



Sunblock extreme

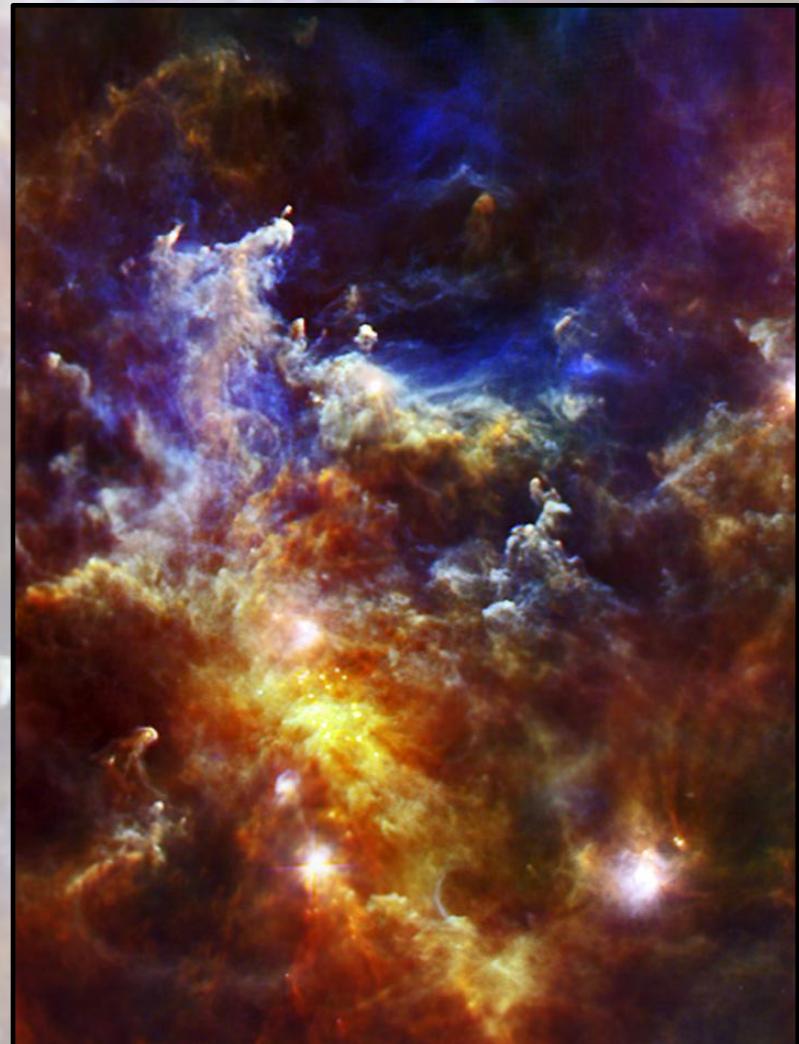
Astrophysics and astrochemistry in
photo-dissociation regions

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Outline

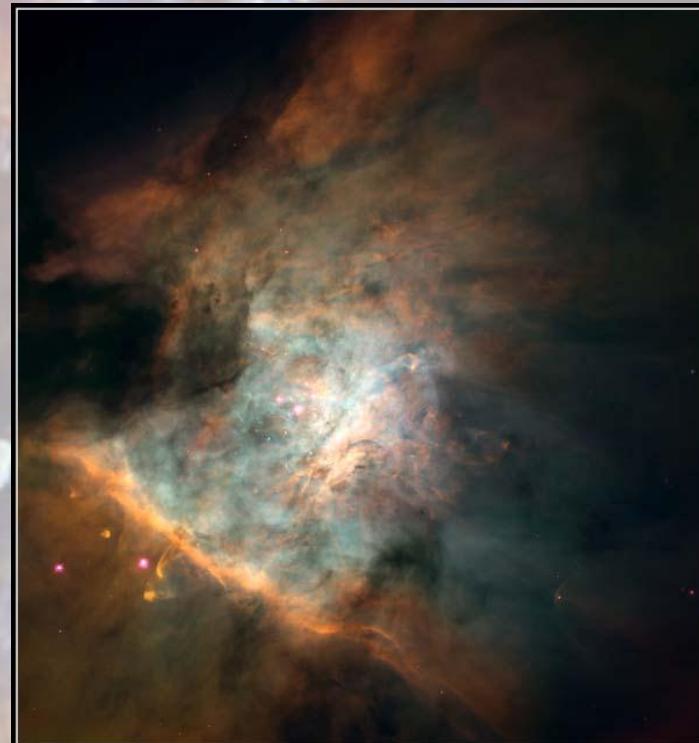
- Introduction
- Modelling
- Observations
- Outlook



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

Introduction

- Introduction
- Modelling
- Observations
- Outlook
- Photo-dissociation Regions



Orion Nebula Mosaic

PRC95-45a · ST Scl OPO · November 20, 1995

C. R. O'Dell and S. K. Wong (Rice University), NASA

HST · WFPC2

Photo-dissociation regions

- Definition

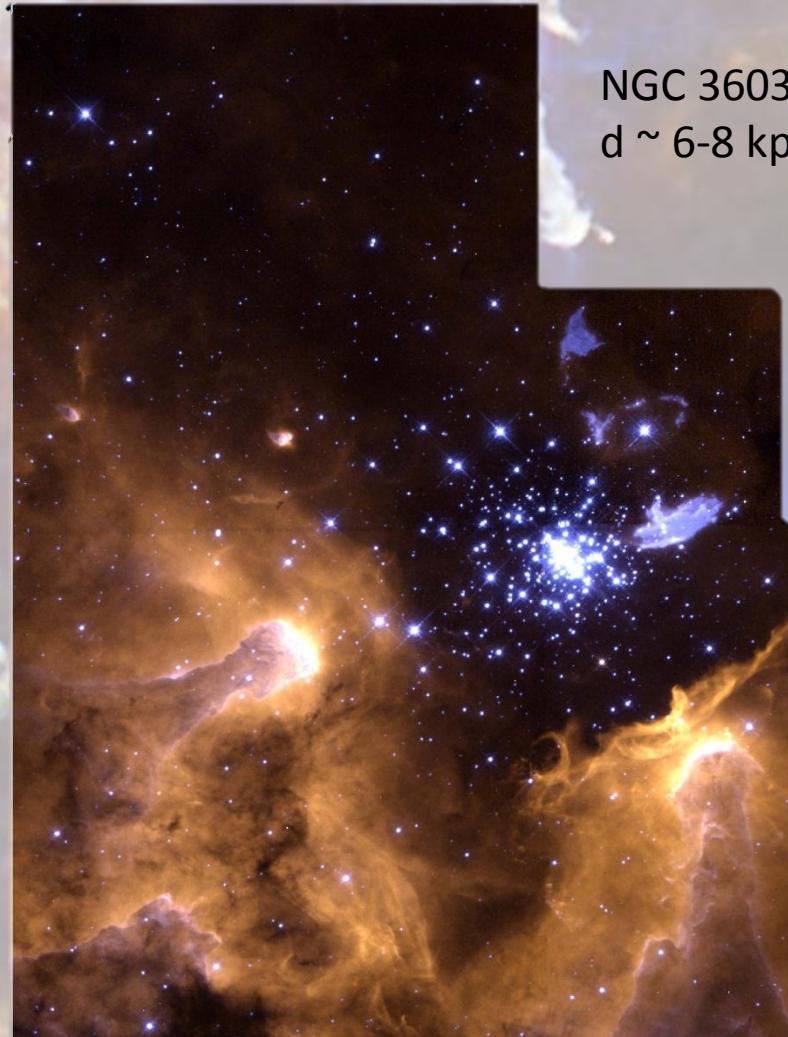
„A PDR is a region where far-ultraviolet (FUV) photons from young, massive stars dominate the physics and chemistry of the interstellar medium“

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



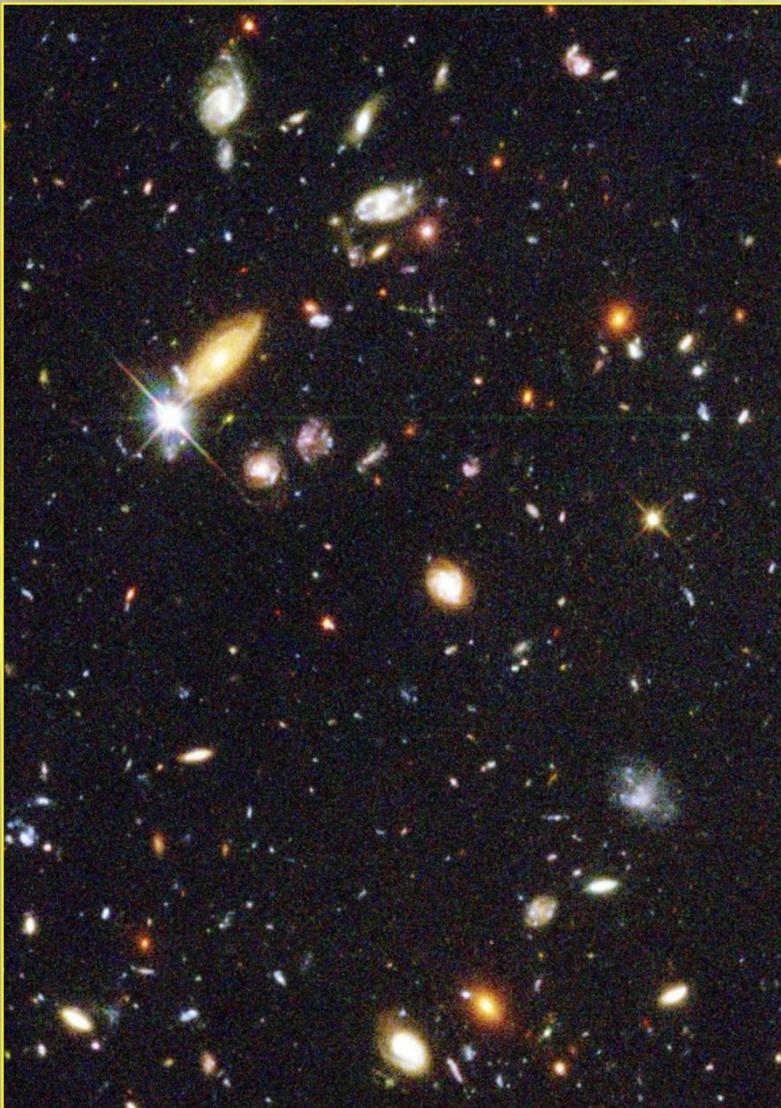
Photo-dissociation regions

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

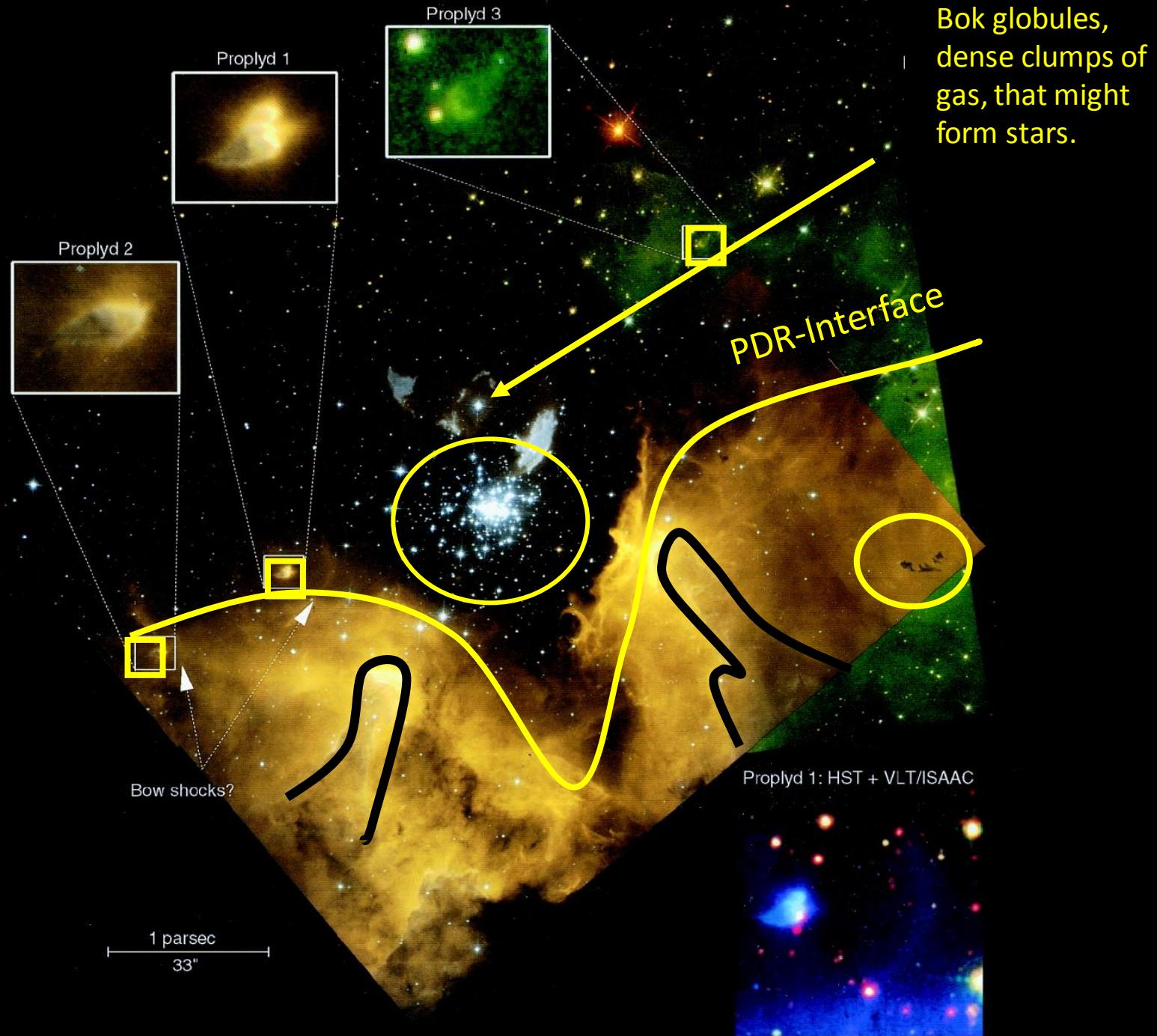


Credit: Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (Univ. Washington), You-Hua Chu (Univ. Illinois Urbana-Champaign), and [NASA](#)

Cycle of matter

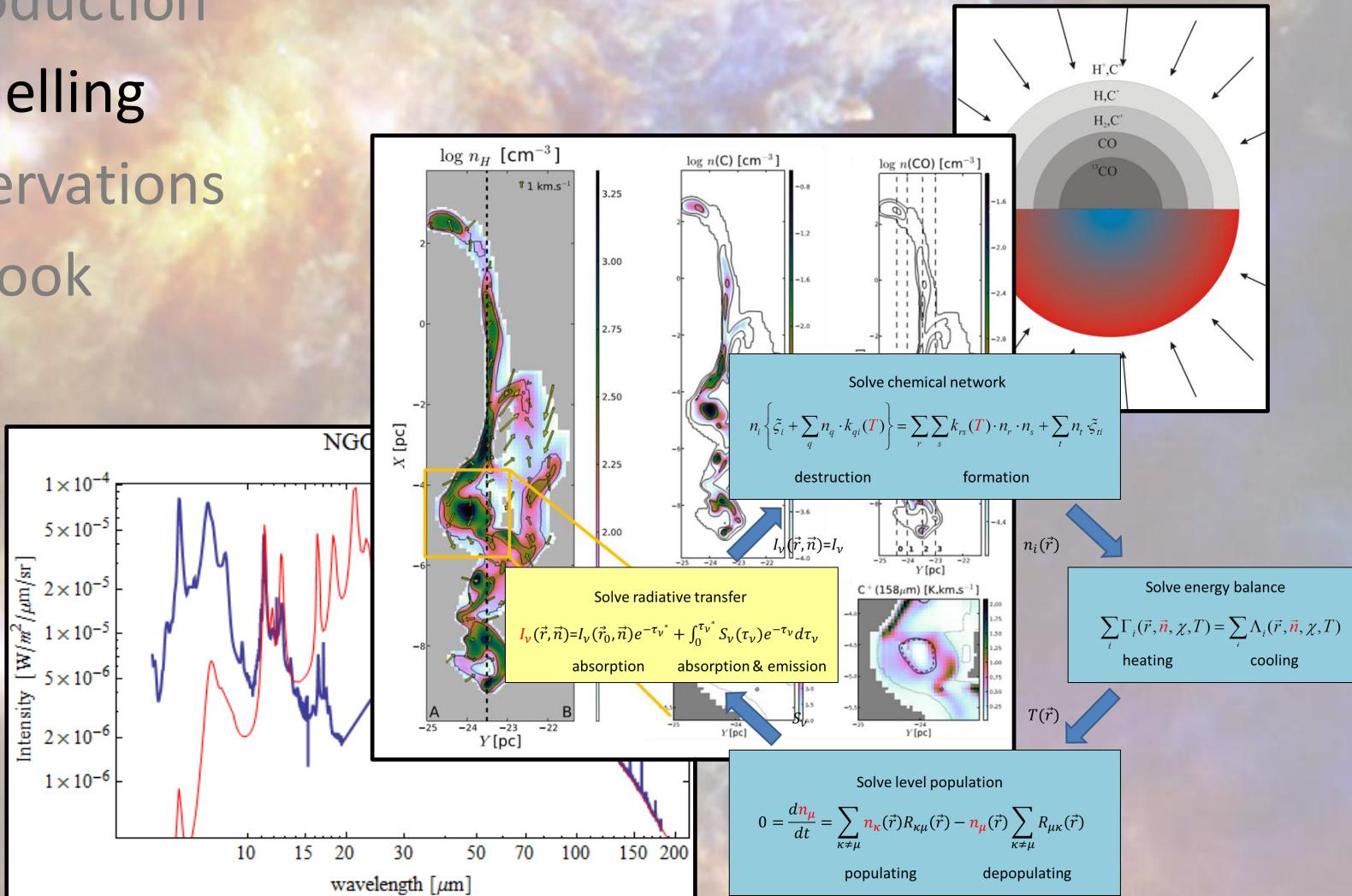


NGC 3603
distance:
6-8 kpc



Modelling

- Introduction
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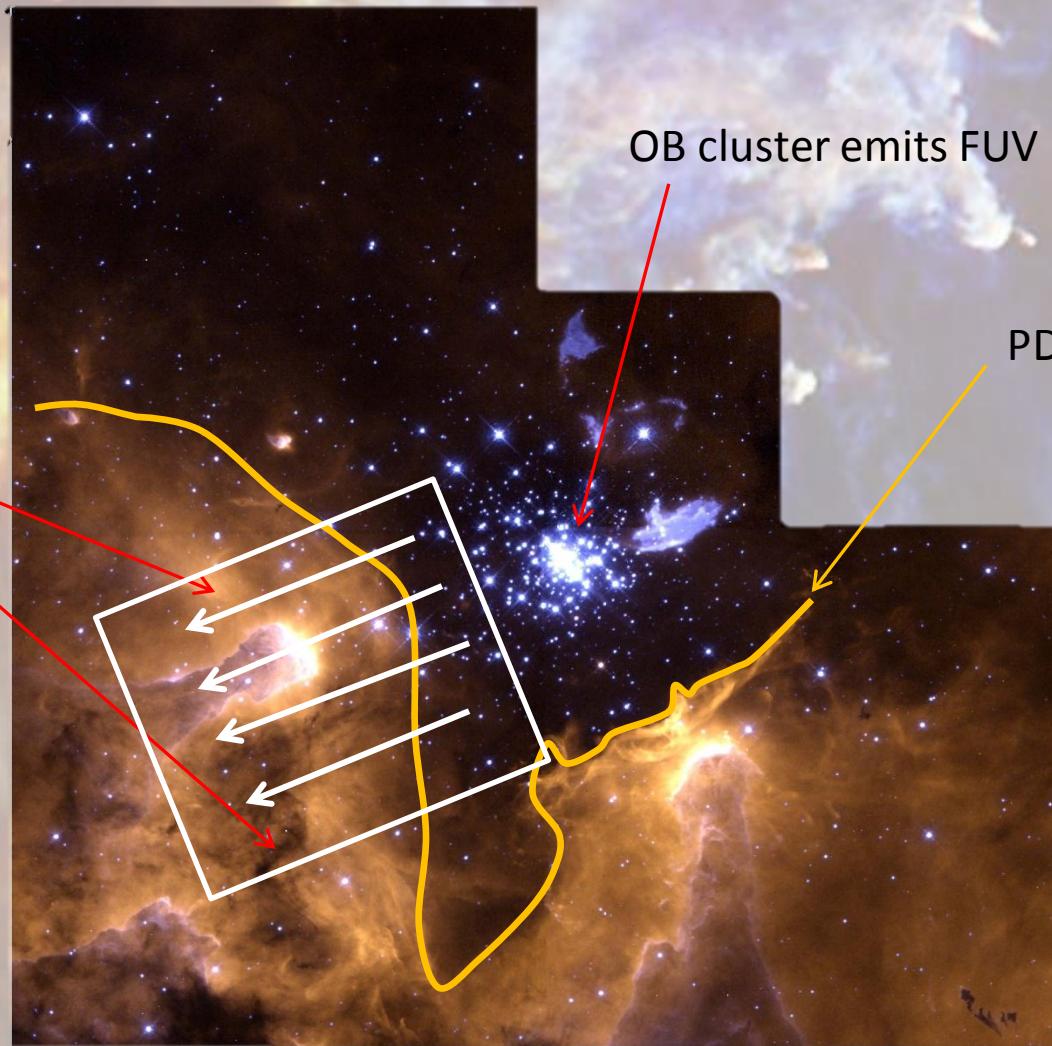


