Nautilus multi-grain model: Impact of cosmic-ray induced desorption on abundances of COMs in the ISM

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Rate equations so far

Most models with grain-surface chemistry have used so-called "**classical grains**", which are characterized by a radius of **0.1μm** and **10^6** binding sites for adsorbates.

With the canonical gas-to-dust mass ratio of 100 and an assumed grain mass density of **3.00 g/cm^3**, the number density of **0.1μm** grains is **$1.33 \times 10^{-12} n_H$**, where **n_H** is the number density of hydrogen in all forms.

However, grains are distributed in various sizes. In addition, they grows with time. Not many full gas-grain chemical simulations have been done to understand how the diversity of grain sizes affects molecular abundances in the cold interstellar medium.

Nautilus multi-grain model

We used 10, 30 and 60 grain sizes.

Radius range of **0.005μm** to **0.25μm**

We used two grain size distributions (MRN and WD)

Flexibility to use different grain surface temperature and other surface properties for different grain sizes

Cosmic-ray-induced desorption rate

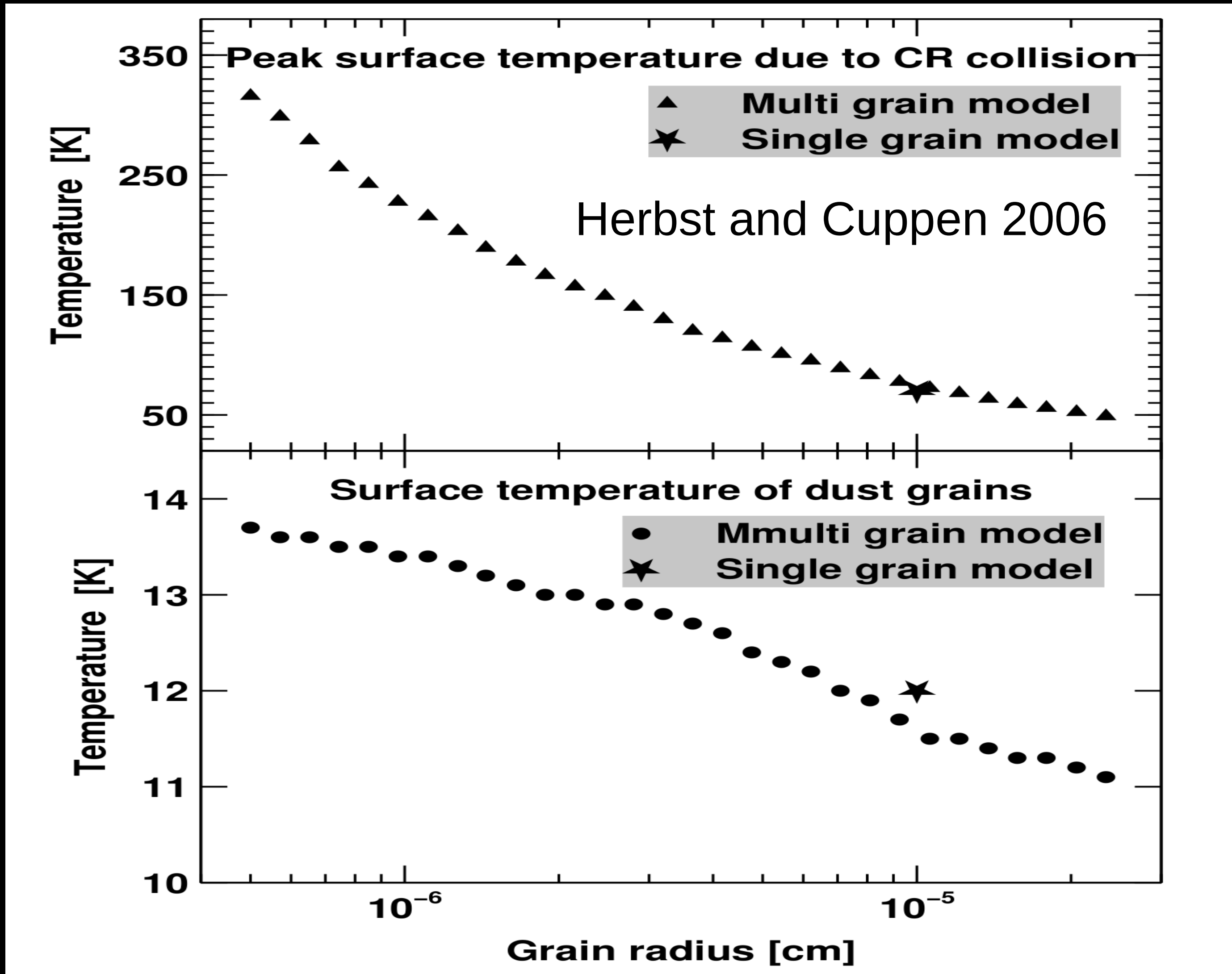
$$k_{crd}(i) = f(T_{max}(i))k_{evap}(i, T_{max}(i))$$

Hasegawa & Herbst (1993).

where $f(T_{max}(i))$ is called duty cycle of the ith grain at elevated temperature $T_{max}(i)$ and $k_{evap}(i,T_{max}(i))$ is the thermal desorption rate for the species on the ith grain at temperature $T_{max}(i)$.

