Revised Models for Cosmic Ray Induced Desorption in Dense Clouds

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Outline of the talk

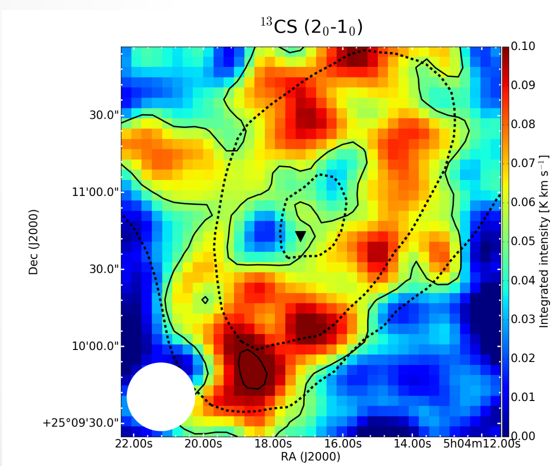
1. Introduction

2. Impact of time-dependent ice abundances on the efficiency of desorption (Sipilä et al. 2021, ApJ 922, 126)

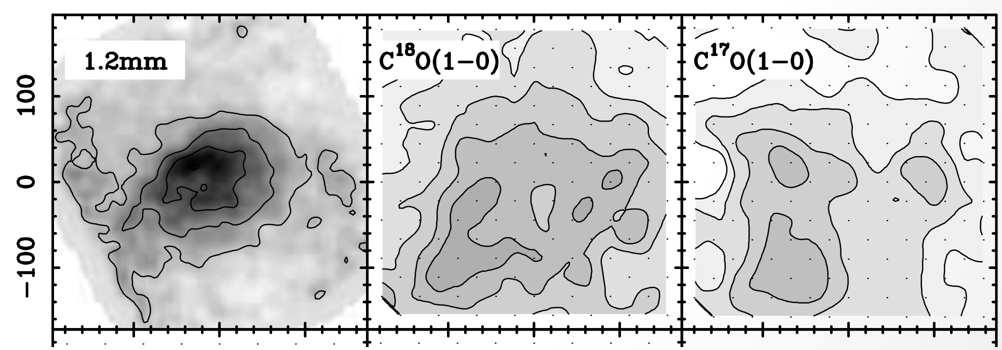
3. New desorption models accounting for variable grain temperatures (in prep.)

4. Conclusions

- collisions of gaseous molecules with interstellar dust grains eventually lead to the formation of ice mantles on the grain surfaces, as the molecules are adsorbed onto the grains
- chemical reactions occurring on (and in) the ice lead to the synthesis of new molecules, which can subsequently be desorbed
- it is clear from observations that desorption must occur: observations point to "valleys" as opposed to "holes" in the abundance distributions of various molecules



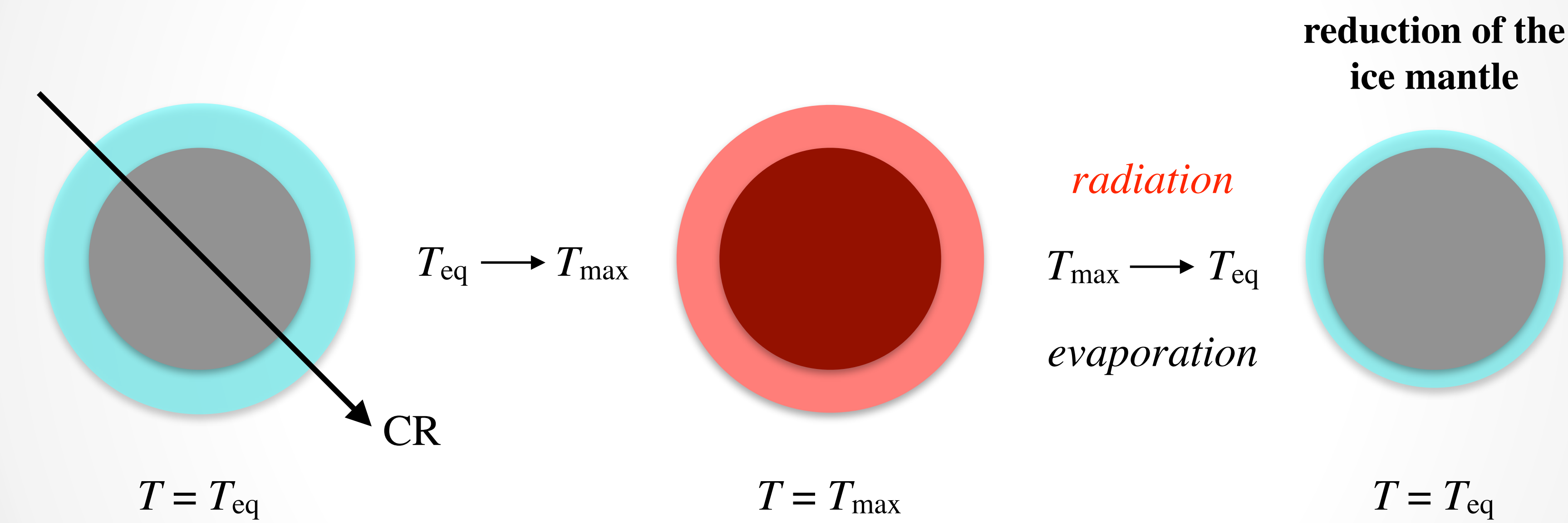
Spezzano et al. (2017)



