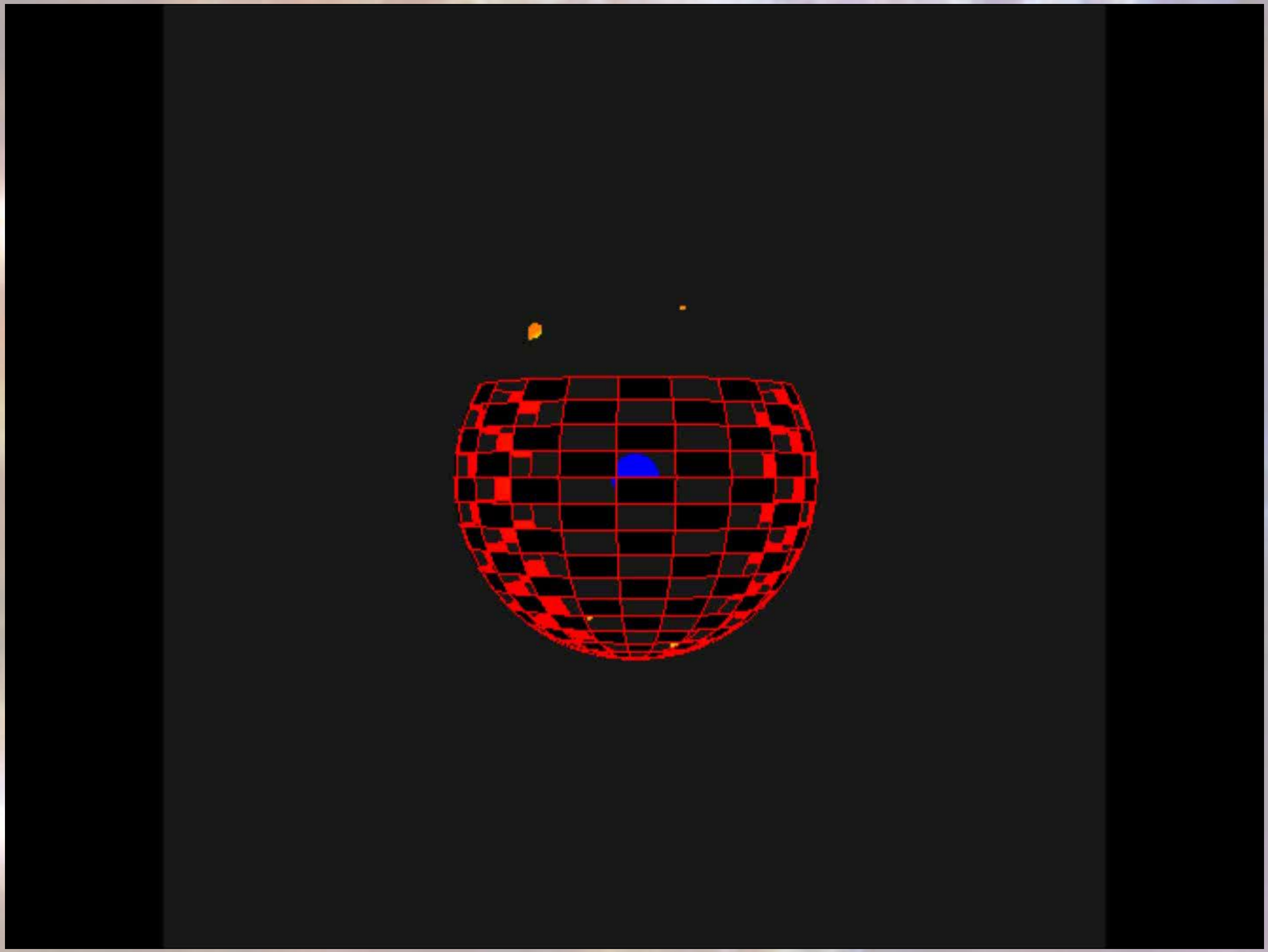
- **Observations**
- Outlook



Lane et al. (1990)

