Modeling the Chemical Distributions of Turbulent Star-Forming Clouds*

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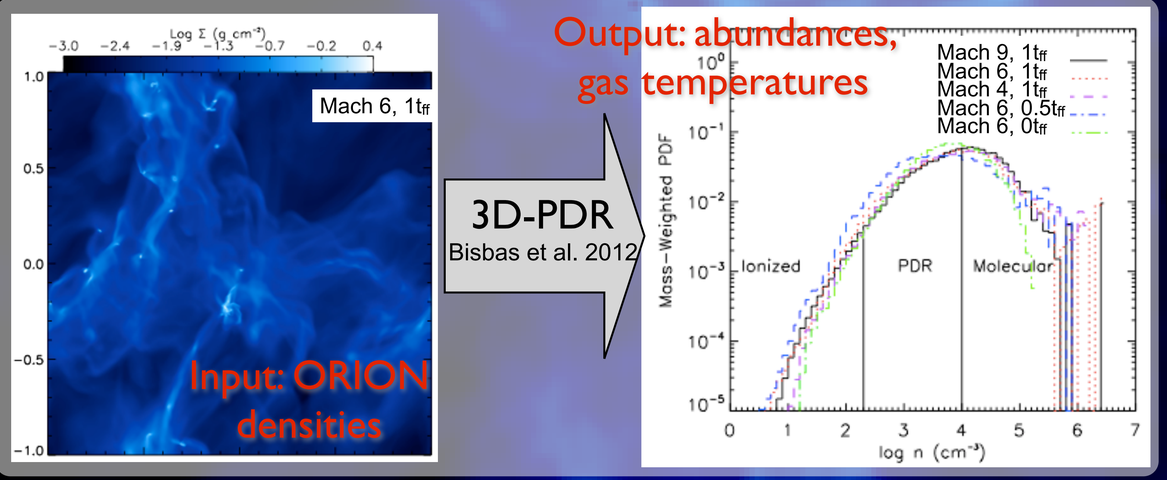
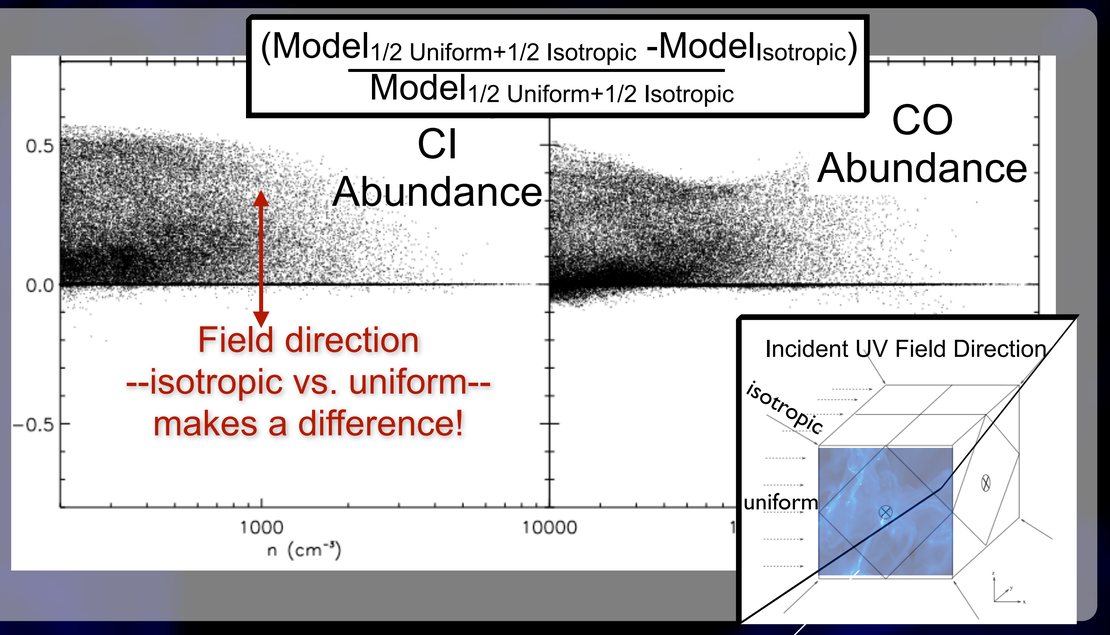
Summary: We use 3D-PDR, a three-dimensional astrochemistry code for modeling photodissociation regions (PDRs), to post-process hydrodynamic simulations of turbulent, star-forming clouds. We focus on the transition from atomic to molecular gas, with specific attention to the formation and distribution of H, C^+, C, H_2 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 H_2 conversion factor.