Tafalla et al. (2002)

- there are several possible desorption mechanisms: thermal desorption, photodesorption, reactive desorption...
- desorption can also be induced by cosmic rays (CRs), via whole-grain heating or localized phenomena (sputtering)
- here we describe a new model for desorption induced by CRs via whole-grain heating, which is here denoted as CRD (cosmic ray induced desorption) for brevity

- consider a CR passing through a grain:



- the efficiency of CRD depends on the ratio of the cooling time of the grain to the average time interval between successive CR strikes

- in a rate-equation gas-grain chemical model, one expresses the CR desorption rate coefficient of a molecule *i* on the grain surface as

$$k_{\mathrm{CR}}(i) = f(a, T_{\mathrm{max}})\, k_{\mathrm{therm}}(i, T_{\mathrm{max}})$$

- almost all current chemical models that consider CRD adopt the description of Hasegawa & Herbst (1993; HH93), who assumed that the ice **consists of a homogeneous layer of a CO analog** and that $\boldsymbol{T_{\mathrm{max}} = 70}$ **K**, which leads to a constant cooling time of $\mathbf{10^{-5}}$ **s** for 0.1 μm grains

- they derived a CR strike interval of $\mathbf{3.16 \times 10^{13}}$ **s**, which yields $f(0.1\ \mu\mathrm{m}, 70\ \mathrm{K}) = \mathbf{3.16 \times 10^{-19}}$

- it is known that interstellar ices are not homogeneous, but consist instead of a variety of molecules such as H_2O, CO, NH_3...

- we reformulated the grain cooling time by considering a time-dependent ice composition:

$$\tau_{\rm cool} = \frac{E_{\rm th}}{\dot{E}} = \frac{E_{\rm th}}{\dot{E}_{\rm evap} + \dot{E}_{\rm rad}}$$

$$\dot{E}_{\rm evap} = N_{\rm des} \sum_i k_{\rm B} E_b(i)\, \theta(i)\, \nu(i)\, \exp(-E_b(i)/T_{\rm max})$$

$$\dot{E}_{\rm rad} = 4\pi a^3 q_{\rm abs} \sigma T_{\rm max}^6$$

- this approach is more accurate than the HH93 one as it is able to describe time-dependent variations in grain cooling time due to the temporally varying ice composition

L85: Léger et al. (1985); P18: Padovani et al. (2018)

Table 2. Values of the transient grain heating interval $\tau_{\rm heat}$ (in seconds) considered in this paper. The scaling factors used to obtain the Fe flux from the proton flux are indicated on the header row. The assumed CR energy range is 0.026 to 70 MeV nucleon^{-1}.

Visual extinction [mag]	P18H $\times 3.1 \times 10^{-4}$	P18L $\times 3.1 \times 10^{-4}$	L85 $\times 1.6 \times 10^{-4}$
0	1.34×10^{11}	4.84×10^{12}	$3.35 \times 10^{13\,(a)}$
5	7.98×10^{11}	8.05×10^{12}	3.07×10^{13}
10	1.15×10^{12}	9.72×10^{12}	3.21×10^{13}
15	1.47×10^{12}	1.11×10^{13}	3.38×10^{13}
30	2.40×10^{12}	1.47×10^{13}	3.97×10^{13}
50	3.62×10^{12}	1.87×10^{13}	4.76×10^{13}
100	6.80×10^{12}	2.74×10^{13}	6.39×10^{13}