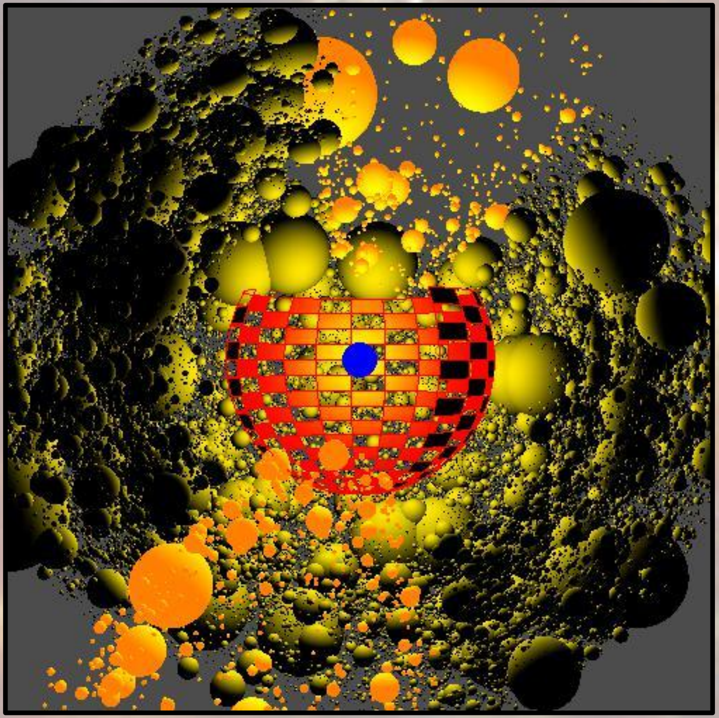

Marston et al. 2007, Spitzer

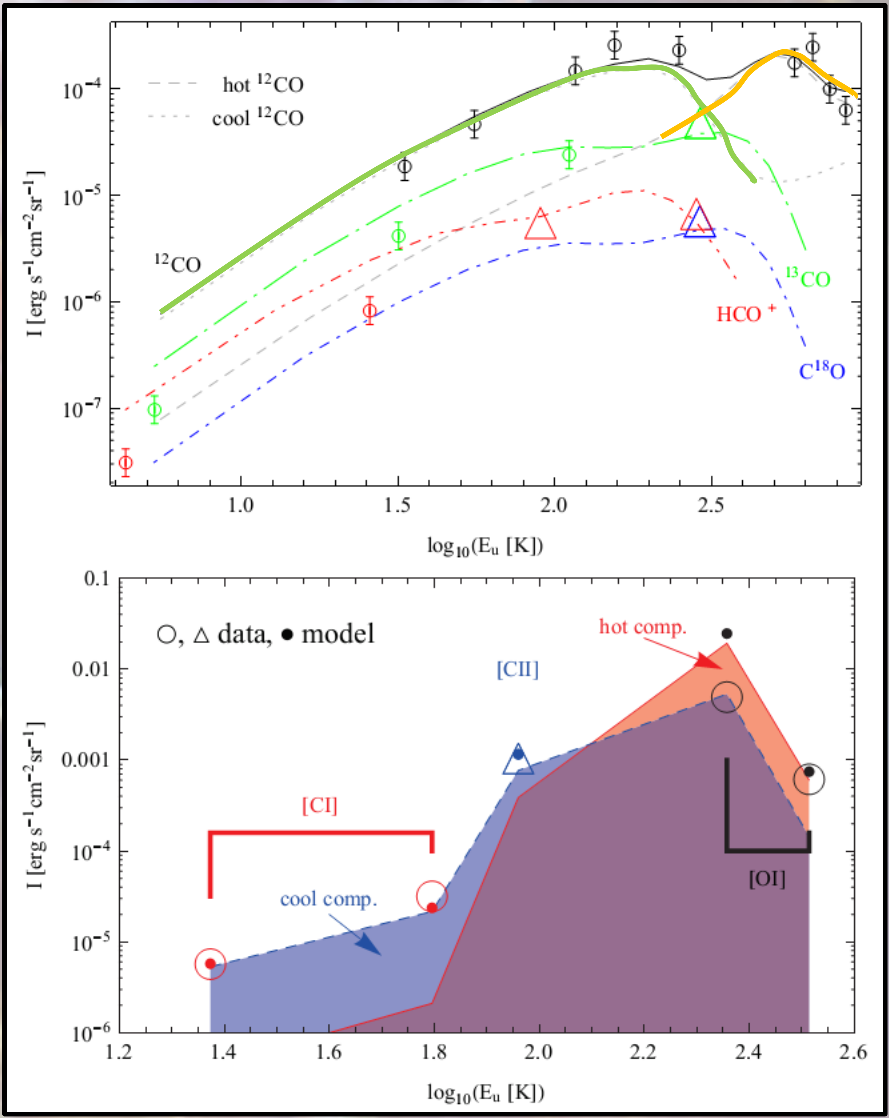
Modeling the embedded blister outflow



blue: central star, red: HII region, yellow & green: molecular clouds (PDRs)