What changes with grain sizes in cold dense cores

Avg. Grain Temperature



MRN and WD grain size distributions

1. MRN Size Distribution:

Mathis, Rumpl & Nordsieck, 1977, ApJ, 217, 425

$$dn_{\rm gr} = C n_{\rm H}\, a^{-3.5}\, da\,, \quad a_{\rm min} < a < a_{\rm max}$$

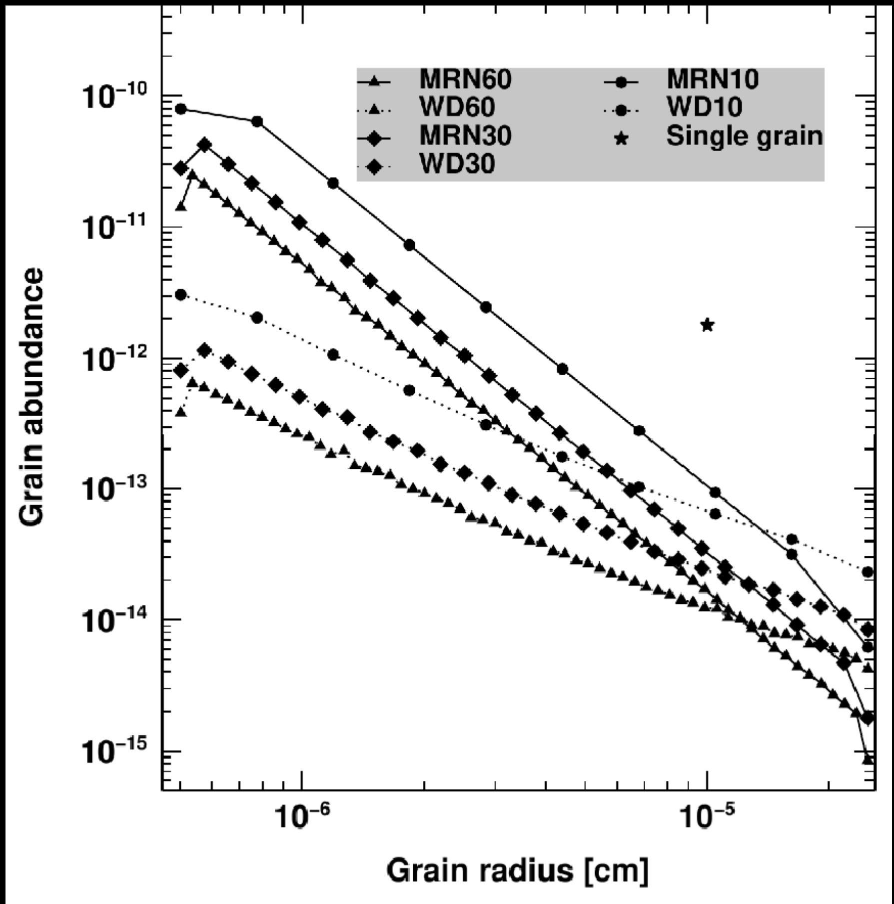
where, n_h is the number density of hydrogen in all form, ***a*** is the grain-radius in ***cm***. This relation is valid between the minimum and the maximum size of the grains a_{min} = 50 Å and a_{max} = 0.25 μm. The grain constant (***C***), is given by $10^{-25.13}(10^{-25.11})\ cm^{2.5}$ for graphite (silicate).

2. WD Size Distribution

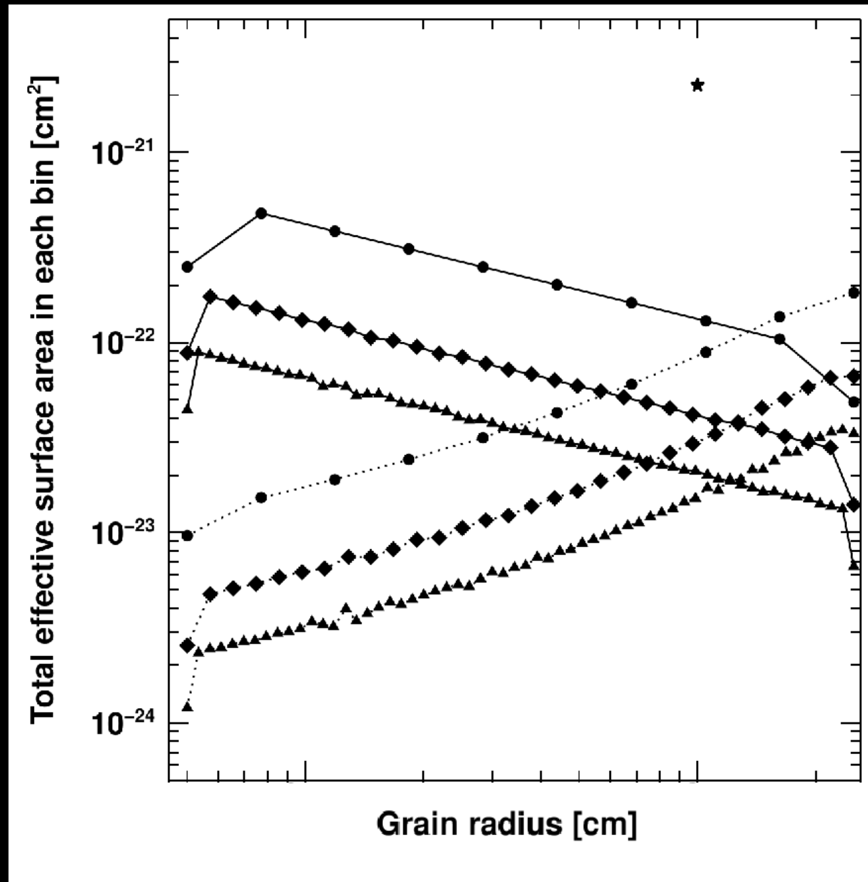
Weingartner and Draine, 2001, ApJ, 548, 296 (WD)