PDR models

molecular cloud
contains gas & dust

OB cluster emits FUV

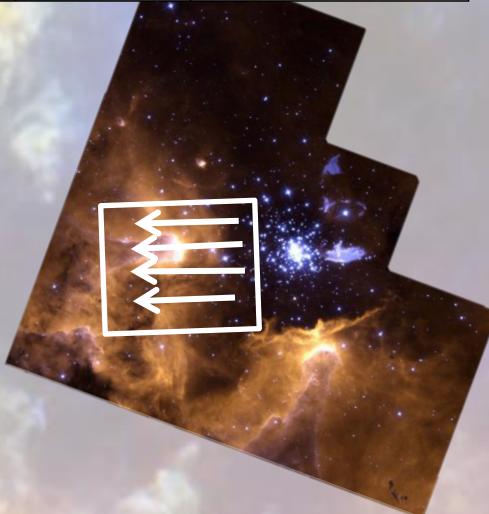
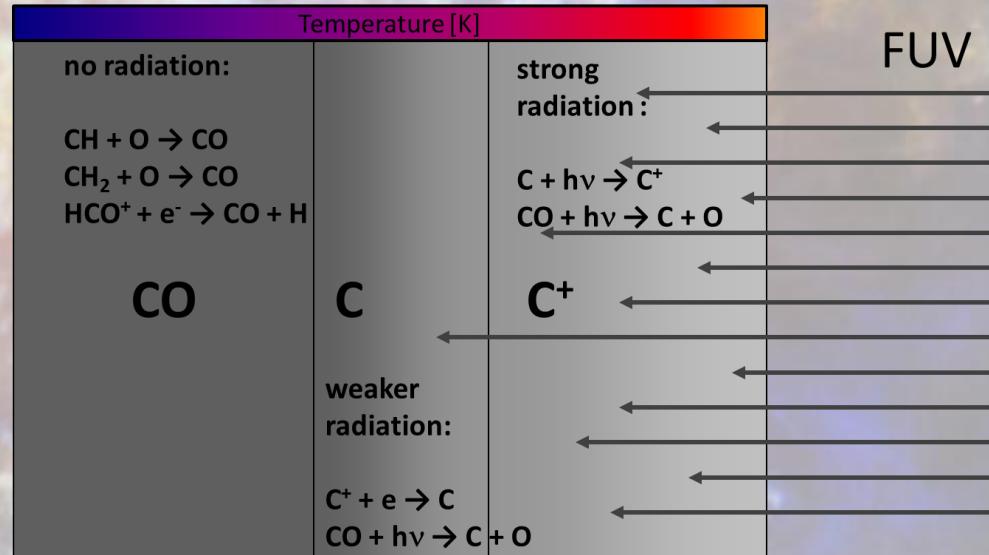
PDR interface



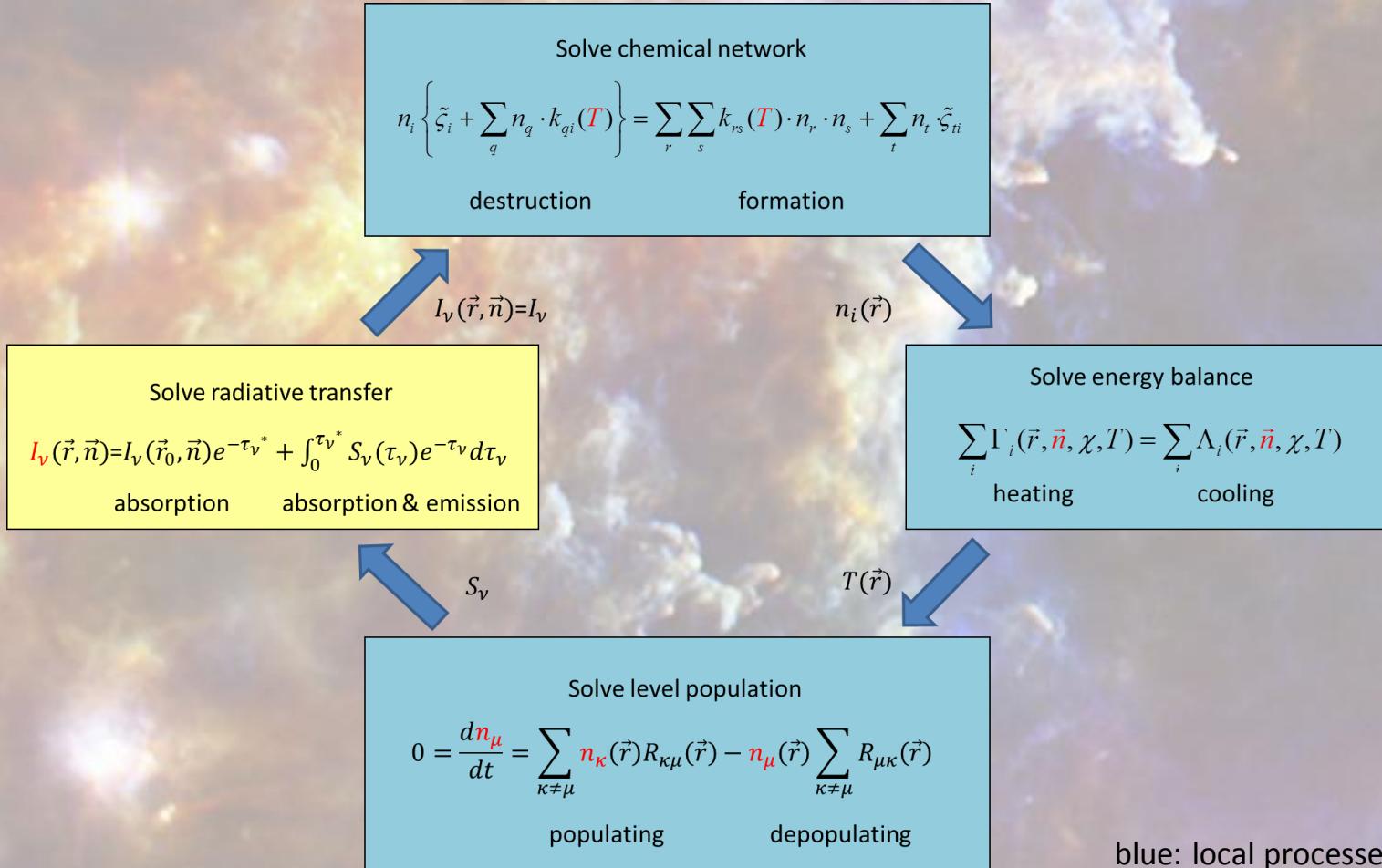
Credit: Wolfgang Brandner (JPL/IPAC), Eva K. Grebel (Univ. Washington),
You-Hua Chu (Univ. Illinois Urbana-Champaign), and [NASA](#)

PDR models

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

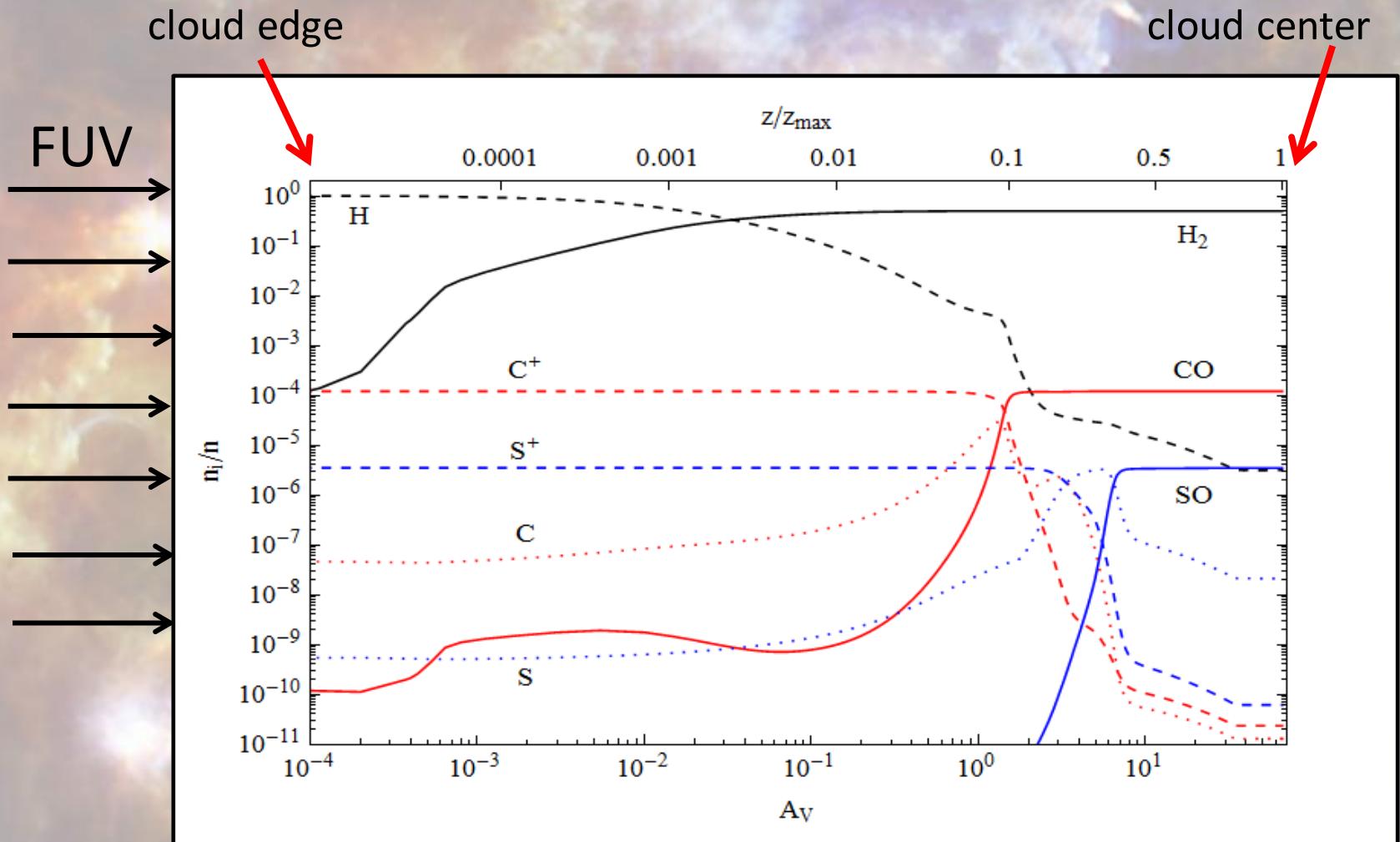


Model scheme



blue: local processes
yellow: non-local processes

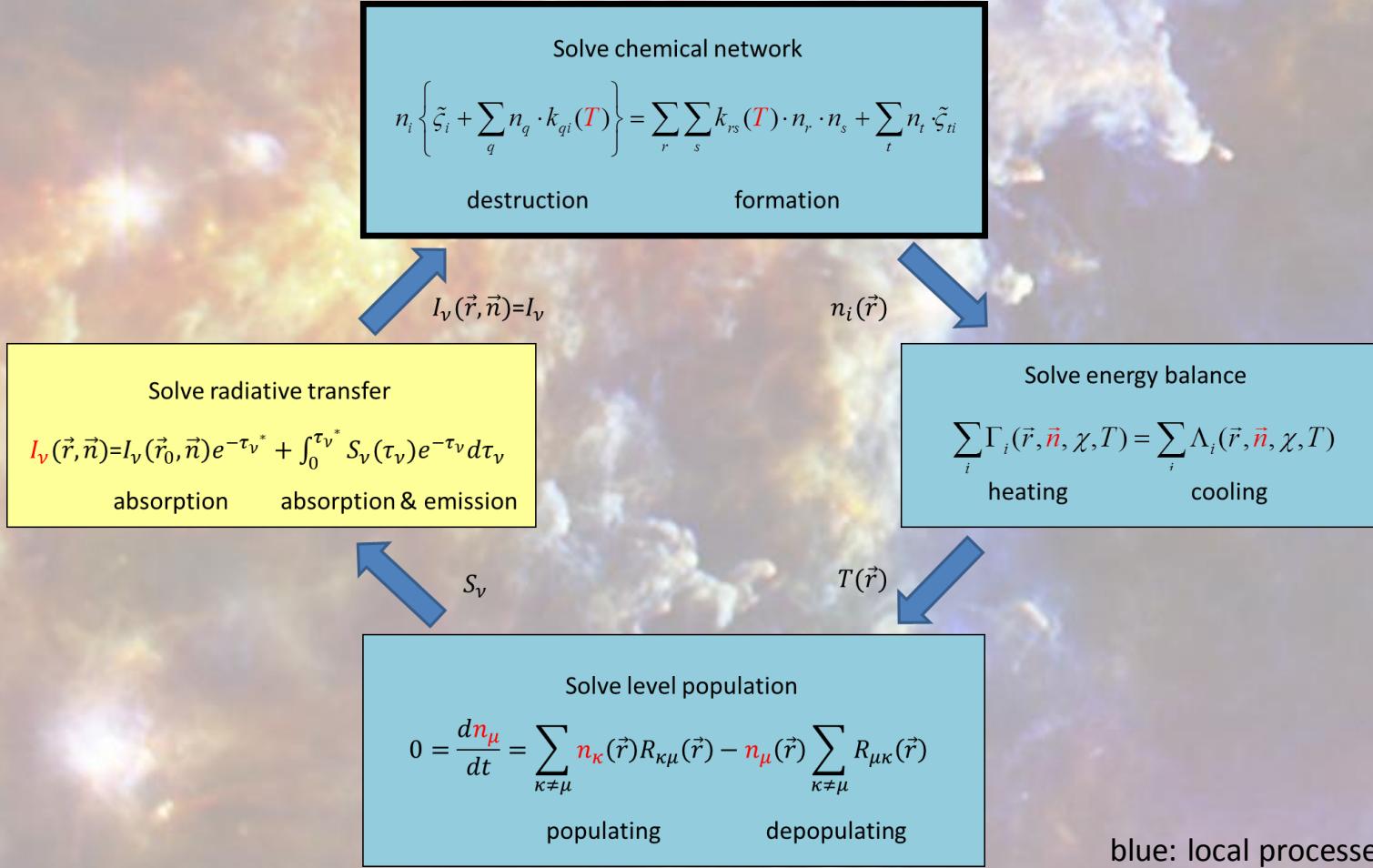
Model outcome



plot flipped, AND Log-Log scale!

A_v : visual extinction

Model chemistry

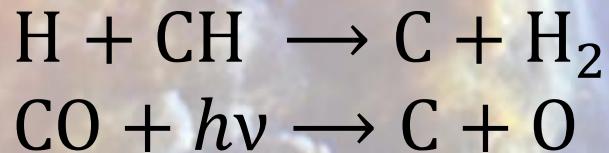


blue: local processes
yellow: non-local processes

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:

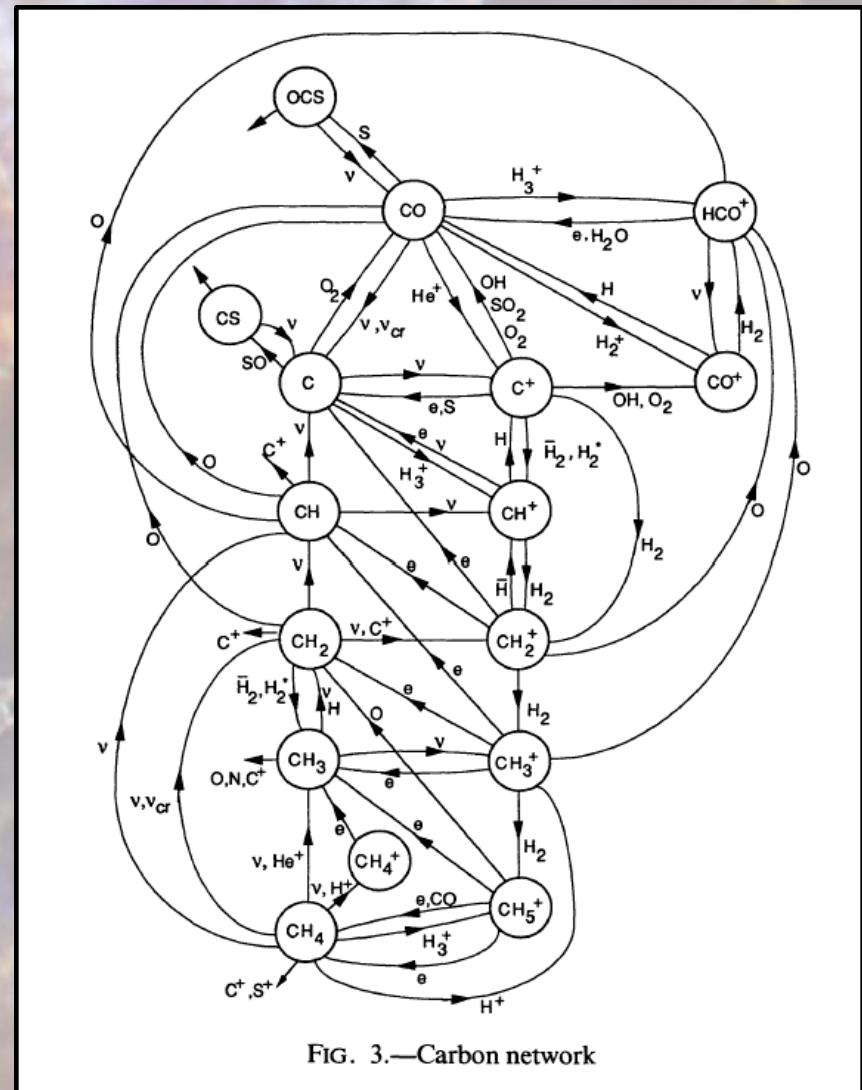
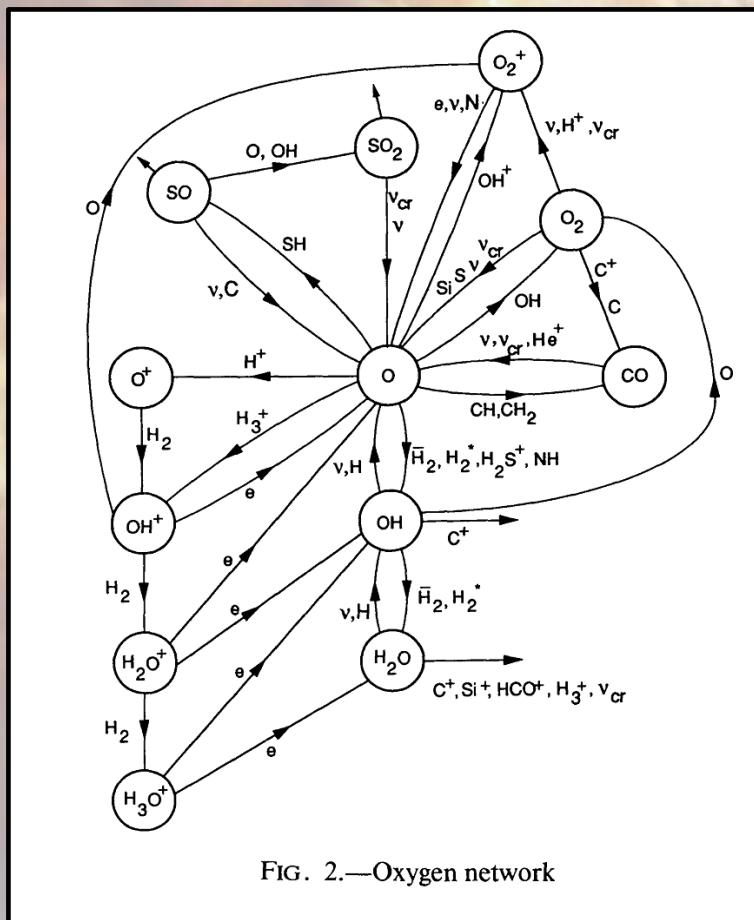