DR 21 C

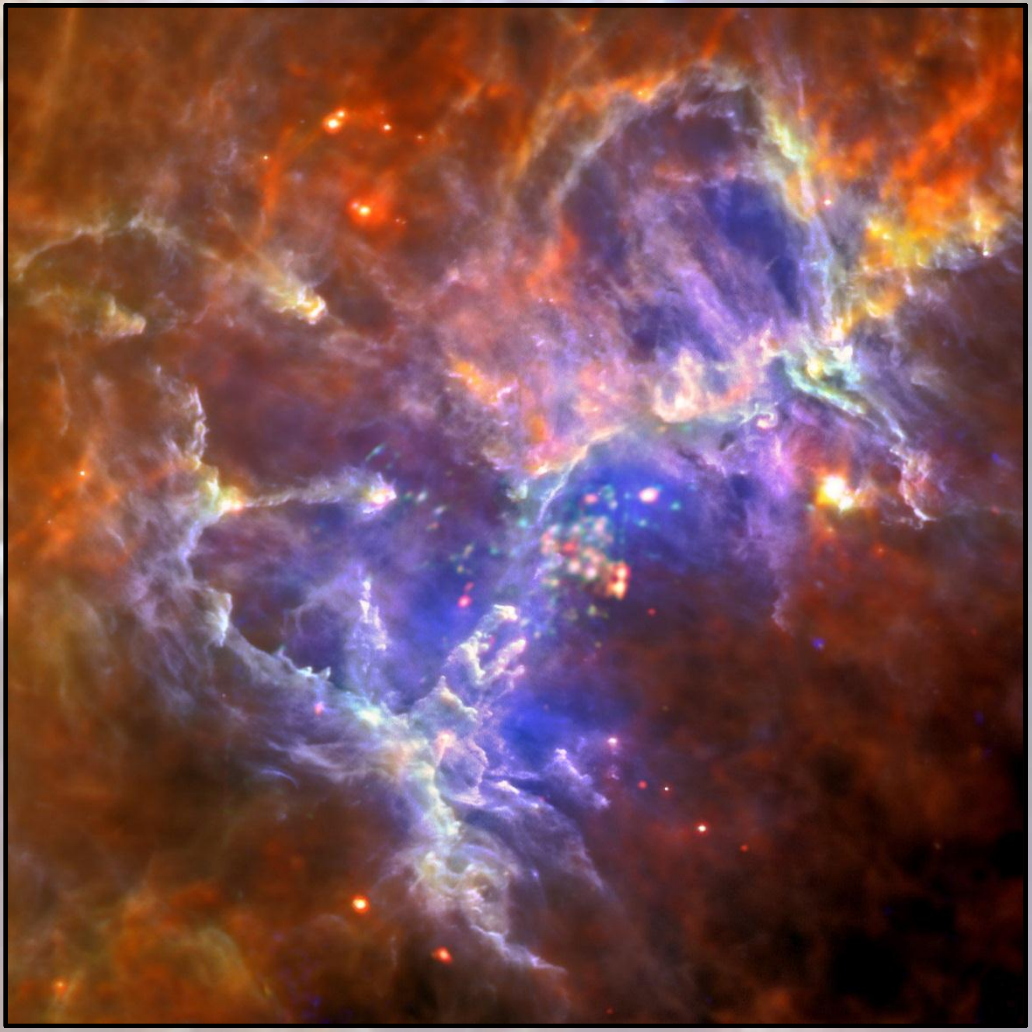




- Two distinct UV fields (10^5 and 300 χ_D)
- Dense clumps facing the blister outflow + clumpy large scale distribution
- Emission can be explained without shock component

Outlook

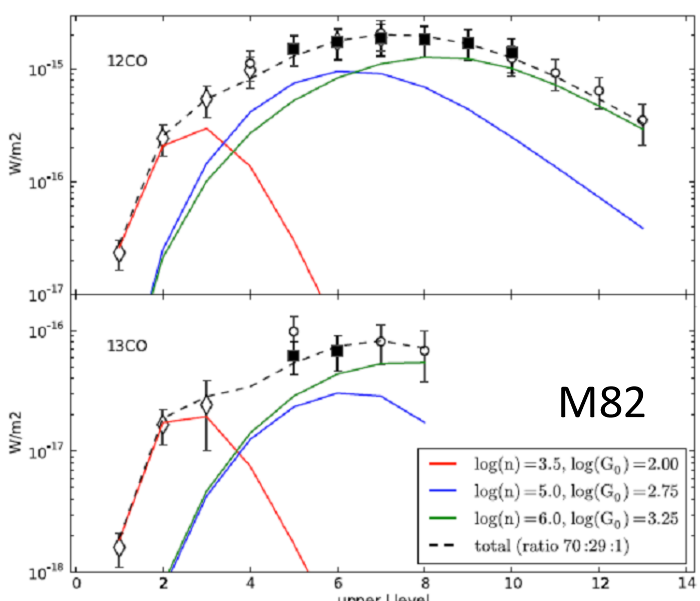
- Introduction
- Modelling
- Observations
- Outlook



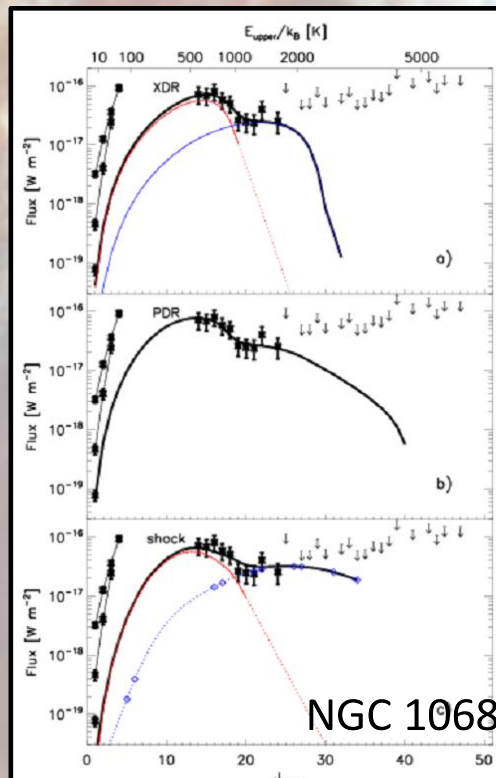
Credits: ESA/Herschel/PACS/SPIRE/Hill, Motte, HOBYS Key Programme Consortium