Feature of grain size distribution

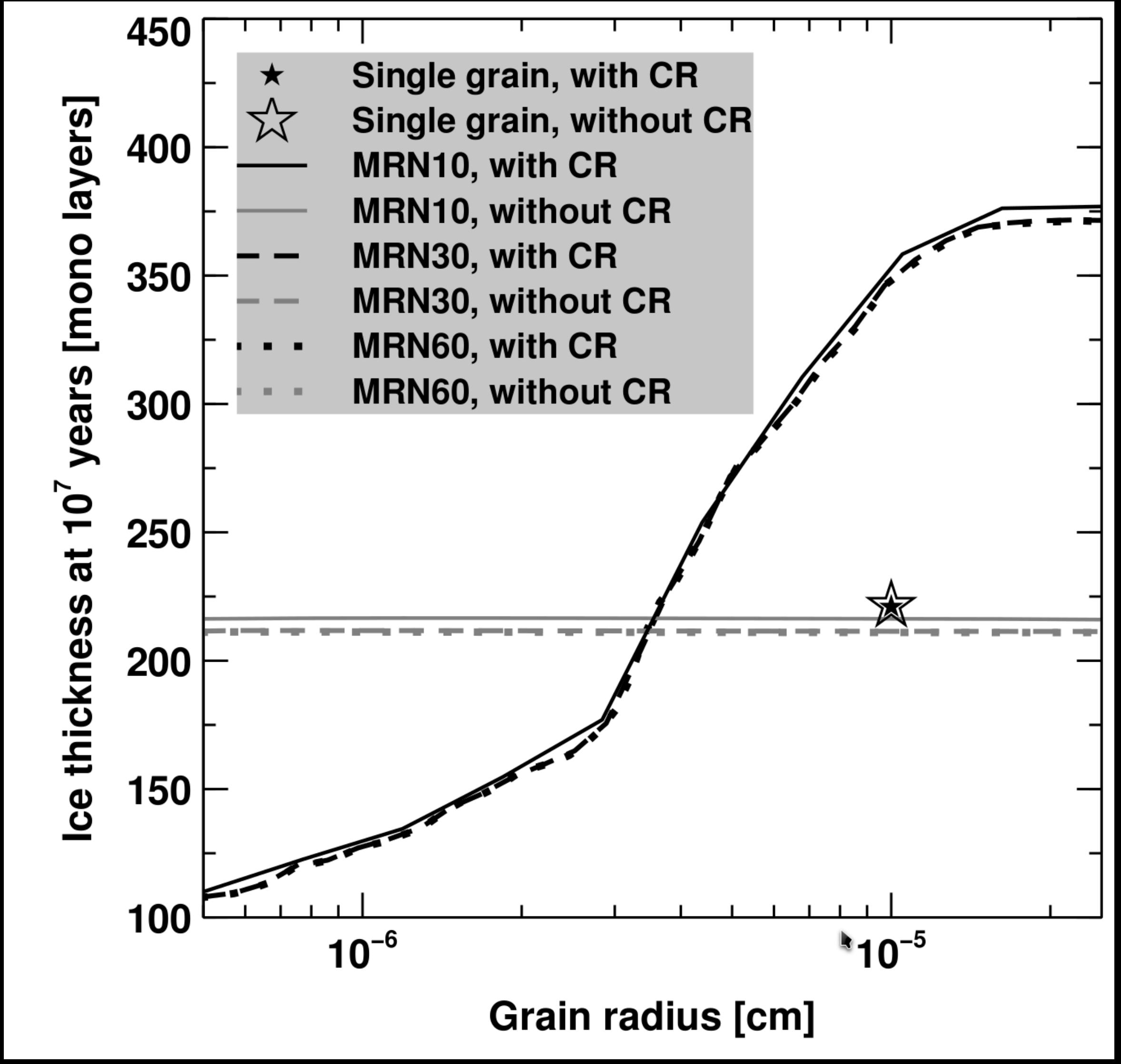
Number density of grain sizes



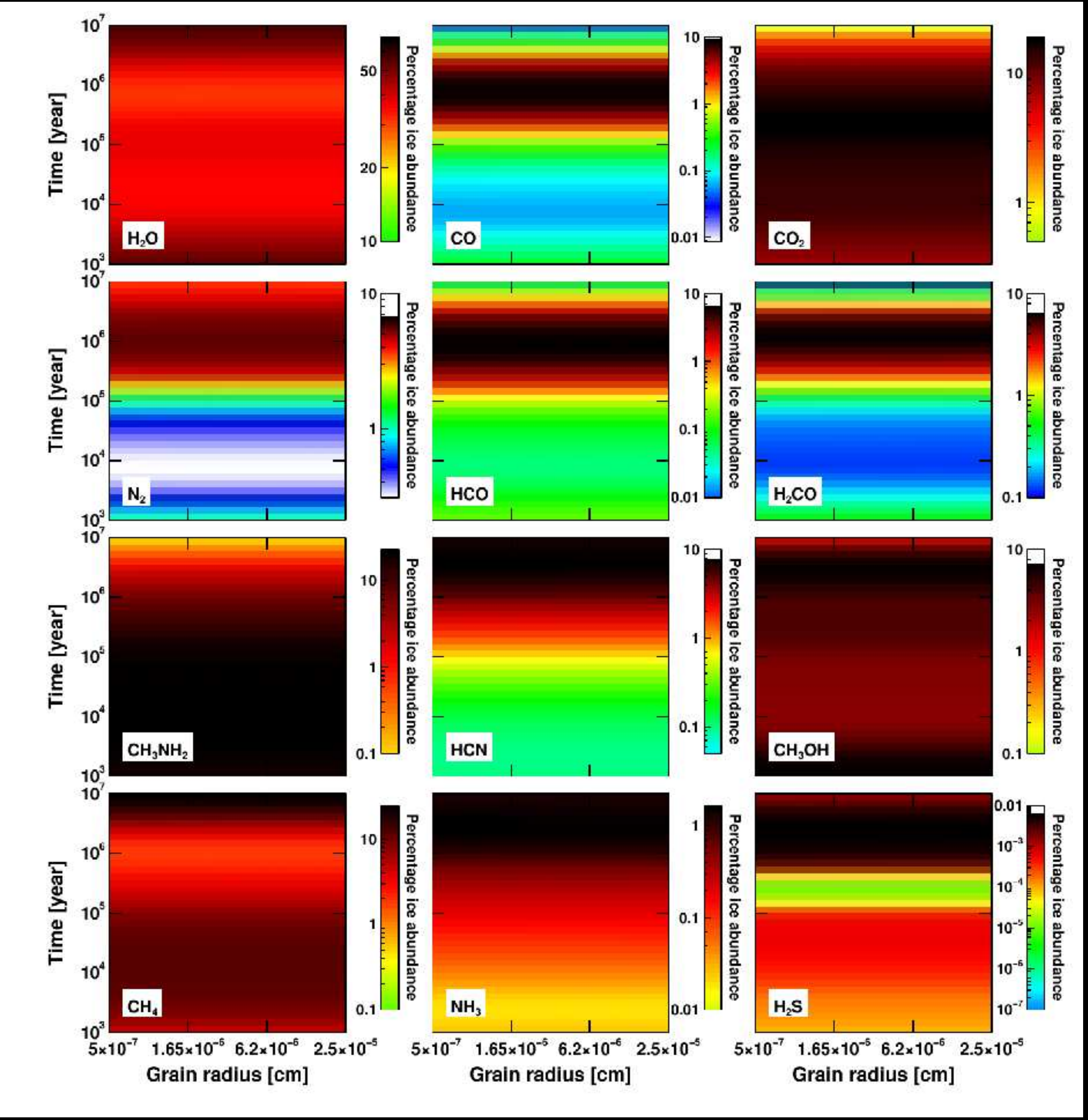
Total effective surface area



