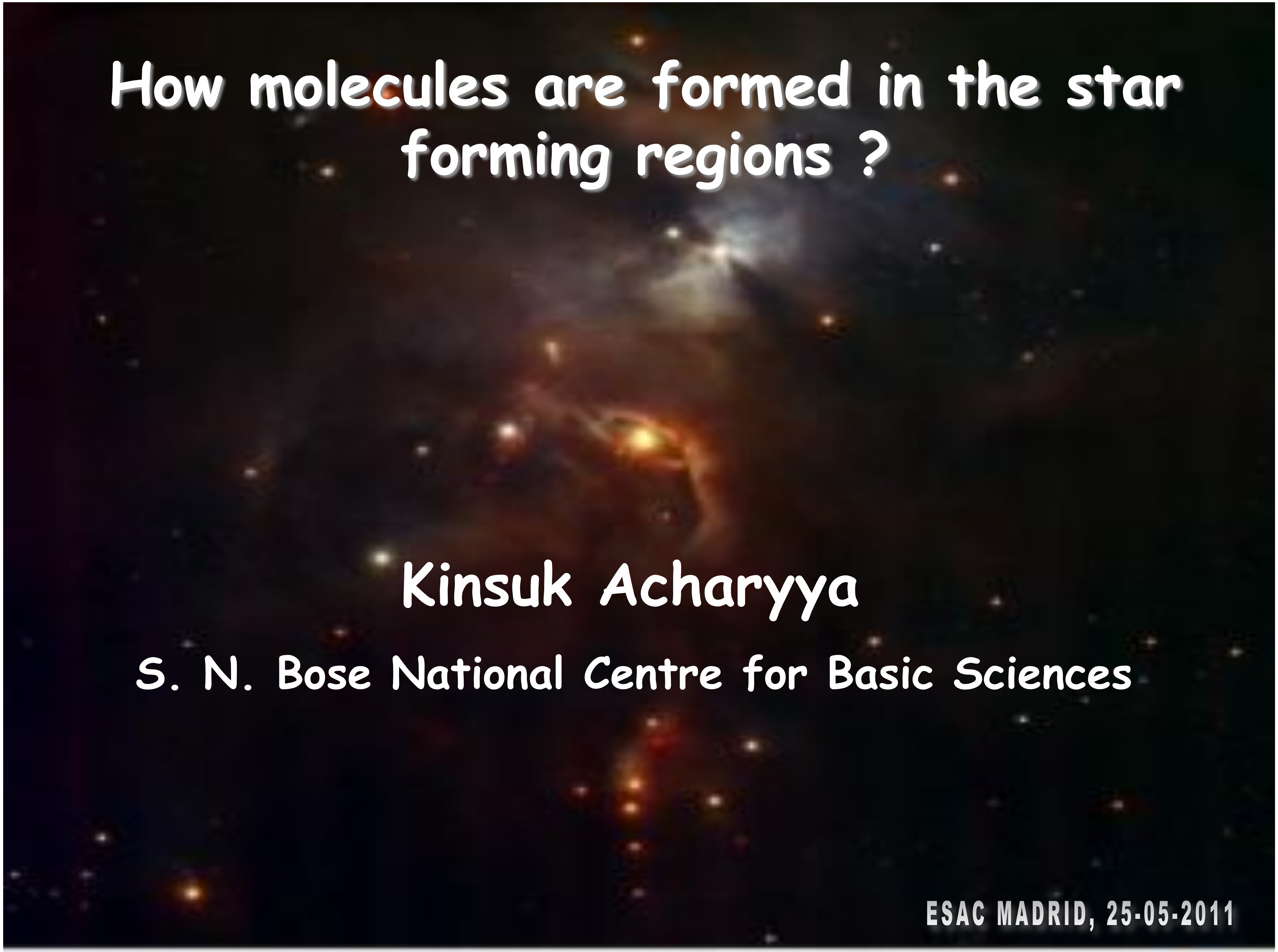
How molecules are formed in the star forming regions ?



Kinsuk Acharyya

S. N. Bose National Centre for Basic Sciences

ESAC MADRID, 25-05-2011

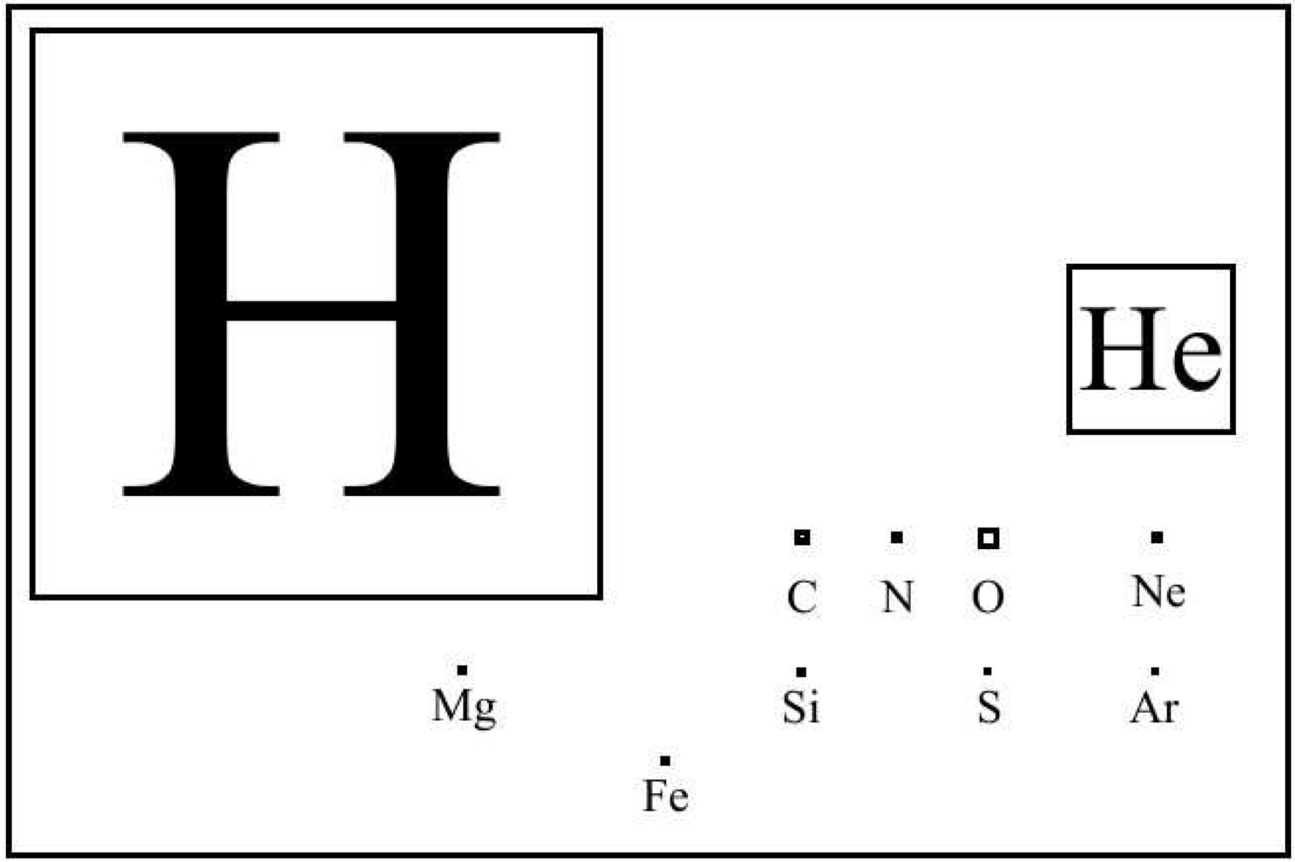
Plan of Talk

- Introduction
- Gas Grain Interaction
- H_2 Formation
- Formation of Water and Methanol
- Effect of grain growth & size distribution
- Conclusions

Interstellar Matter

Comprises gas and dust

By mass, 99% is gas and 1% is dust.



Diffuse cloud

- $n \sim 10 - 10^2\ \mathrm{cm}^{-3}$
- $T \sim 30 - 80$ K
- Low-density clouds in the ISM that can easily be penetrated by energetic radiation such as the UV radiation.

Tarantula Nabulae

Dark Cloud

- T ~ 10 K
- n ~ 10^3 - 10^6 cm^{-3}
- Not penetrated by optical and UV photons. Little ionisation. Material is mostly molecular, dominant species is H_2.

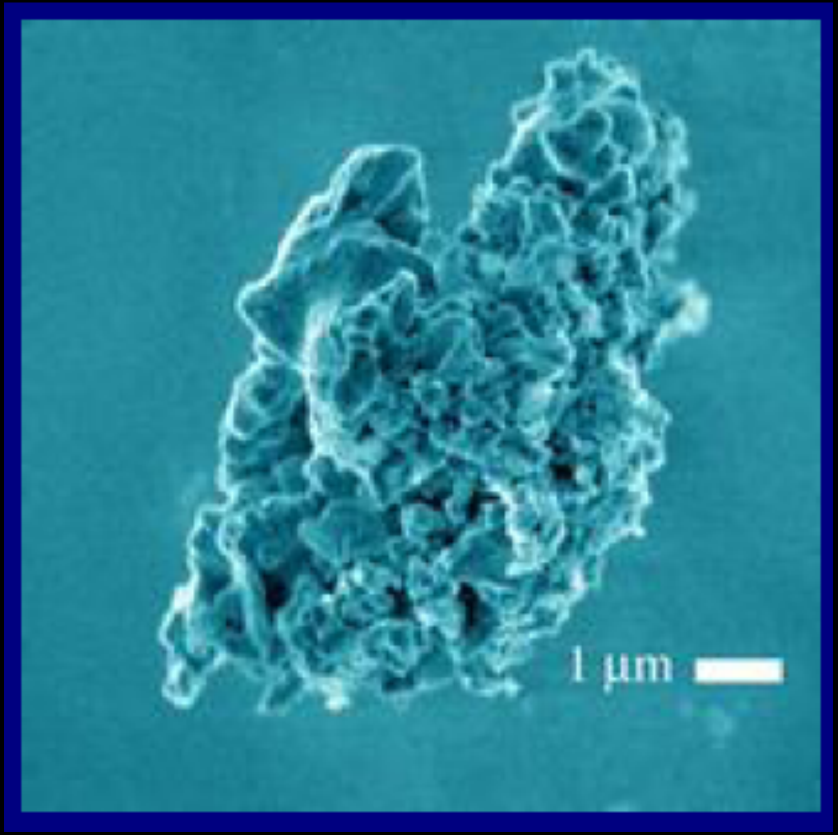
Dark Cloud B 68

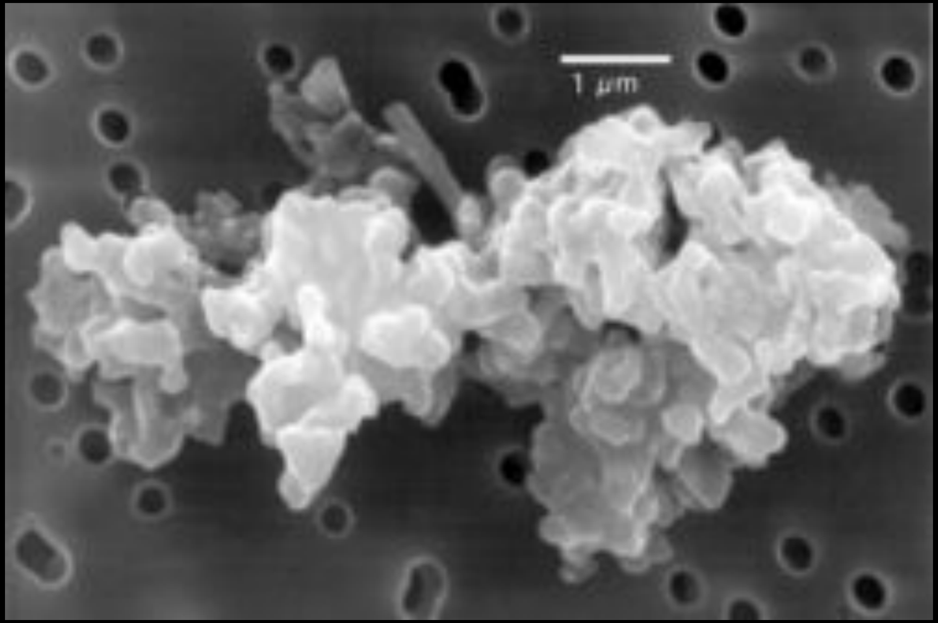
Giant Molecular Cloud (GMC)

- T ~ 10-50 K
- n ~ 10^4 - 10^7 cm^{-3}
- Material is mostly molecular.