Outlook

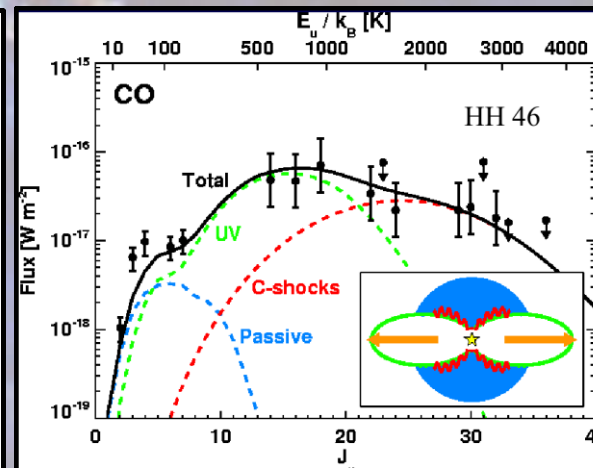
- Recent instrument missions opened up the FIR spectral window and allowed for the first time to directly observe many PDR tracers.
- PDR models again struggle to explain CO emission.



Loenen et al. 2010



Hailey-Dunsheath at al. 2012

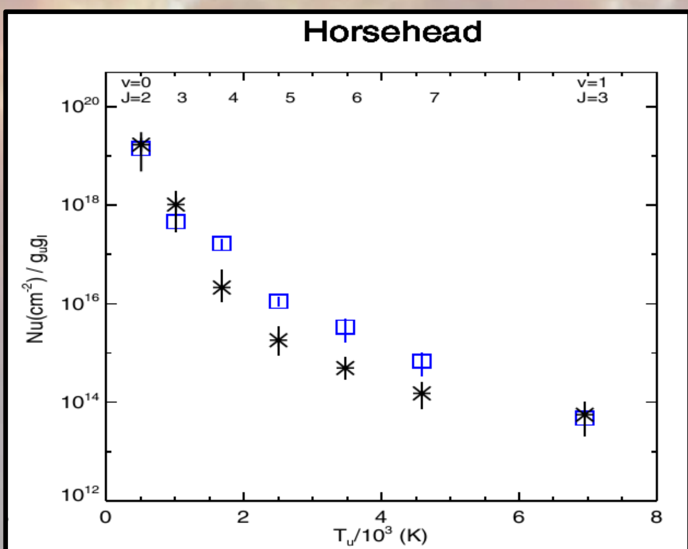


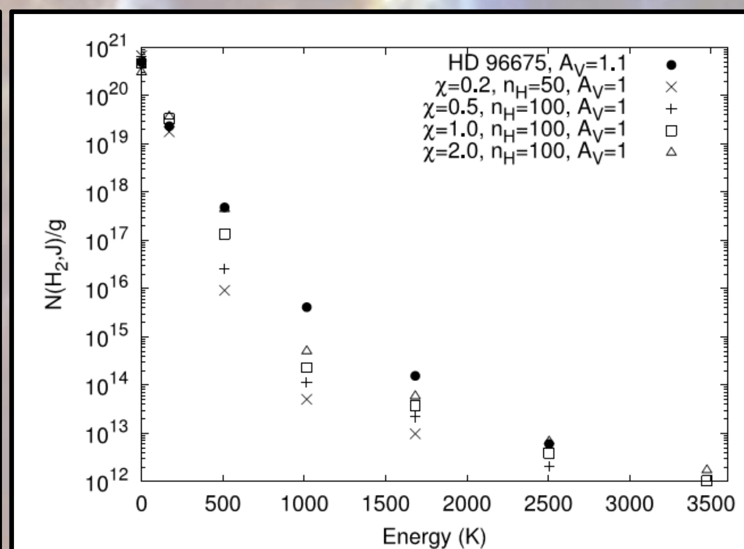
Visser at al. 2012, van Kempen et al. 2010

High-J CO lines reveal new insights into the local physics!

Outlook

- Recent instrument missions opened up the spectral FIR window and allowed for the first time to directly observe many PDR tracers.
- PDR models <u>again</u> struggle to explain CO emission and H_2 emission.
- This already taught us many new details on the local physical and chemical conditions and the dominant processes in PDRs.





H_2 emission remains difficult to reproduce in PDR models, but recent missions taught us a lot about H_2 formation.