Results: Impact of CR-induced desorption



Results: no CR



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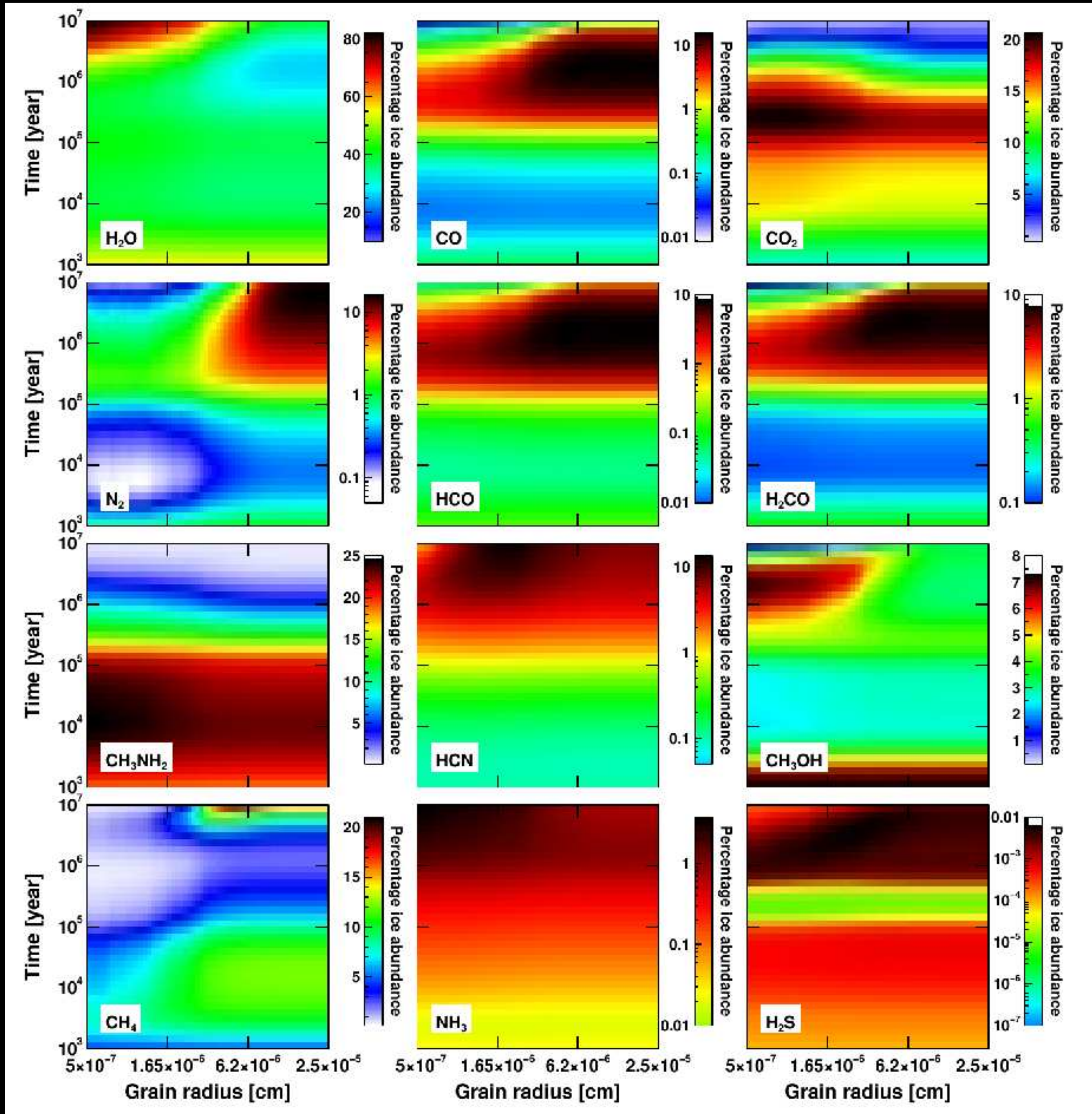
Results: with CR