Enlarged view of the OMC2.

Analog of interstellar dust grains



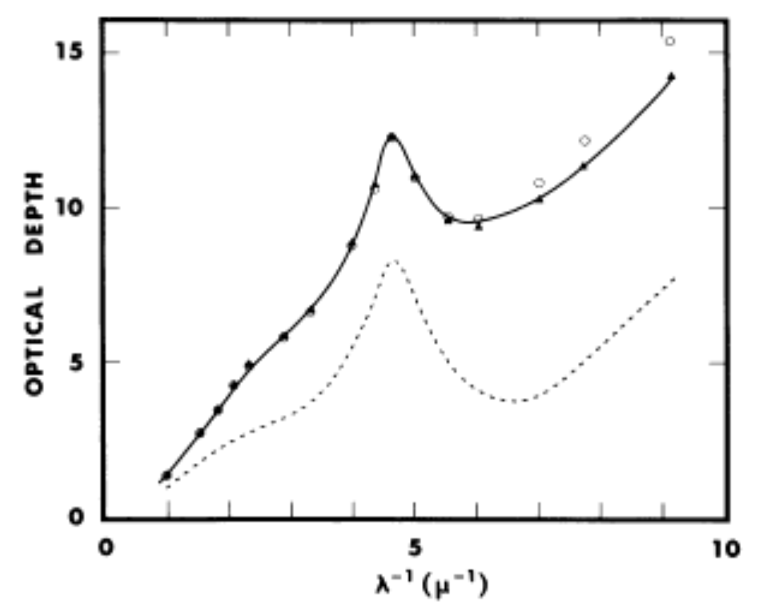


✓sizes

The blockage is most effective when there is an approximate match of particle size to wavelength.

UV extinction implies small (~ 100 nm) grains

Visual Extinction implies normal (~ 1000 nm) grains.



The interstellar extinction curve

Size Distribution of dust grains

- $n(a)da \sim a^{-3.5}da$

- Mass dust/Mass gas ~ 0.01

- Dense gas – **larger** grains with icy mantles

- **Normal** – $n_d/n \sim 10^{-12}$

Low density

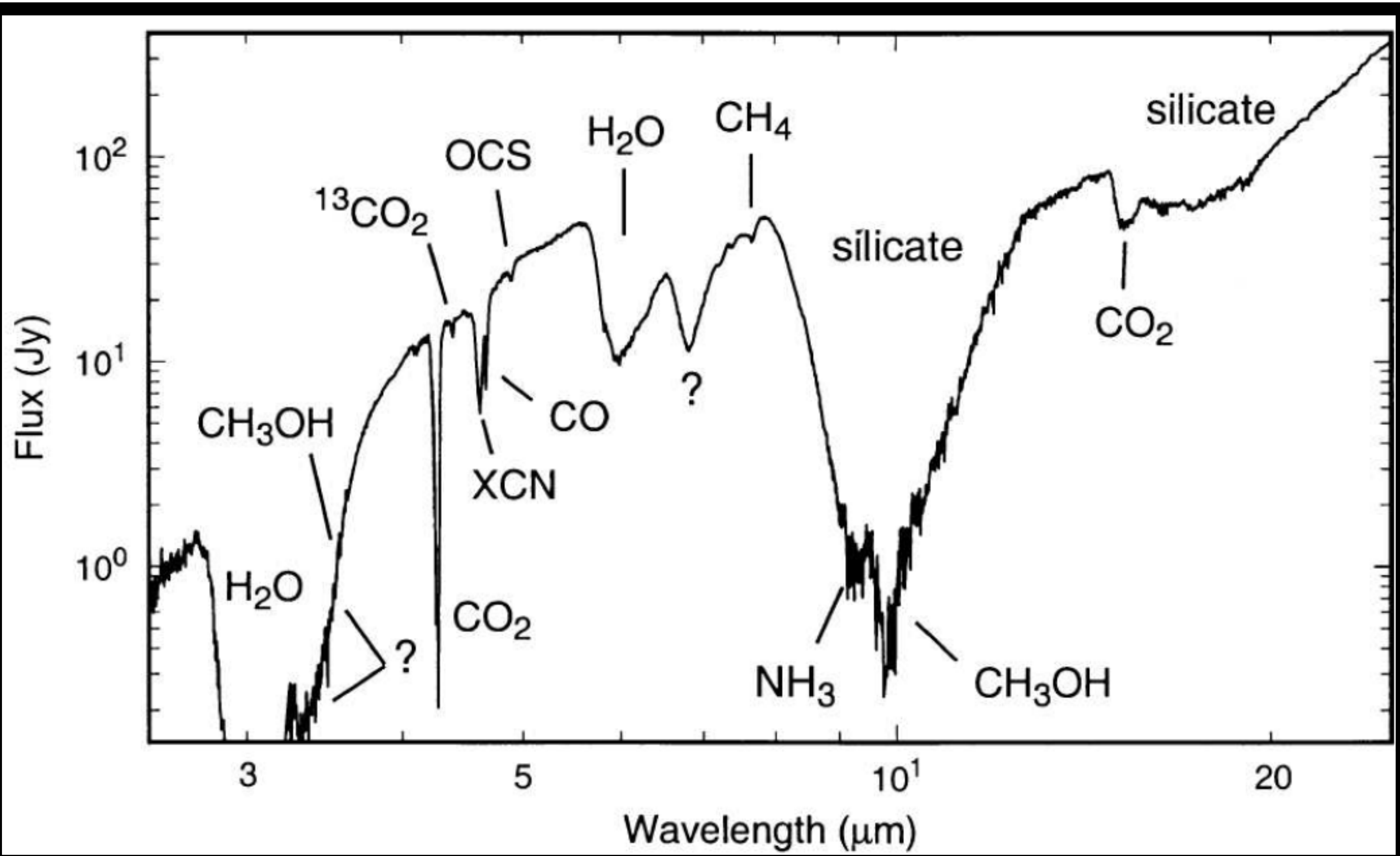
Low temperature

Perhaps not a great place chemistry !!

Interstellar Organic Molecules

CH+	**HCN**	H2CO	**HC3N**	CH3OH	**HC5N**	HCOOCH3	**HC7N**
CS	HNC	H2CS	HOCHO	CH3CN	CH3CCH	CH3C3N	**HC9N**
CO	HCO	H2CN	CH2NH	CH3NC	CH3NH2	CH3COOH	**HC11N**
CN	OCS	HNCO	CH2CO	CH3SH	CH3CHO	CH2OHCHO	C2H5CN
C2	CH2	HNCS	NH2CN	NH2CHO	CH2CHCN	H2C6	CH3C4H
CH	**C2H**	**C3H**	**C4H**	**C5H**	**C6H**		CH3C5N
CO+	C3	*c*-C3H	c-C3H2	H2C4	c-C2H4O		CH3OCH3
CF+	CO2	C3N	H2C3	**HC3NH+**	CH2CHOH		C2H5OH
	C2O	C3O	CH2CN				CH3COCH3
	C2S	C3S	HCCNC				OHCH2CH2OH
	HCO+	CH3	HNCCC				NH2CH2COOH?
	HOC+	C2H2	CH4				
	HCS+	**HOCO+**	**H2COH+**				
		HCNH+					

- Around 150 molecules detected in various star forming regions



ISO-SWS spectrum of YSO W33A. Various absorption features due to silicate grain cores and icy mantles are shown. Gibb *et al.* 1999

- Around 20 species are detected on the interstellar grains.

How these molecules are formed ?

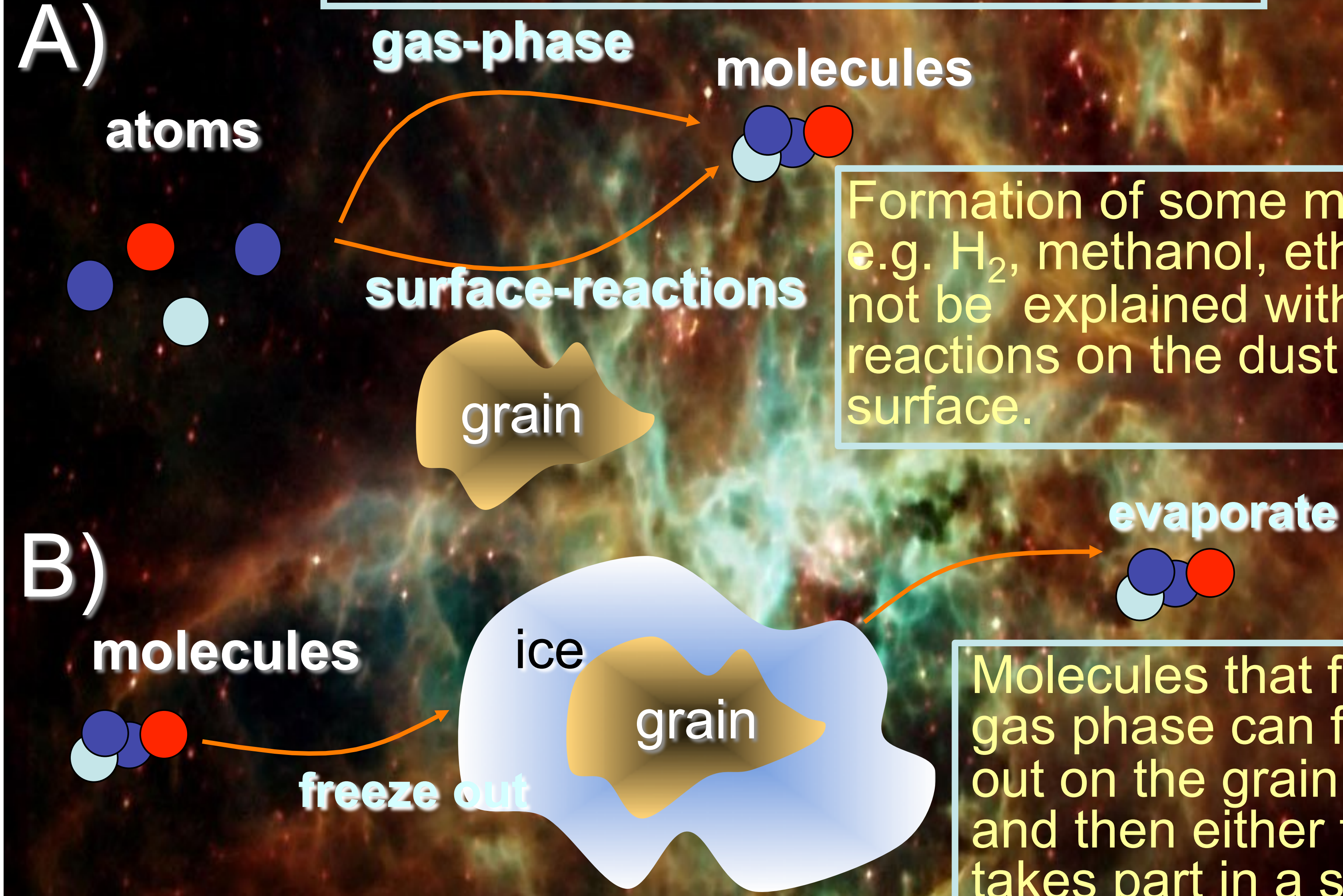
These molecules are formed in both the

interstellar gas (gas phase chemistry)

and

dust grains (surface chemistry).