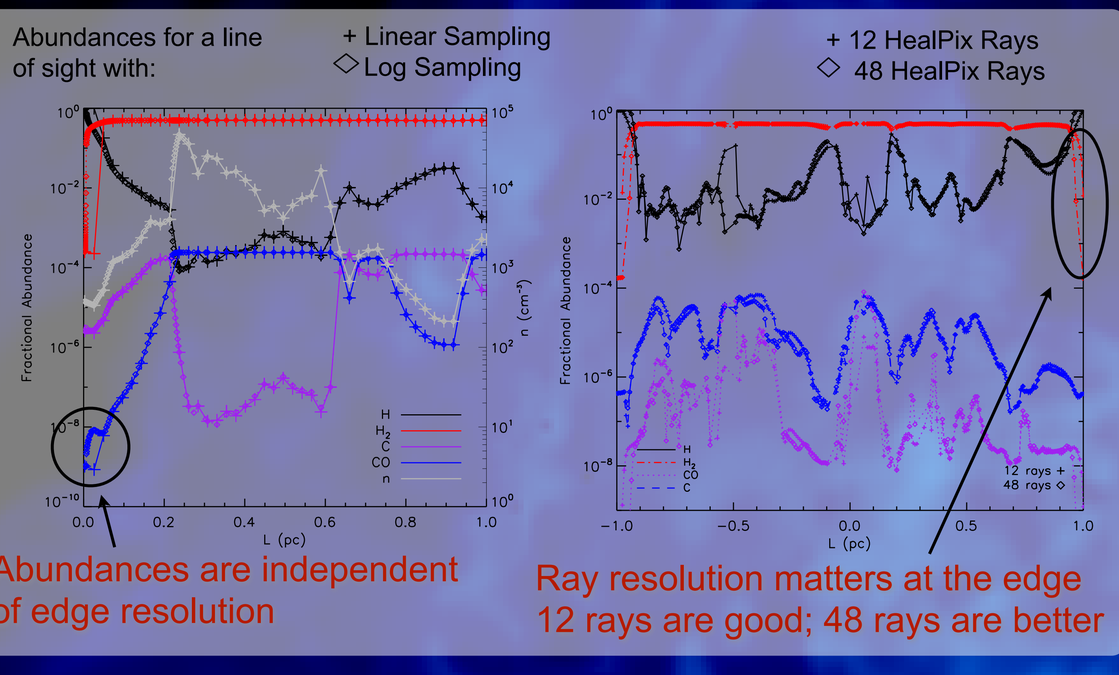
Method: Post-Processing with 3D-PDR



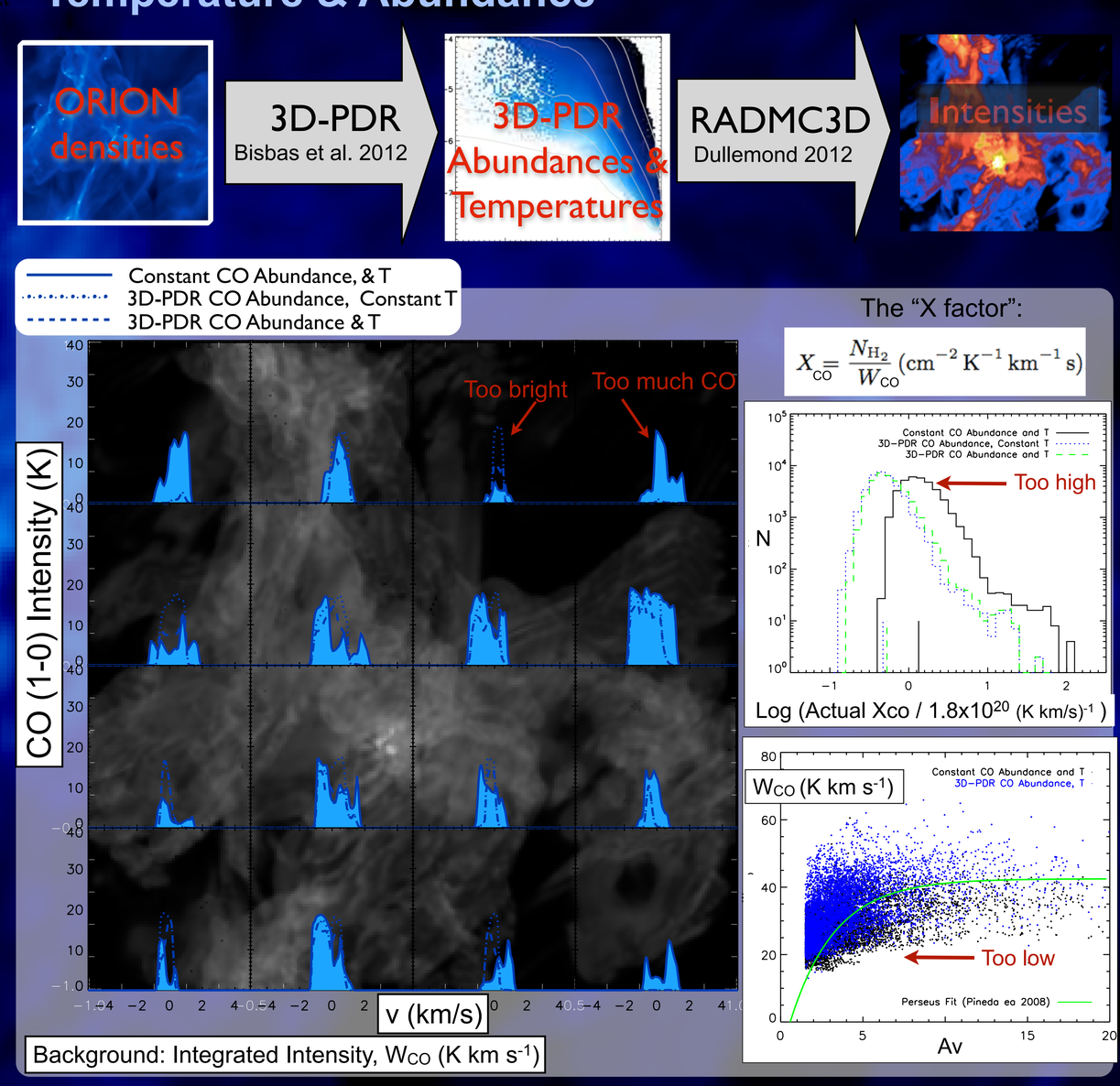
External UV Field: Uniform vs. Isotropic