- Described by reaction rates

$$R_{\text{C}} = R_{\text{H}_2} = k \times n_{\text{H}} \times n_{\text{CH}}$$

$$R_{\text{C}} = R_{\text{O}} = \zeta \times n_{\text{CO}}$$

Chemical networks

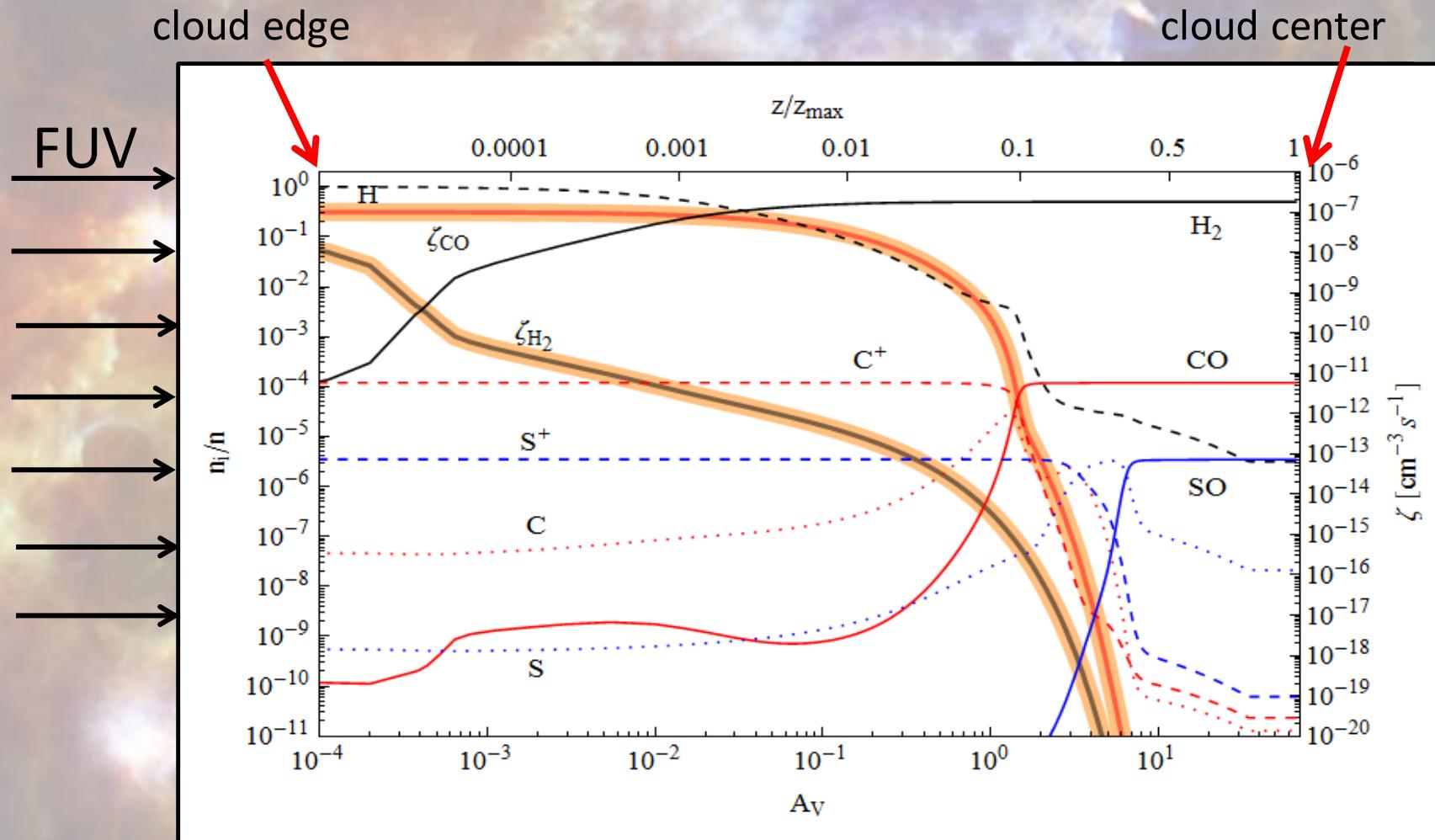


Model chemistry

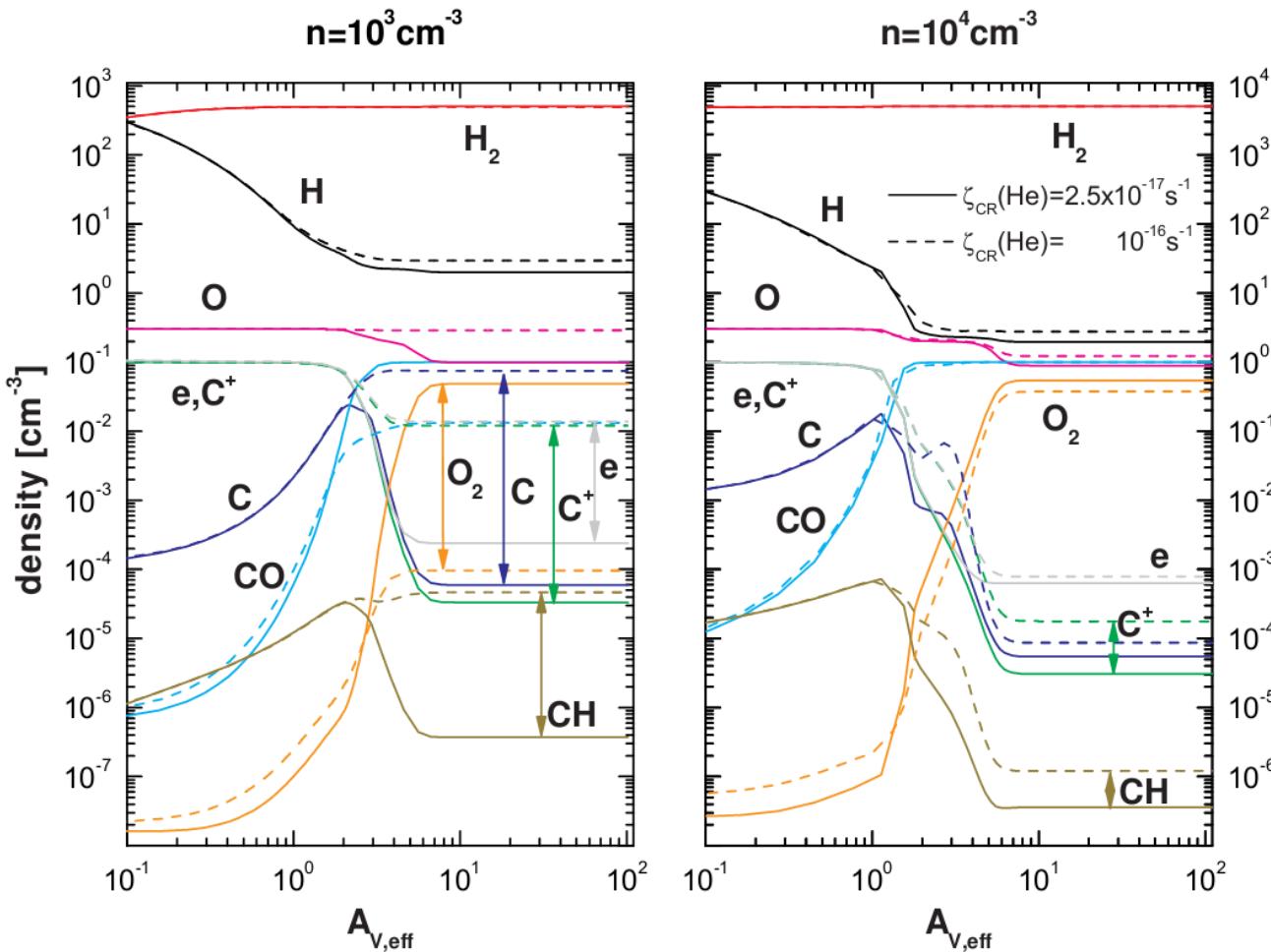
$$\frac{dn_i}{dt} = n_i \left\{ \tilde{\zeta}_i + \sum_q n_q k_{qi} \right\} - \sum_r \sum_s k_{rs} n_r n_s + \sum_t n_t \tilde{\zeta}_{ti}$$

- density n_i (species $i=1, \dots, N$),
hundreds of species, thousands of reactions
 - reaction rate coefficients:
 $k_{xy}(T_{gas}=5-5000\text{ K}, T_{dust}=5-500\text{ J}), \zeta_z(J)$
 - 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 H₂ and CO



Model non-linearity



Non-linear system:

Slight input changes may affect the outcome significantly

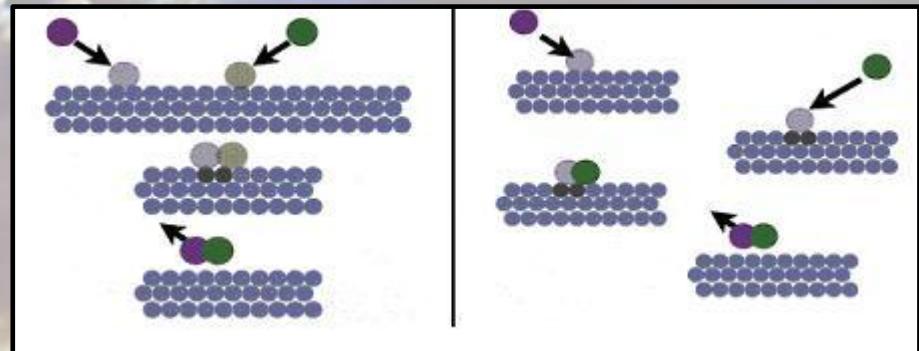
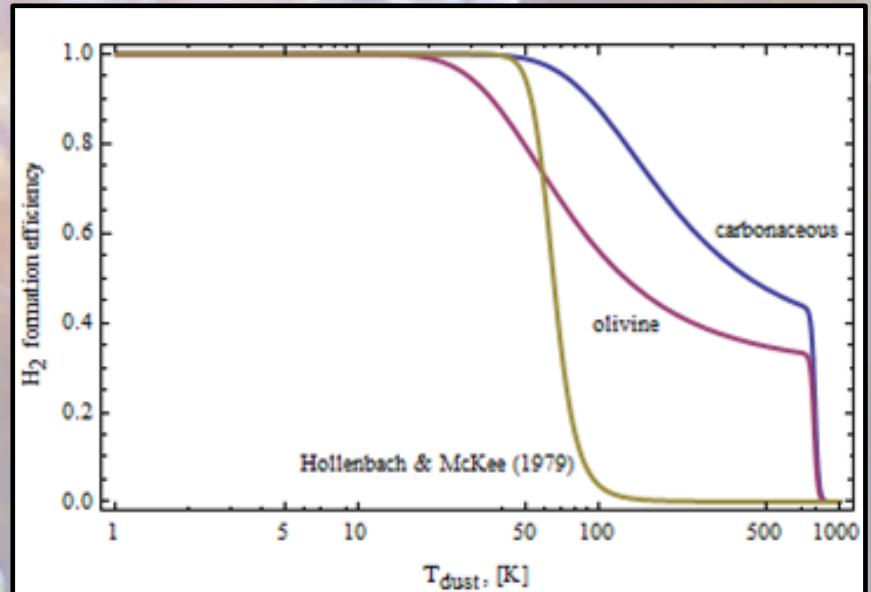
Changing only one process:

$\zeta_{\text{CR}}(\text{He})$ 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



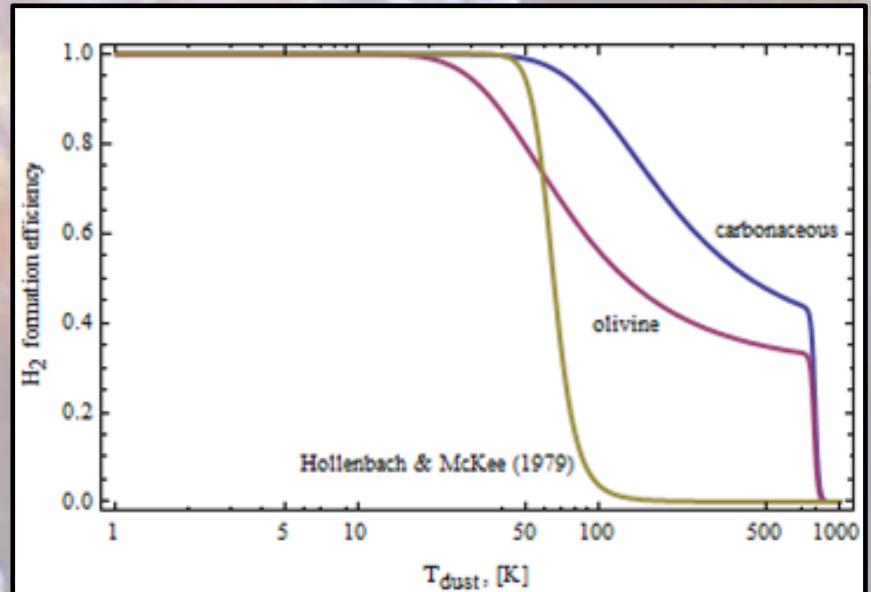
Langmuir-Hinshelwood

Elay-Rideal

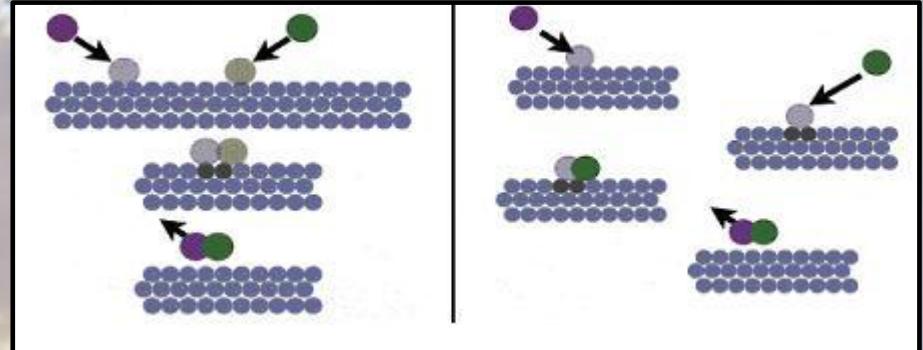
H₂ formation

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

Röllig et al. 2012, A&A, in press



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



Langmuir-Hinshelwood

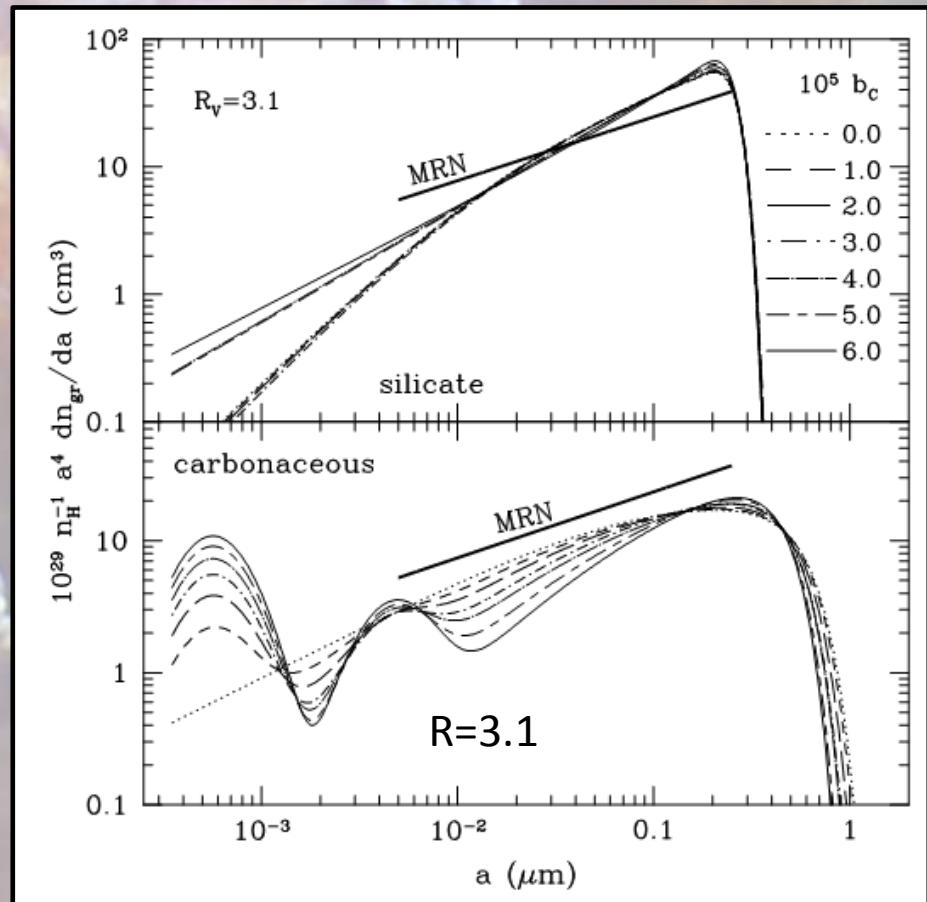
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Weingartner & Draine 2001, ApJ, 548