Gas Grain interaction

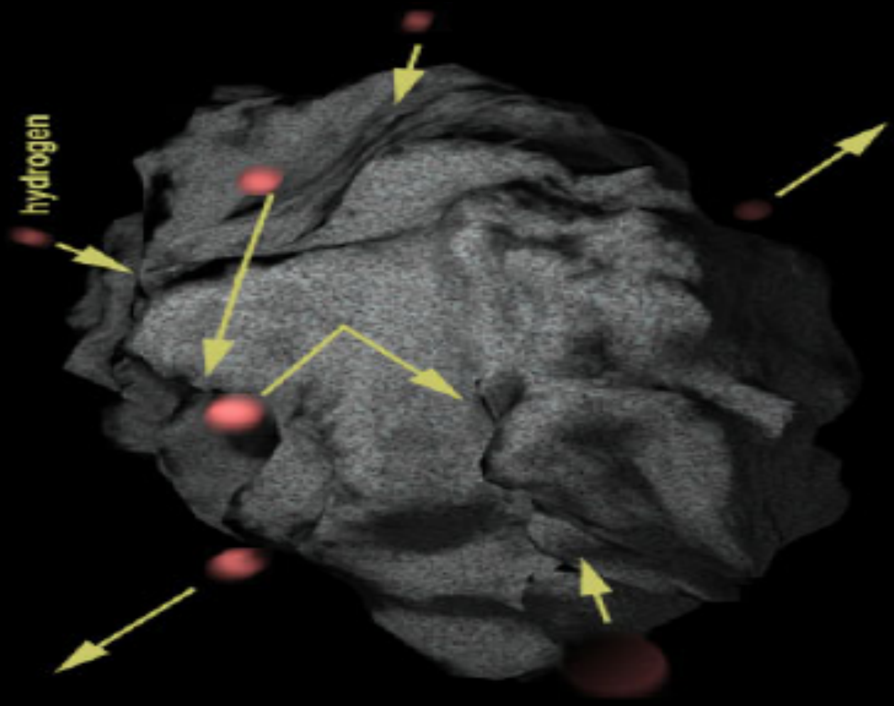


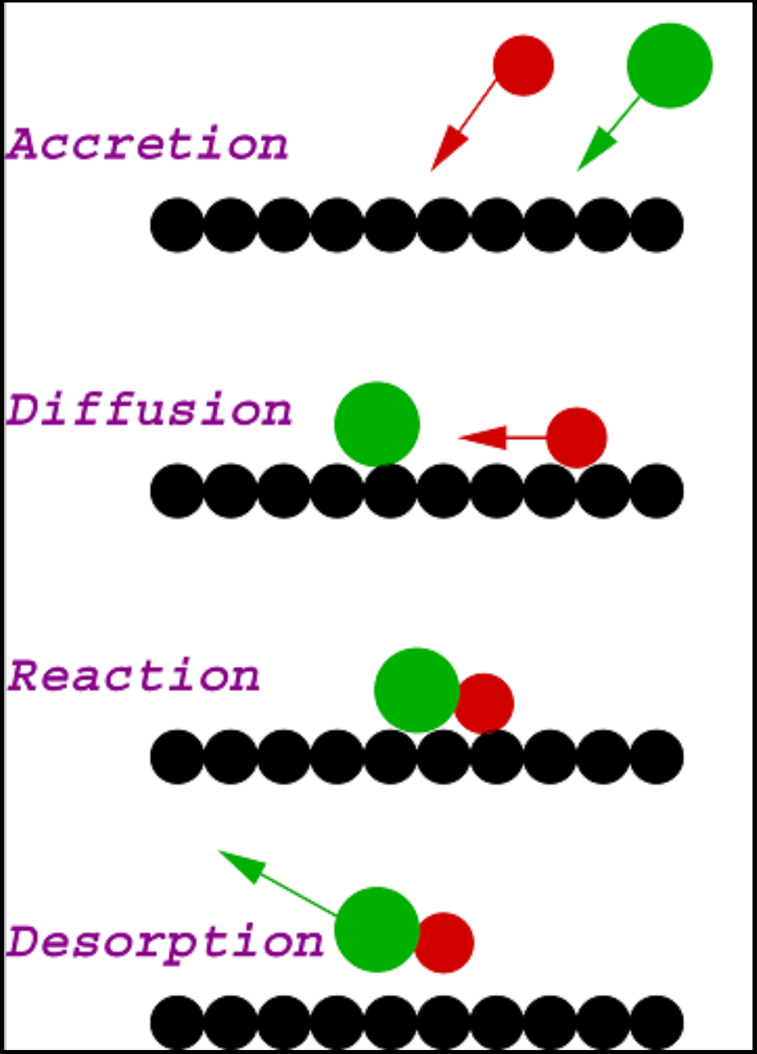
Formation of some molecules: e.g. H_2, methanol, ethanol can not be explained with out reactions on the dust grain surface.

Molecules that forms in gas phase can freeze out on the grain surface and then either they takes part in a surface reaction or evaporates during grain heating.

Basic Physical Process on Grain Surfaces

There are ESAC, MADRID, 5/25/2011four major physical processes involved during a gas-grain interaction.



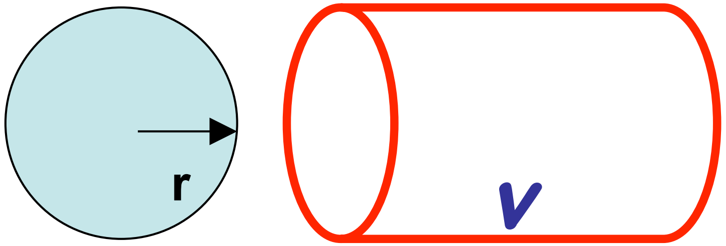


Basic Physical Process on Grain Surfaces

There are four major physical processes involved during a gas-grain interaction.

Accretion: In this step molecules are accreted on the grain surface. The accretion rate (F_h) is given ,

$$F_h = S \, \boxed{\pi r^2} \, v \, n_x \, \boxed{n_d}$$



S= **sticking co-efficients**

r = Radius of the grain,

v = $(8KT/\pi m_x)^{1/2}$ = The thermal velocity,

n_x = the number density of any species 'x' and

n_d = is the grain number density

Second step is the **diffusion,**

Accreted species then diffuse or tunnel through different binding sites. The time scale t_{hop} for any absorbed species to migrate from one surface site to an adjacent site via thermal diffusion is,

$$t_{hop} = \nu_0^{-1} \exp(E_b/KT_d),$$

T_d = dust temperature and $\nu_0 = (2n_sE_d/\pi^2 m_x)^{1/2}$ = is the characteristic frequency for the absorbed species, for most of the species it is $\sim 10^{12}\ s^{-1}$

n_s = the surface density of sites and. It is $\sim 10^{15}\ cm^{-2}$

The diffusion time t_{diff} required for an adsorbed particles to sweep over a number of sites equivalent to the whole grain surface is,

$t_{diff} = \enclose{circle}{N_s}\, t_{hop}$, **N_s is the total no. of sites of grain**

Third step is **surface reaction**,

If surface reaction rate is R_{diff} is defined as the inverse of the t_{diff}, the surface reaction rate $R_{i,j}(s^{-1})$ between surface species i and j occurring due to classical diffusion can be expressed as,

$$R_{i,j} = k_{i,j}\,(R_{diff\ i} + R_{diff,j,})$$

$k_{i,j}$ is the probability for the reaction to occur upon a encounter. **For exothermic reactions with out activation energy** $k_{i,j}$ **is unity**. For **reactions with activation energy** it could be approximated by the **exponential portion of the quantum mechanical tunnelling** through a rectangular barrier of thickness a,

$$k_{i,j} = \exp[-2(a/h)(2\mu E_d)^{1/2}]$$

Hasegawa, Herbst, and Leung, 1992, APJS, 82, 167

The fourth and final step is the **desorption.**

Every molecules have their own time period depending on their adsorption energy after that they desorbs from the grain surface.

The **thermal desorption time scale** is given by,

$$t_{desorb} = \nu_0^{-1} \exp(E_d/KT_d)$$

Grain Surface Time-scales

Accretion time: $t_c = [v_H(\pi r^2 n_d)]^{-1} \sim 10^9/n(\mathrm{cm}^{-3})$ years

Thermal hopping time: $t_h = v_0^{-1}\exp(E_b/kT)$

Tunnelling time: $t_t = v_0^{-1}\exp[(4\pi a/h)(2mE_b)^{1/2}]$

Thermal desorption time $t_{ev} = v_0^{-1}\exp(E_D/kT)$

Here $E_b \sim 0.3E_D$, so hopping time < desorption time

For H at 10K, $E_D = 300$K, $E_b = 100$, $t_h \sim 7 \times 10^{-9}$ s, $t_d \sim 500$ s

For O and C, $E_b \sim 240$ K $E_D \sim 800$K, $t_h \sim 0.025$ s, $t_d = 5 \times 10^{22}$ s

- Accretion time scale is large.
- Hopping time for smaller atoms like H is very small. Therefore, reaction is almost instantaneous if it finds an reactant partner.
- Heavier atoms are immobile.
- Thermal desorption is in-efficient.
- We need some other mode of desorption.

Non Thermal Desorption

Other than the thermal energy, there are two sources of photons in the interstellar cloud:

(i) the background radiation field and

(ii) cosmic ray generated internal photons.

The background field mainly consists of UV and visible photons. They are effective in the diffuse cloud but their role in the dense cloud is very limited and only at large times.

But the cosmic ray generated internal photons can play an affective role in the dense cloud.

These photons can heat up the grain and also can dissociate species on the grain surface.

$$r_{CR,d} = I_0 Y_{pd} \boxed{(\pi a^2)}$$

Öberg et al., 2009, AA, 296, 2810

$$r_{CR,d} = D\nu_0 \left(\boxed{\frac{a}{0.1\mu m}} \right)^2 \exp(-E_d / KT_c)$$

Hasegawa & Herbst, 1993, MNRAS, 261, 83

$$r_{UV,d} = G_0 Y_{pd} \boxed{(\pi a^2)} \exp(-\gamma A_V)$$

Öberg et al., 2009, AA, 296, 2810

I_0 (10^4 photons $cm^{-2}s^{-1}$) is UV photon flux for typical galactic cosmic ray photons

Y_{pd} is the photo-desorption yield

D (3.19×10^{-19}) duty cycles of the grain at elevated temperature.