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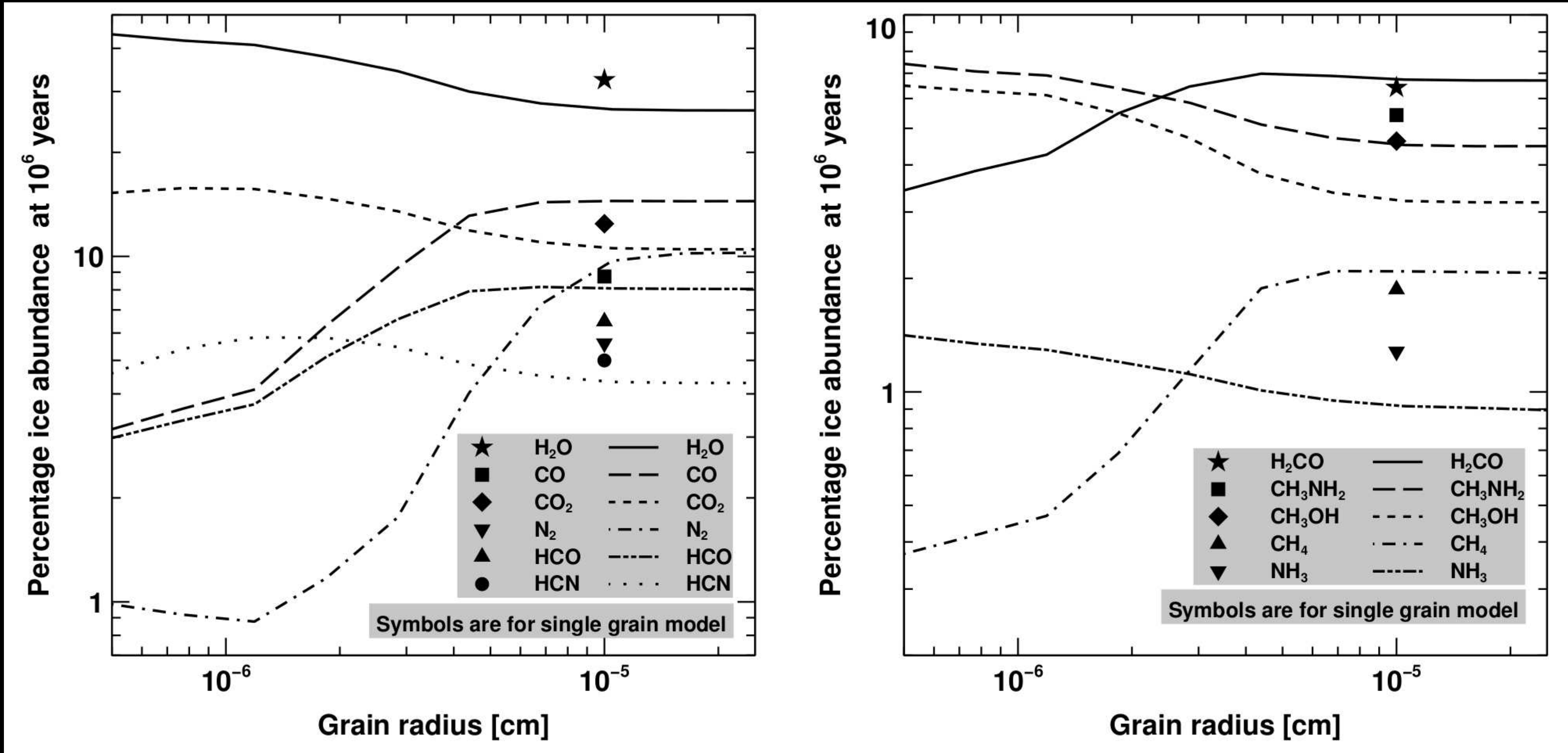
Results: Impact of CR-induced desorption