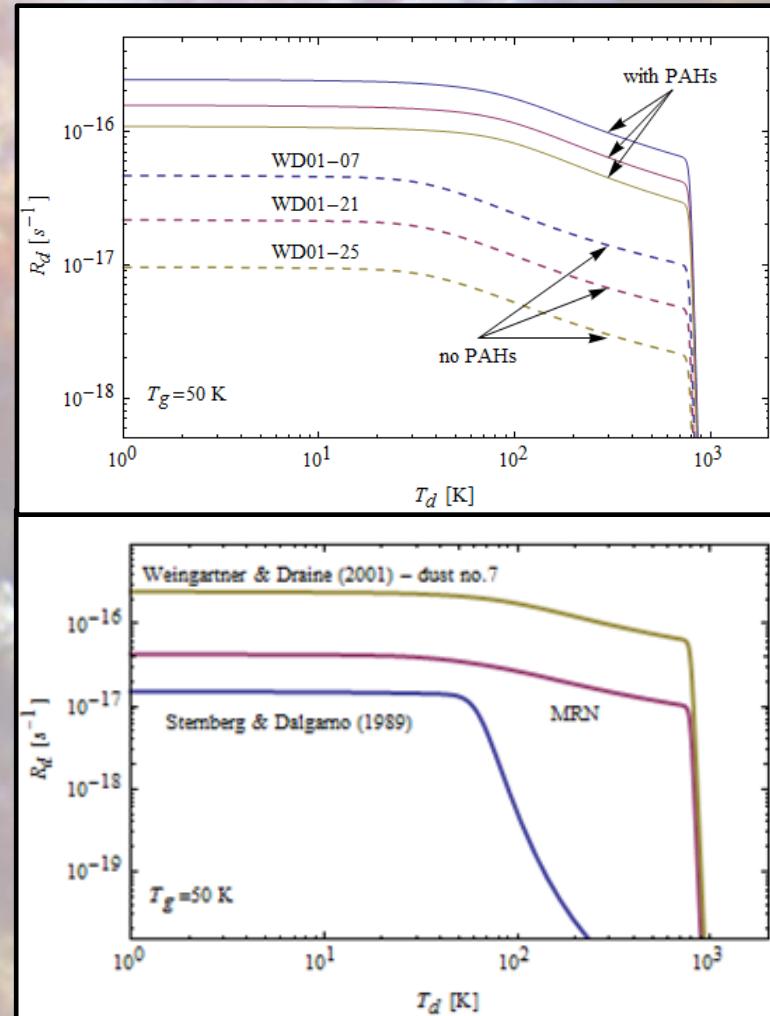


H₂ formation

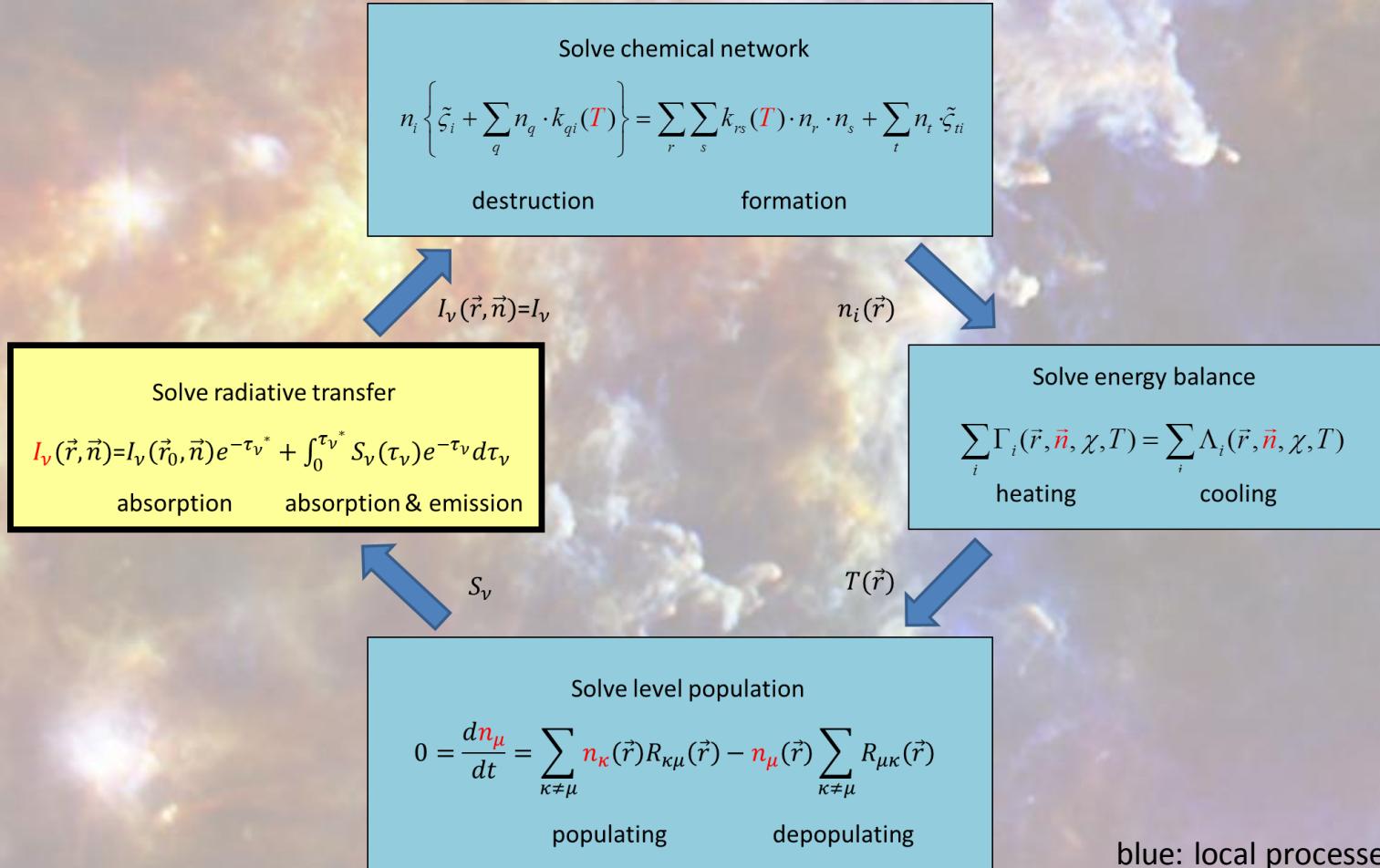
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- depends on grain material

Real properties of interstellar dust grains are unknown !

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



Radiative Transfer



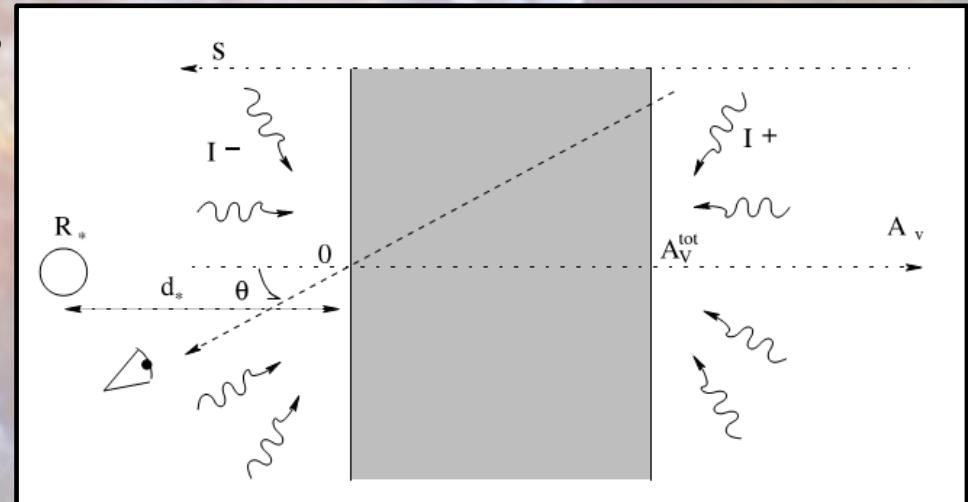
blue: local processes
yellow: non-local processes

Radiative Transfer

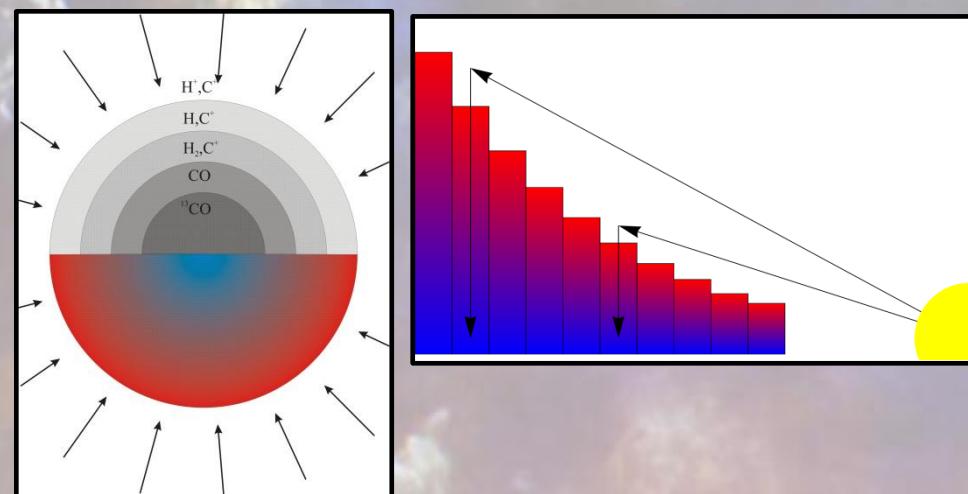
- Radiative transfer describes the propagation of photons through a medium along a line of sight.
 - RT accounts for absorption and emission processes.
 - RT couples physical & chemical conditions of different volume elements along line of sights
- non-local problem
- model geometry becomes important

Model geometry

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

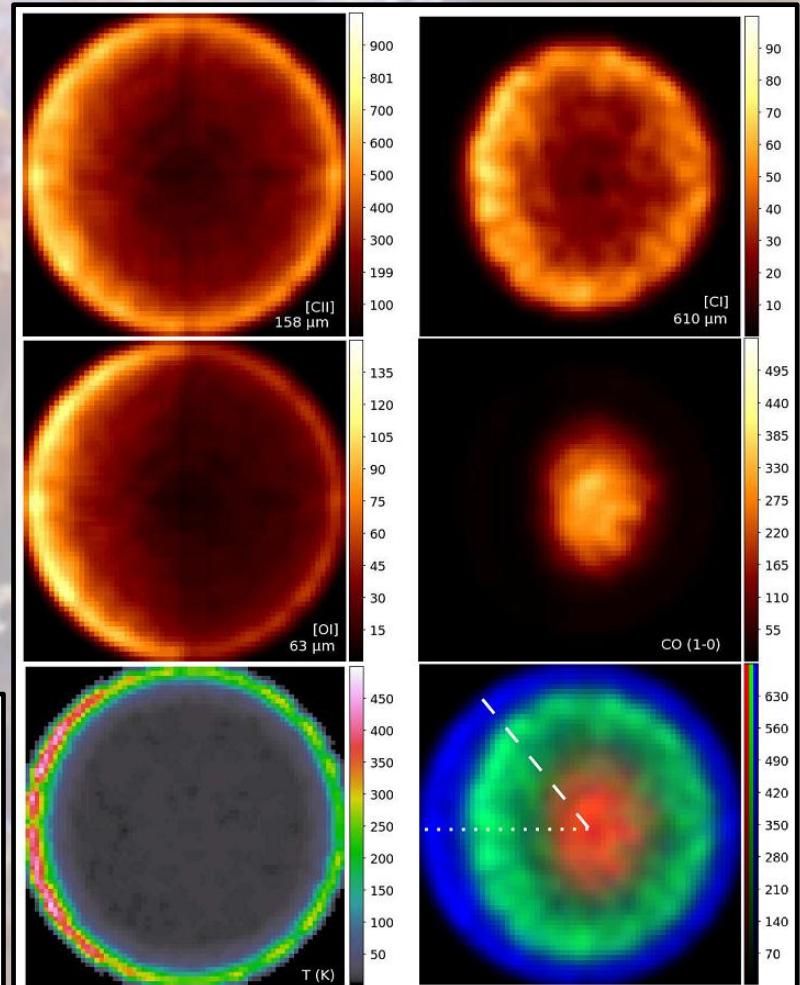
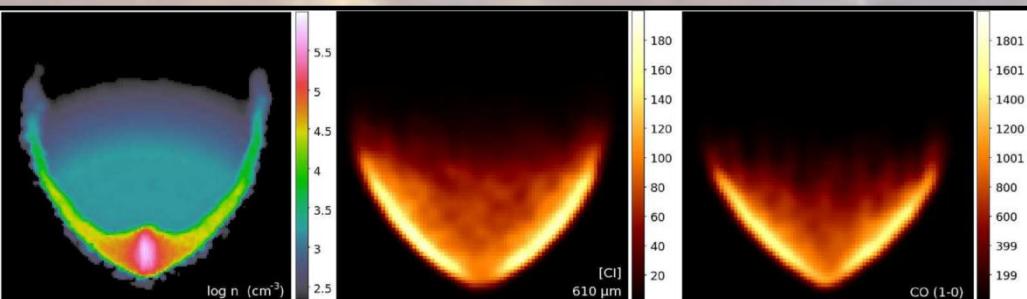


Le Petit et al. 2006, ApJSS 164



Model geometry

- Numerous configurations
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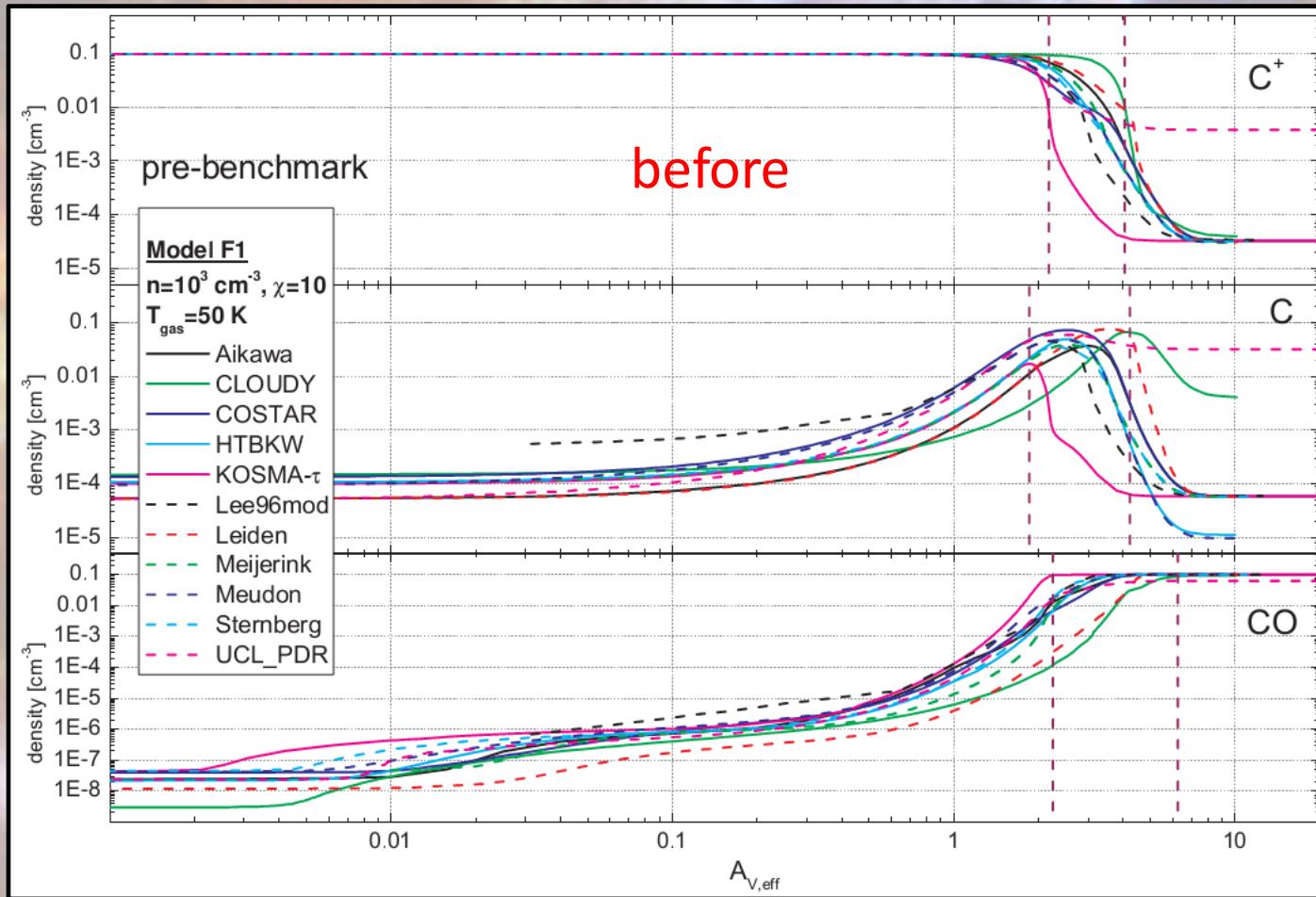


PDR model benchmark

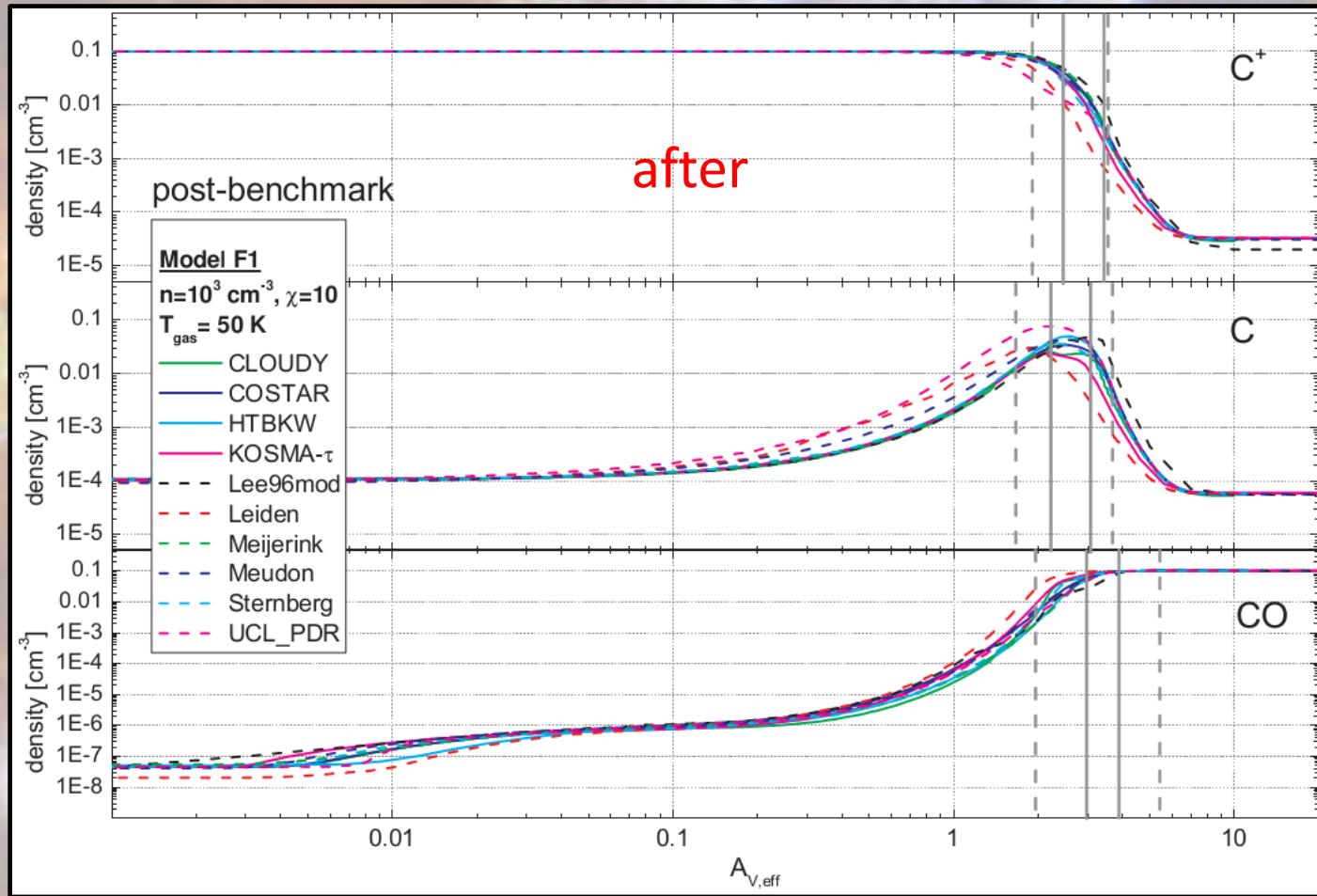
- Large international effort to compare model results from 10 different numerical PDR codes.
- All codes restricted to a minimum common functionality.
- 8 (very) simplified toy-models were calculated
- first and only database of reference PDR model results