G_0 (10^8 photons $cm^{-2}s^{-1}$) is the un-attenuated photon flux

T_c (70 K) is elevated temperature

γ is the measure of UV extinction relative to the visual extinction

A_v (10) is the visual extinction

Around 600 different gas phase species and 8,000 reactions are considered.

$$\frac{dn_g(i)}{dt} = \underbrace{\sum_i \sum_j \underbrace{K_{ij}}_{\text{Rate constants}} n_g(l) n_g(j)}_{\text{Formation Pathways}} - \underbrace{n(i) \sum_i K_{ij} n_g(j)}_{\text{Destruction Pathways}} - \underbrace{r_{acc}(i)}_{\boxed{\text{Accretion Term}}} + \underbrace{r_{des}(i) n_s(i)}_{\text{Desorption Term}},$$

Inputs:

- Gas Temperature (T_g) = 10 K
- Grain Temperature (T_d) = 10 K
- Visual Extinction Co-efficient (A_V) = 10
- Number Density of total hydrogen (n_H) = 2×10^4 cm^{-3}
- Gas phase reaction cross-sections are taken OSU database
- Initial atomic abundance

Species	H_2	He	C^+	N	O	S^+
n_i/n_H	0.5	0.14	7.3(-5)	2.14(-7)	1.76(-4)	8.0(-8)

Species	Na^+	Mg^+	Si^+	P^+	Cl^+	Fe^+
n_i/n_H	2.0(-9)	7.0(-9)	8.0(-9)	3.0(-9)	4.0(-9)	3.0(-9)

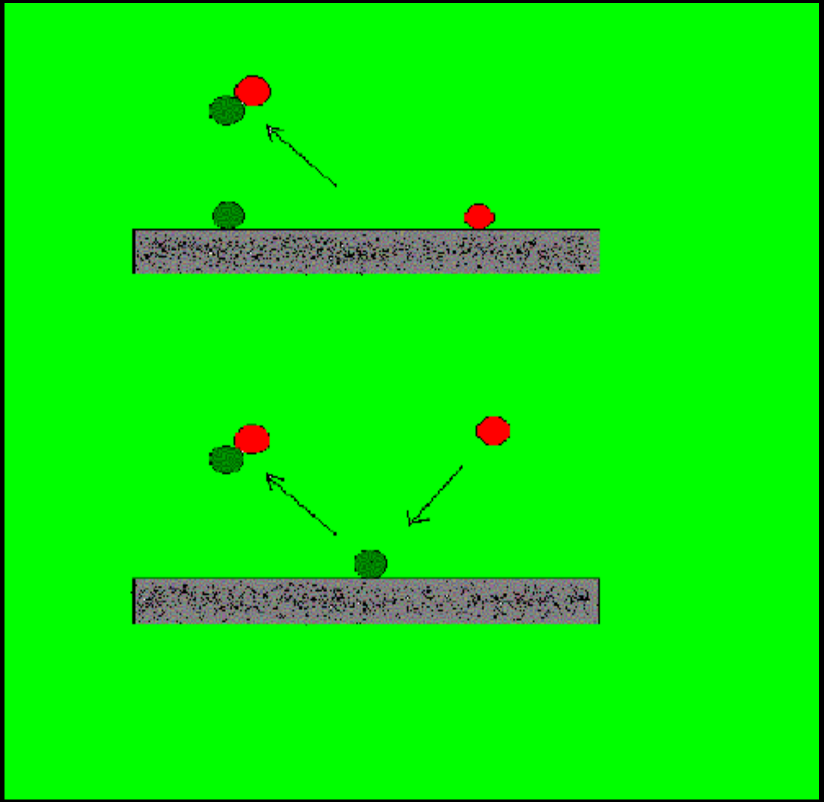
A test case : H_2 formation

Formation of Molecular Hydrogen

Gas-Phase formation:

$H + H \rightarrow H_2 + h\nu$ very slow, insignificant in ISM

Grain surface formation:



Langmuir-Hinshelwood

(surface diffusion)

Eley-Rideal

(direct hit)

Grain Surface Chemistry

❖ Deterministic (Rate Coefficient) Approach:

Basics: We have to define an effective rate coefficient based on mobility (velocity) and mean free path before interaction (cross-section).

Technique: We have to solve the set of coupled ODEs which describe grain surface and gas phase abundances (approximately doubles the no. of ODEs)

Problem: Rate equations depend on an average being a physically meaningful quantity – ok for gas but not for grains

4 grains + 2 H atoms – average = 0.5 H atoms per grain

BUT reaction cannot occur unless both H atoms are actually on the same grain

Grain Surface Chemistry

- Stochastic (Accretion Limit) Approach:

Basics: Reaction on the surface can only occur if a particle arrives while one is already on the surface – the rate of accretion limits chemistry

Technique: Monte-Carlo method – attach probabilities to arrival of individual particles and fire randomly at surface according to these probabilities

Caselli et al. 1998, ApJ, 495, 309

Agreement between rate and MC poor for low values of n(H) – as expected

Solution?: We can Improve method of calculating surface rate coefficients

Problem: Modifications cannot be a priori – you need a MC calculation – and these are 'impossible' for large numbers of species

Caselli et al. 1998, ApJ, 495, 309

Grain Surface Chemistry

- Stochastic (Accretion Limit) Approach:

Solution?: Master Equation

Reaction depends on the probabilities of a particular number of species being on the grains e.g. PH(0), PH(1), PH(2), … PH(N), PO(0), PO(1), …

Biham et al. 2001, ApJ, 553, 595

Green et al. 2001, A&A, 375, 1111

Technique: Integrate the rates of change of probabilities, eg dPH(i)/dt

Problem: Formally, one has to integrate an infinite number of equations

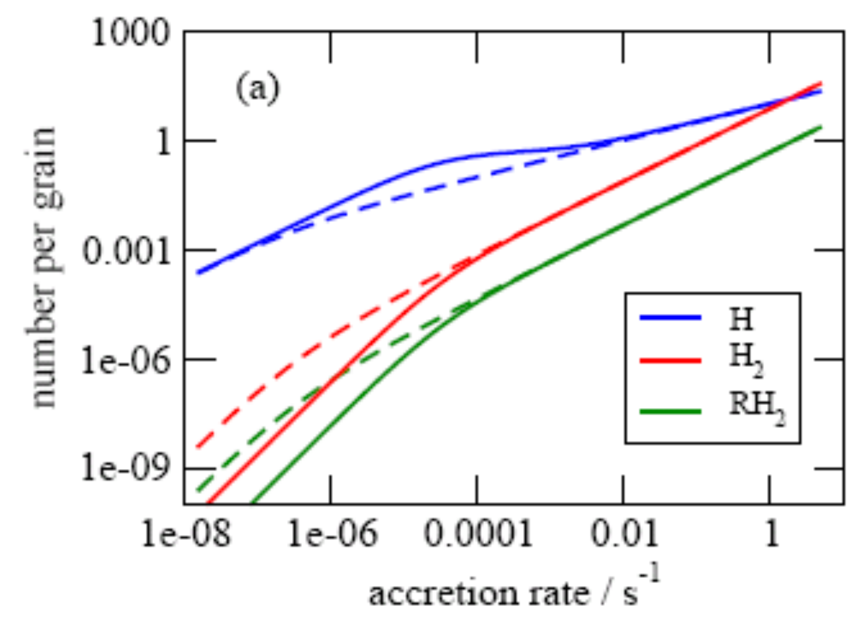
For a system of H only:

$$\begin{aligned} dP(i)/dt = {} & k_{fr}[P(i-1) - P(i)] \\ & + k_{ev}[(i+1)P(i+1) - iP(i)] \\ & + 0.5k_{HH}[(i+2)(i+1)P(i+2) \\ & \quad - i(i-1)P(i)] \end{aligned}$$

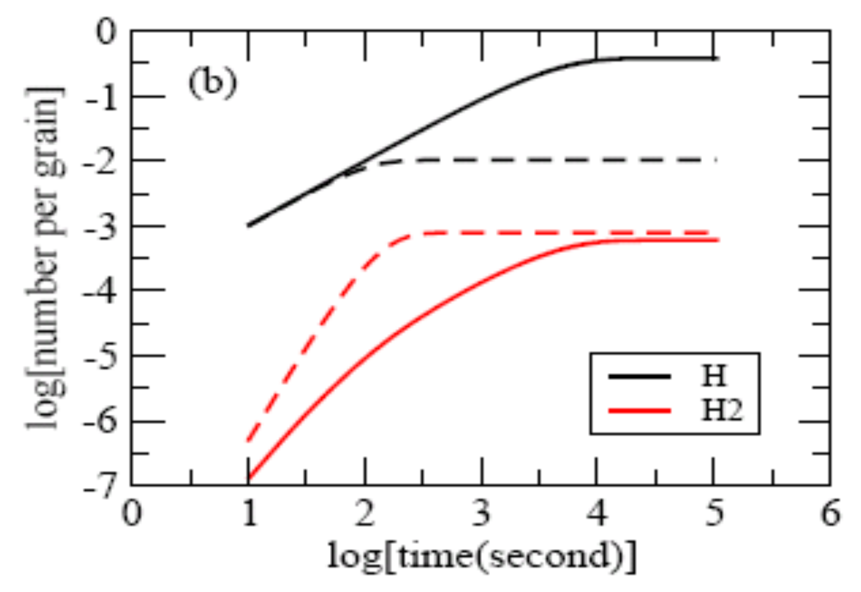
for all I = 0 to infinity

For larger systems, eg O, OH, H_2O, H, H_2, the ODEs get very complex – even the steady state solution is difficult to solve

H_2 on Grains



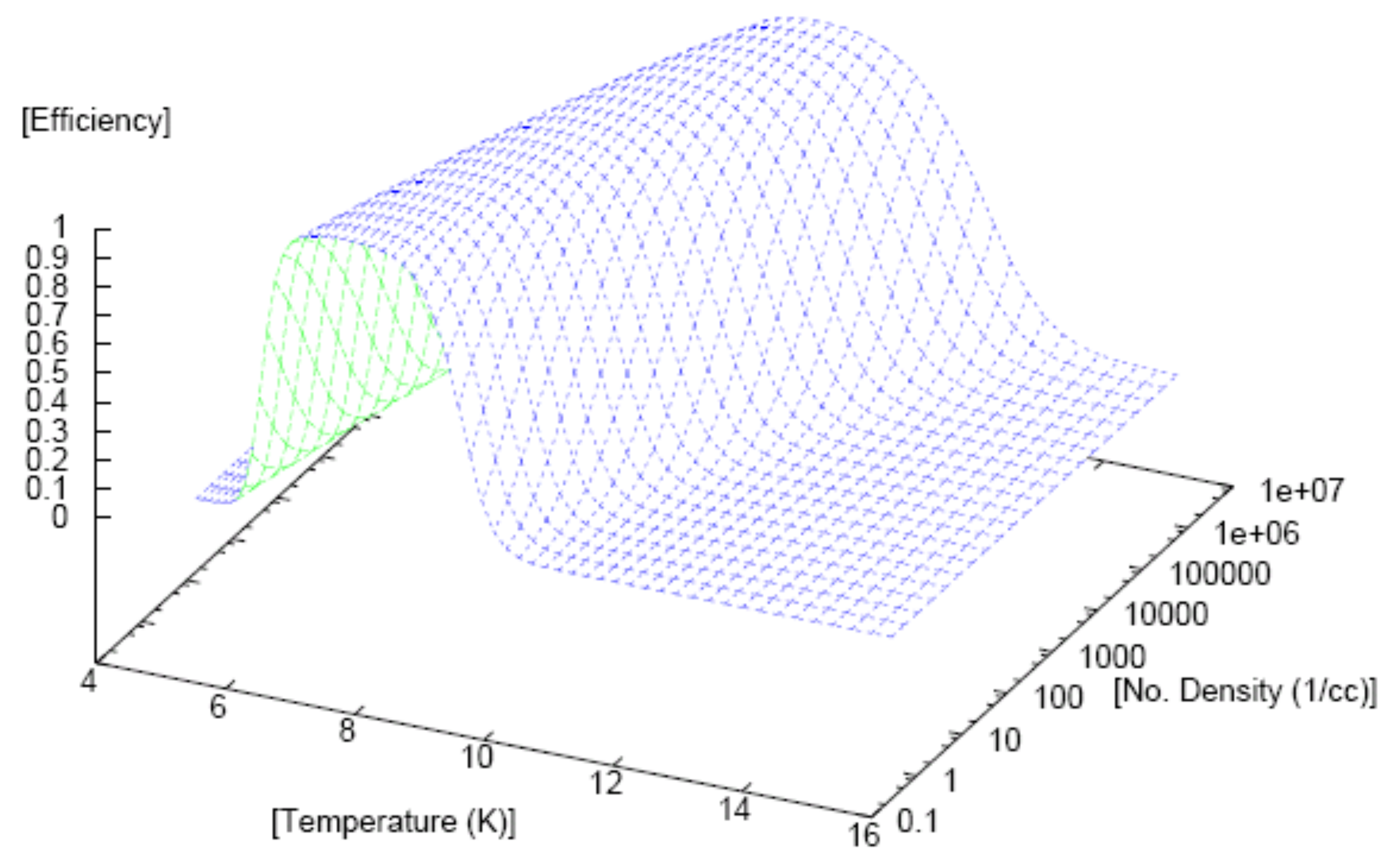
Variation of saturation values of the number of H, H_2 and recombination rate (RH_2). Rate equation results are shown dotted lines and master equation results are shown in solid line.



