Modeling the Chemical Distributions of Turbulent Star-Forming Clouds*

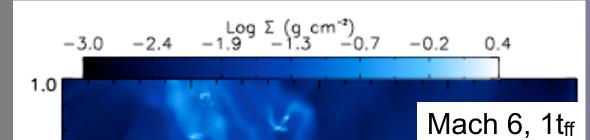
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*Offner, Bisbas, Viti & Bell 2013, ApJ, 770, 49 and Offner, Bisbas, Viti & Bell, 2013 in prep. 1. Hubble Fellow, Yale University, 2. University College London, 3. Centro de Astrobiologia (CSIC-INTA)

Summary:

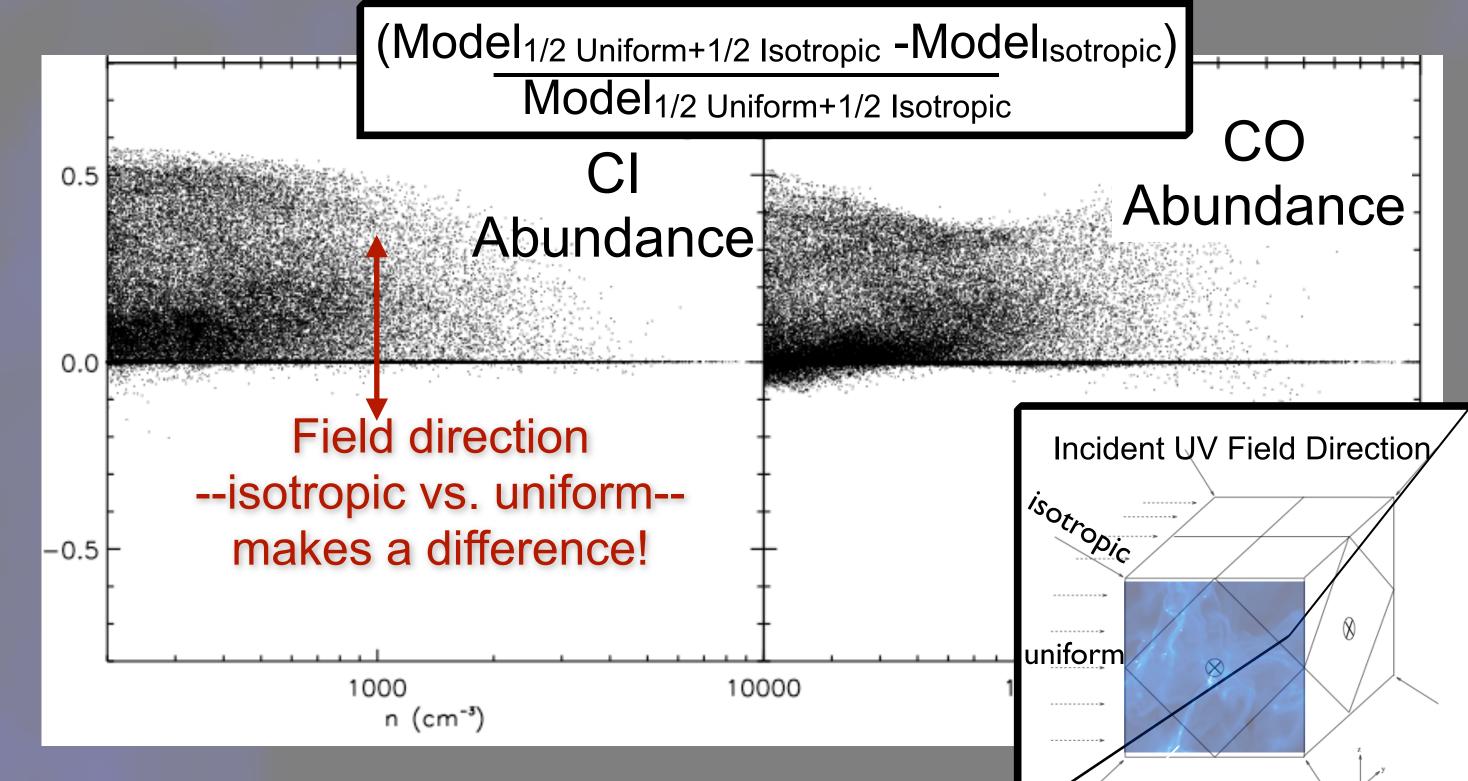
We use 3D-PDR, a three-dimensional astrochemistry code for modeling photodissociation regions (PDRs), to post-process hydrodynamic simulations of turbulent, star-forming clouds. We focus on the transition from atomic to molecular gas, with specific attention to the formation and distribution of H, C⁺, C, H₂ and CO. We investigate the effect of geometry and simulation parameters on chemical abundances. For a uniform external radiation field, we find similar distributions to those derived using a one-dimensional PDR code. However, we demonstrate that a three-dimensional treatment is necessary for a spatially varying external field. Finally, we use RADMC-3D to compute CO emission and explore the effect of spatially varying temperature and abundance on X_{CO}, the CO to H₂ conversion factor.