- we also considered variations of the heating interval adopting different CR spectra
- our new model uses only quantities included in any rate-equation based gas-grain chemical model that tracks the ice composition time-dependently, making it easy to apply; one only needs to replace the (constant) $f(a,T_{\rm max})$ term by $\tau_{\rm cool}/\tau_{\rm heat}$ in the CRD rate coefficients

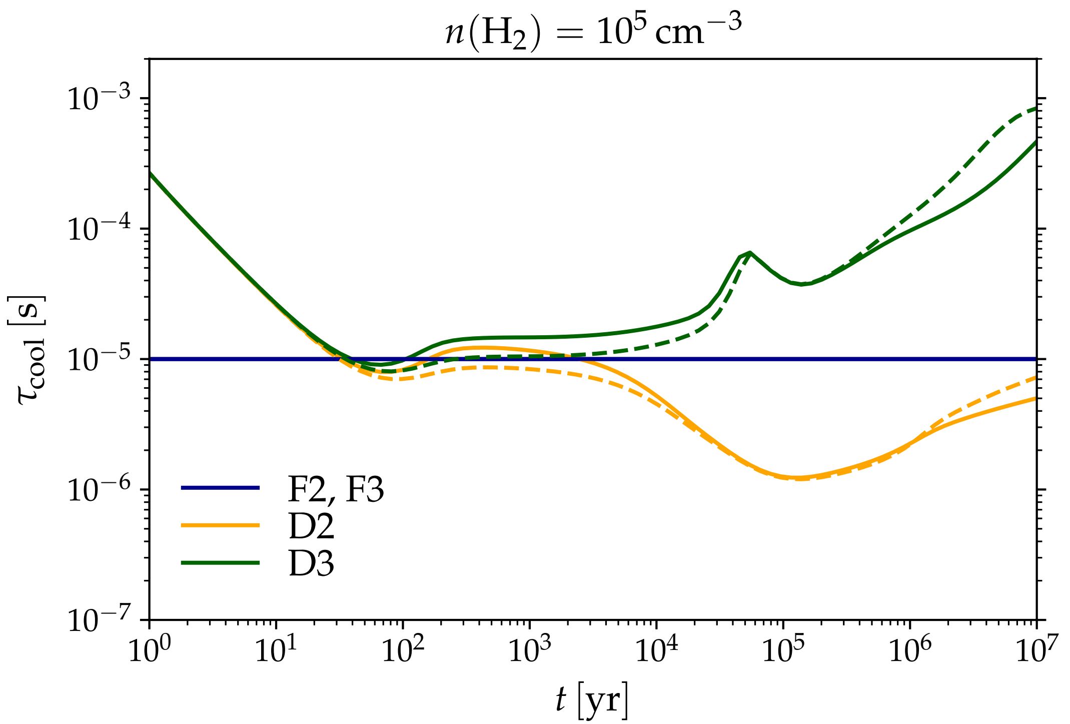
- we studied the effect of our new CRD model on the results of chemical simulations in physical conditions corresponding to molecular clouds and cores, adopting **two-phase** and **three-phase** gas-grain models

Model	Description
F2	Fiducial model, two-phase ice chemistry, grain cooling following HH93
D2	As F2, but with dynamic grain cooling
F3	Fiducial model, three-phase ice chemistry, grain cooling following HH93
D3	As F3, but with dynamic grain cooling