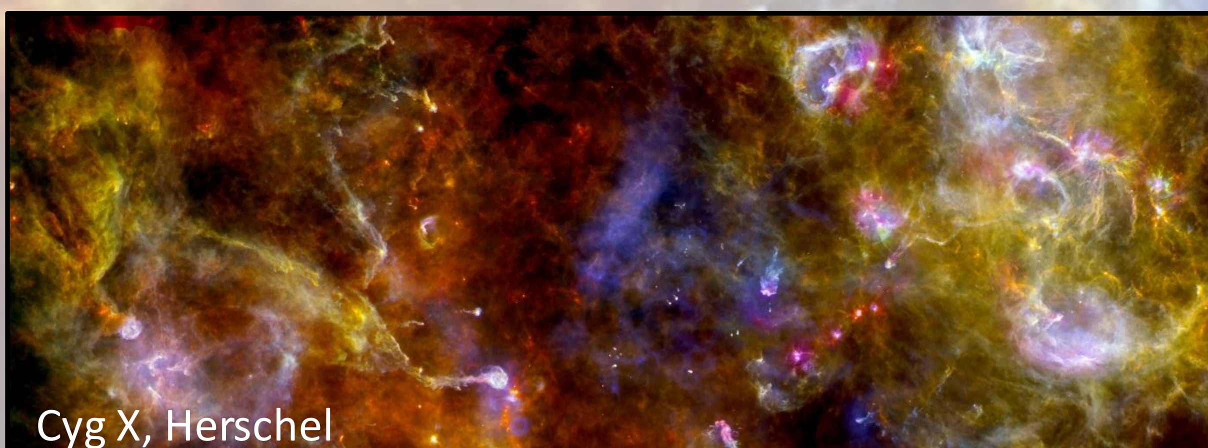
Habart at al. 2011

Outlook

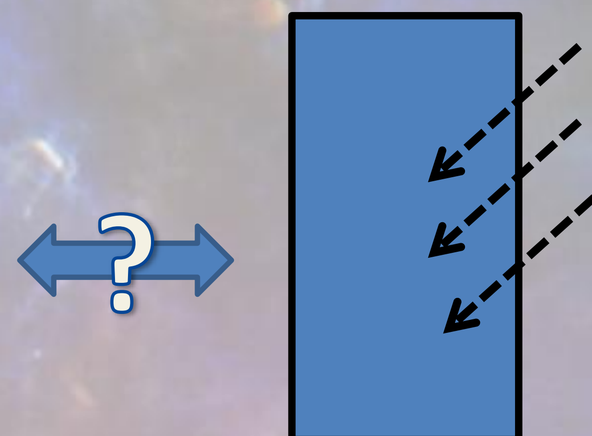
- Reproducing the chemistry of light hydrides (OH, CH^+, H_2O,…) remains a challange – more discoveries waiting.
- Laboratory data is desperately missing (collision rates, line frequencies, chemical reaction rates,..).

→ The universe remains wonderfully complex.

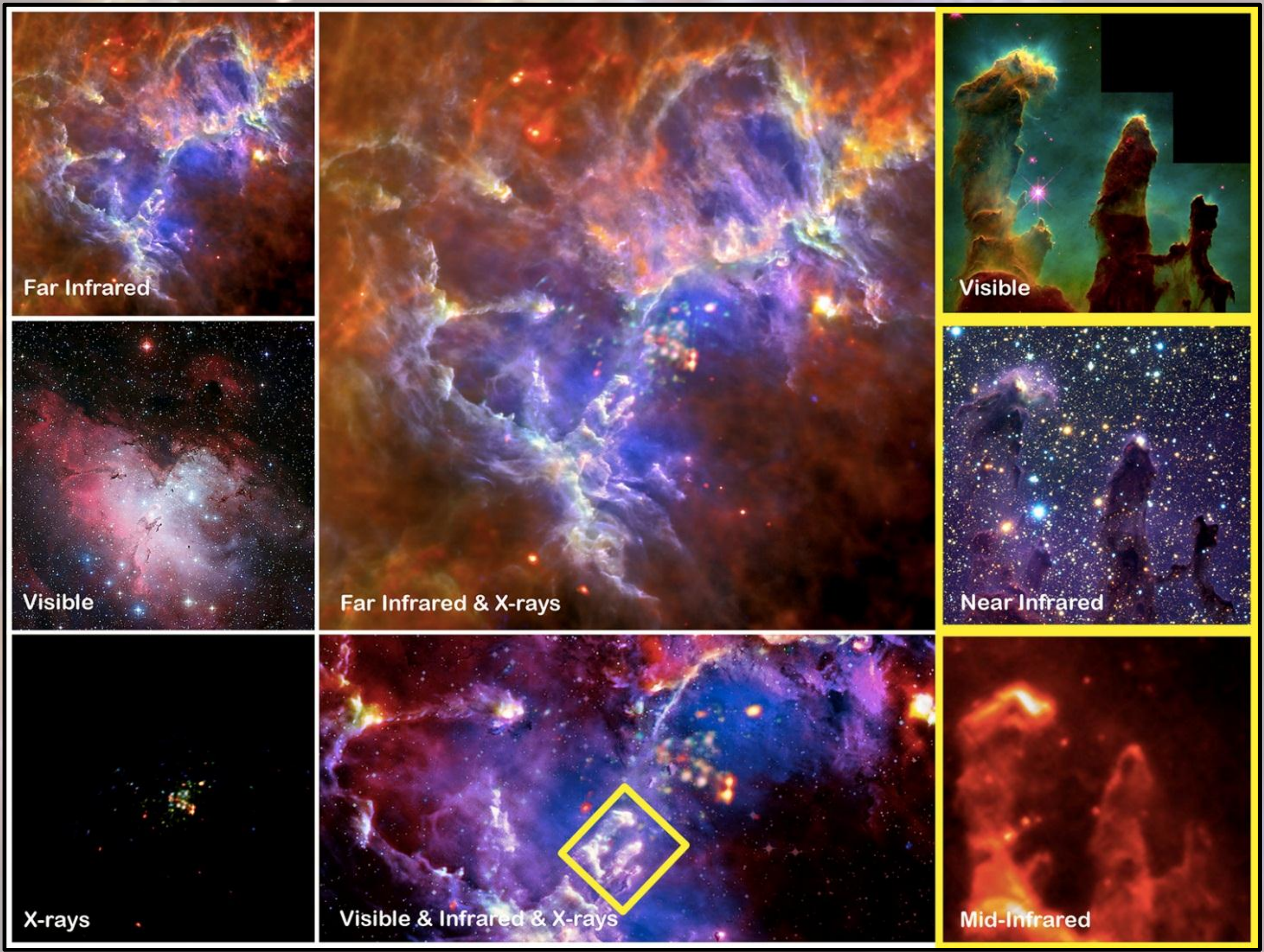
→ Amazing how far we already got with our simple model attempts.