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

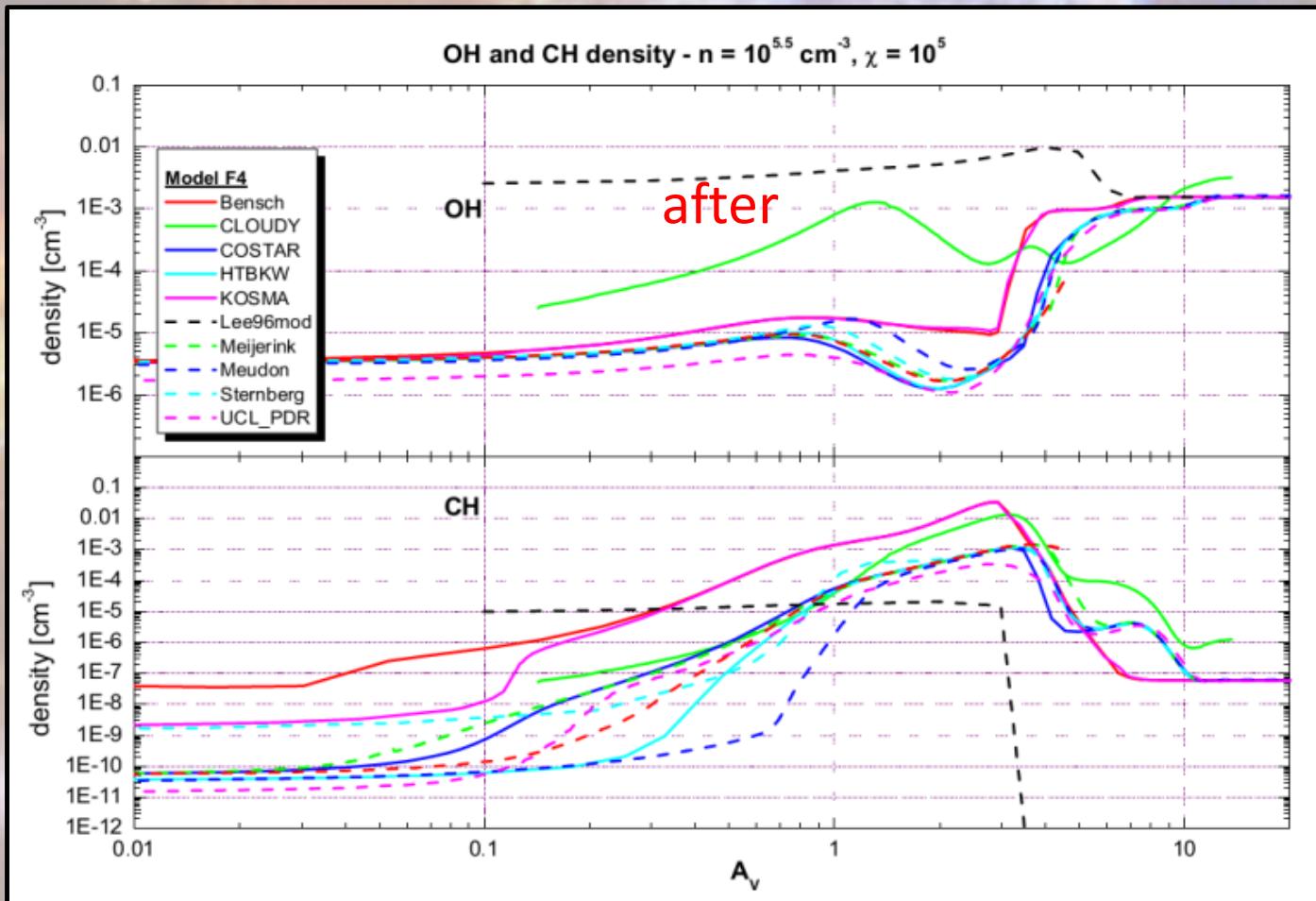
PDR model benchmark



PDR model benchmark



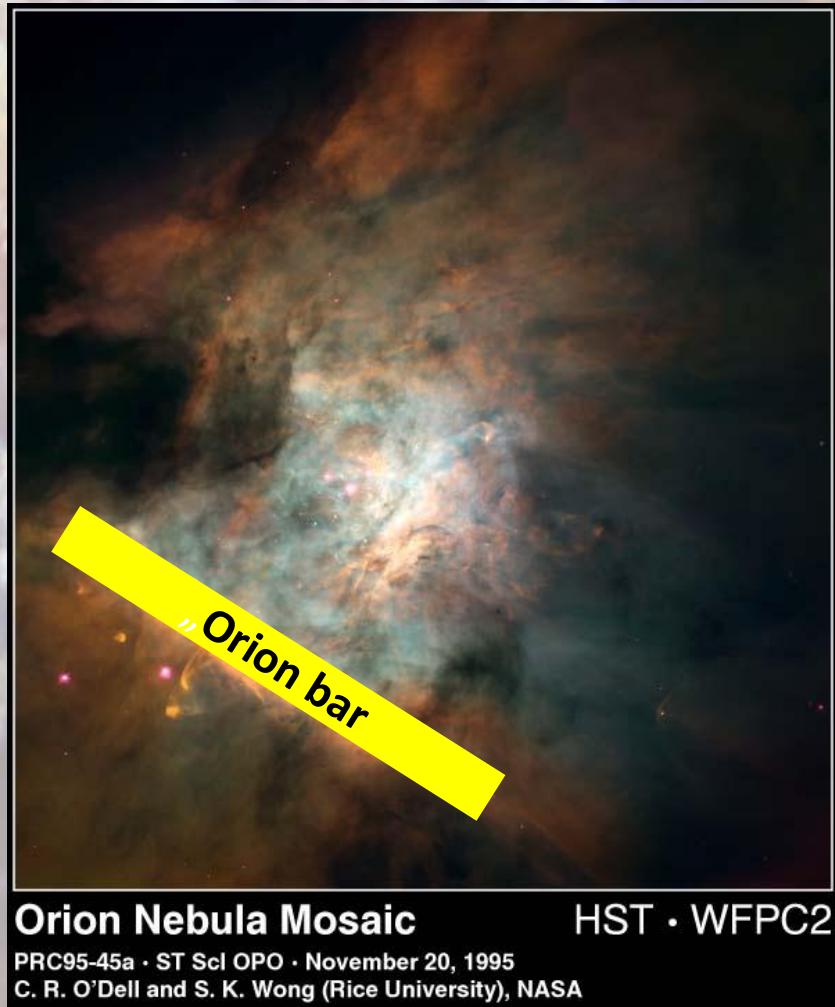
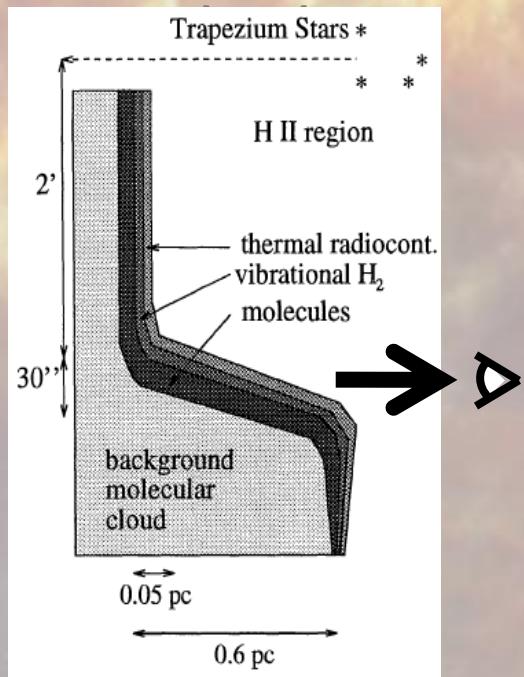
PDR model benchmark



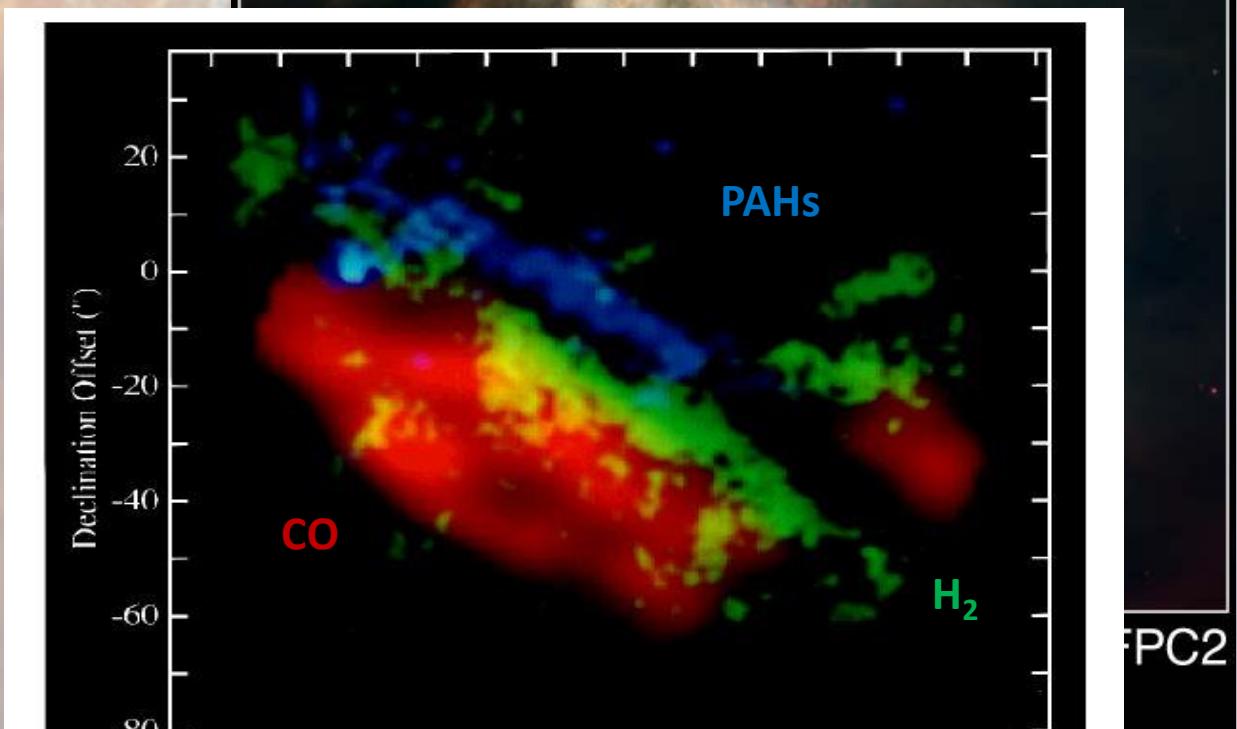
Light hydride chemistry largely unknown, but a lot of progress since then.

Orion bar

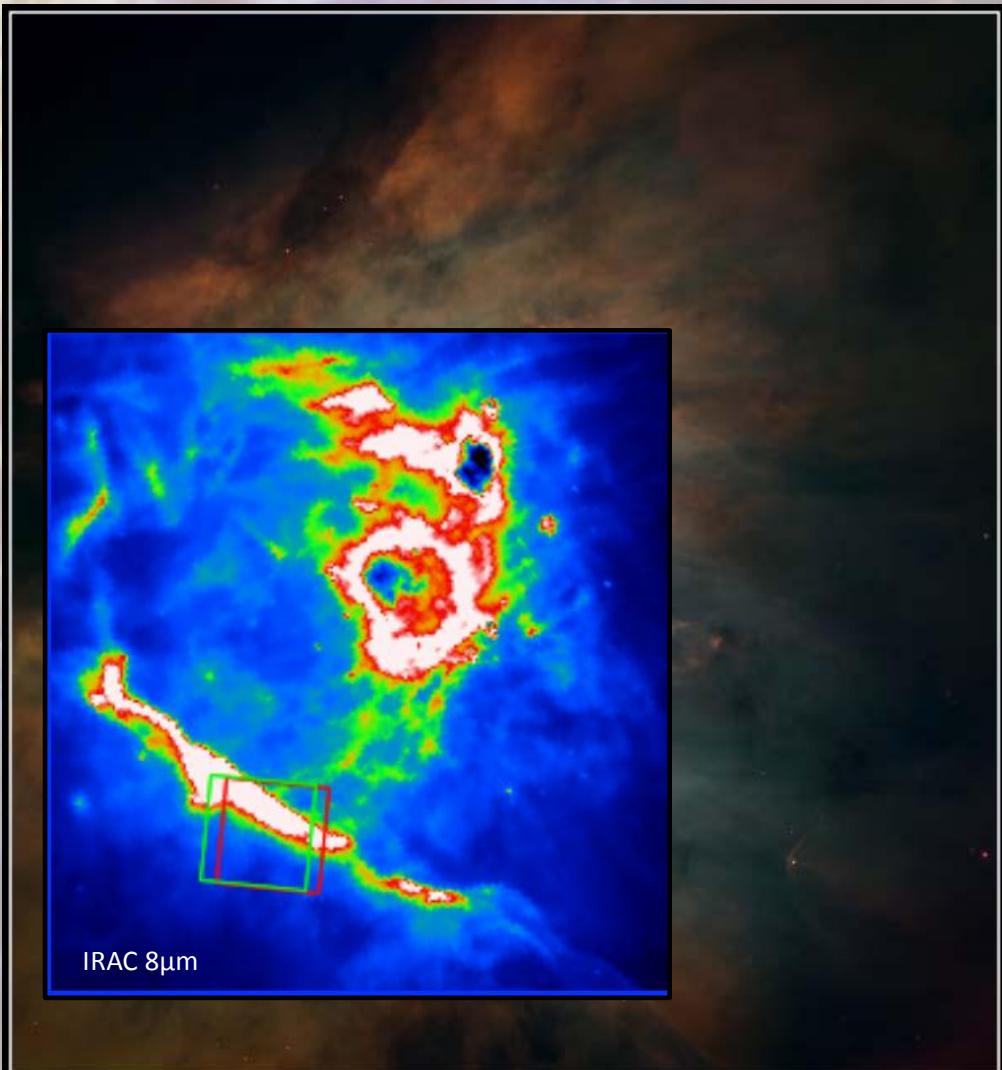
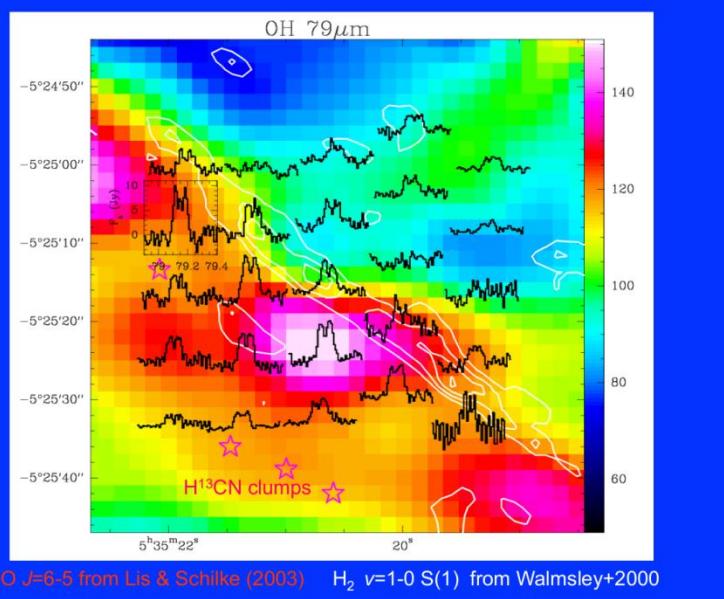
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Orion bar PDR



Orion bar



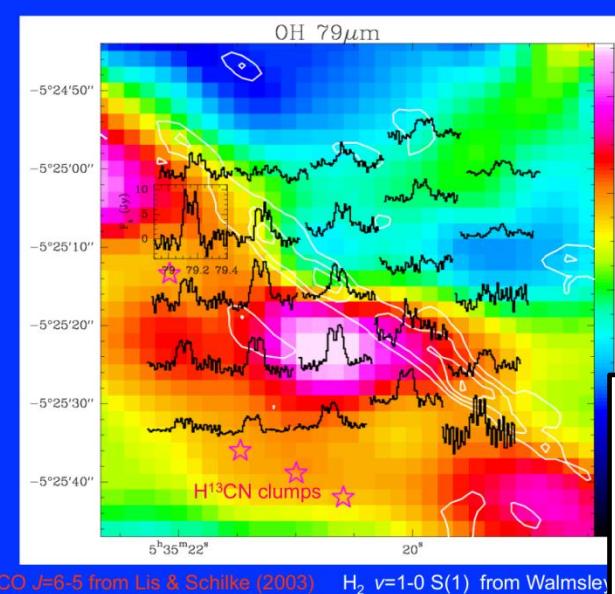
Orion Nebula Mosaic

PRC95-45a · ST Scl OPO · November 20, 1995

C. R. O'Dell and S. K. Wong (Rice University), NASA

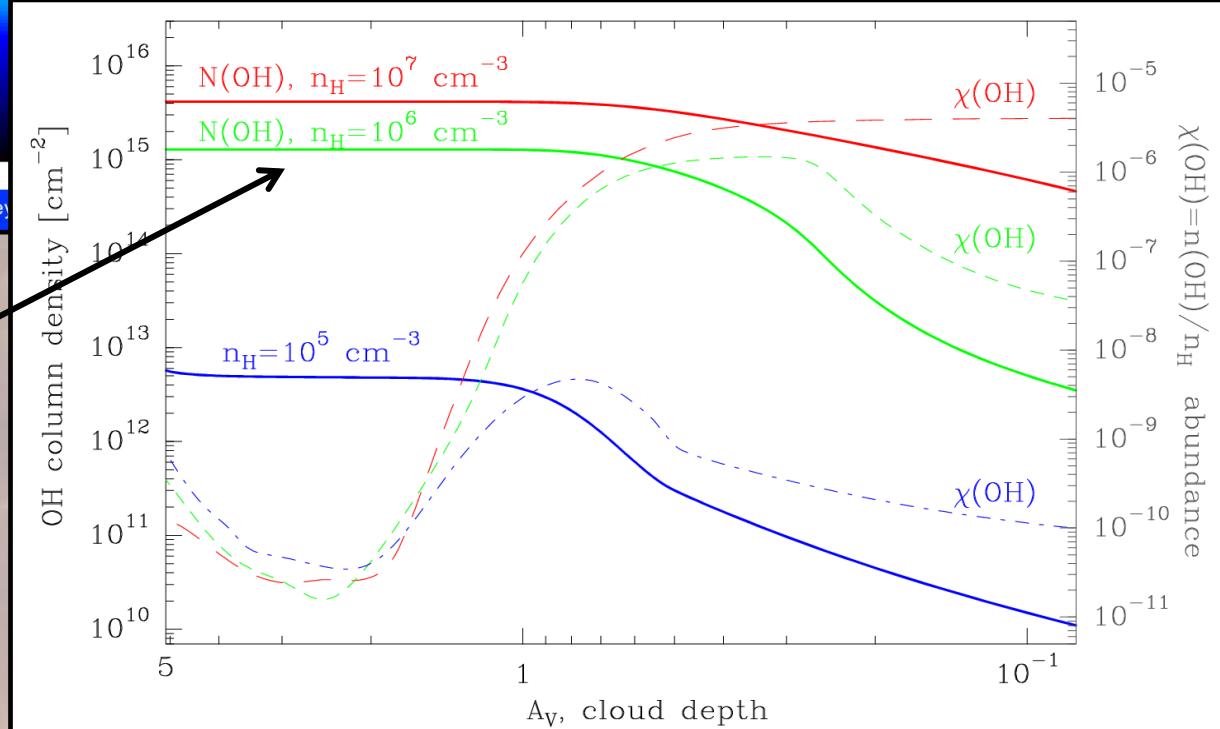
HST · WFPC2

Orion bar: OH measurements



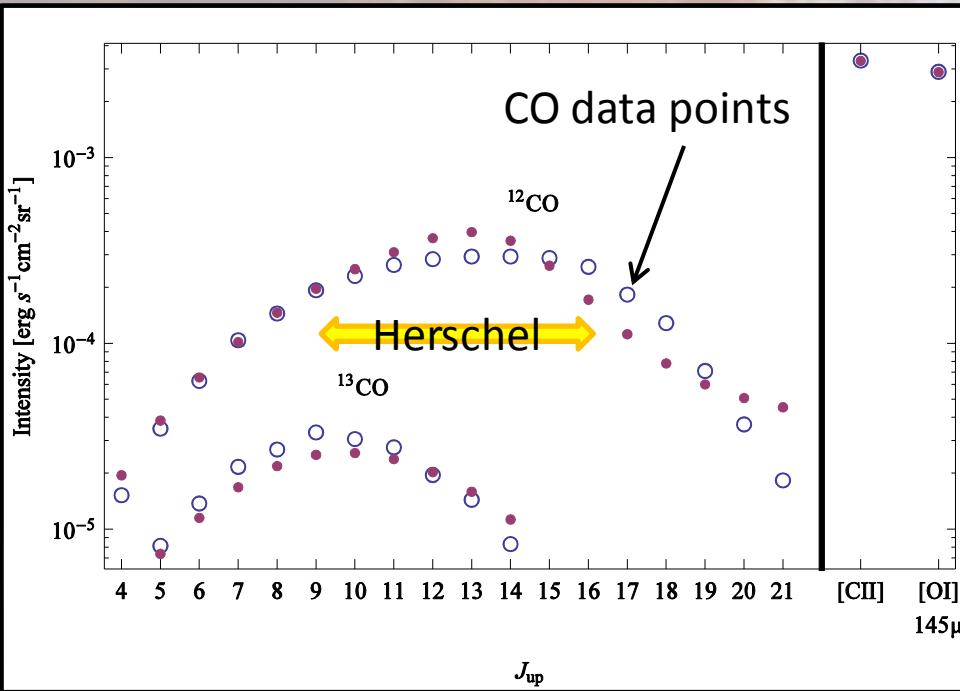
very high gas density required to reproduce the observed amount of OH in PDR models

