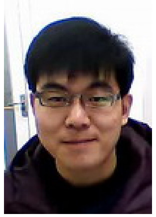
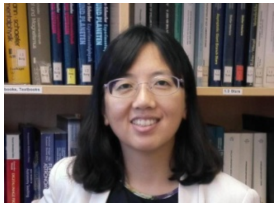
Modeling the effects of grain motion, charging and size distribution to interstellar chemistry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Introduction

Discrepancies between obs. and astro-chem. models persist. E.g., we also found in a sample of MSFRs:
(*Ge, He, Chen & Takahashi   2014MNRAS.445.1170G*)

(**1.28×10^{-7}**)

X(**CH_3OH**) : X(**$HCOOCH_3$**) : X(**CH_3OCH_3**) = 1.00 : **0.42 : 2.36**

But in the molecular cloud warm-up chemical model, the predicted ratios were

(**10^{-5}**)

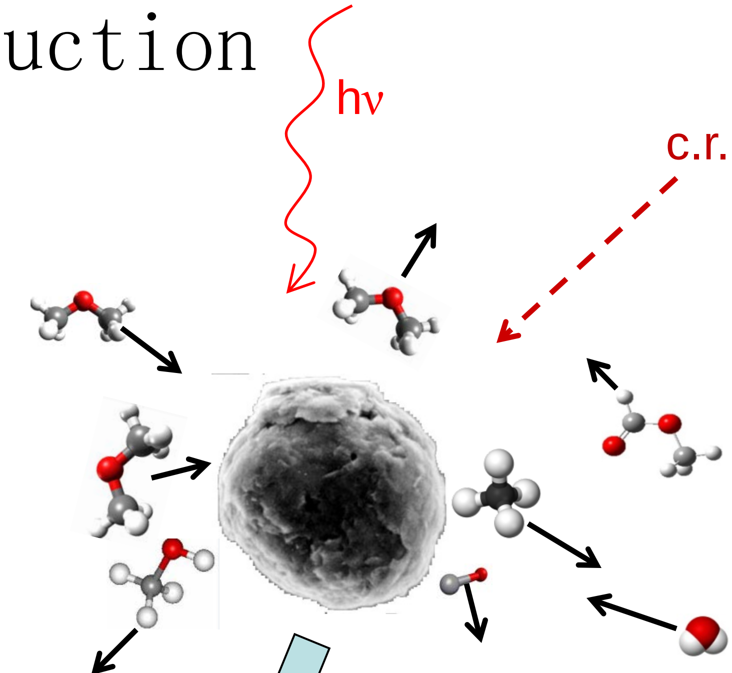
X(**CH_3OH**) : X(**$HCOOCH_3$**) : X(**CH_3OCH_3**) ≈ 1.00 : **0.01 : 0.006**

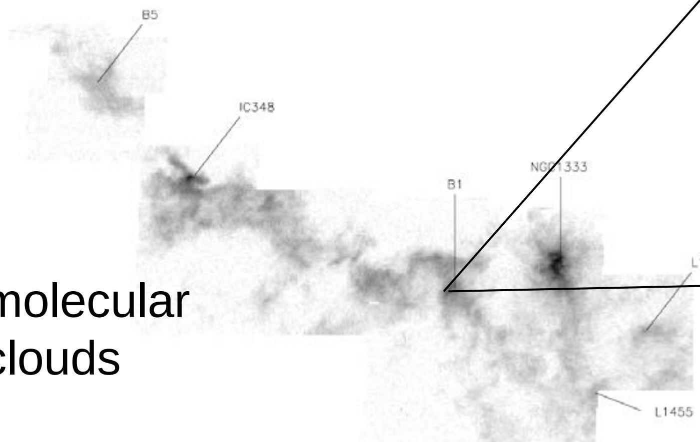
(Garrod 2013ApJ...765...60G)

More examples in: Wakelam+ 2010SSRv..156...13W
Caselli & Ceccarelli 2012A&ARv..20...56C

Introduction

Various ways to improvement:





molecular clouds

Cloud parameters in DC, hot cores, discs, …

Reaction networks & parameters (e.g., many Brazilian talks)

Physics of surface processes & grain properties (e.g., Chang's talk)

Physics in gas-grain interaction

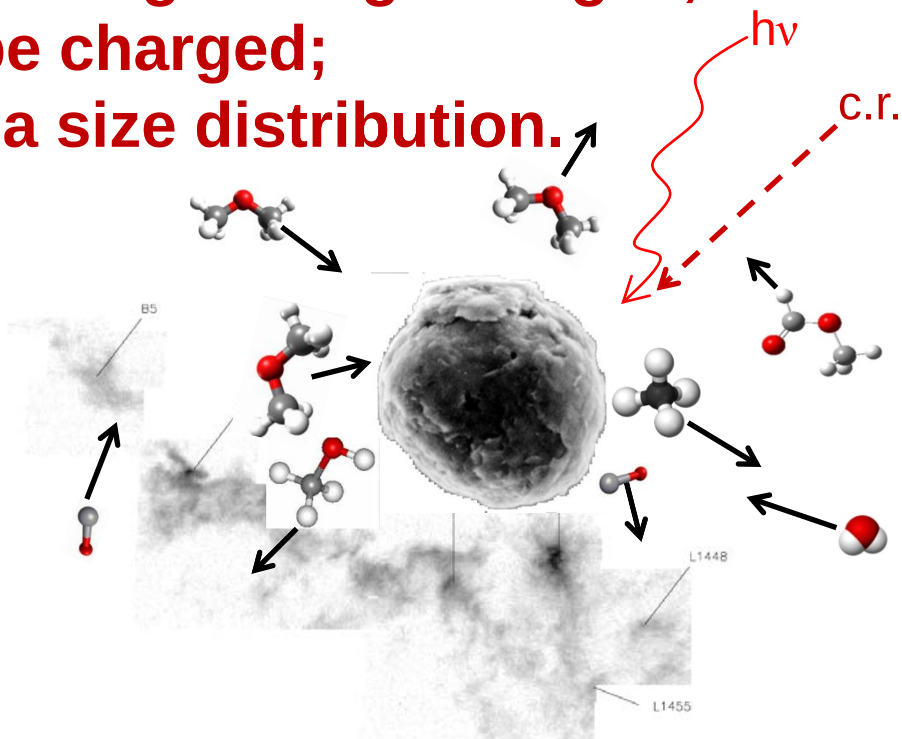
Introduction

How to improve the gas-grain interaction?

In a classical picture of gas-grain interaction:
neutral grains of a single size standing still in gas.

In reality:

1) **Grains are moving through the gas;**
2) **Grains can be charged;**
3) **Grains have a size distribution.**



1. Chemical effects of grain motion+Cha

Grains are moving through the gas in turbulent clouds (Yan+ 2004ApJ...616..895Y):

Grain acceleration due to:

- Hydro-drag
- Gyro-resonance (in turbulent B field)