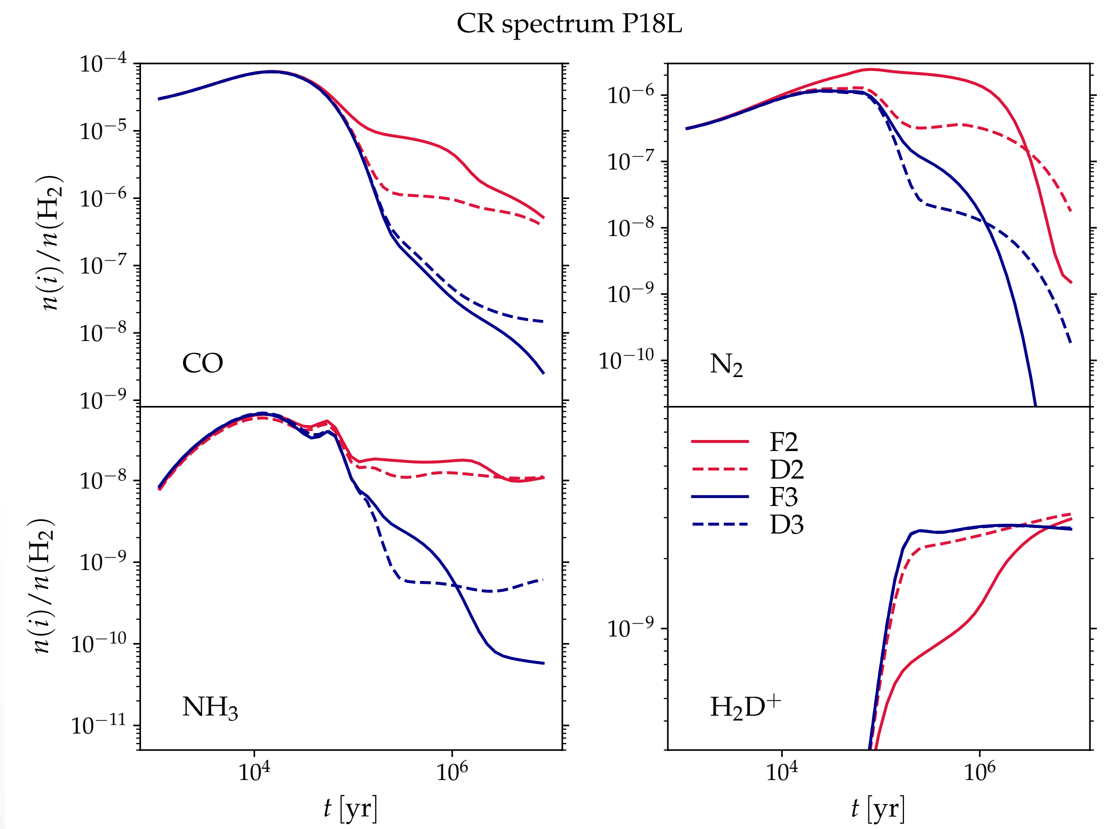
Table 1. Binding energies of the chemical species that participate in the cooling.

Species	Binding energy [K]
H	450
C	800
N	800
CH	925
N_2	1000
CO	1150
CH_4	1300
O	1390
oNH_3	5534
pNH_3	5534
oH_2O	5700
pH_2O	5700
others	3000

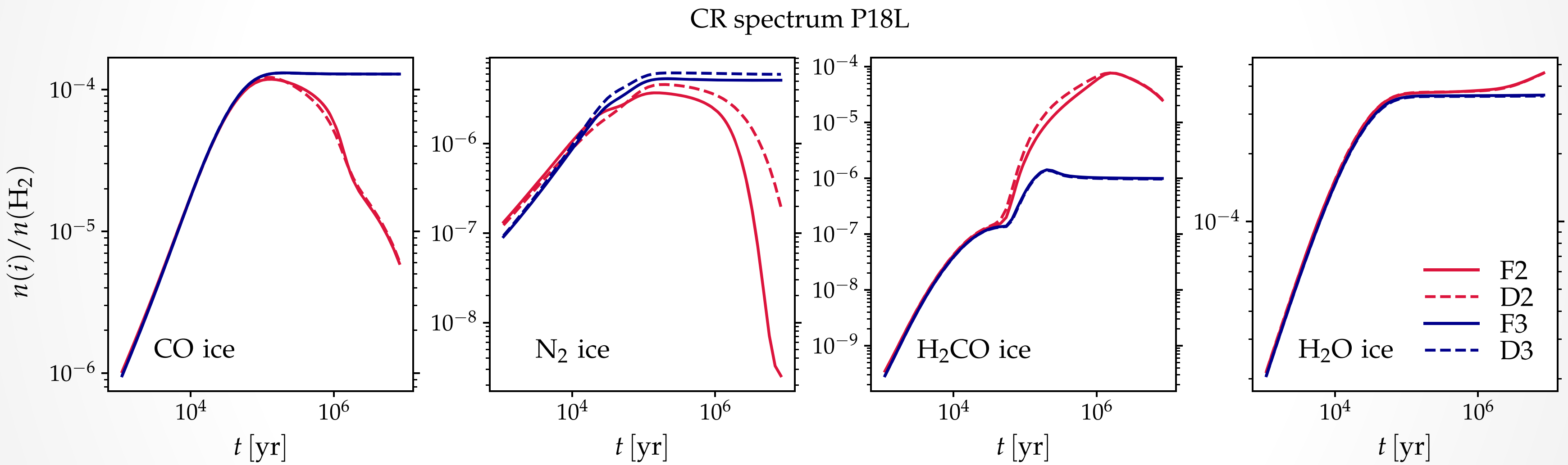
- grain cooling time in HH93 vs. our new model, at constant density