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



Orion bar model results

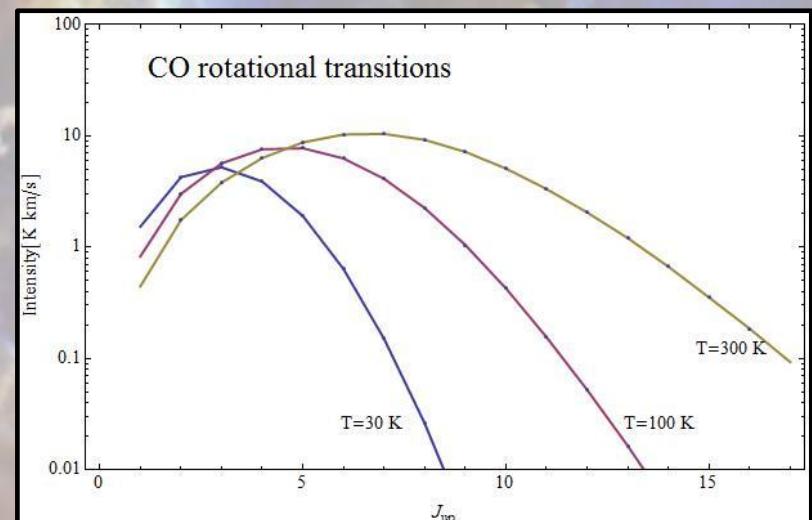
For the first time full J-ladder up to J=21 available.



Spectral line energy distribution SLED

Population of rotational quantum states of CO depends on the local excitation conditions ($T, n_{\text{CO}}, \tau, \dots$).

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

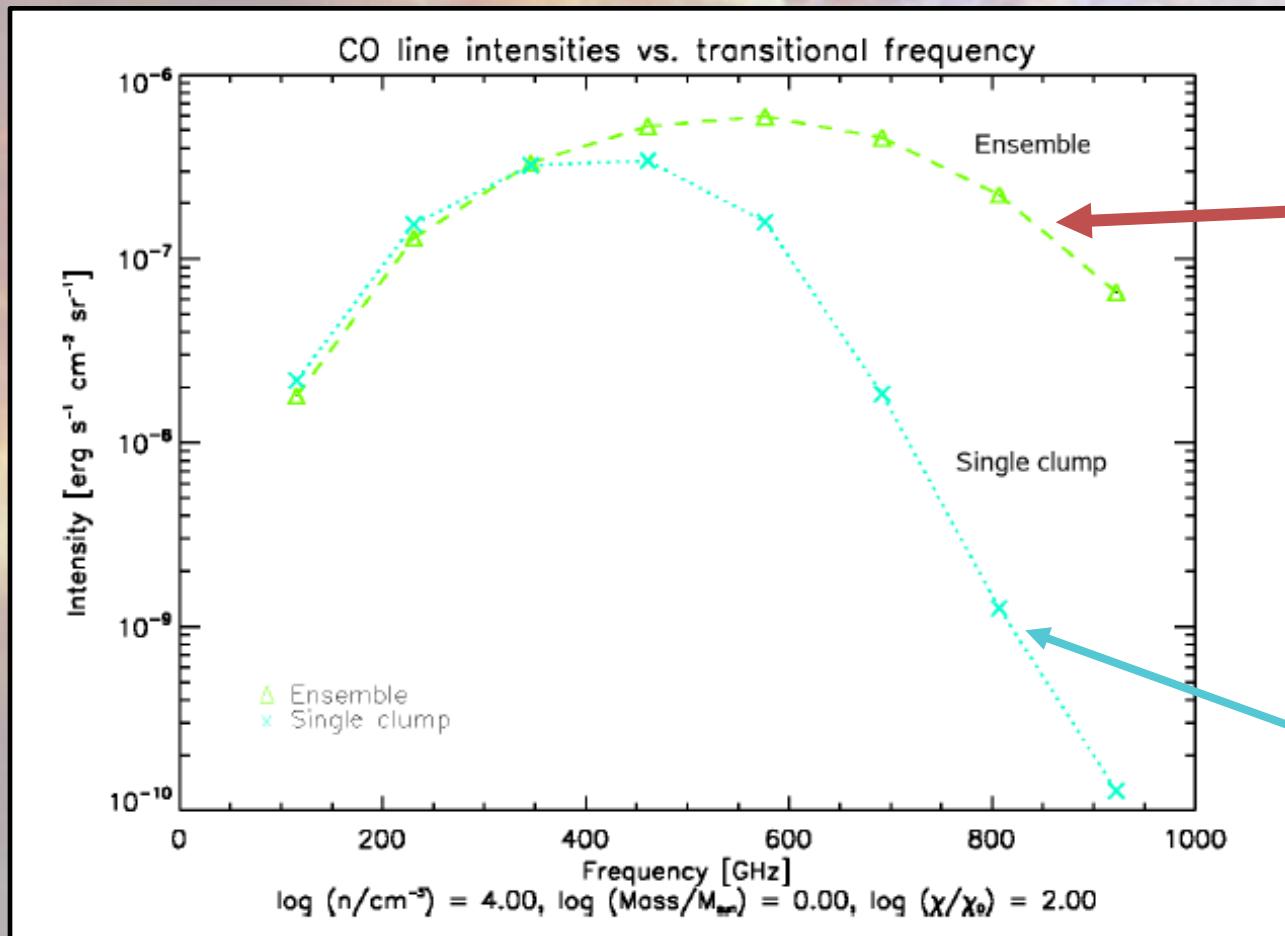


CO: linear rotator

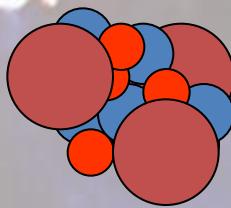
→ allowed transitions $\Delta J = \pm 1$

escape prob. simulation: homogeneous slab of gas

Clumpy Molecular Clouds

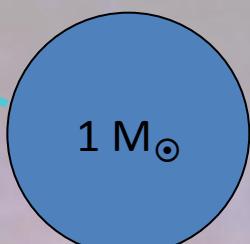


fractal structure
with larger surface to
volume ratio



$$\sum M_i = 1 M_{\odot}$$

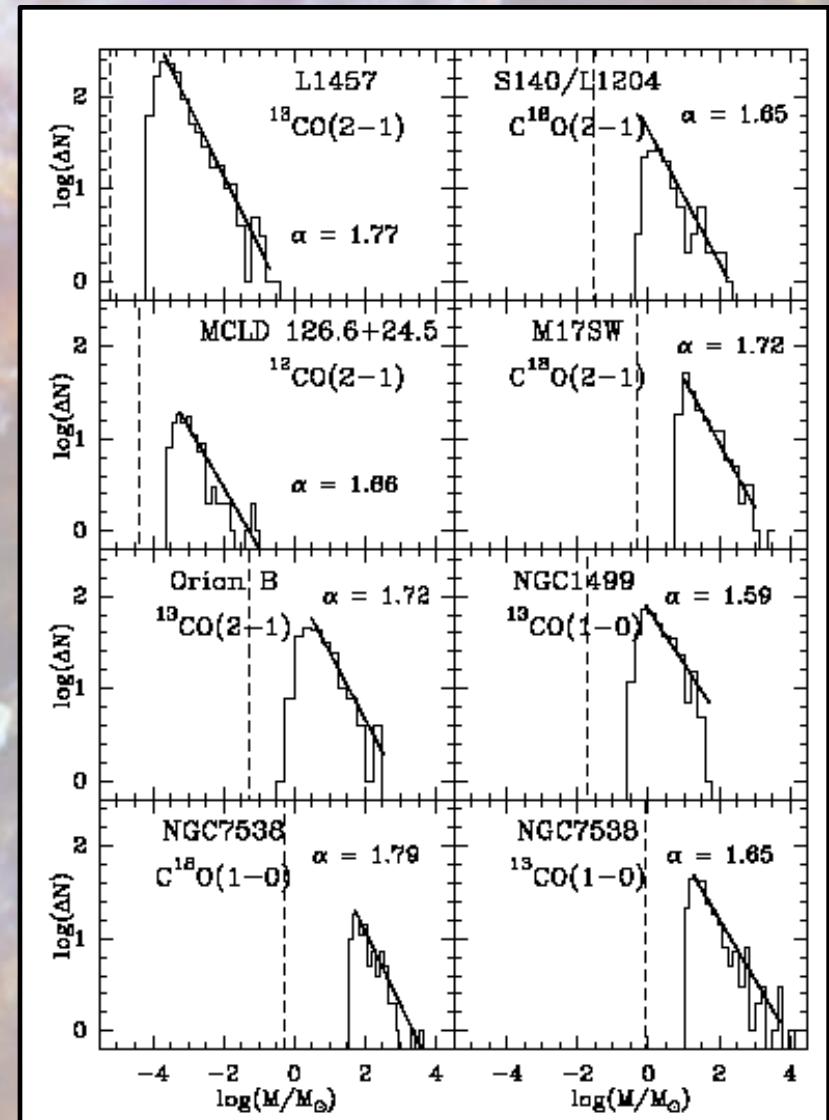
monolithic clump



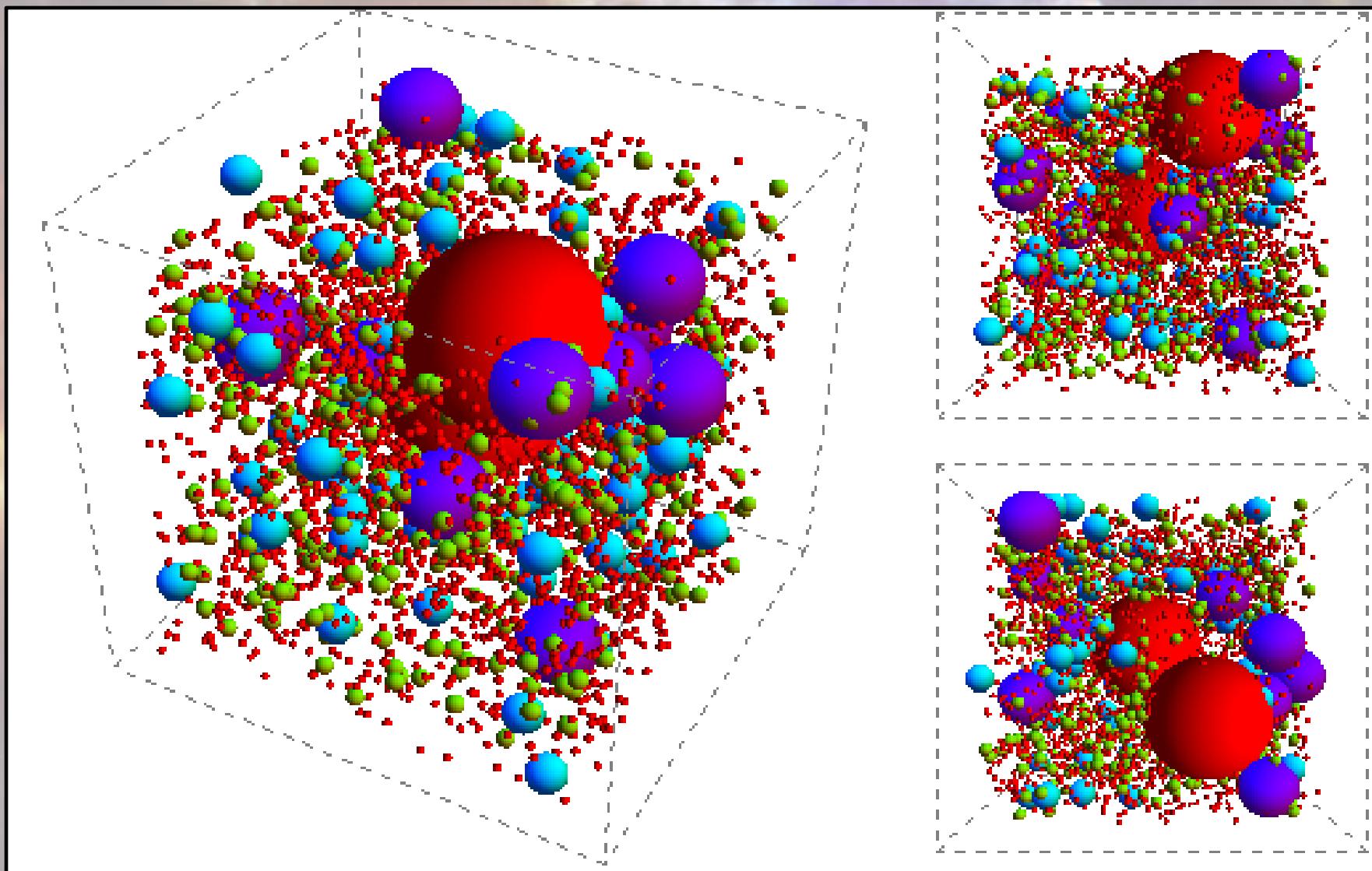
Clumpy Molecular Clouds

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

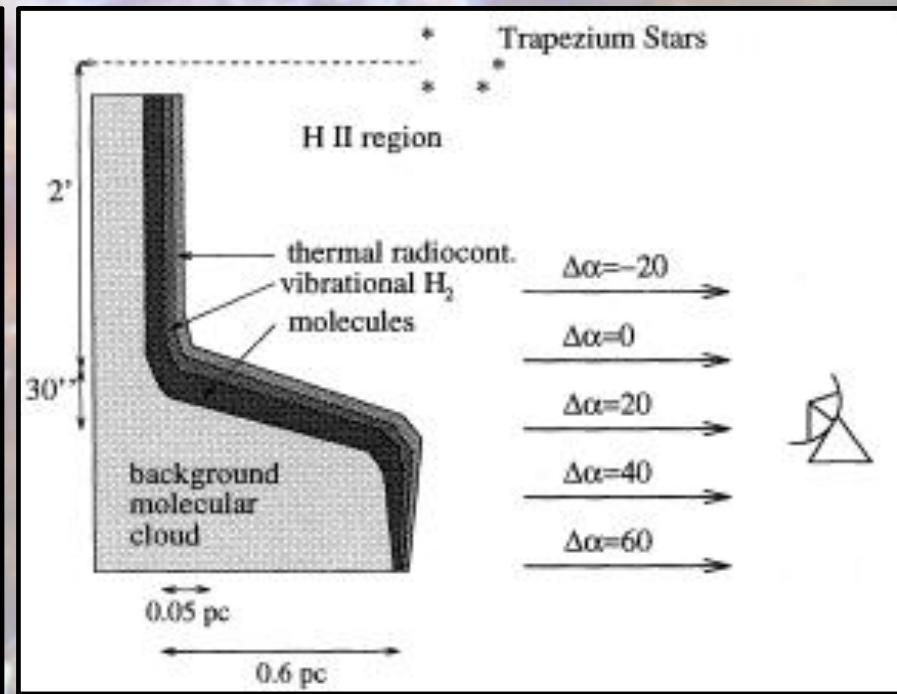
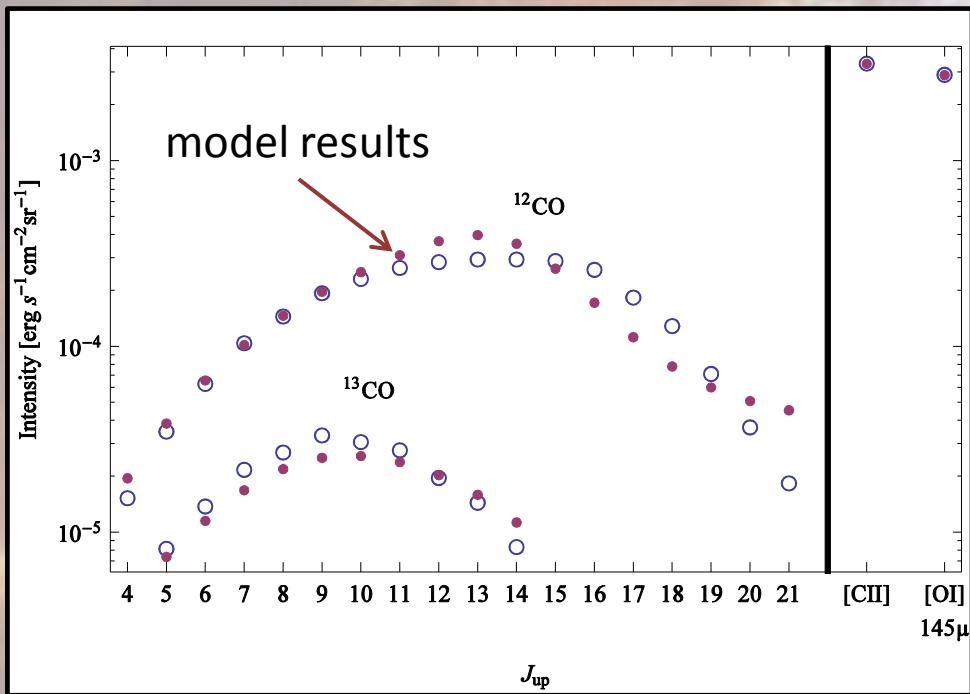
(Kramer et al. 1998)



Clumpy clouds



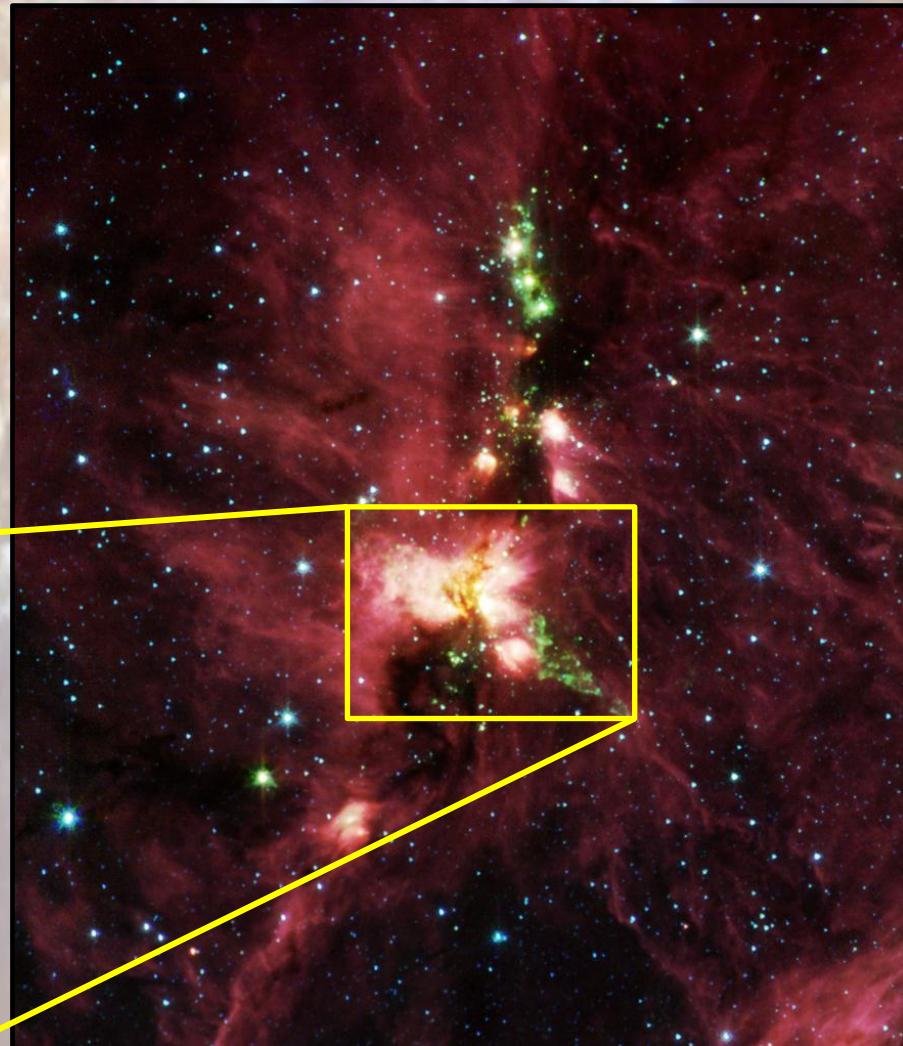
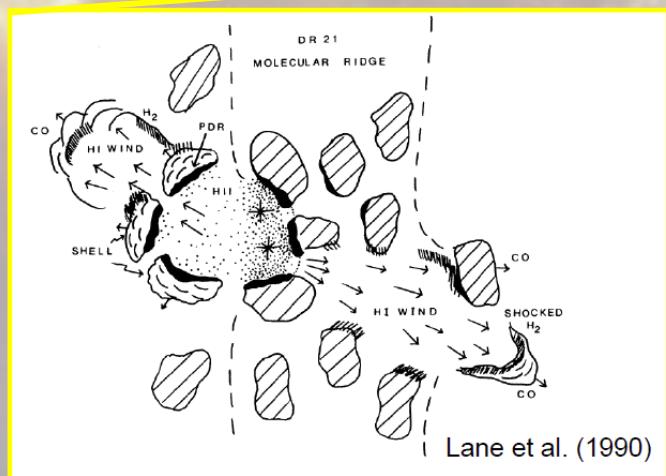
Orion bar model results



- ^{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 $6.5 \times 10^{22} \text{ cm}^{-2}$ and a $(9.6'')^2$ pixel implies a mass of $0.2 M_\odot$ \rightarrow model mass $\sim 0.3 M_\odot$
- reasonable model FUV strength!