Cyg X, Herschel



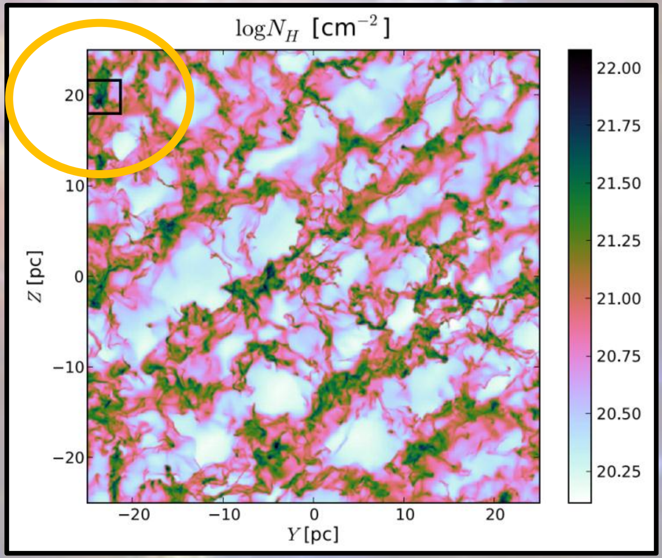
Thank you!



Credit: European Space Agency, European Southern Observatory, NASA

Model geometry

- Numerous configurations
  - Cloud geometry
    - plane-parallel (1D)
    - spherical (1D)
    - disk (1D+1D)
    - full 3-D
  - Illumination
    - isotropic
    - uni-directional