- abundances of selected **gas-phase** molecules as a function of time in a 0D physical model ($n(H_2) = 10^5$ cm^{-3}, T = 10 K, A_V = 10 mag)



- total ice abundances **do not change significantly** when switching from static to dynamic CRD



- we have developed a new numerical description of CRD which accounts for time-dependent changes in ice composition, and describes the desorption process well in a wide variety of physical conditions

- we found that using dynamic CRD **decreases** gas-phase abundances in two-phase chemical models, but **increases** them in three-phase chemical models

- ice abundances are not strongly affected when switching from static to dynamic CRD, though the effects are (marginally) larger toward lower volume densities

- we have so far considered models with a fixed transient maximum temperature; in reality one expects instead a spectrum of $T_{\max}$ values

- we are currently working on modifying the 2021 CRD model by simulating the effect of variable $T_{\rm max}$

- this requires a change in the CRD rate coefficient:

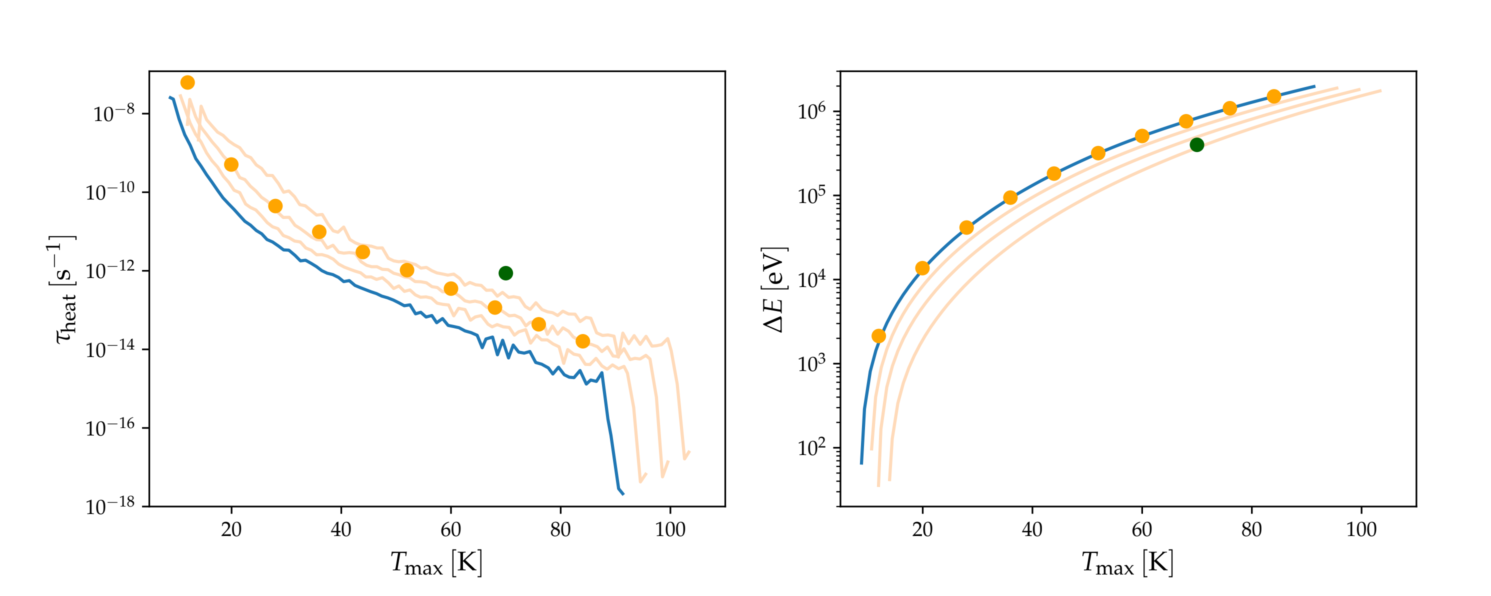
2021: $$k_{\rm CRD}(i) = \min\left(f(a, T_{\rm max})\, k_{\rm therm}(i, T_{\rm max}), \tau_{\rm heat}^{-1}\right)$$