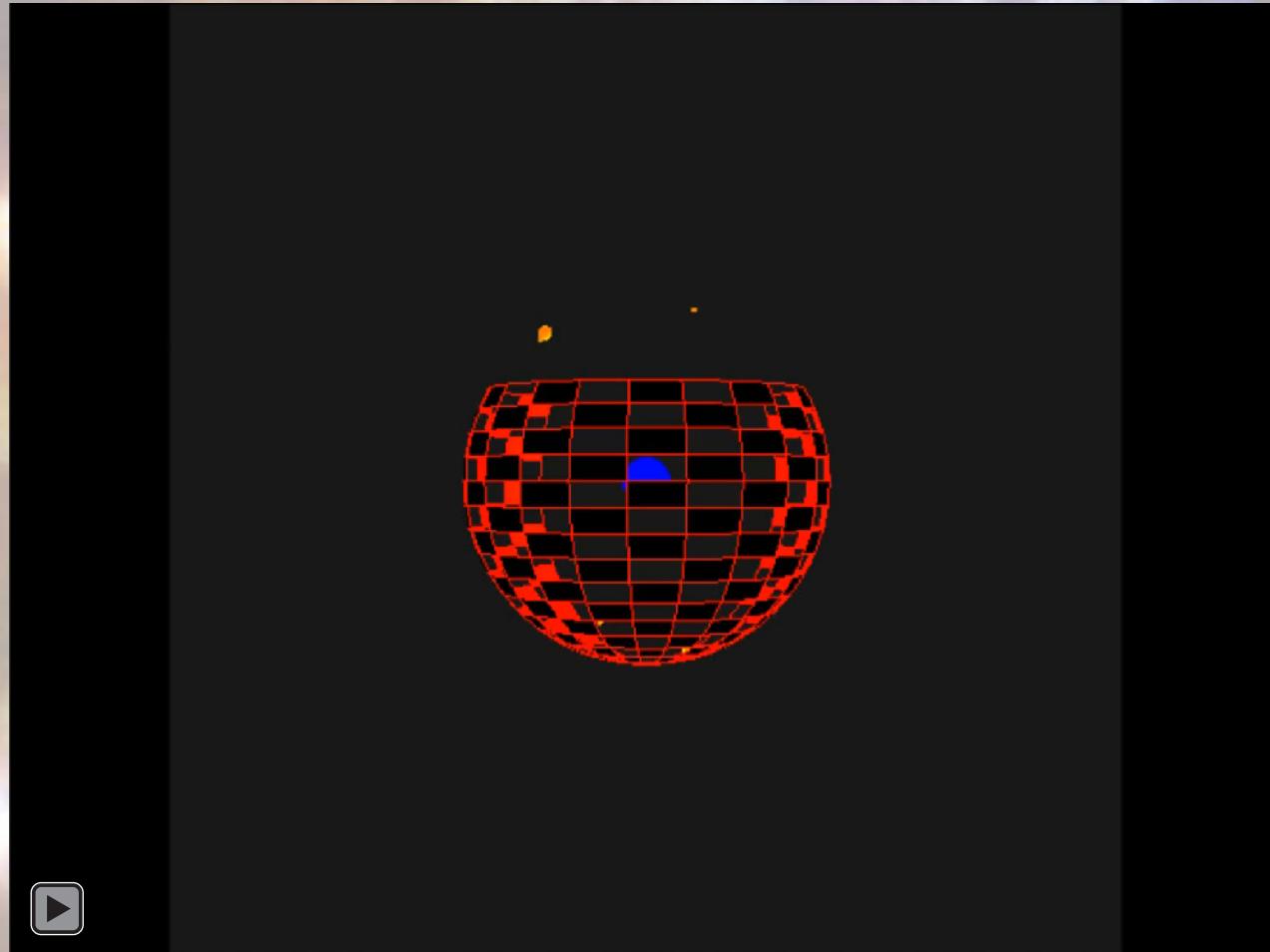
DR 21 C

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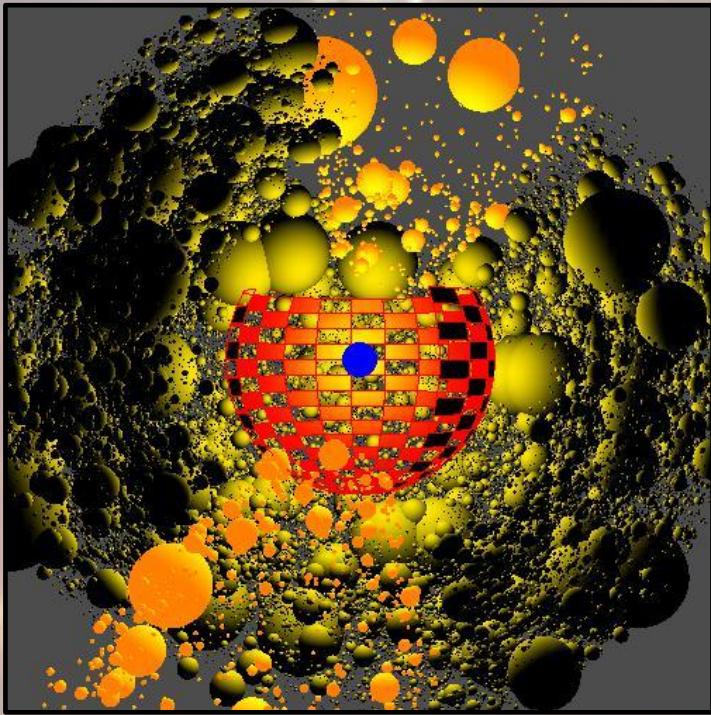
Marston et al. 2007, Spitzer

Modeling the embedded blister outflow

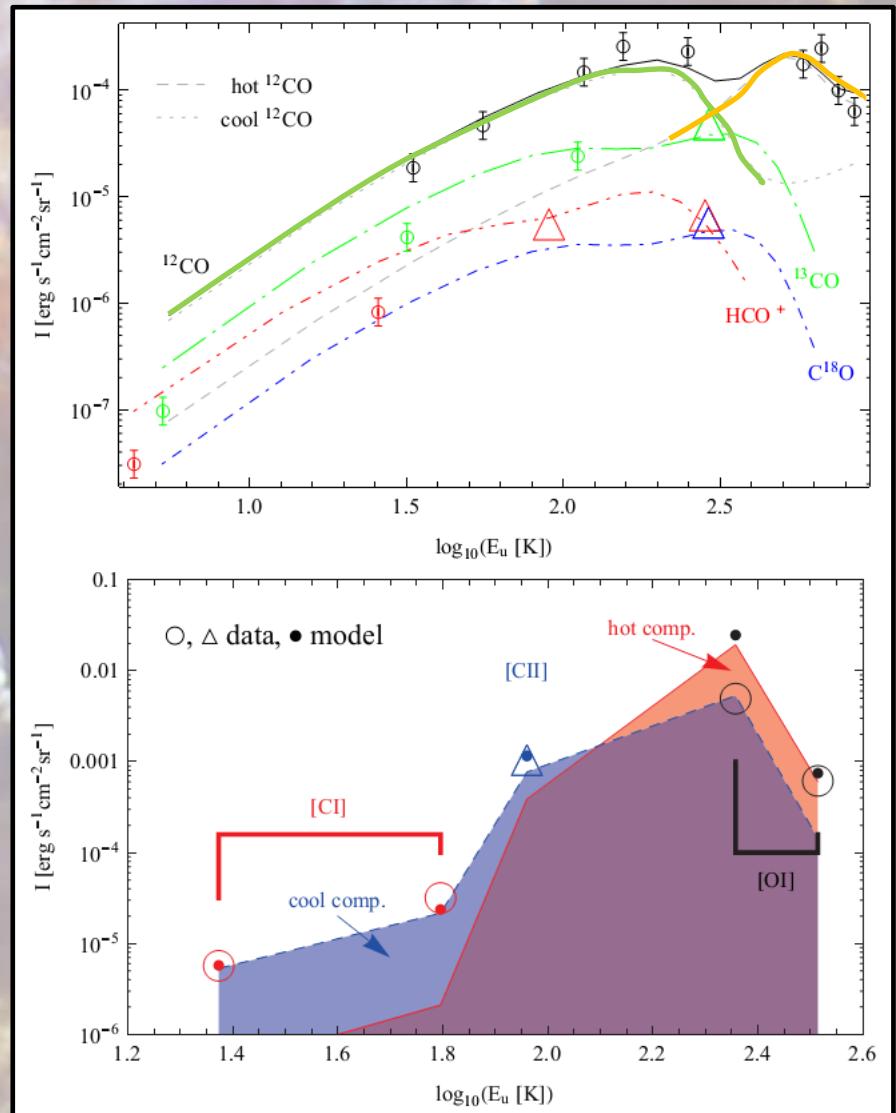


blue: central star, red: HII region, yellow & green: molecular clouds (PDRs)

DR 21 C

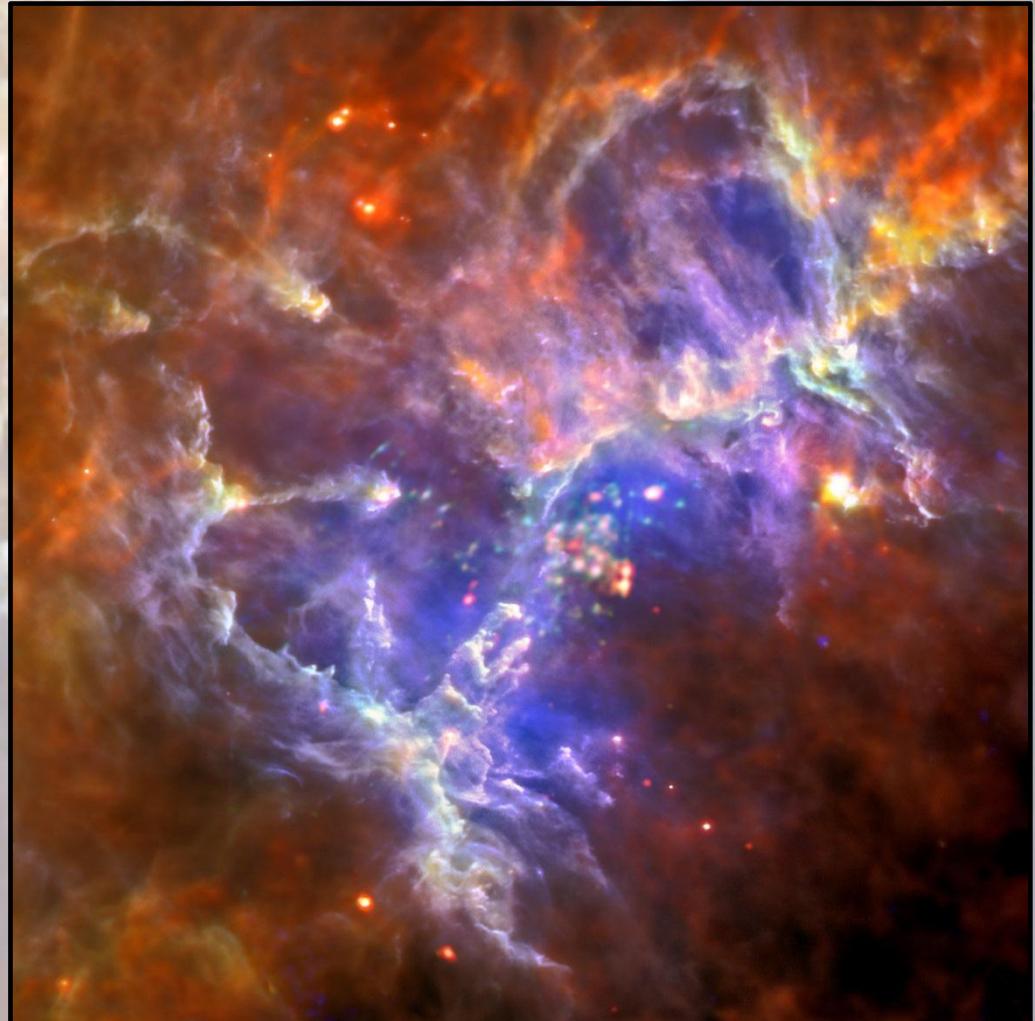


- Two distinct UV fields (10^5 and $300 \chi_D$)
- Dense clumps facing the blister outflow + clumpy large scale distribution
- Emission can be explained without shock component



Outlook

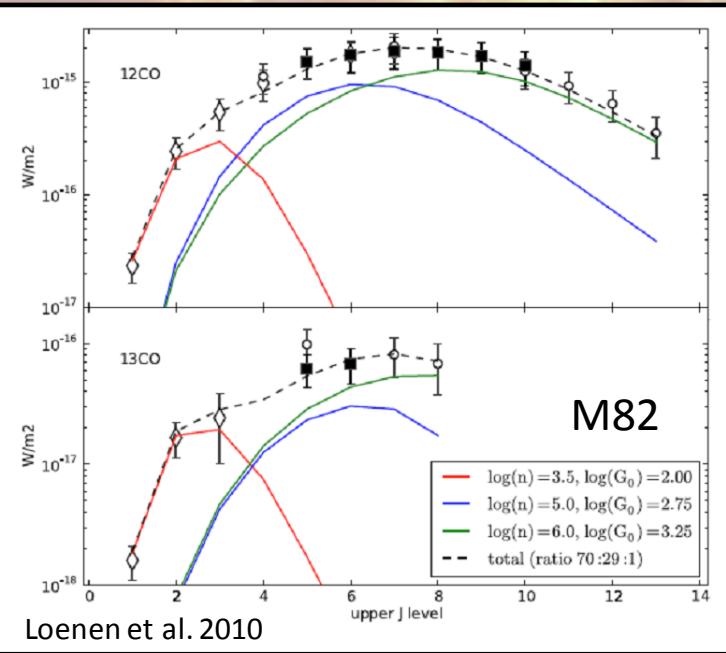
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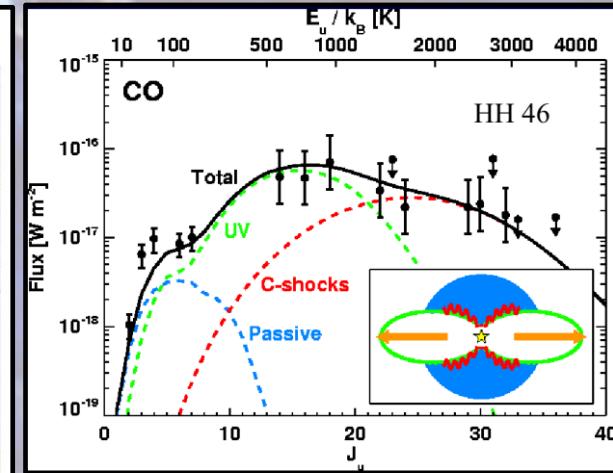
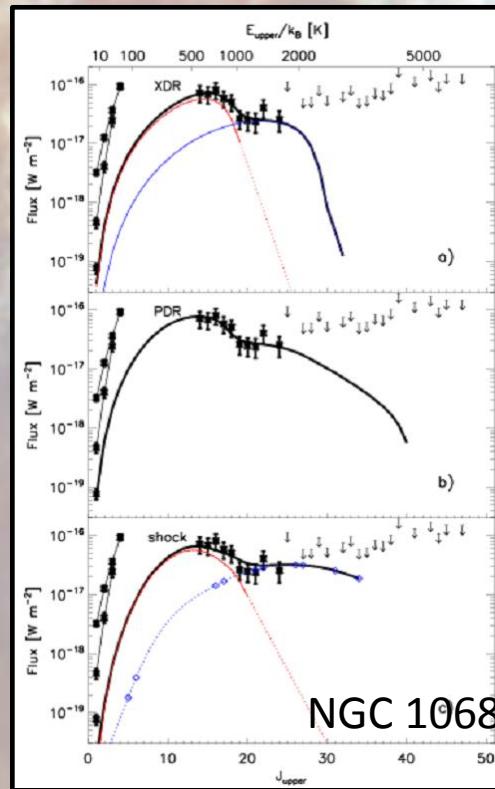
Credits: ESA/Herschel/PACS/SPIRE/Hill, Motte, HOBYS Key Programme Consortium

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.