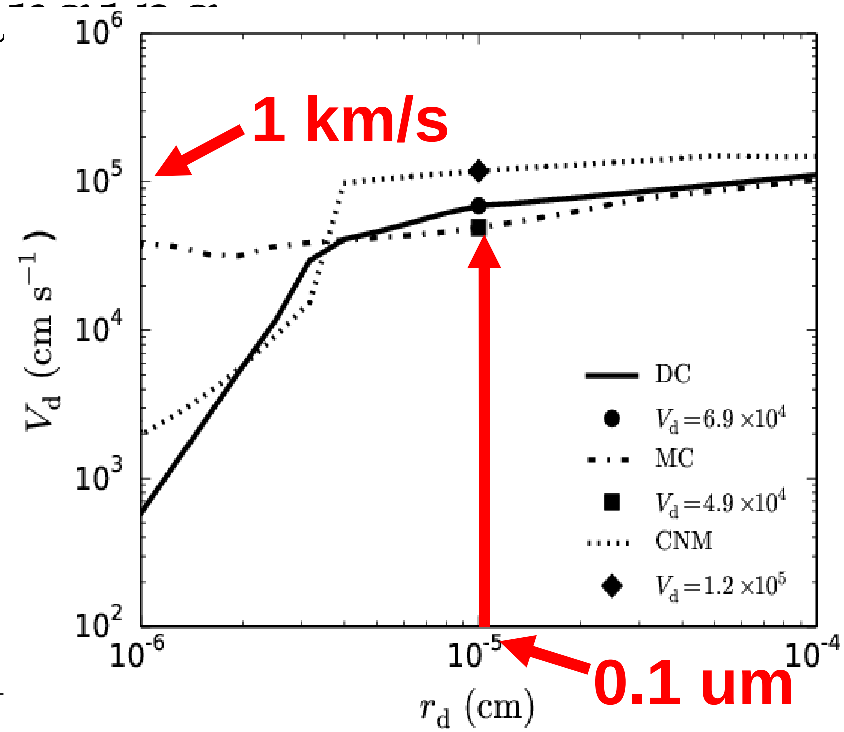


Table 1

Model (1)	T (K) (2)	T_d (K) (3)	n_H (cm^{-3}) (4)	V_d (km s^{-1}) (5)	A_V (mag) (6)	χ (χ_0) (7)
DC	10	10	10^4	0	7.5	1.0
DCv	10	10	10^4	0.69	7.5	1.0
MC	25	15	300	0	2.5	1.0
MCv	25	15	300	0.49	2.5	1.0
CNM	100	18	30	0	0.0	1.0
CNMv	100	18	30	1.20	0.0	1.0

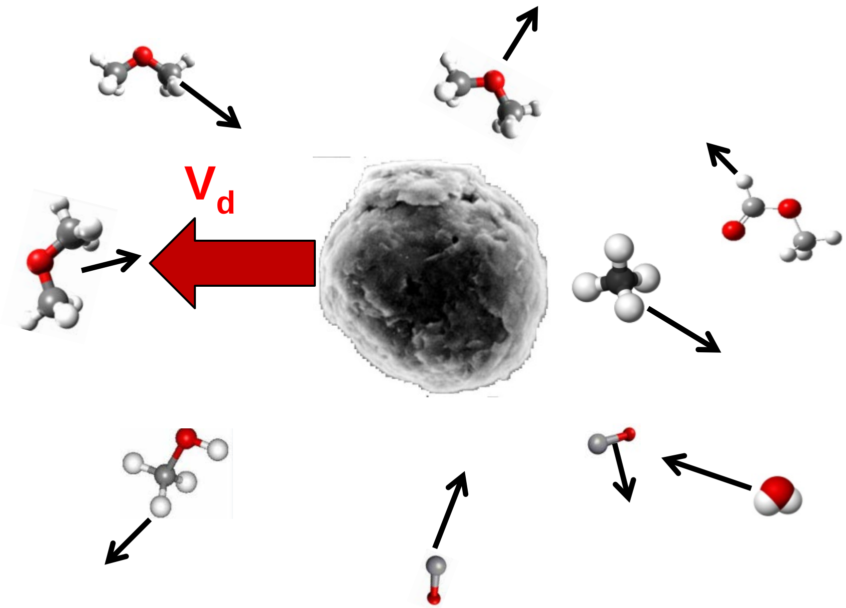
Dark clouds

Molecular clouds

Cold neutral medium

1. Chemical effects of grain motion+Charging

Grains motion → gas accretion



Accretion speed increases:

$$V_{\rm imp}(i) = V_{\rm t}(i) = \sqrt{8k_{\rm b}T/(\pi m_i m_{\rm p})}.$$

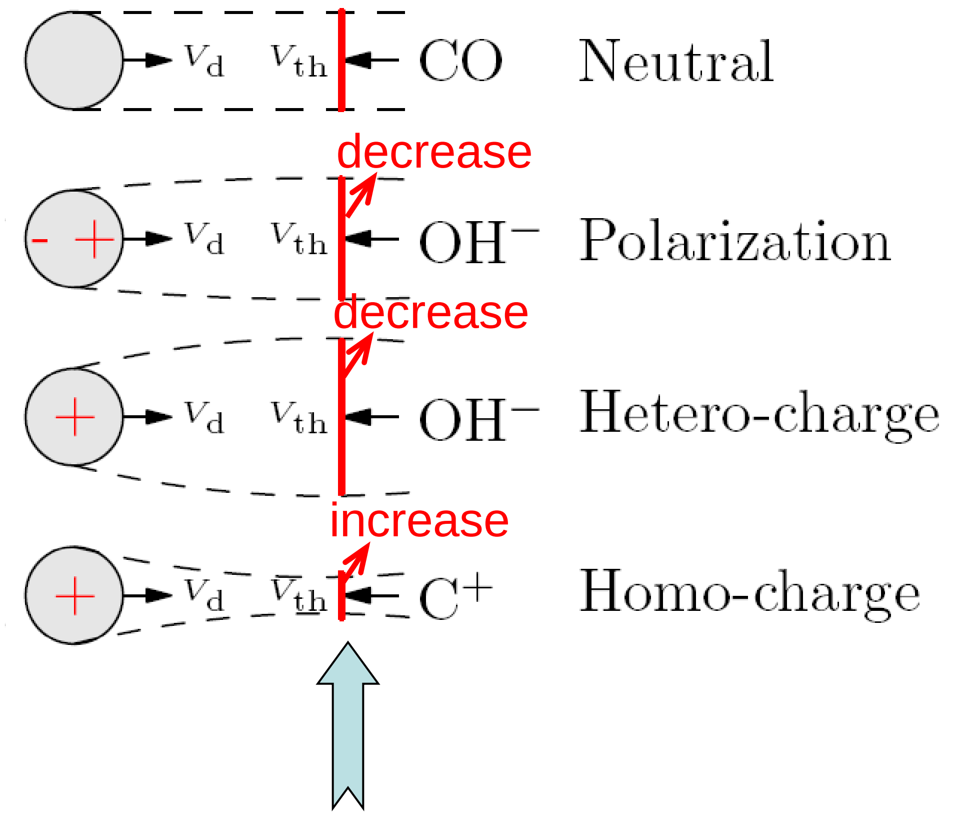
$$V_{\rm imp}(i) = \sqrt{V_{\rm d}^2 + V_{\rm t}(i)^2},$$

Accretion cross-section?:

... next page

1. Chemical effects of grain motion+Charging

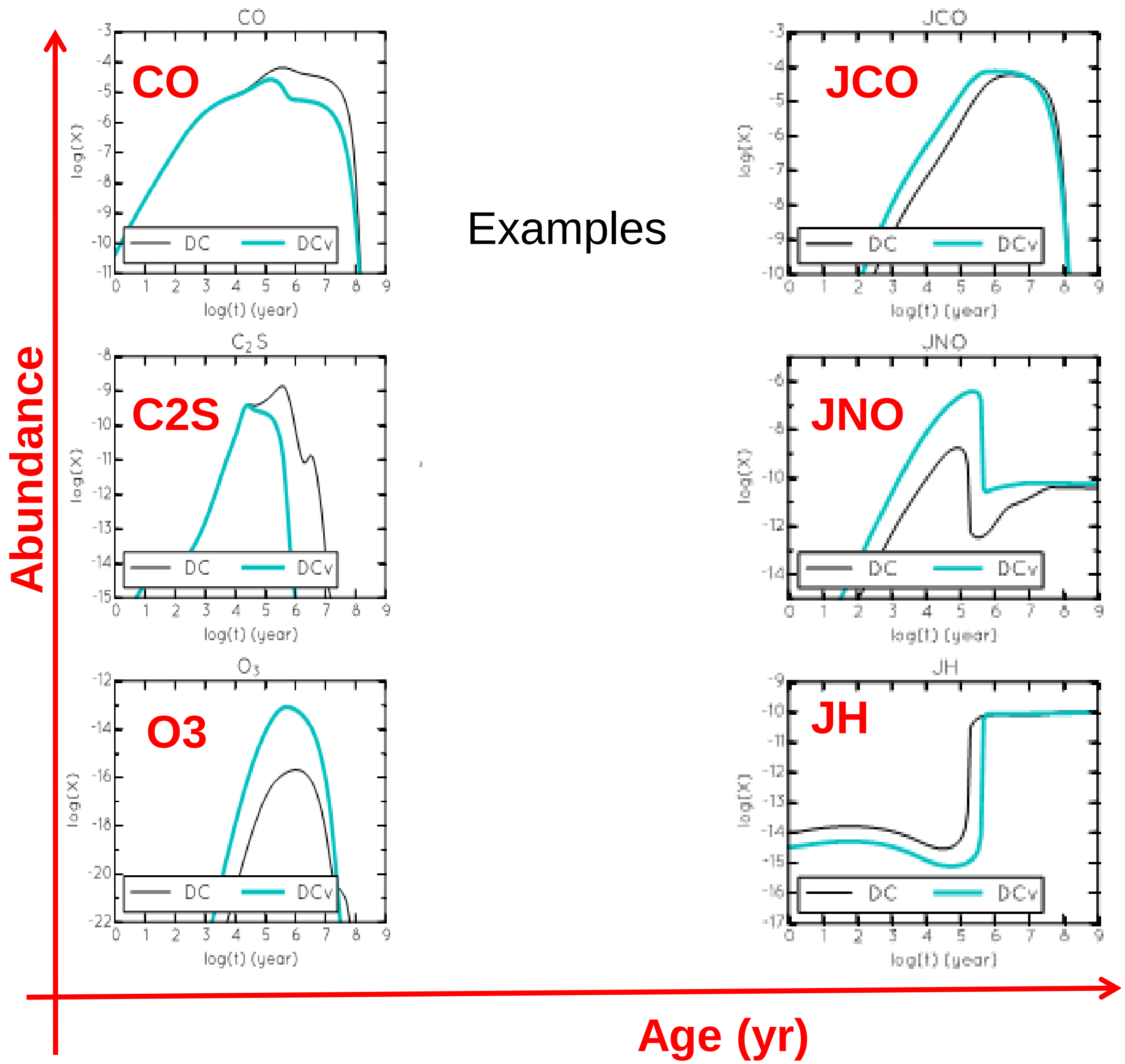
Change of accretion cross section by grain motion:



Draine & Sutin (1987ApJ...320..803D)

1. Results: Dark cloud (DC)

Typical cases in gas phase **Typical cases on grain surface**

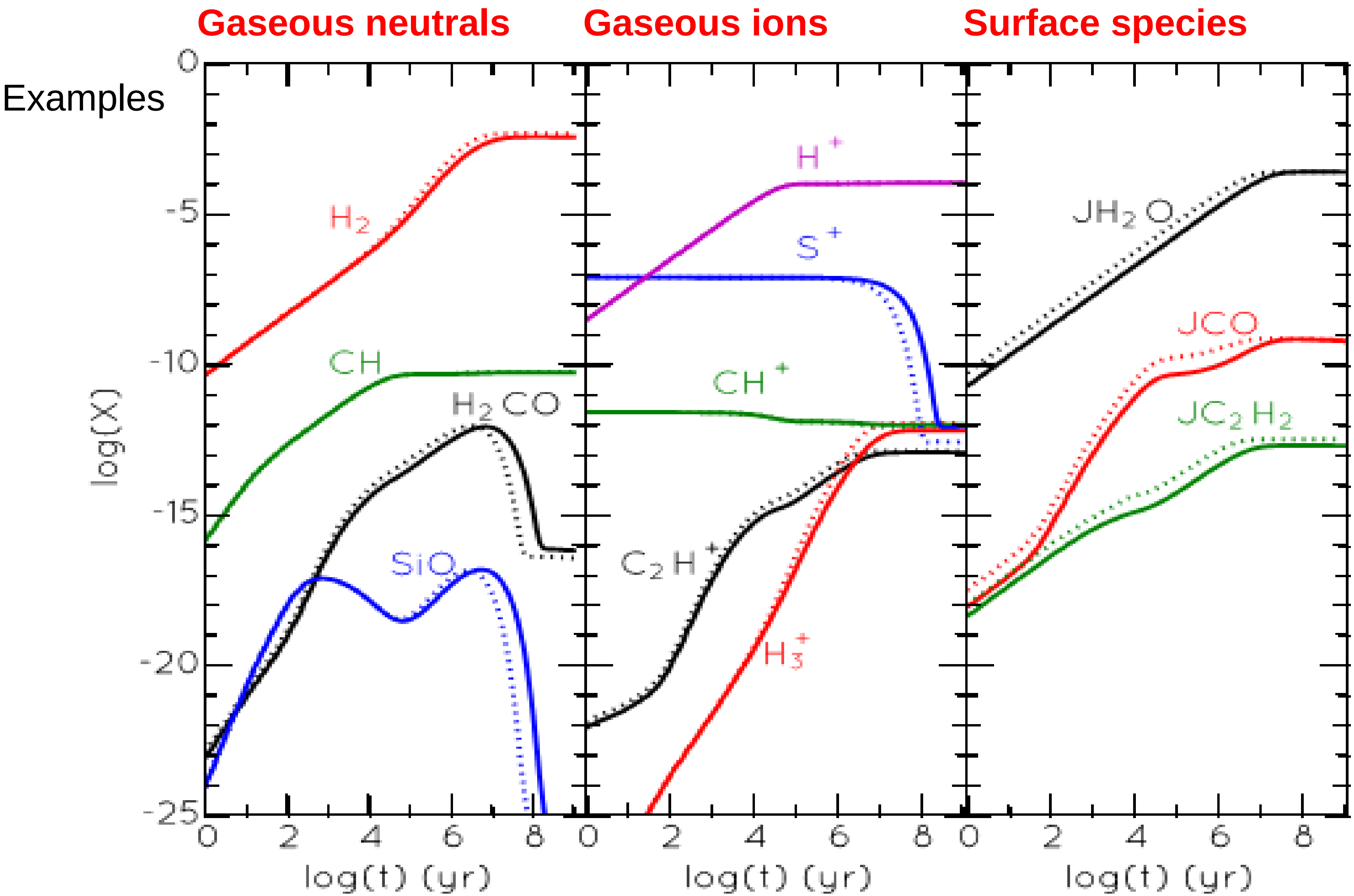


Our ggchem F90 code:
Rate equation,
Single grain size,
Chem. Network:
- 655 species
- 6067 reactions

(Benchmarked against Semenov et al. 2010)

Added physics:
- Grain charging
- Ion accretion
- Photo-electron ejection *(Weingartner & Draine 2001ApJS..134..263W)*