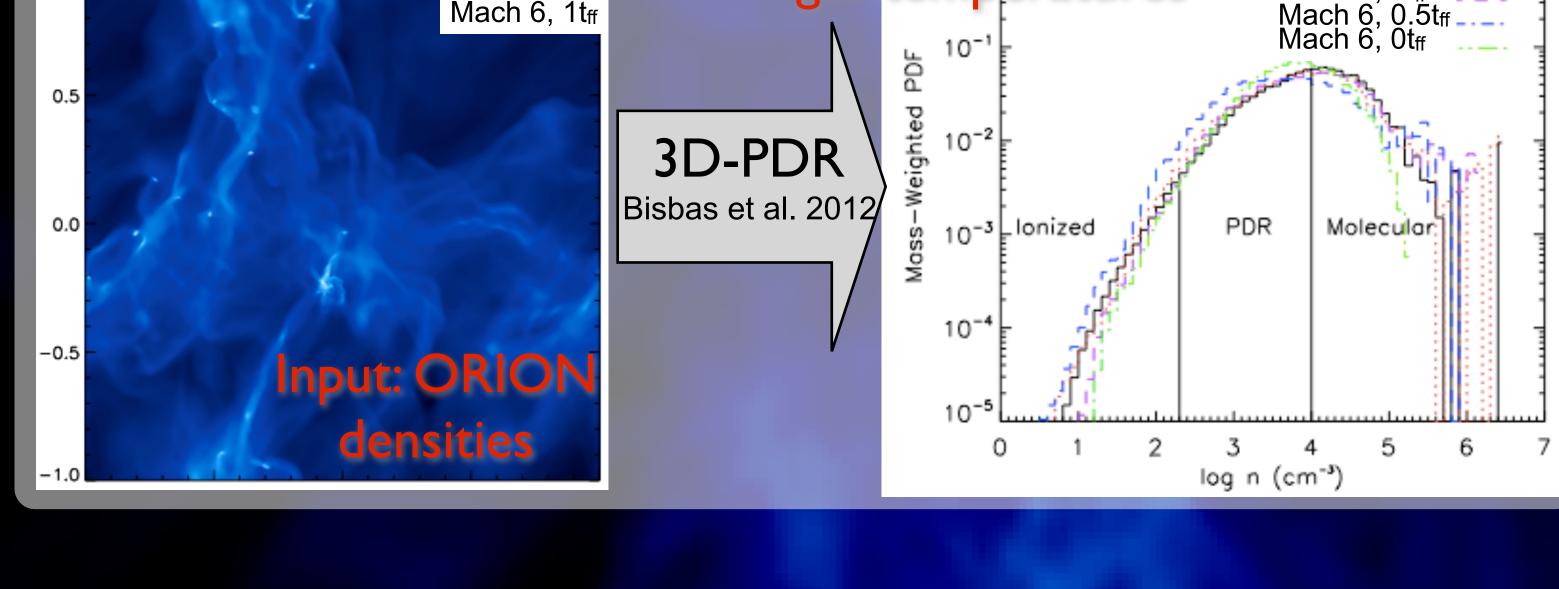
Method: Post-Processing with 3D-PDR



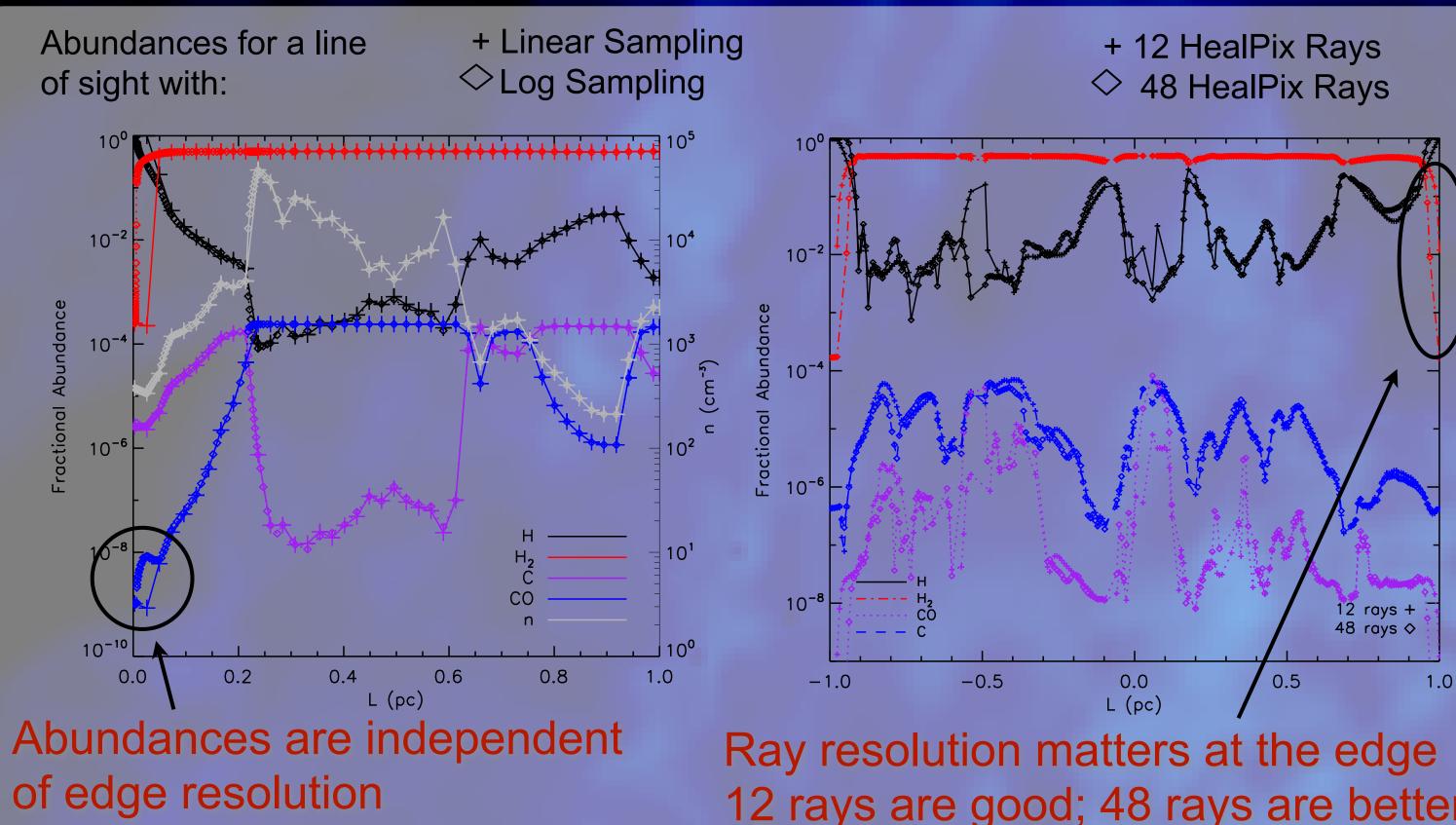
Output: abundances, temperatures

External UV Field: Uniform vs. Isotropic





Verification



CO Line Profiles: 3D-PDR vs. Constant **Temperature & Abundance**







Too high