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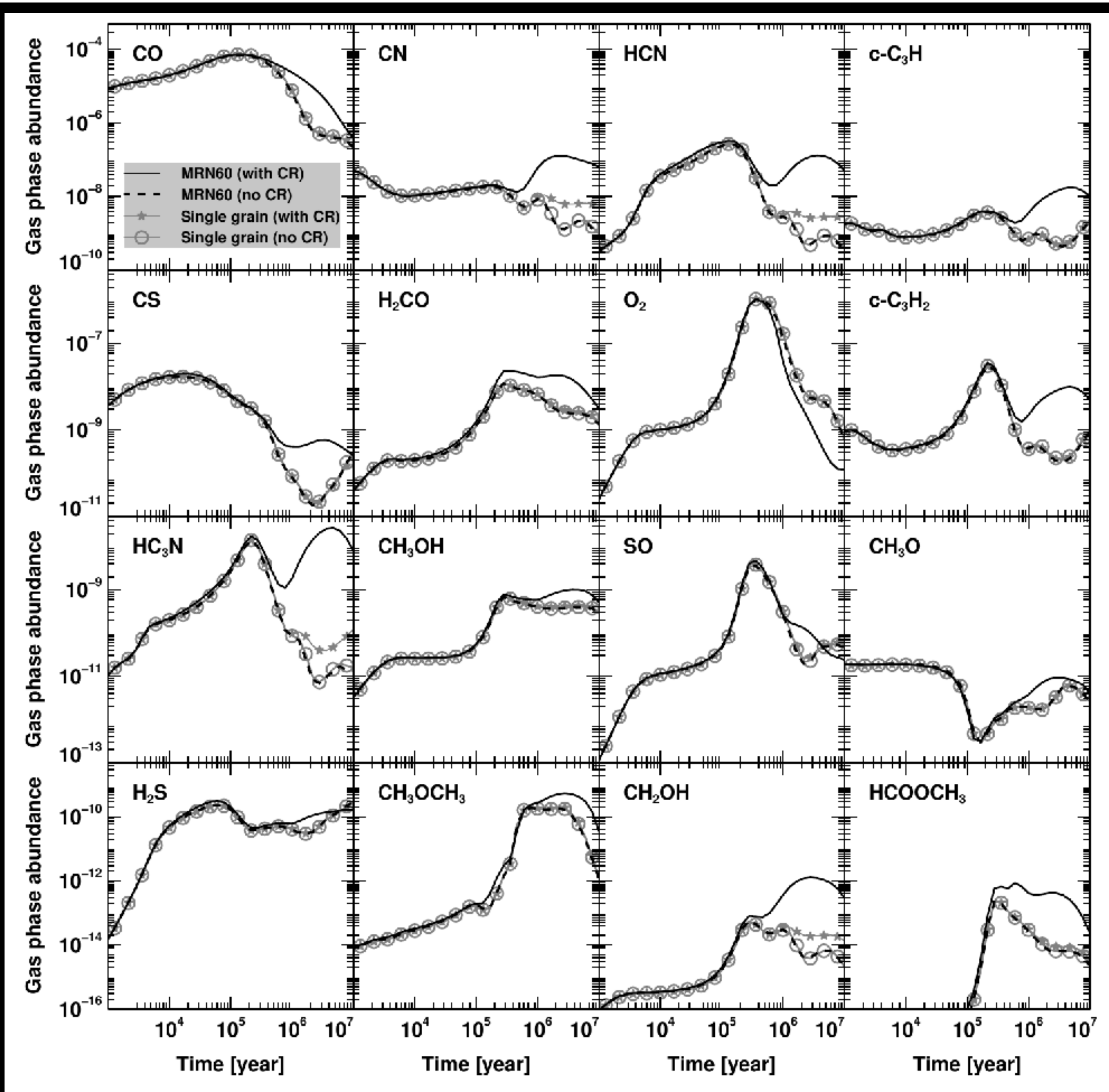
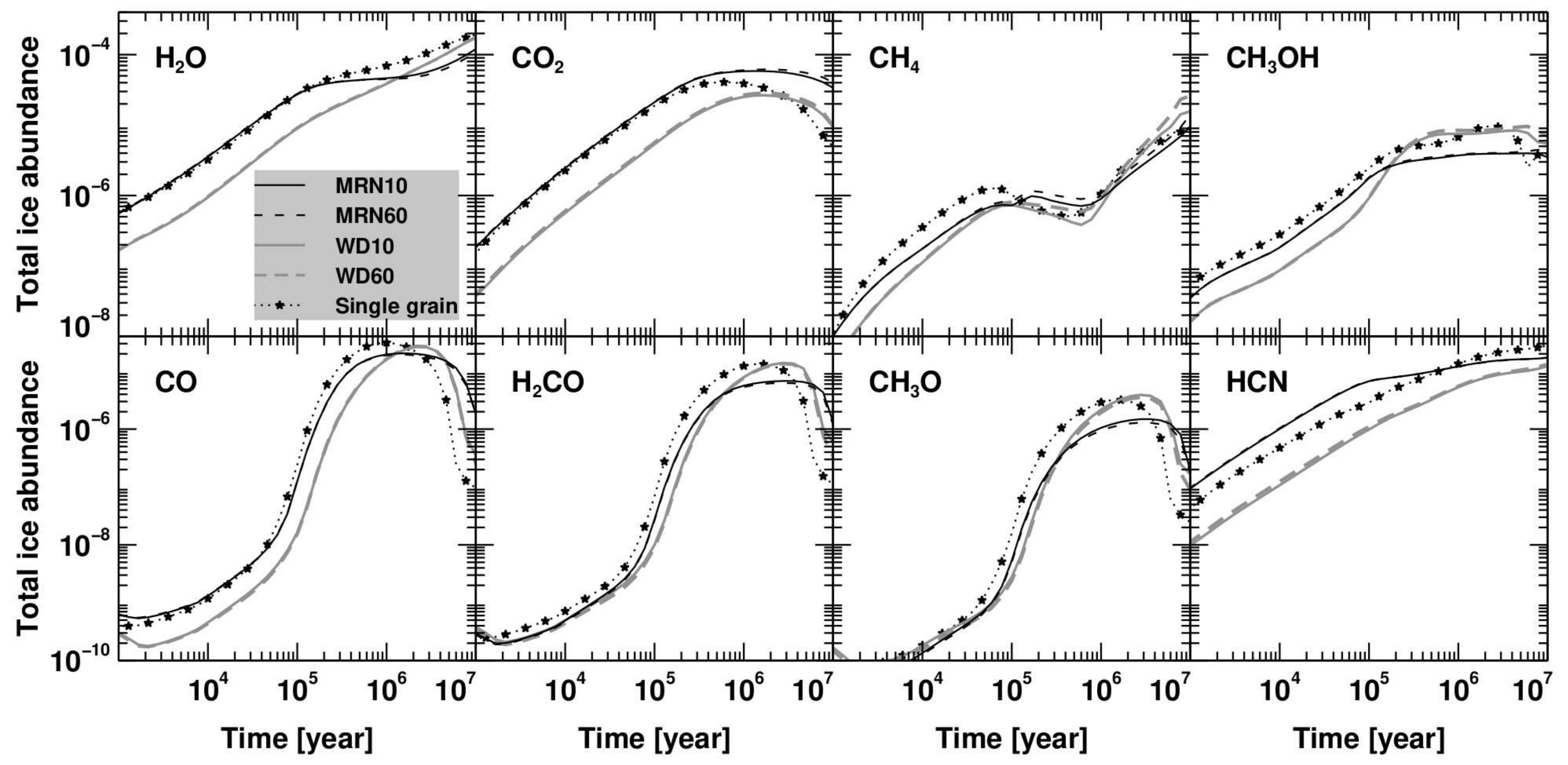
Results: Impact of CR-induced desorption