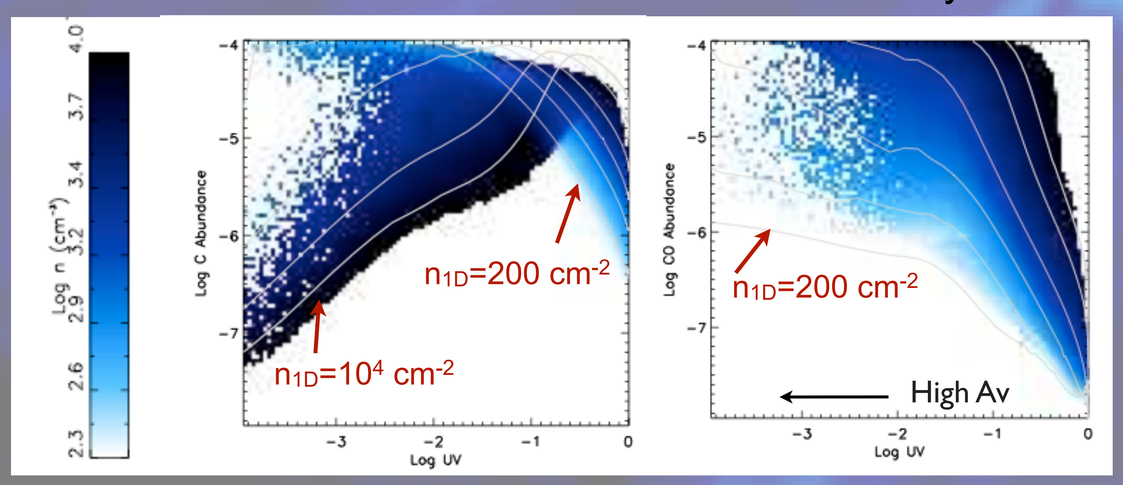
Verification



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



1D vs. 3D Modeling



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}.**