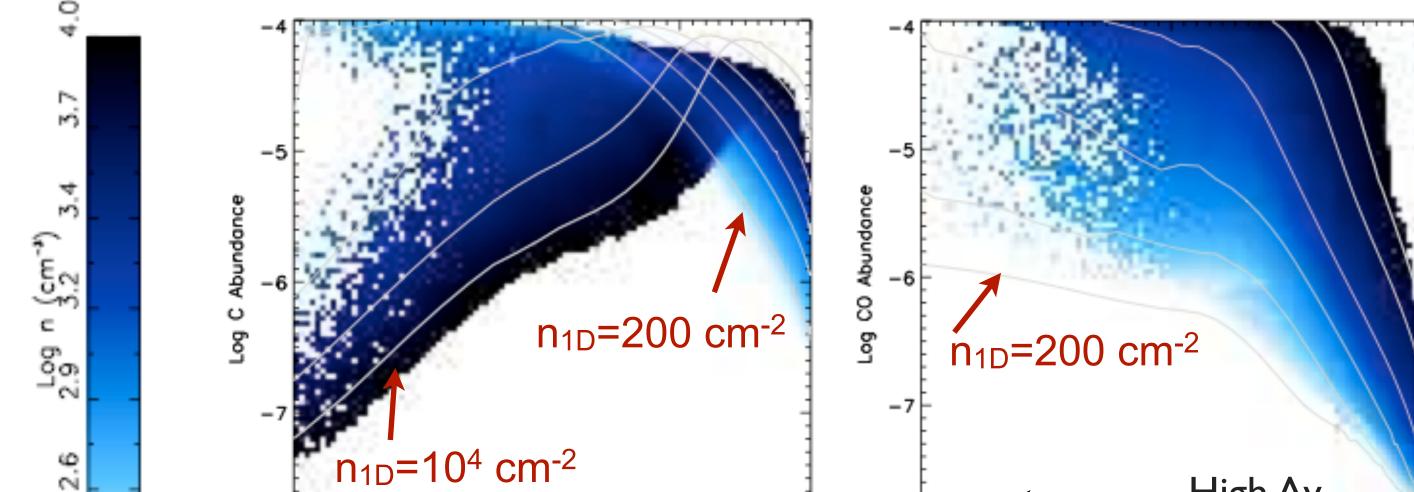
Av

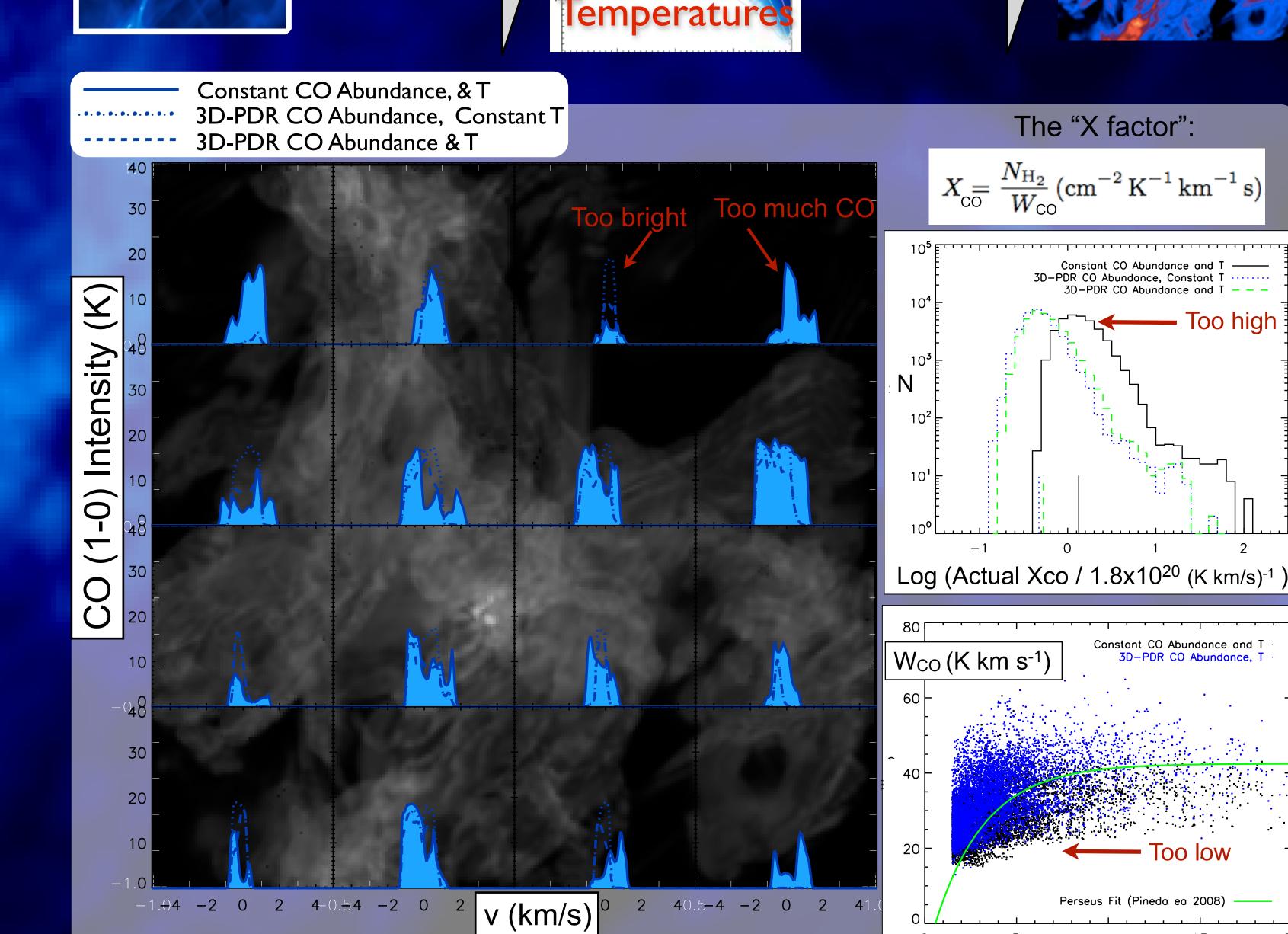
Ray resolution matters at the edge 12 rays are good; 48 rays are better

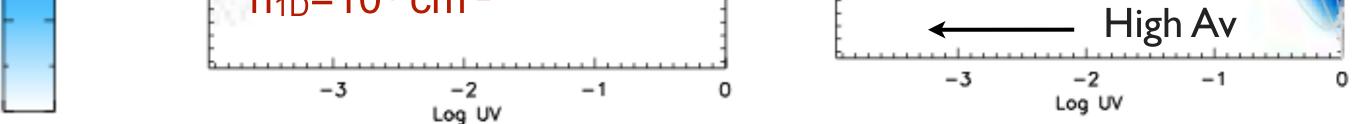
1D vs. 3D Modeling

F) N

Abundance vs. UV field vs. Mean Density







lines = ID PDR calculations with constant density, incident UV

 Once the local UV field is computed from the 3D information, the chemistry is a 1D problem.

• The spread in abundances at a given UV depends on the range of densities present.

Background: Integrated Intensity, W_{CO} (K km s⁻¹)

Conclusions

• **3D-PDR** results are converged in grid resolution and ray angular resolution. • Computing the UV field is a 3D problem; the chemistry is approx. a 1D problem. • The incident field direction, even for simple field geometries, affects the abundances. • PDR chemistry is necessary to accurately model CO line emission and X_{CO}.