Results: Impact of grain size distribution



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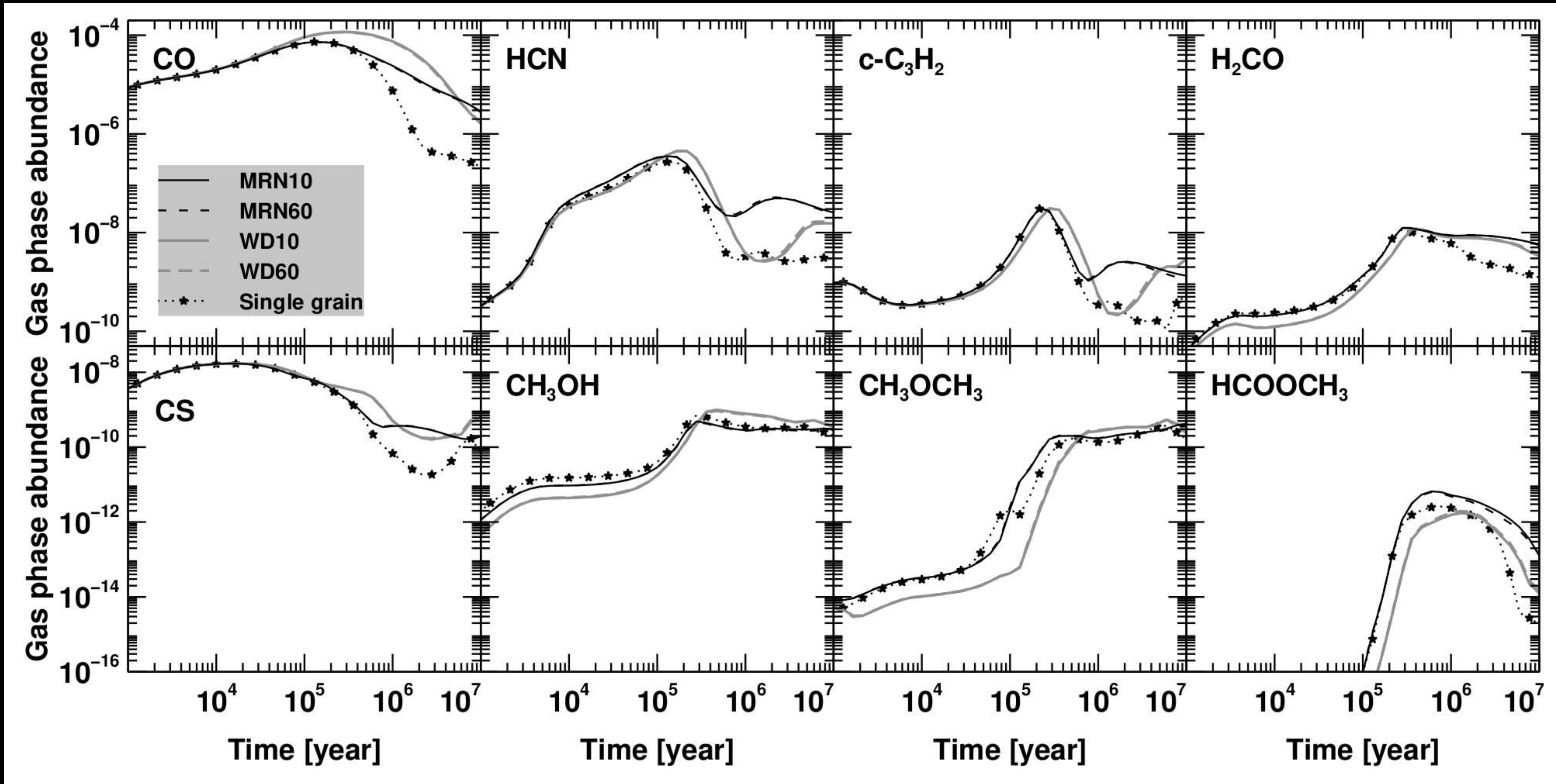
Results: Impact of grain size distribution