1. Results: Molecular cloud (MC)



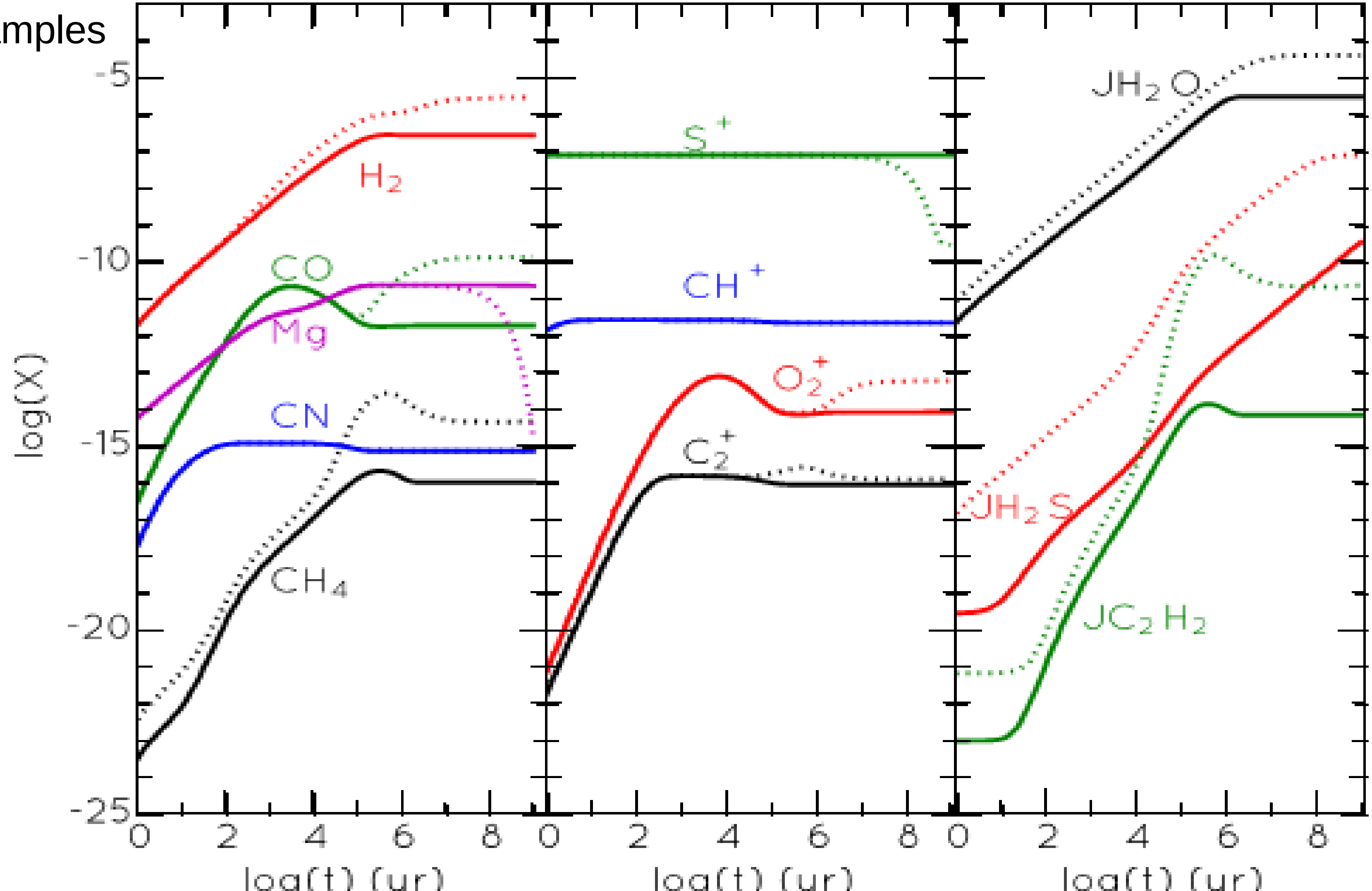
Full line: no grain motion;
Dotted line: with grain motion.

Grain motion effect is small in MC.

1. Results: Cold neutral medium (CNM)

Gaseous neutrals　　Gaseous ions　　Surface species

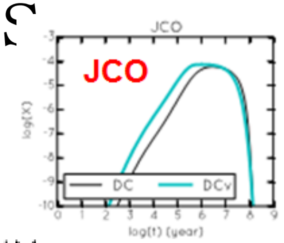
Examples

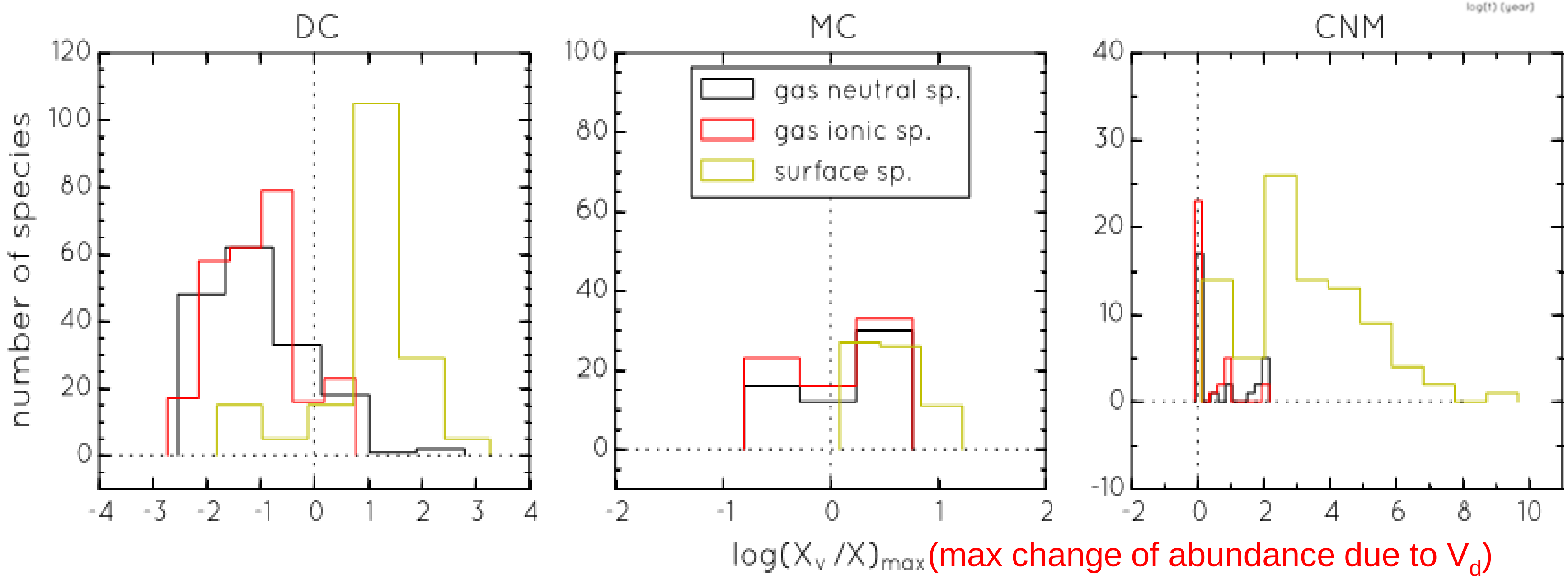


Full line: no grain motion;
Dotted line: with grain motion.

grain motion effect can be quite big.