Time evolution oh H and H_2 numbers on a grain with both rate (dashed) and master (master) equation method.

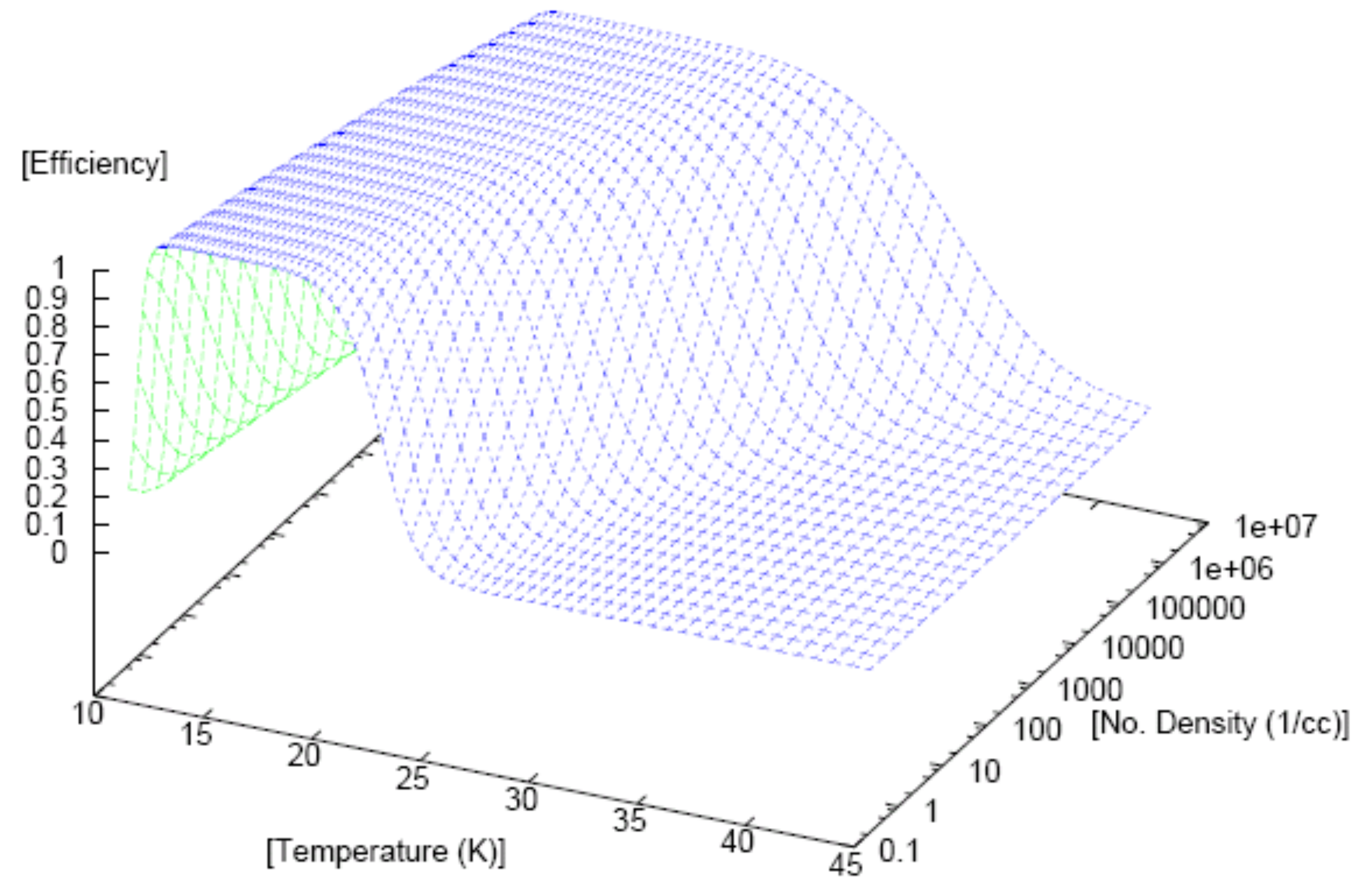
Acharyya et. Al., 2005, MNRAS

Olivine Grains

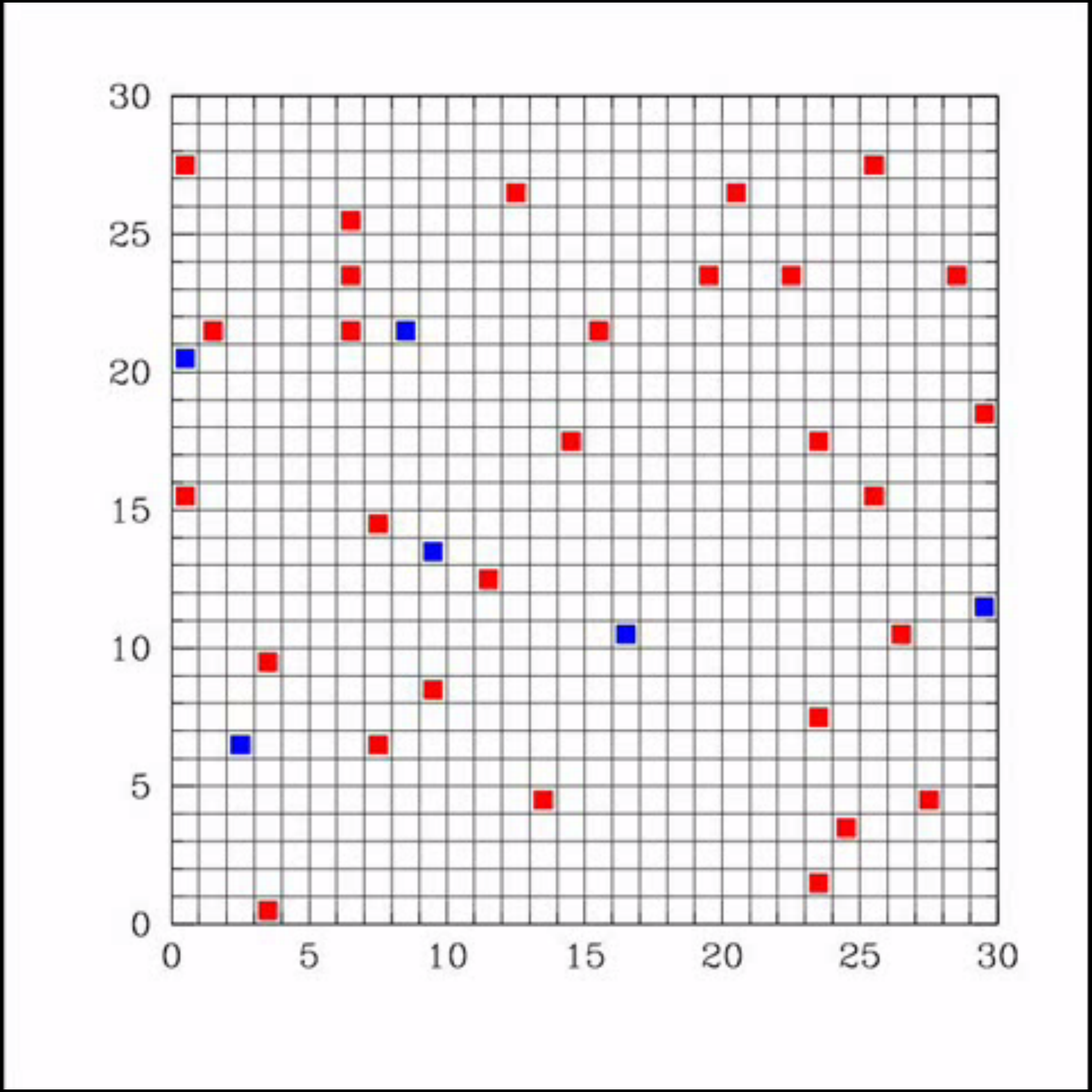


Recombination efficiency (η) of H_2 as a function of the grain temperature and the number density n_h in the ambient gas of T_{gas} =90 K

Carbonaceous Grains



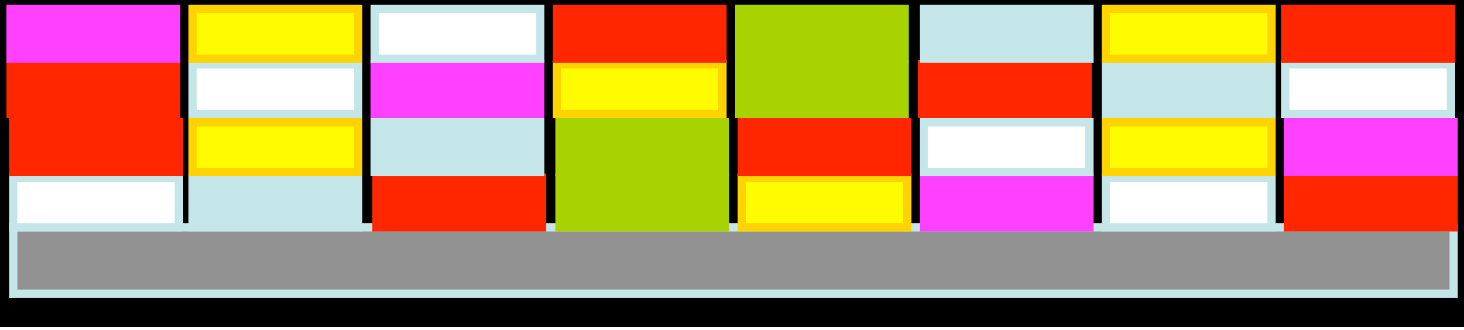
Recombination efficiency (η) of H_2 as a function of the grain temperature and the number density n_h in the ambient gas of T_{gas} =90 K