Levrier et al., 2012, A&A 544

- The model geometry is determined by the field of application

Model geometry

- Numerous configurations
  - Cloud geometry
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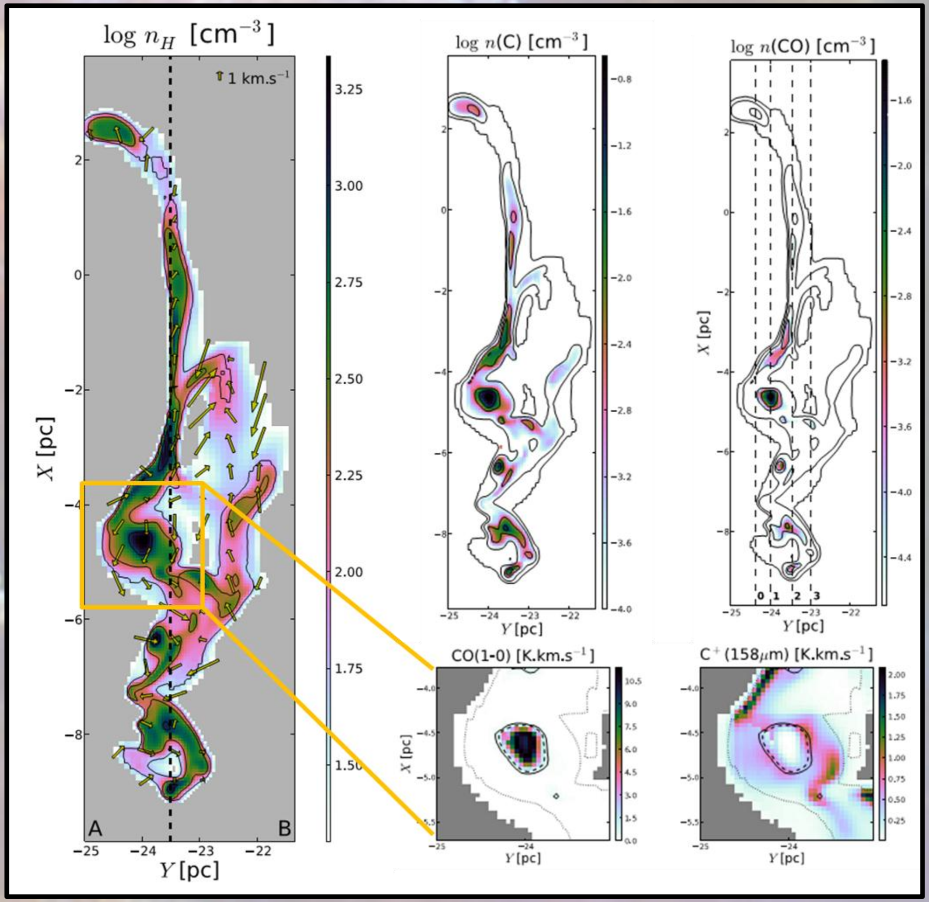
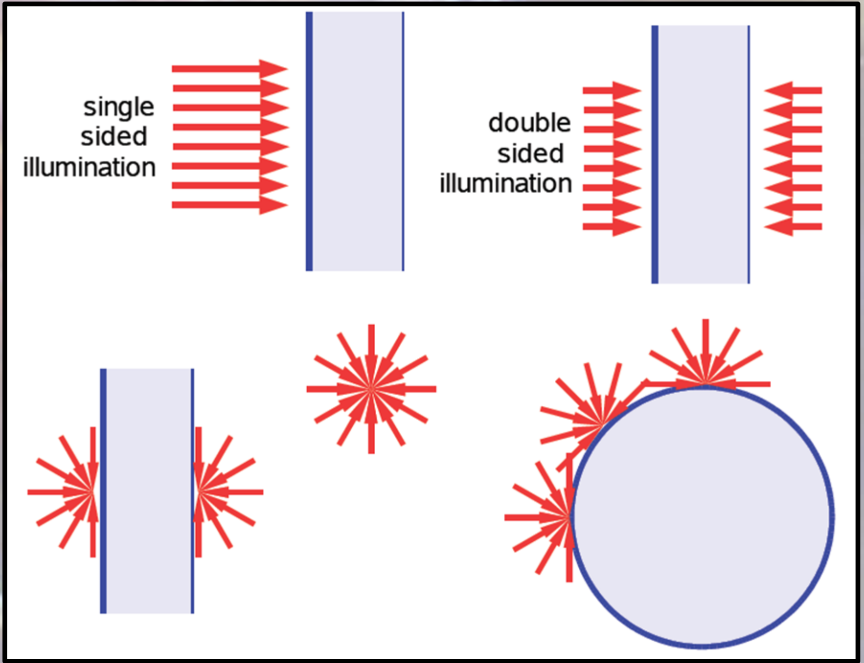
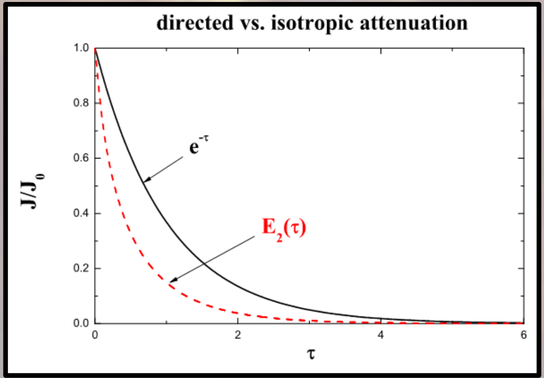


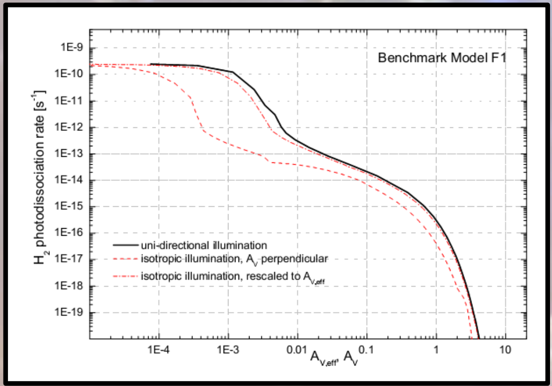
Post-processed MHD simulations, Levrier et al., 2012, A&A 544

Geometry of the Radiation Field

- Numerous configurations
  - Cloud geometry
    - plane-parallel (1D)
    - spherical (1D)
    - disk (1D+1D)
    - full 3-D
  - Illumination
    - isotropic
    - uni-directional
  - Clumpiness