1. Compare grain motion effects in different cloud models



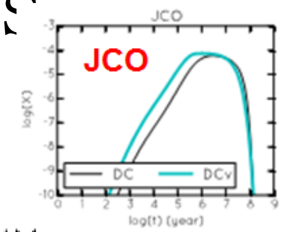


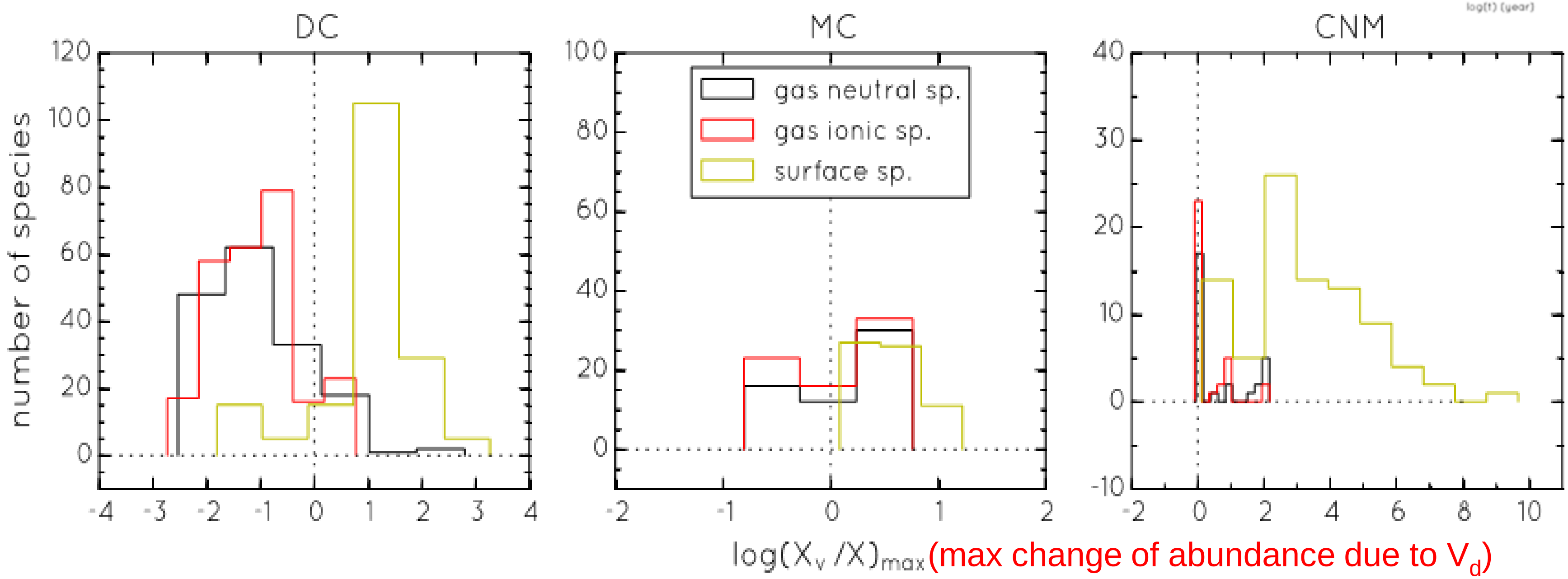
DC:
- **gas phase decreases;**
- **surface increases;**
- **Mostly 1-2 orders of magnitude**

MC:
changes are all small.

CNM:
- **most gas unaffected;**
- **all others increase;**
- **surface -- increase by up to more than 6-7 orders of magnitude**

1. Compare grain motion effects in different cloud models

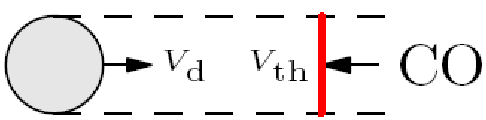


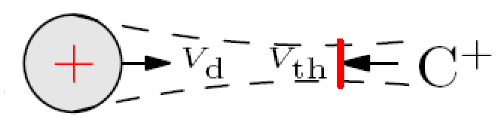


Neutral grains accrete neutral particles.

Intermediate case.

G20+ accrete cations

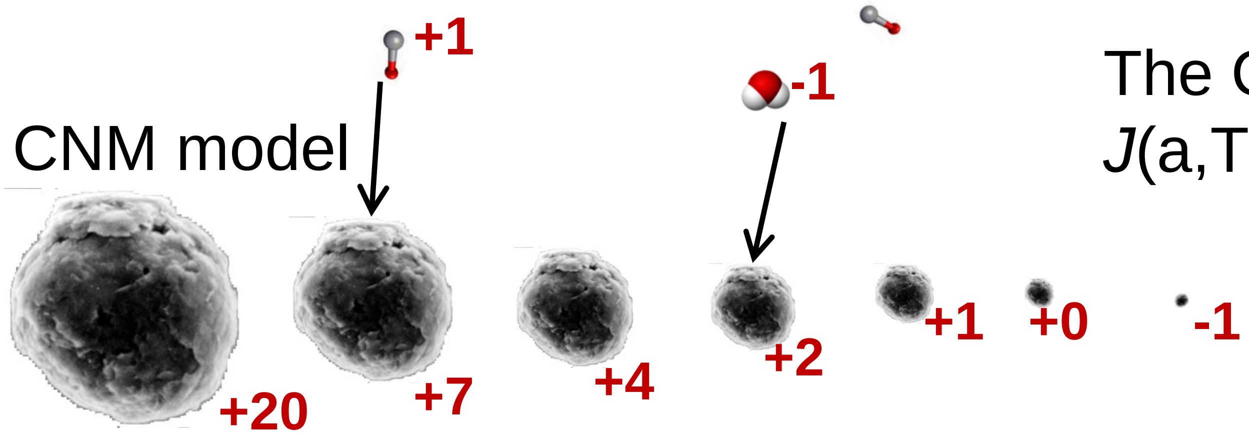




See more details in our paper:
Ge, He & Yan 2016MNRAS.455.3570G

2. Grain charging + size distribution

In a CNM model

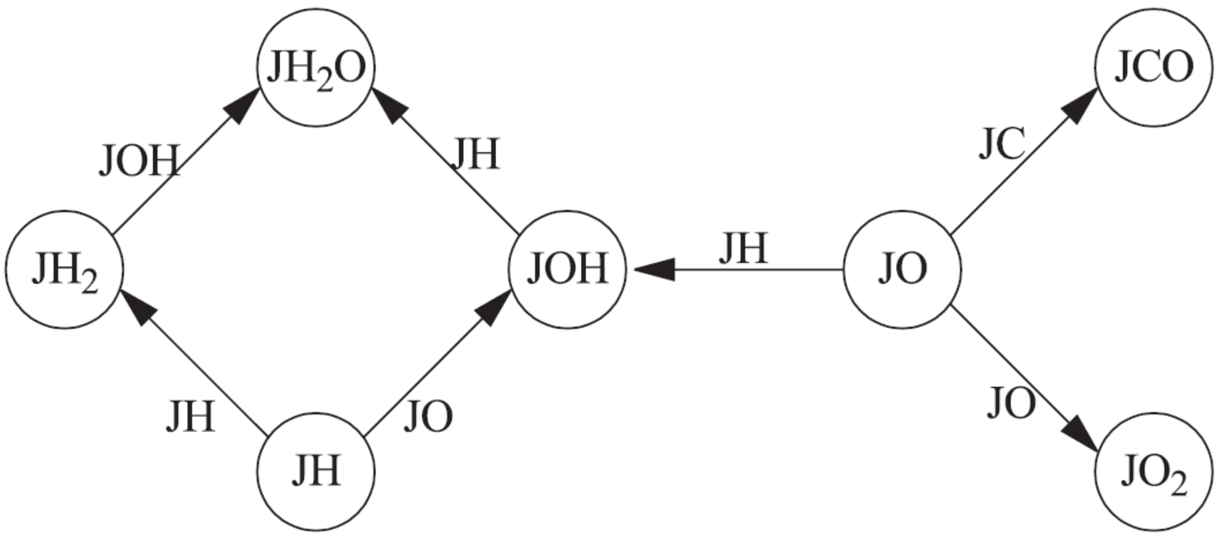


The Coulomb factor:
$J(a, T_d, Z, q_i)$.

Td higher for smaller grains in CNM models → affects surface reactions and desorption!

We expect chemical differentiation among grain sizes.

2. Grain charging + size distribution



Reduced surface network:
Ices related to H, C, O.

Our ggchem F90 code:
Modified rate equation
Full gas network:
- 655 species

Reduced surface network.

Added physics:
- Grain charging
- Ion accretion
- Photo-electron ejection

No grain motion.