2022: $$k_{\rm CRD}(i) = \underline{\sum_j} \min\left(f(a, T_{\rm max}^j)\, k_{\rm therm}(i, T_{\rm max}^j), (\tau_{\rm heat}^j)^{-1}\right)$$

- in addition, we require calculations of the frequencies of the heating events associated with different CR species

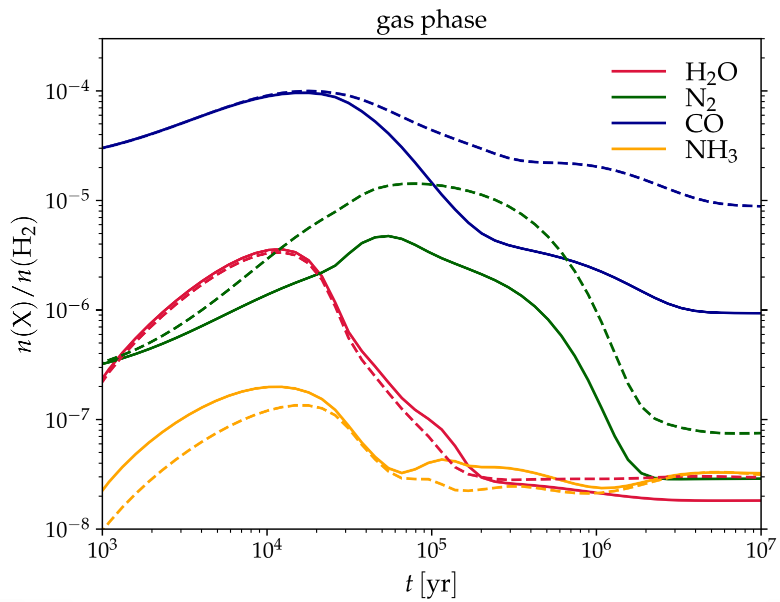
- for our initial simulations, we adopted the heating frequency & T_{max} data from Kalvāns (2022, ApJS 259, 68)

- values calculated using the Padovani et al. (2018) "High" model

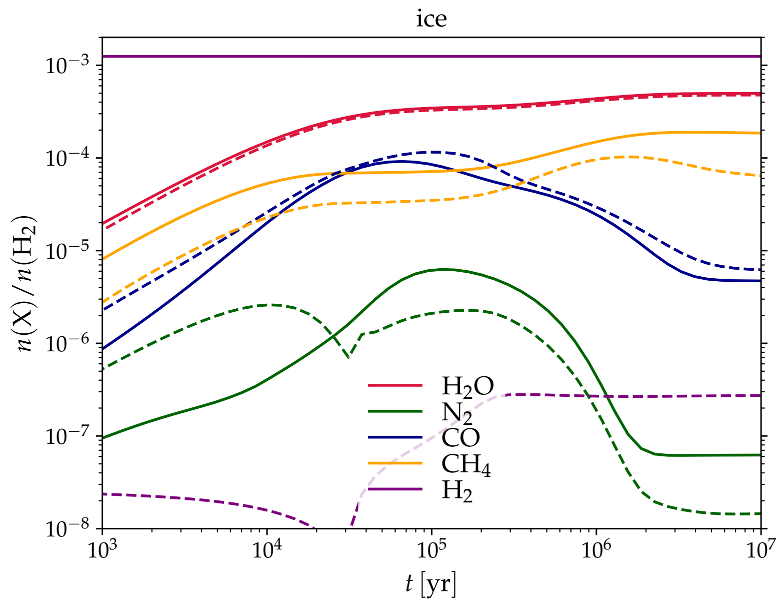


- sample of gas-phase abundances as a function of time at constant density & kinetic temperature ($n(H_2) = 10^5$ cm^{-3}, $T = 10$ K)

- cosmic ray ionization rate set to **10^{-16} s^{-1}**, following the adoption of P18H



- ice abundances at the same physical conditions



CONCLUSIONS

- the dynamic CRD model (Sipilä et al. 2021) allows for a more accurate representation of CRD, compared to earlier models where the time-dependent ice content is not taken into account, using only the quantities that are inherently included in any gas-grain chemical model

- we are working on revising the 2021 model, where $T_{\rm max}$ is allowed to vary

- the first results from the latest model already indicate potential solutions to some outstanding issues, such as the "H_2 problem"

- the main caveat is that the simulations results are highly dependent on the choice of the CR spectrum, and on how the CR flux is attenuated

- going even further, one may consider the effect of variations in ice thickness etc.