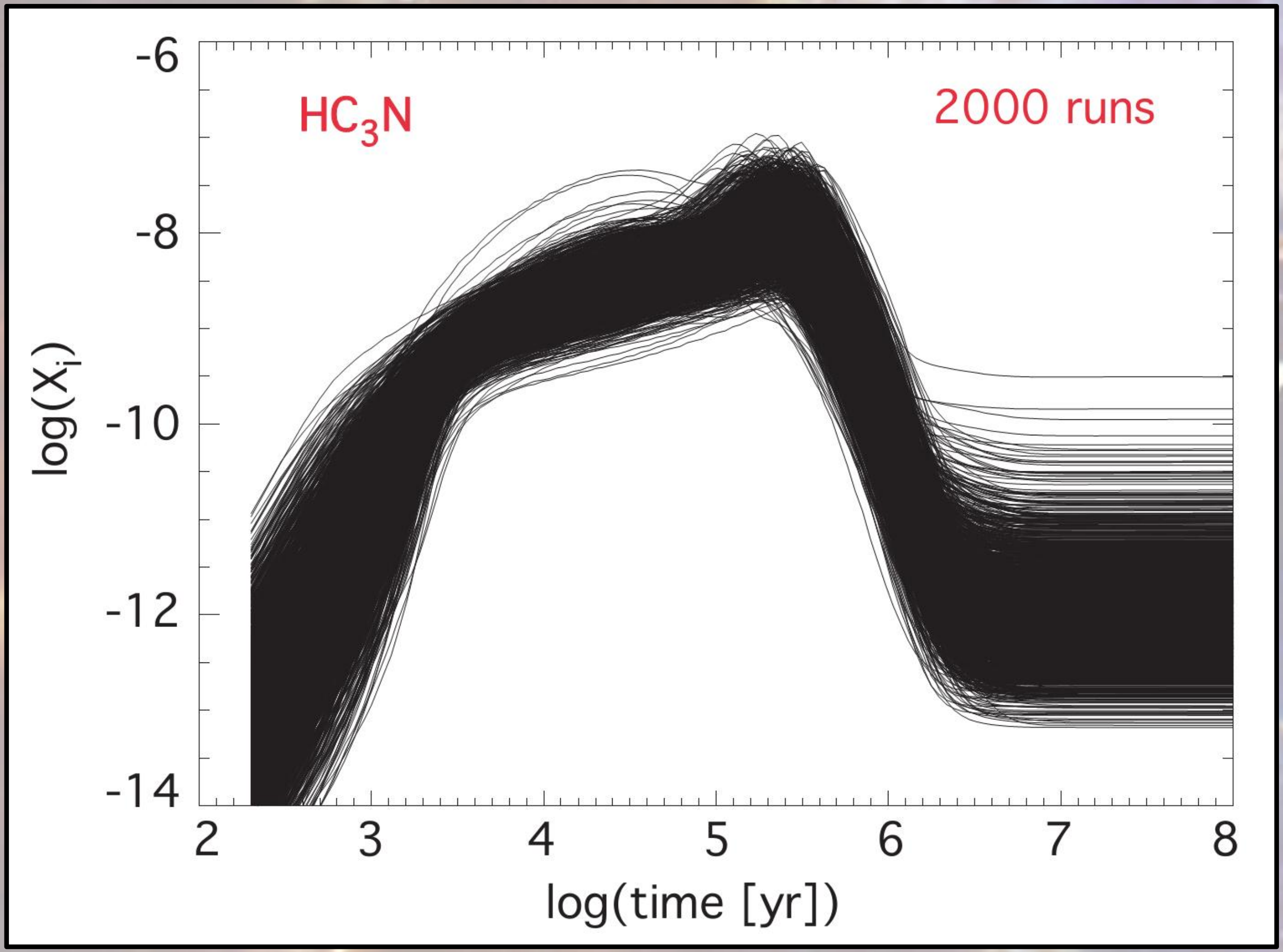






Röllig et al. 2007, A&A, 467

Model chemistry



Wakelam et al, 2010, Space Sci. Rev. 156

Non-linear system:

Slight input changes may affect the outcome significantly

uncertain rate coefficients (errors: smaller than 25%, ..., larger than a few 1000%)

Model physics

- radiative transfer
  - dust properties
    - size distribution & composition
  - self shielding
    - shielding rates vs. full computation
  - turbulence/clumpyness
    - micro/meso/macro-turbulence
- energy balance
  - heating & cooling effects
    - PE heating, H_2 formation heating, H_2 vib. deexcitation
  - optical depths
  - collisional rates
    - line + continuum cooling
- model parameters
  - density
    - $n=10^3\text{-}10^7$ cm^{-3}
  - FUV intensity
    - $\chi=1\text{-}10^6$
  - mass
    - $M=10^{-3}\text{-}10^3\ M_\odot$
  - CR ionization rate
    - $\zeta_{CR}= 10^{-17}\text{-}10^{-14}$ s^{-1}