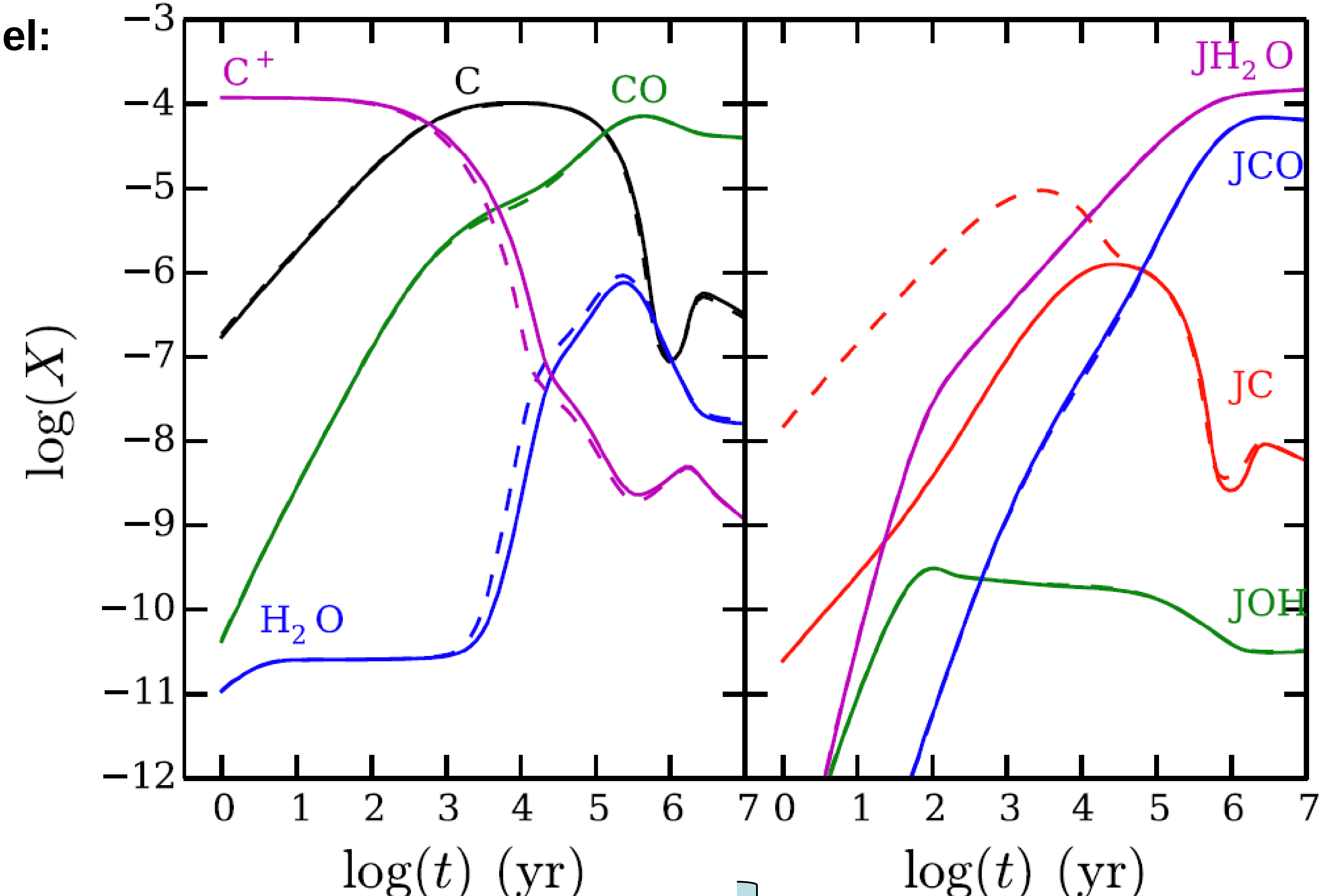
2. Results: Abundances

Dark Cloud **model:**

Change of X:

Gas: < 10

Surface:
can enhance
by > 100



Full line: single size grains
Dashed lines: multiple size grains

Same total grain surface area

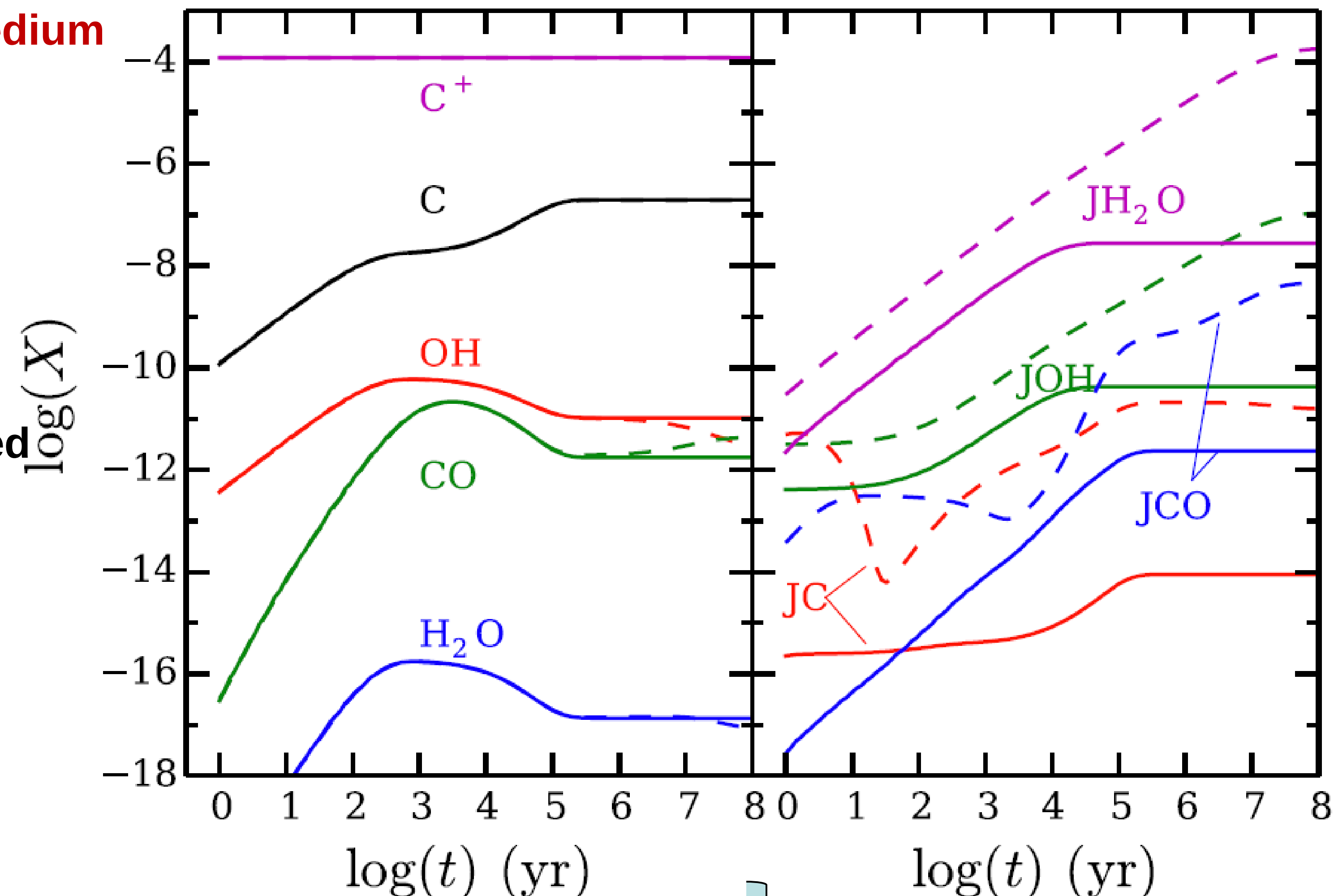
2. Results: Abundances

Cold Neutral Medium model:

Change of X

Gas: < 10

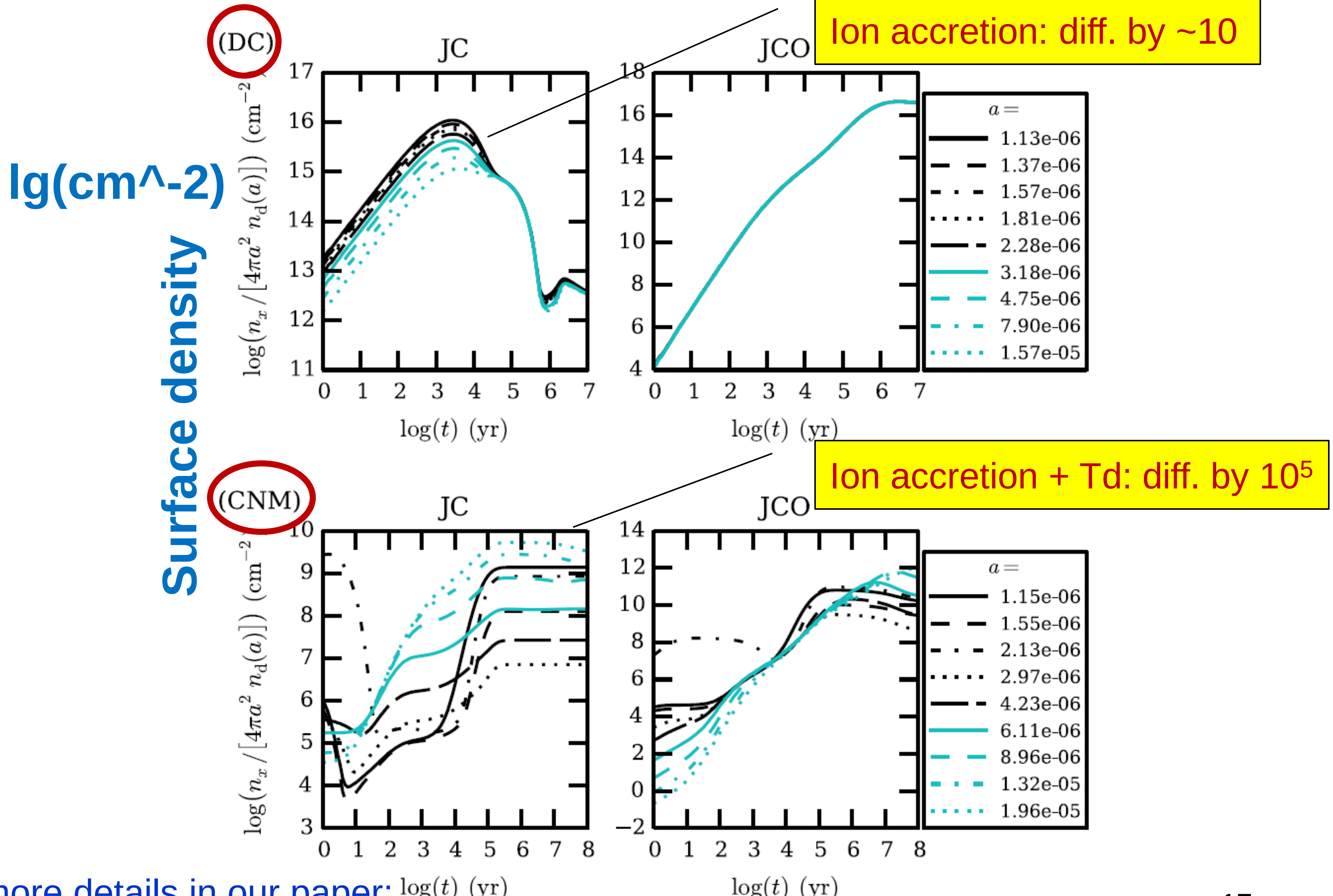
Surface:
Can be enhanced by 10^4



Full line: single size grains
Dashed lines: multiple size grains

Same total grain surface area

2. Results: Areal abundances



See more details in our paper:
Ge, He & Li 2016MNRAS.460..L50G

Take home points

1) Grain motion + charging
➔ abundance changes up to more than 6 orders of magnitude.

2) Grain charging + size distribution
➔ enhance ice abundance up to 4 orders of magnitude.
➔ areal density can be different across grain sizes by up to 5 orders of magnitude.

3) A proper treatment of gas-grain interaction (grain motion, charging, size distribution, Td variation, …) is important!

4) Do the such models explain obs. better? That's our next step…

Thanks!

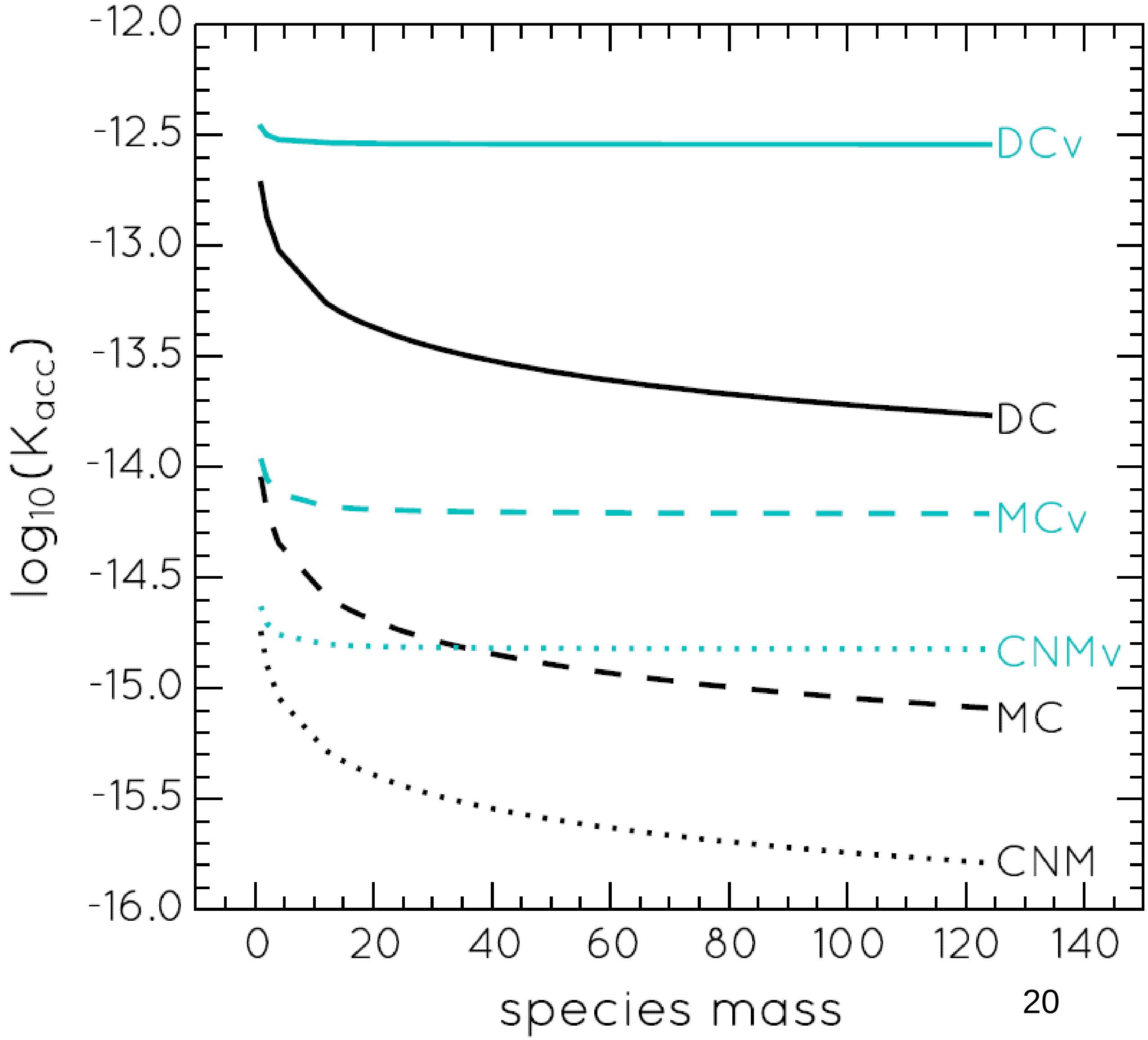
How grain motion affect accretion?

Accretion of
neutral species:

1) Enhanced;

2) Heavy species enhanced more;

3) More enhanced DC model than in MC or CNM.



How and how fast do grains move?