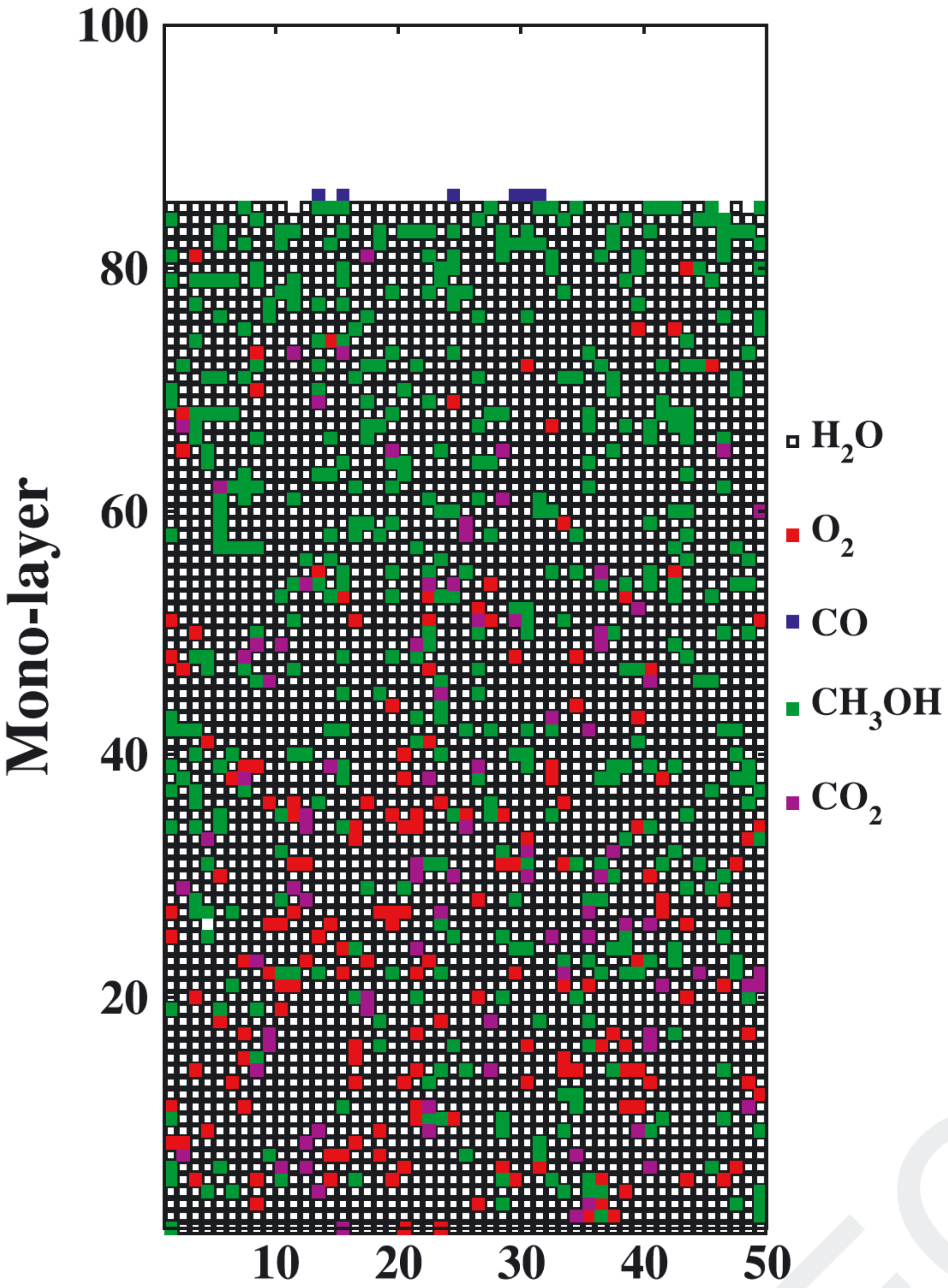


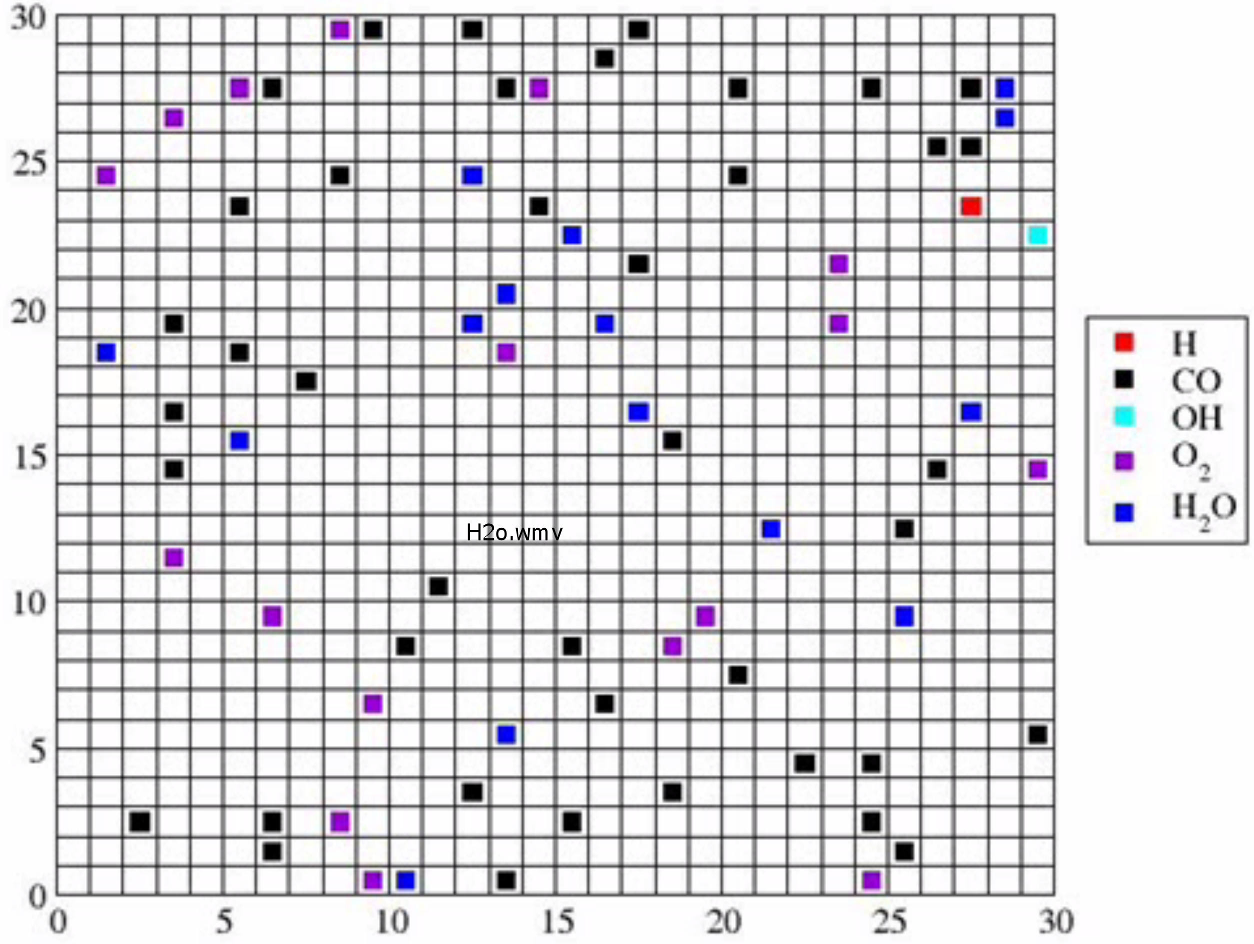
Chakrabarti, Das, Acharyya and Chakrabarti, 2006, A&A,457, 167

Water, Methanol in star forming regions

1. We concentrated on water, methanol and carbon dioxide, because it constitutes nearly 90 per cent of the grain mantle.
2. How the final production of these molecules depend on the relative gas-phase abundances of oxygen (O) and carbon monoxide (CO).
3. We constrained the relevant parameter space that reproduces these molecules close to the observed abundances.
4. We have considered accretion of only H, O and CO on the grains and used the Monte Carlo method.
5. We allow the formation of multi-layers on the grains and incorporate the freeze-out effects of accreting O and CO.