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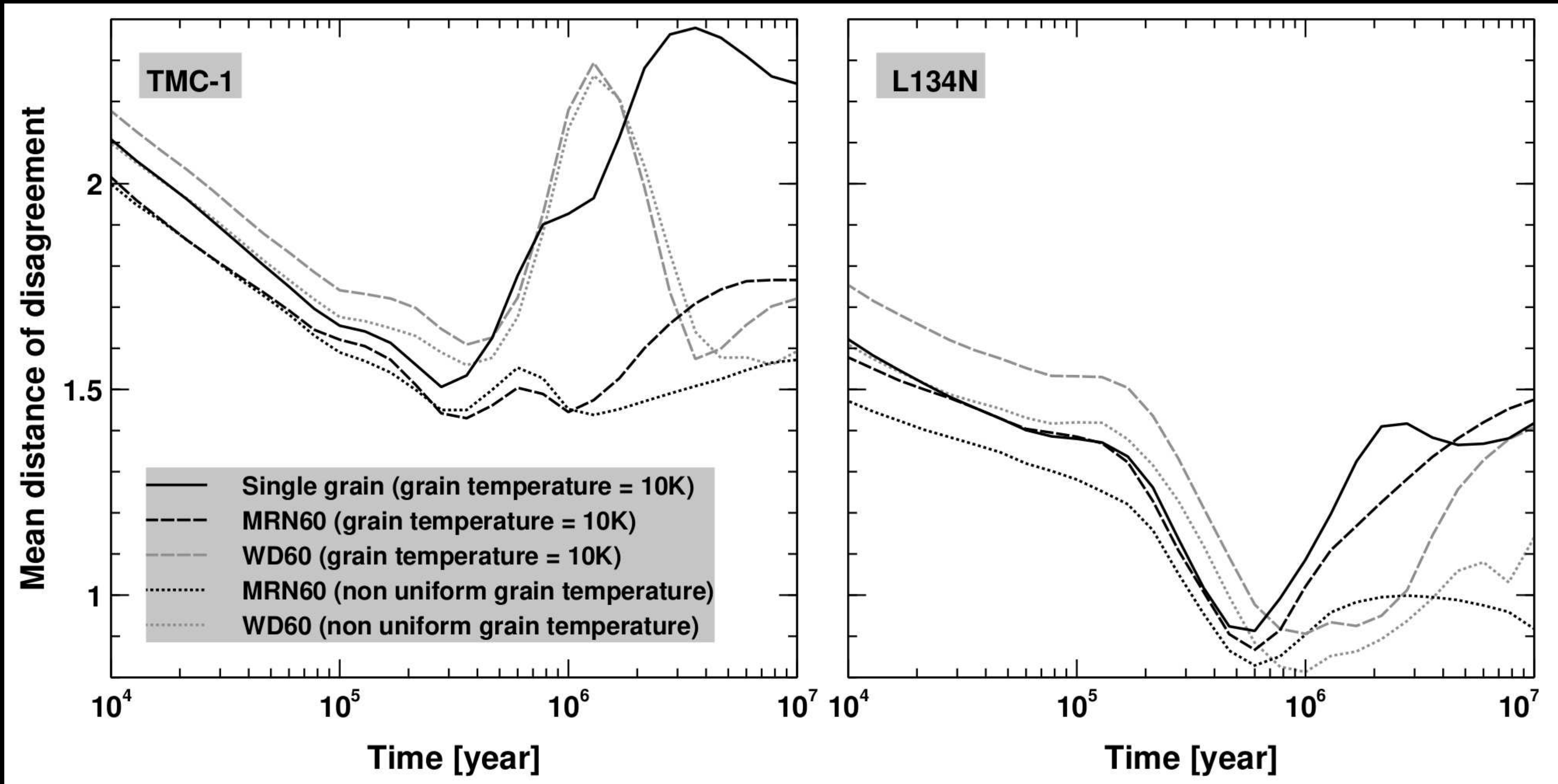
Results: Comparison with observation

$$D(t) = \frac{1}{N_{obs}} \sum_i |[log[n(X_i,t)] - log[n(X_i^{obs})]]|$$

[Wakelam et al. 2006]



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Conclusions

The ice composition is different on different grain sizes. Cosmic ray-induced desorption play an important role in determining ice composition.

The choice of the MRN or the WD distributions strongly affects the abundances of most of the species. The cosmic ray induced desorption is the most effective in the MRN distribution case

Considering a non-uniform surface temperature for the different grain sizes strongly impacts the overall gas and the ice compositions. The difference in the chemical compositions between the smaller and the bigger grains are even stronger

In our model, methanol is very abundant on small grains and more desorption from the small grains could account for the observed gas phase abundances. Similar results were found for CH_3O, CH_3CCH, HCOOH, and CH_3OCH_3

The MRN distribution gives a better agreement with TMC-1 observations considering a uniform or a non-uniform dust temperature while both the MNR and the WD distributions give a better agreement with L134N with a non-uniform dust temperature

Thank You

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