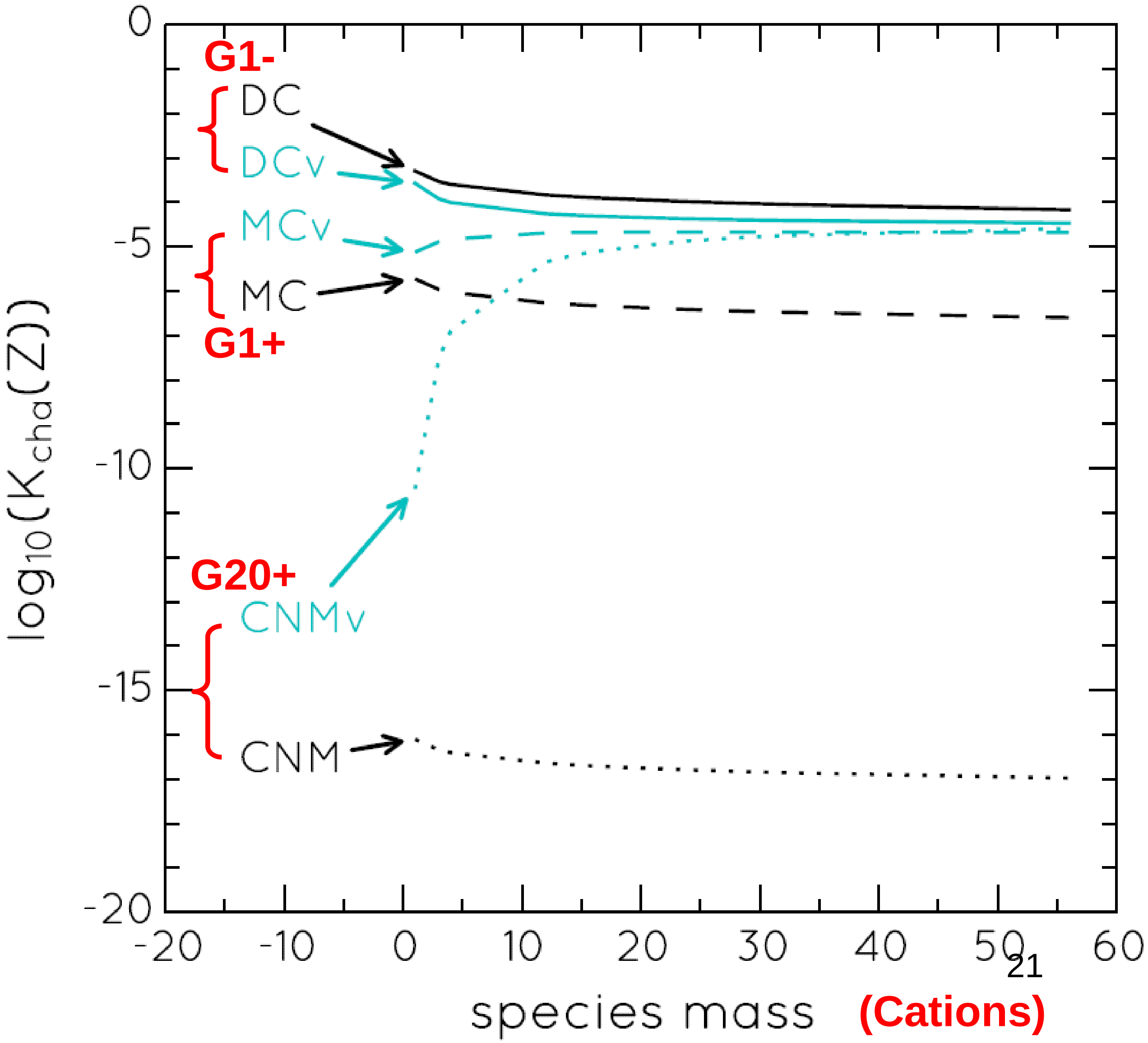
Accretion of

ionic species:

1) Weakened in DC;

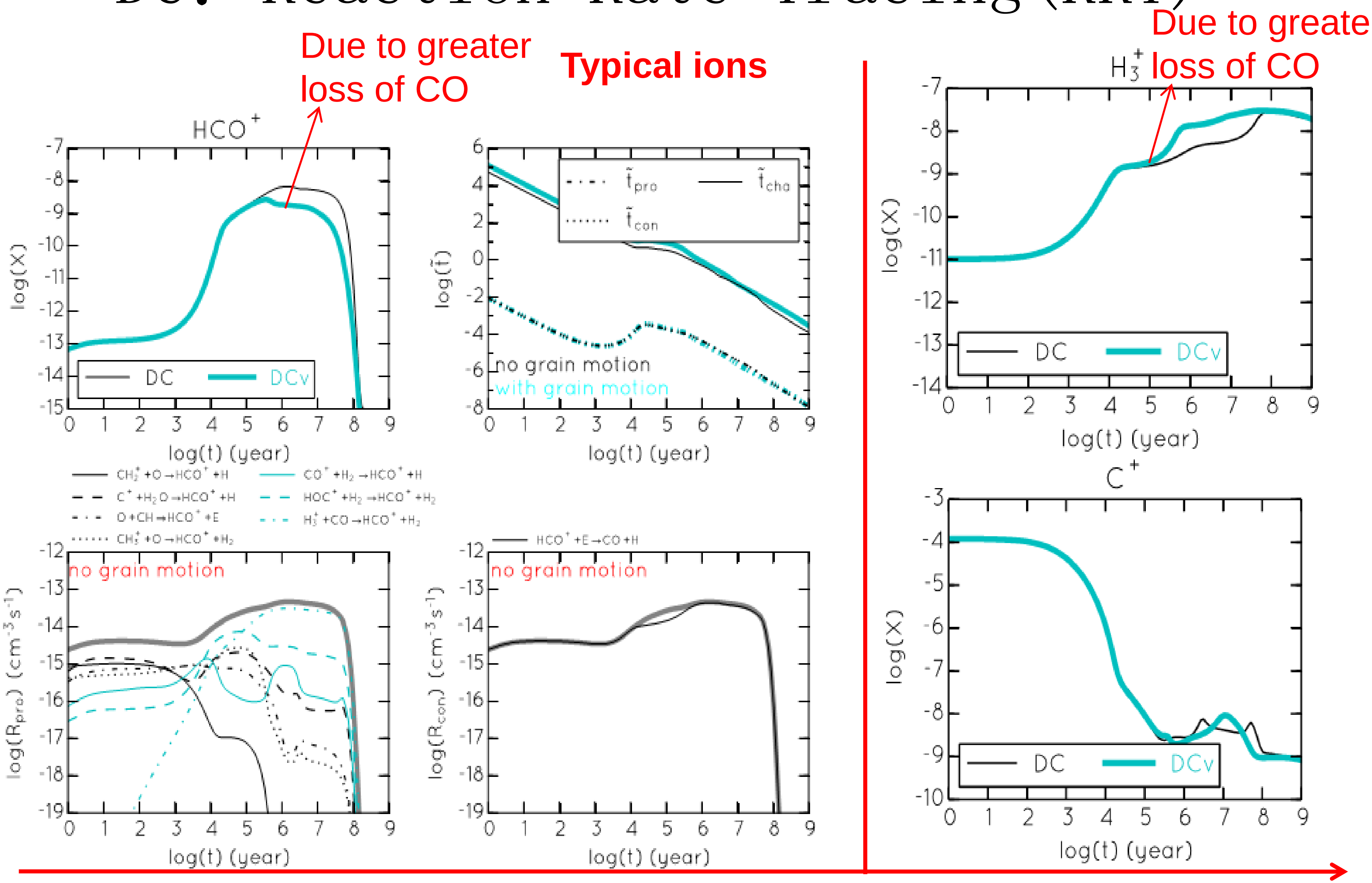
2) Enhanced in MC;

3) Greatly enhanced in CNM.



DC：Reaction Rate Tracing(RRT)

Typical ions



Age (yr)

Ge et al. 2015MNRAS.455.3570G

Average grain charges for different grain sizes