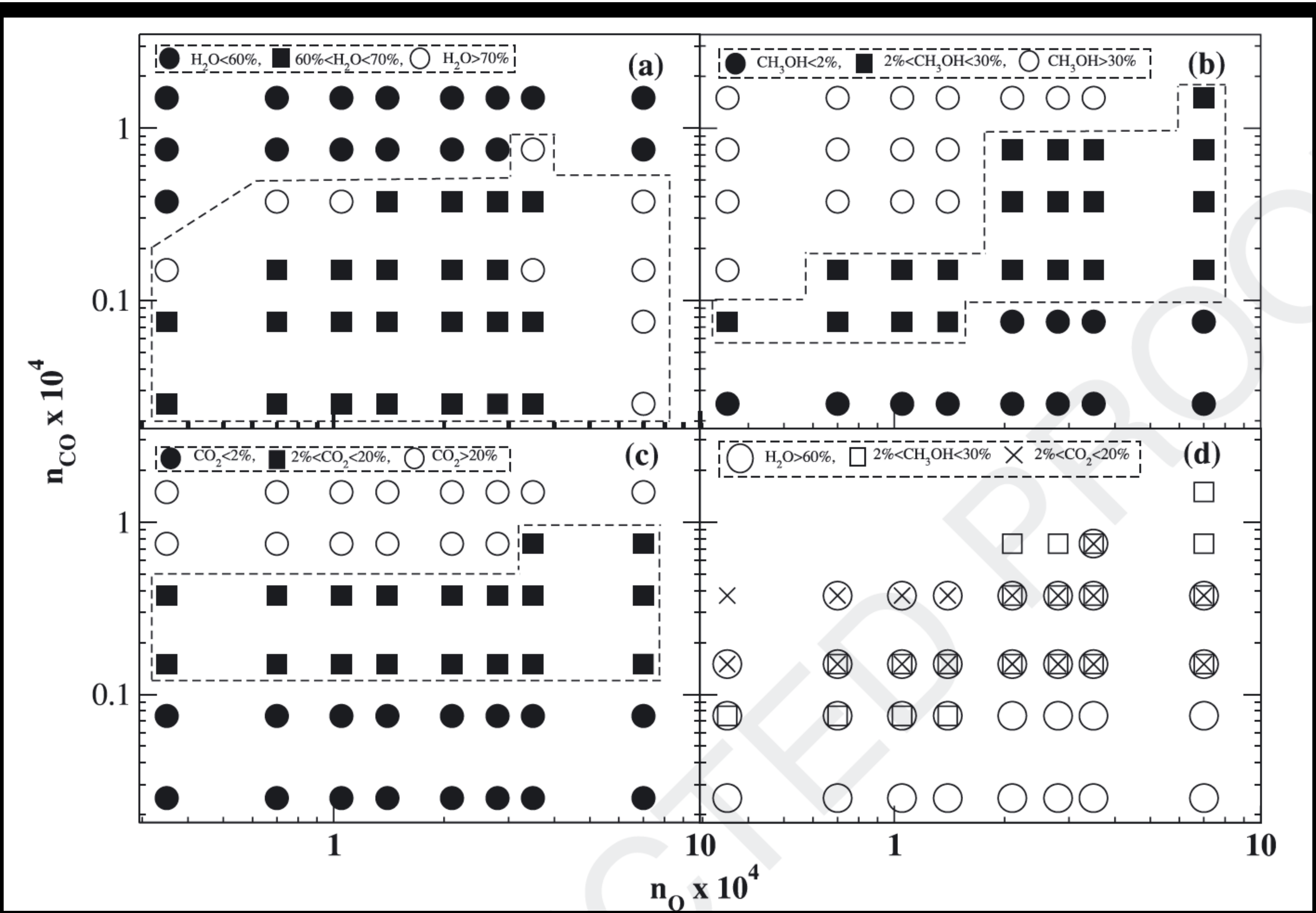



100
80
60
40
20
Mono-layer
10
20
30
40
50
H$_2$O
O$_2$
CO
CH$_3$OH
CO$_2$



Das, Acharyya, Chakrabarti, 2008, A&A, 486, 209

Initial gas-phase oxygen	Species	Initial gas-phase CO = 7.5(-5)	Initial gas-phase CO = 3.75(-5)	Initial gas-phase CO = 1.5(-5)
7.0(-5)	H_2O	100 [5.3(-5)]	100 [6(-5)]	100 [6.4(-5)]
	CO	3 [1.6(-6)]	1 [6.1(-7)]	0.5 [2.9(-7)]
	H_2CO	0.2 [8.8(-8)]	0.05 [3(-8)]	0.02 [1.1(-8)]
	CH_3OH	116 [6.1(-5)]	52.3 [3.2(-5)]	20 [1.3(-5)]
	CO_2	22.7 [1.2(-5)]	8.6 [5.2(-6)]	2.8 [1.8(-6)]
	O_2	5 [2.6(-6)]	3.6 [2.2(-6)]	3 [2(-6)]
1.05(-4)	H_2O	100 [7.5(-5)]	100 [8.8(-5)]	100 [9.4(-5)]
	CO	0.8 [5.8(-7)]	0.4 [3.7(-7)]	0.3 [2.4(-7)]
	H_2CO	0.05 [4(-8)]	0.01 [1.2(-8)]	0.01 [7(-9)]
	CH_3OH	70.3 [5.3(-5)]	33.4 [2.9(-5)]	13 [1.2(-5)]
	CO_2	20.7 [1.5(-5)]	7.8 [6.8(-6)]	2.5 [2.4(-6)]
	O_2	7 [5.3(-6)]	5.4 [4.7(-6)]	4.6 [4.4(-6)]
3.5(-4)	H_2O	100 [2.1(-4)]	100 [2.3(-4)]	100 [2.1(-4)]
	CO	0.1 [2.1(-7)]	0.02 [4.5(-8)]	0.02 [3.5(-8)]
	H_2CO	0.01 [1.9(-8)]	0.0 [4.8(-9)]	0.0 [1.6(-9)]
	CH_3OH	19.4 [4.1(-5)]	9.5 [2.2(-5)]	3.3 [6.8(-6)]
	CO_2	14.3 [3(-5)]	6.2 [1.4(-5)]	2.5 [5.2(-6)]
	O_2	24.2 [5.1(-5)]	21.7 [5(-5)]	23.7 [4.9(-5)]
7.0(-4)	H_2O	100 [2.4(-4)]	100 [3.4(-4)]	100 [3.6(-4)]
	CO	0.03 [8.4(-8)]	0.02 [6.5(-8)]	0.00 [3.7(-8)]
	H_2CO	0.00 [1.2(-8)]	0.00 [4.8(-9)]	0.00 [1.1(-9)]
	CH_3OH	8.5 [2.2(-5)]	4.9 [1.7(-5)]	2 [7.1(-6)]
	CO_2	15 [3.8(-5)]	5.7 [2(-5)]	2.1 [7.6(-6)]
	O_2	63 [1.6(-4)]	48.6 [1.7(-4)]	46.8 [1.7(-4)]



The parameter space in which the formation of water, methanol and CO2 is studied. The regions in which these molecules are produced within the observed limits (favourable zones) are marked on the parameter space. (d) The favourable zone is the common zone when (a–c) are superimposed.

1. When the number density of accreting O is less than three times that of CO, methanol is always overproduced.
2. Using the available reaction pathways it appears to be difficult to match the exact observed abundances of all three molecules simultaneously.
3. Only in a narrow region of parameter space are all three molecules produced within the observed limits.
4. Furthermore, we found that the incorporation of the freeze-outs of O and CO leads to an almost steady state on the grain surface. The mantle thickness grows anywhere between 60 and 500 layers in a period of two million years.

Effect of size distribution and grain growth

More complex chemistry

Grain Size Distributions

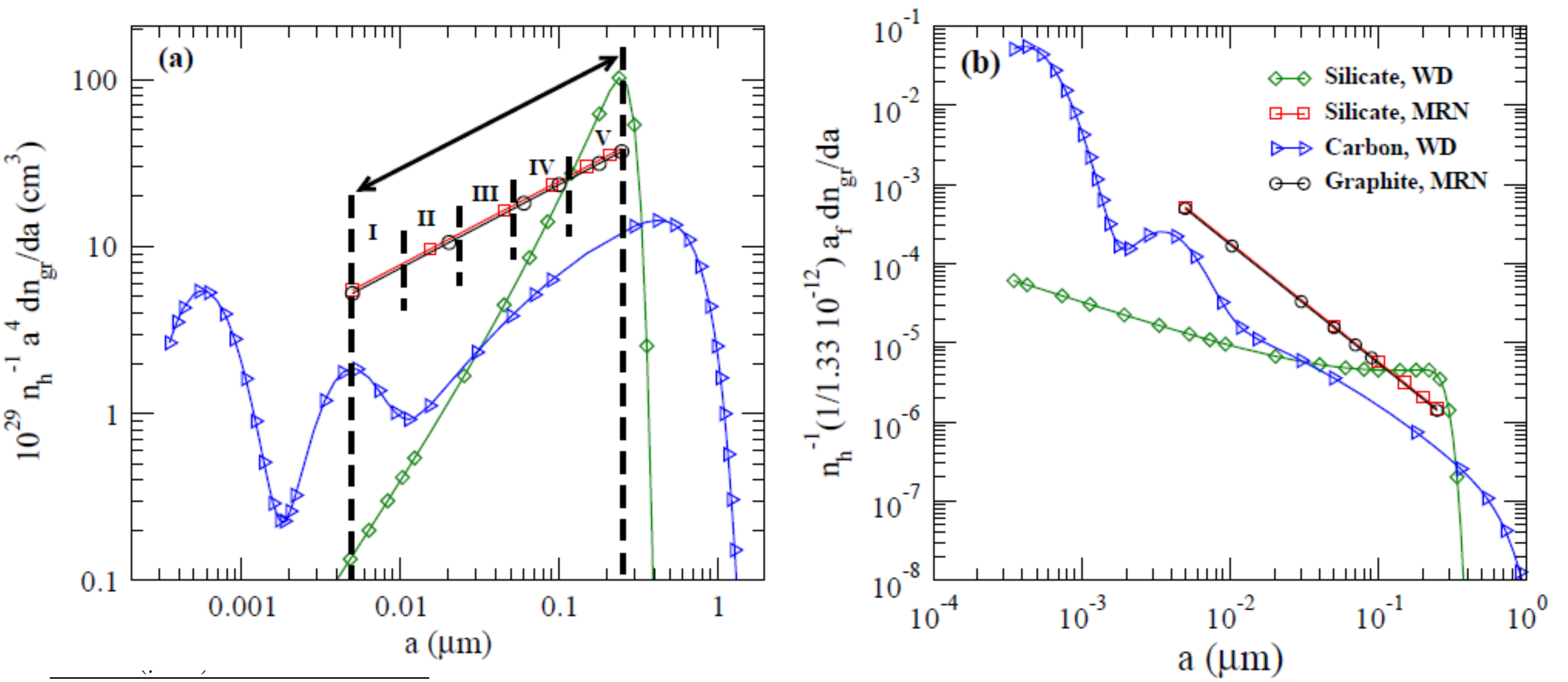
1. MRN Size Distribution:

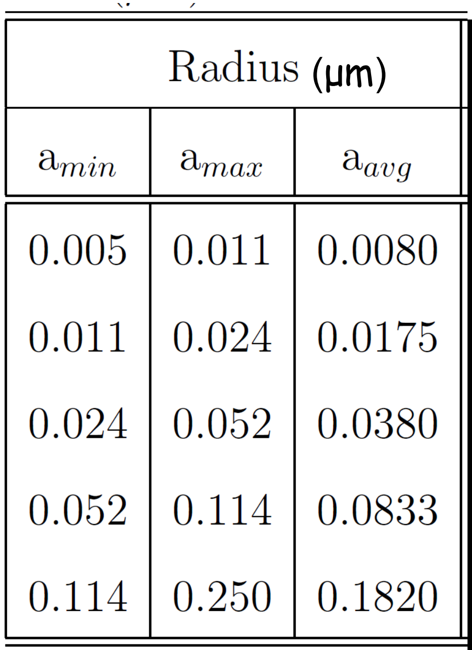
$$dn_{\rm gr} = C n_{\rm H}\, a^{-3.5}\, da\;, \quad a_{\rm min} < a < a_{\rm max}$$

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 $10^{-25.13}$ $(10^{-25.13})$ $cm^{2.5}$ for graphite (silicate).

2. WD Size Distribution

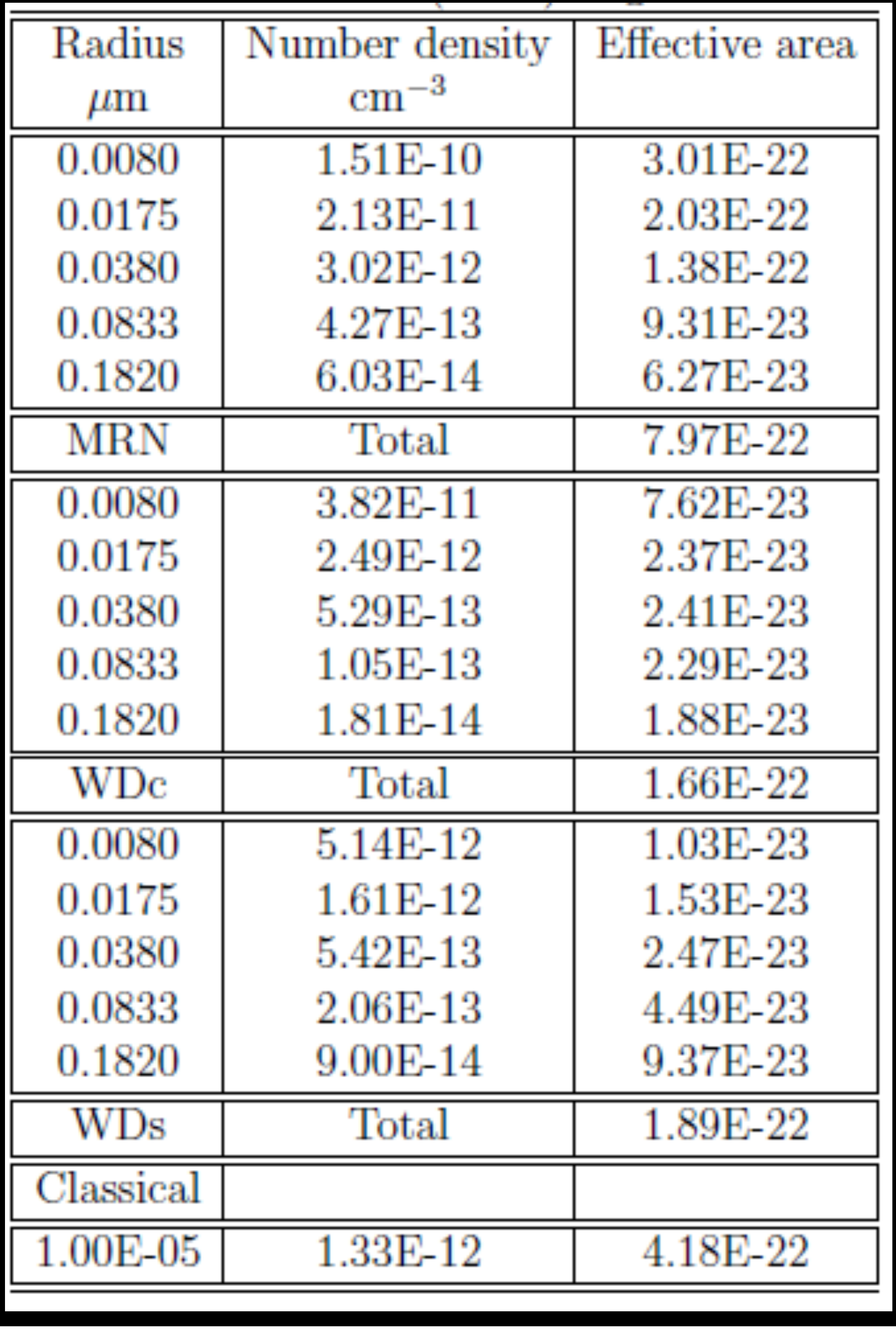
Mathis, Rumpl & Nordsieck, 1977, ApJ, 217, 425 (MRN)
Weingartner and Draine, 2001, ApJ, 548, 296 (WD)