Hailey-Dunsheath et al. 2012

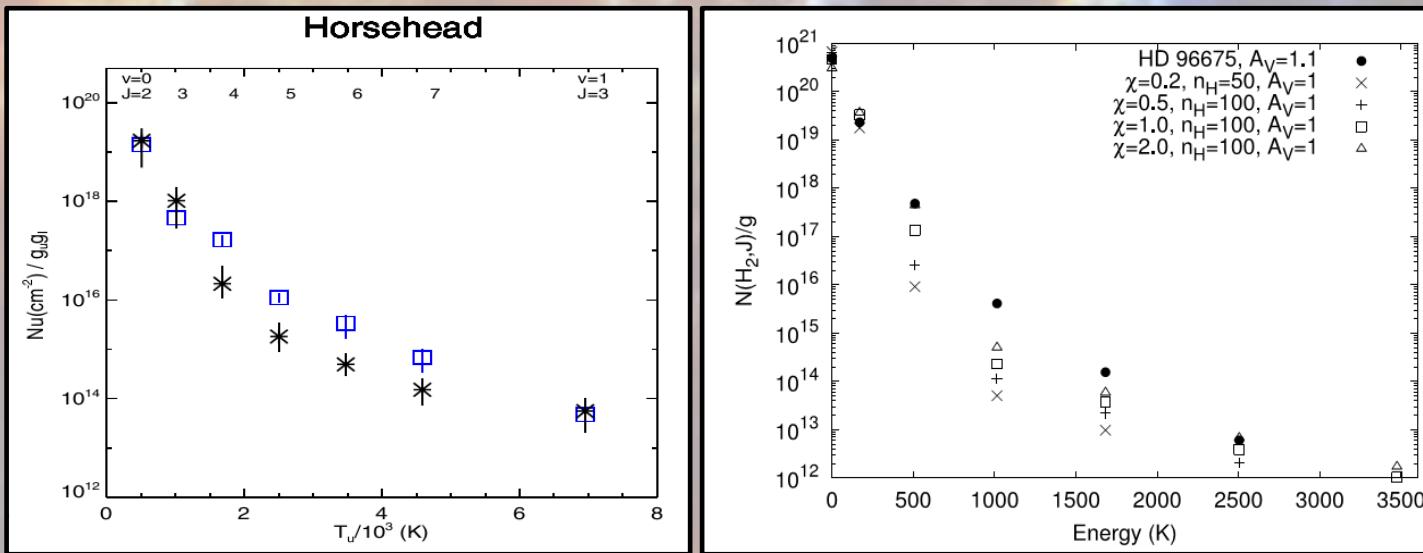


Visser et al. 2012, van Kempen et al. 2010

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

Outlook

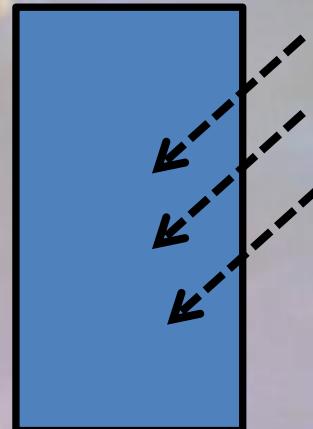
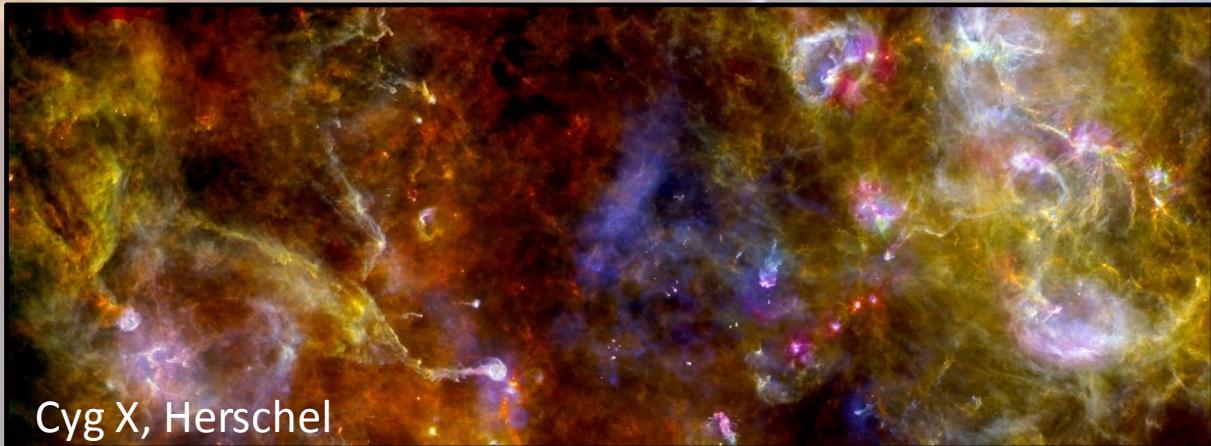
- Recent instrument missions opened up the spectral FIR window and allowed for the first time to directly observe many PDR tracers.
- PDR models again struggle to explain CO emission and H₂ emission.
- This already taught us many new details on the local physical and chemical conditions and the dominant processes in PDRs.



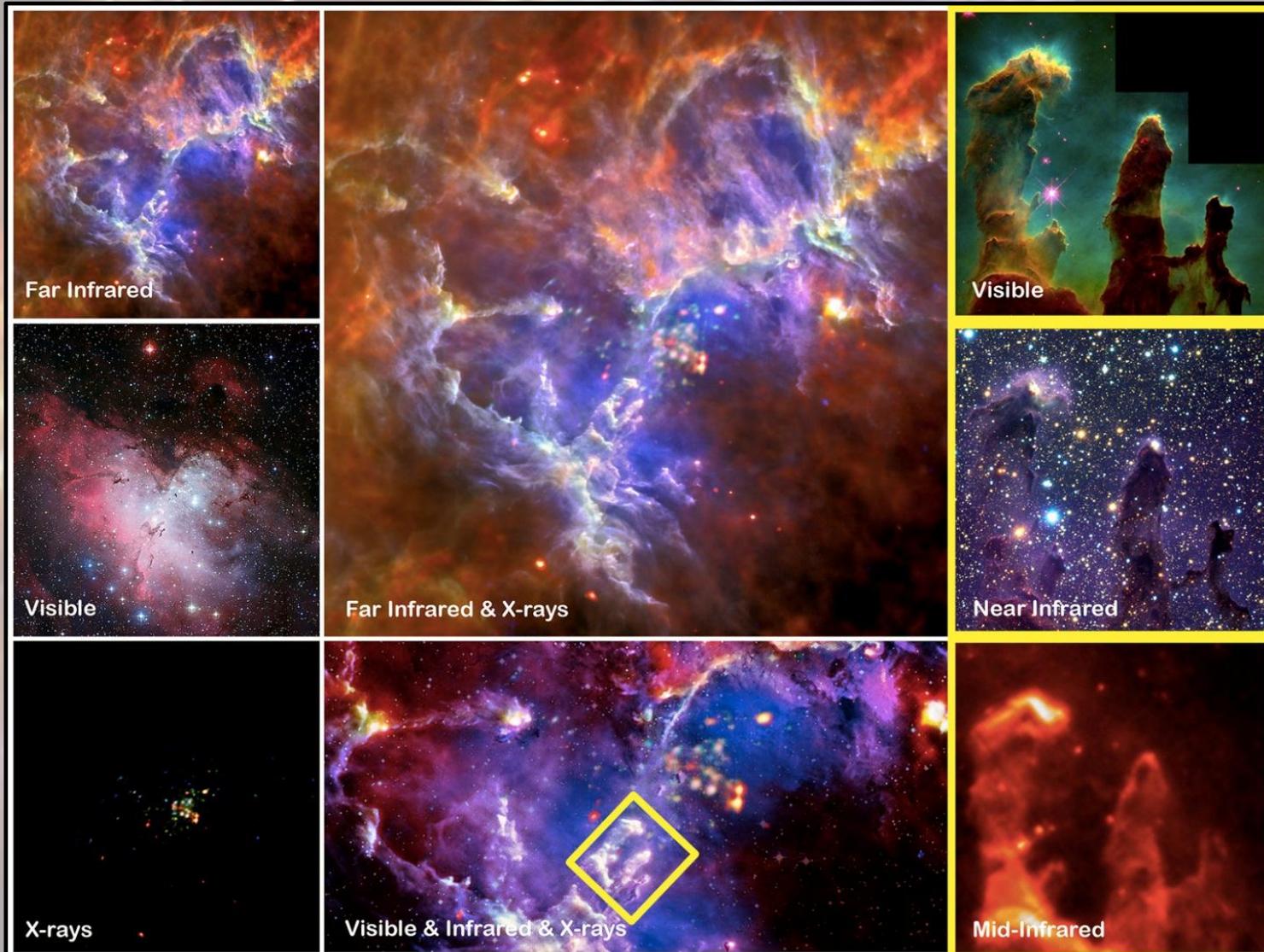
H₂ emission remains difficult to reproduce in PDR models, but recent missions taught us a lot about H₂ formation.

Outlook

- Reproducing the chemistry of light hydrides (OH , CH^+ , $\text{H}_2\text{O}, \dots$) remains a challenge – 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.



Thank you!



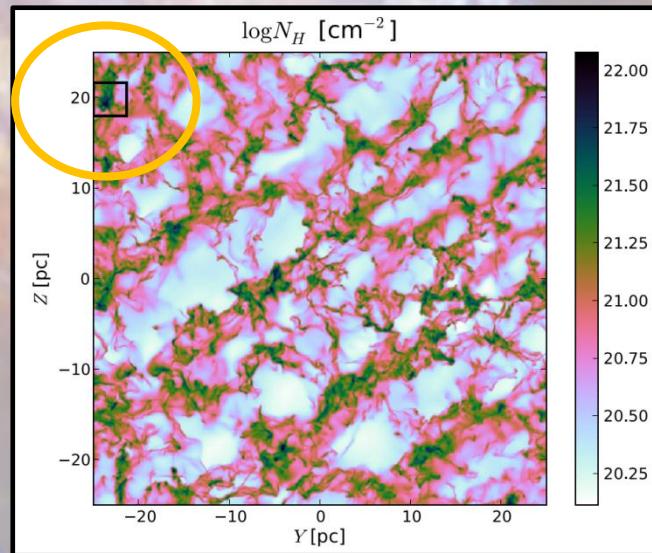
Credit: European Space Agency, European Southern Observatory, NASA





Model geometry

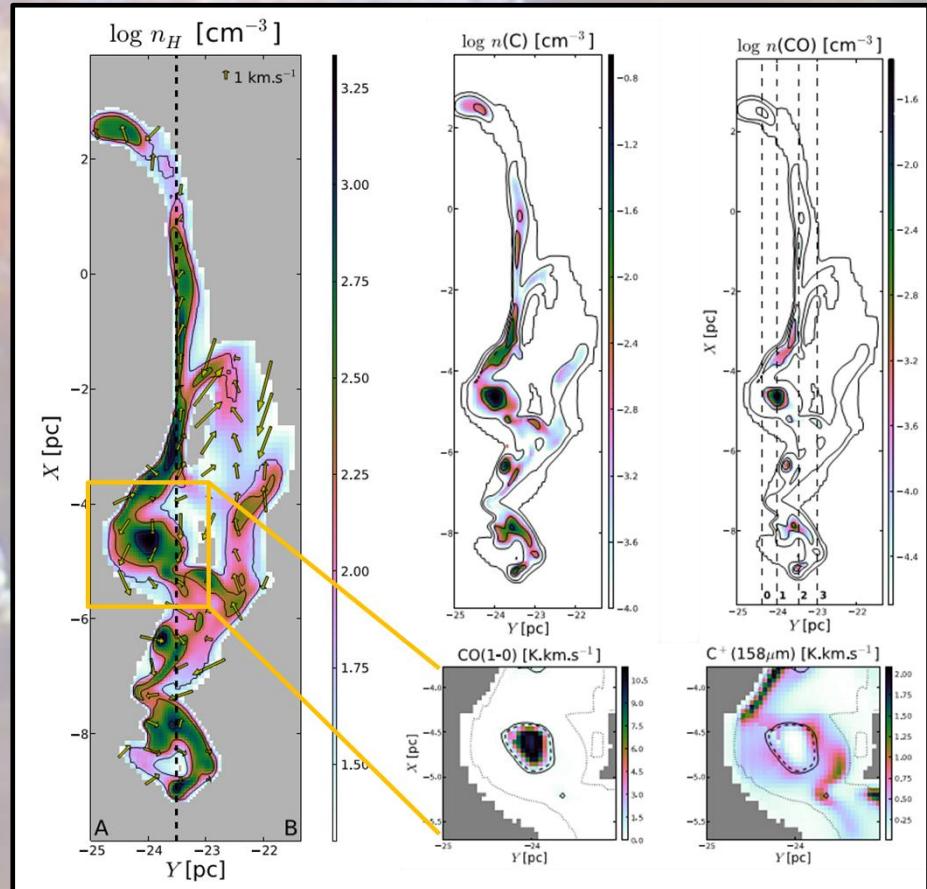
- Numerous configurations
 - Cloud geometry
 - plane-parallel (1D)
 - spherical (1D)
 - disk (1D+1D)
 - full 3-D
 - Illumination
 - isotropic
 - uni-directional
- The model geometry is determined by the field of application



Levrier et al., 2012, A&A 544

Model geometry

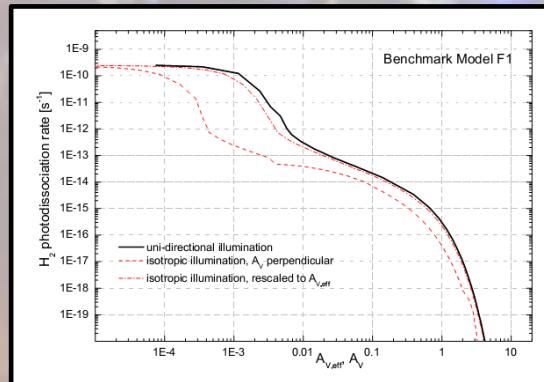
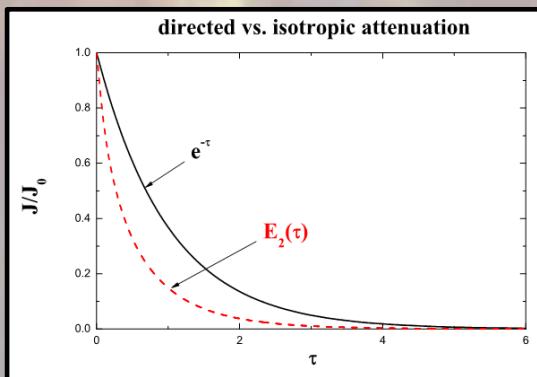
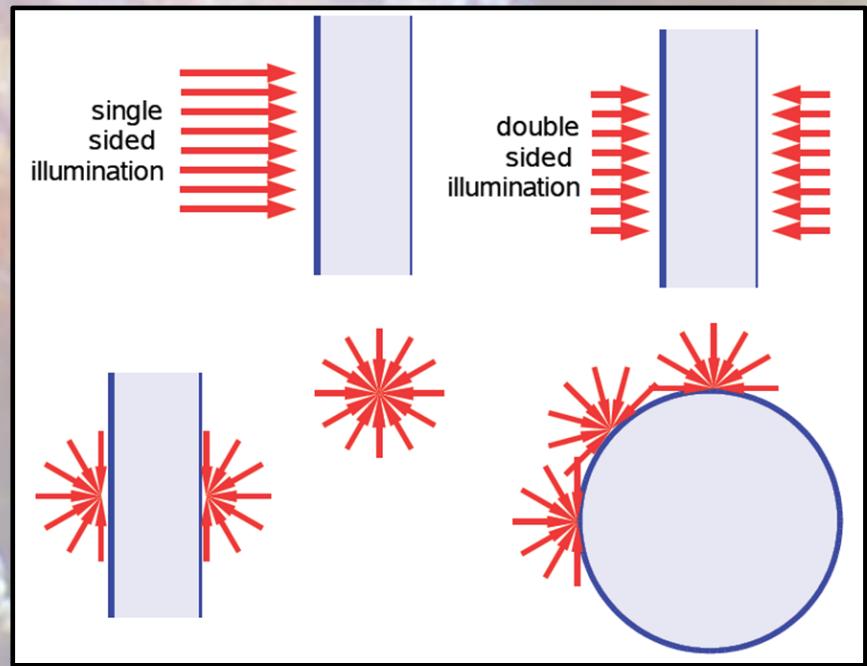
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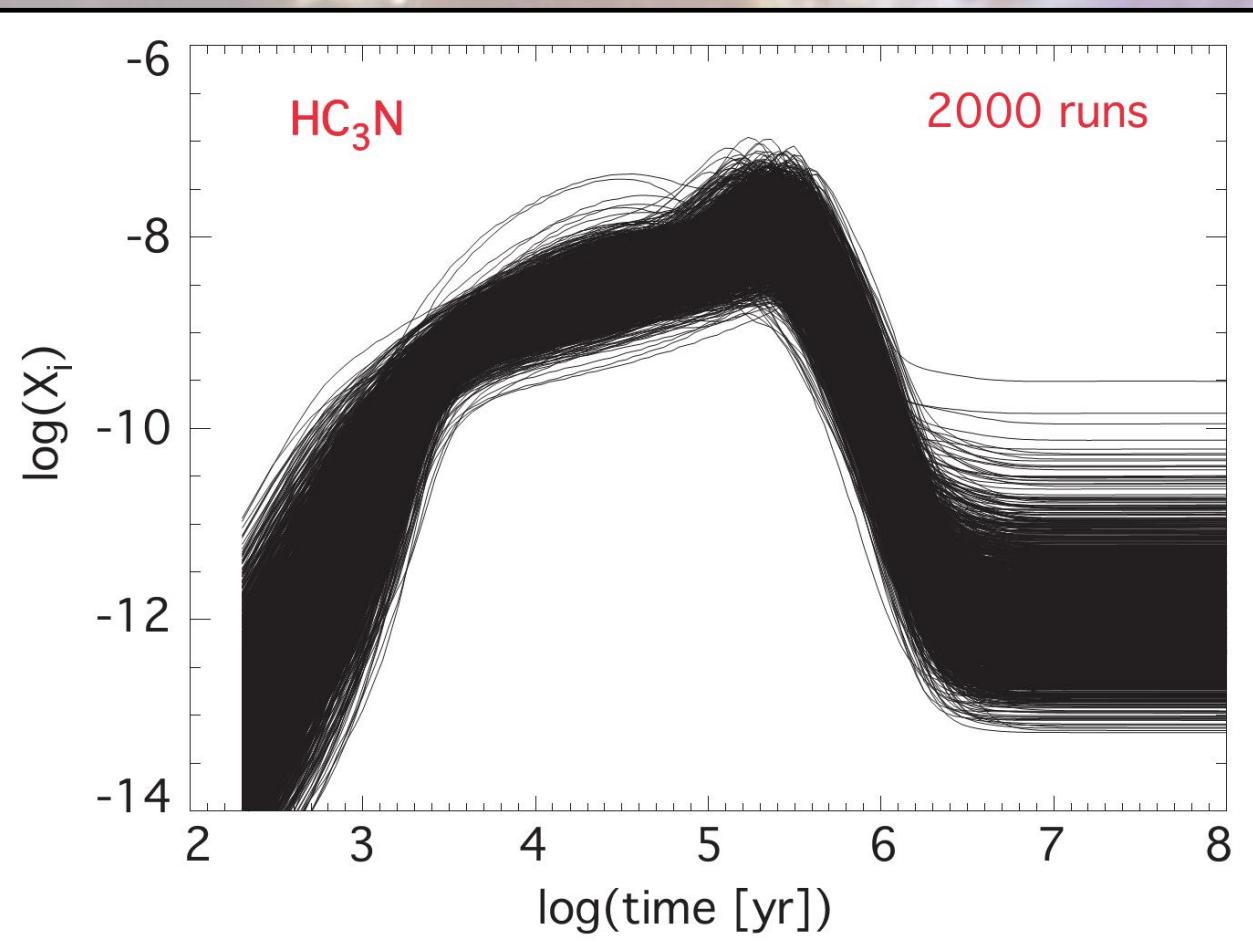
Post-processed MHD simulations, Levrier et al., 2012, A&A 544

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



Model chemistry



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
 - self shielding
 - turbulence/clumpyness
 - size distribution & composition
 - shielding rates vs. full computation
 - micro/meso/macro-turbulence
- energy balance
 - heating & cooling effects
 - optical depths
 - collisional rates
 - PE heating, H₂ formation heating, H₂ vib. deexcitation
 - line + continuum cooling
- model parameters
 - density
 - FUV intensity
 - mass
 - CR ionization rate
 - $n = 10^3 - 10^7 \text{ cm}^{-3}$
 - $\chi = 1 - 10^6$
 - $M = 10^{-3} - 10^3 M_{\odot}$
 - $\zeta_{\text{CR}} = 10^{-17} - 10^{-14} \text{ s}^{-1}$