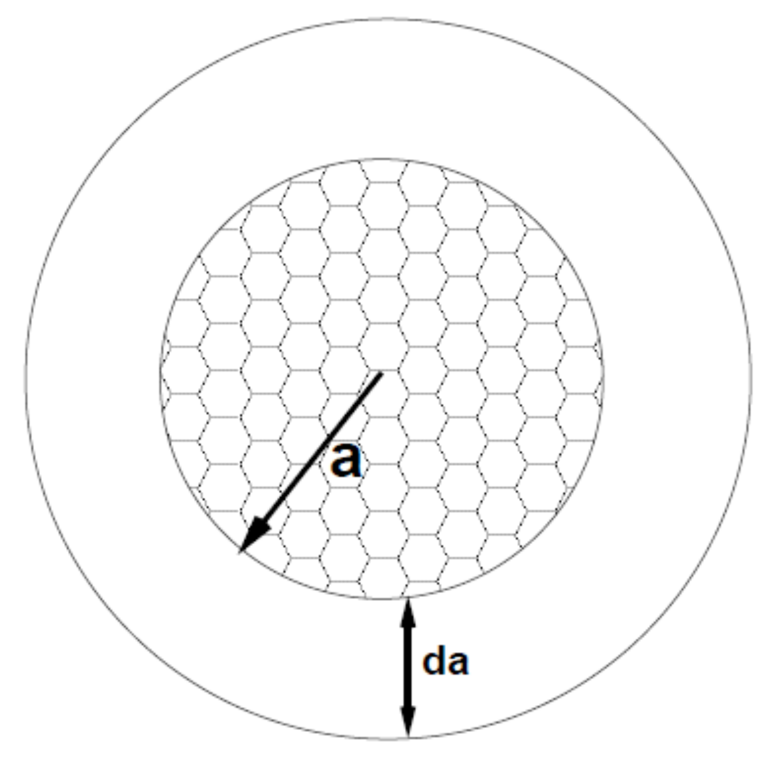


Radius (μm)		
a_{min}	a_{max}	a_{avg}
0.005	0.011	0.0080
0.011	0.024	0.0175
0.024	0.052	0.0380
0.052	0.114	0.0833
0.114	0.250	0.1820

To simplify the computation, we assumed that only five types of grains exist. Their number densities are estimated self-consistently from the area under the curve given by the MRN and WD distribution

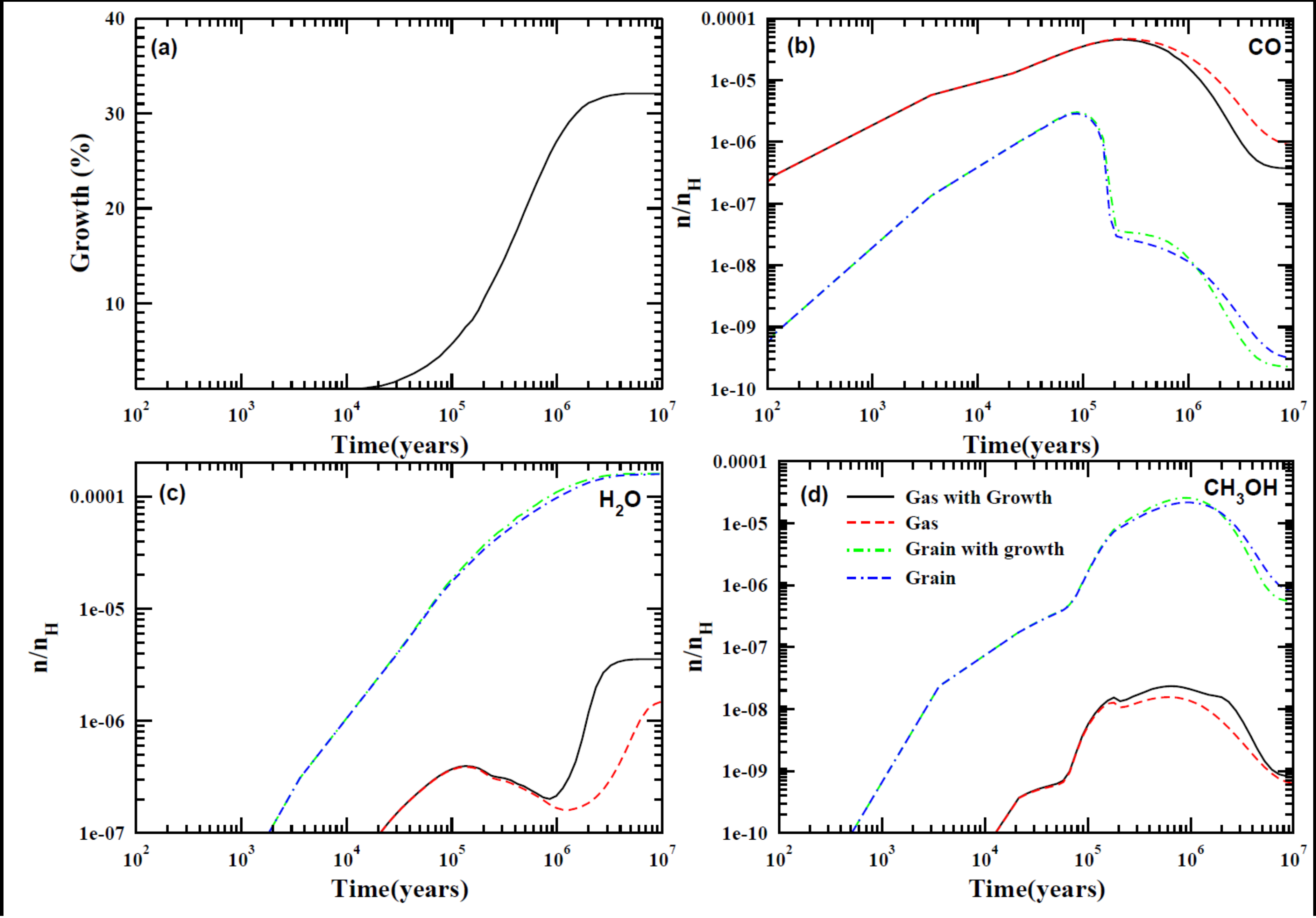


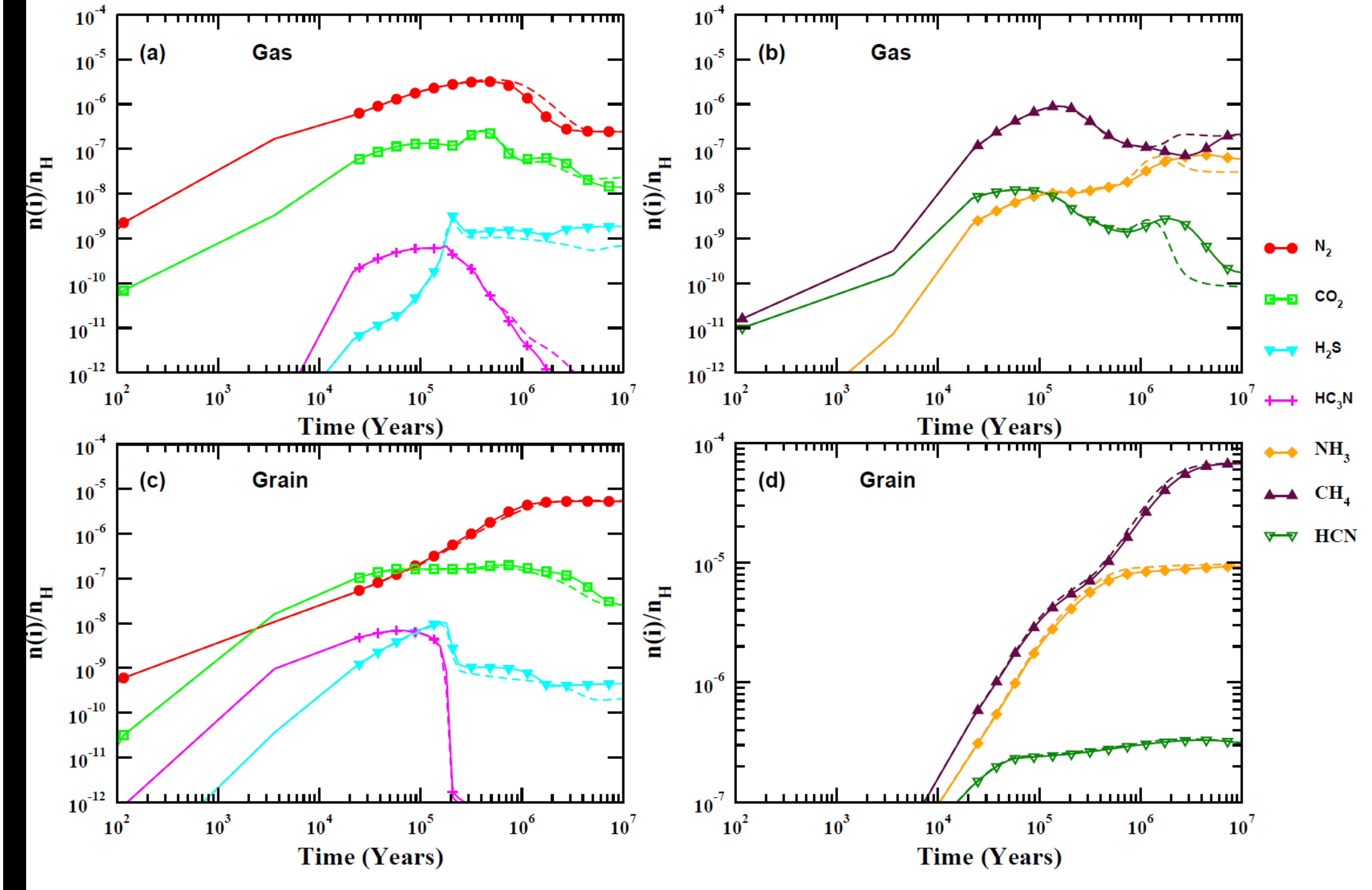
Radius µm	Number density cm^{-3}	Effective area
0.0080	1.51E-10	3.01E-22
0.0175	2.13E-11	2.03E-22
0.0380	3.02E-12	1.38E-22
0.0833	4.27E-13	9.31E-23
0.1820	6.03E-14	6.27E-23
MRN	Total	7.97E-22
0.0080	3.82E-11	7.62E-23
0.0175	2.49E-12	2.37E-23
0.0380	5.29E-13	2.41E-23
0.0833	1.05E-13	2.29E-23
0.1820	1.81E-14	1.88E-23
WDc	Total	1.66E-22
0.0080	5.14E-12	1.03E-23
0.0175	1.61E-12	1.53E-23
0.0380	5.42E-13	2.47E-23
0.0833	2.06E-13	4.49E-23
0.1820	9.00E-14	9.37E-23
WDs	Total	1.89E-22
Classical		
1.00E-05	1.33E-12	4.18E-22

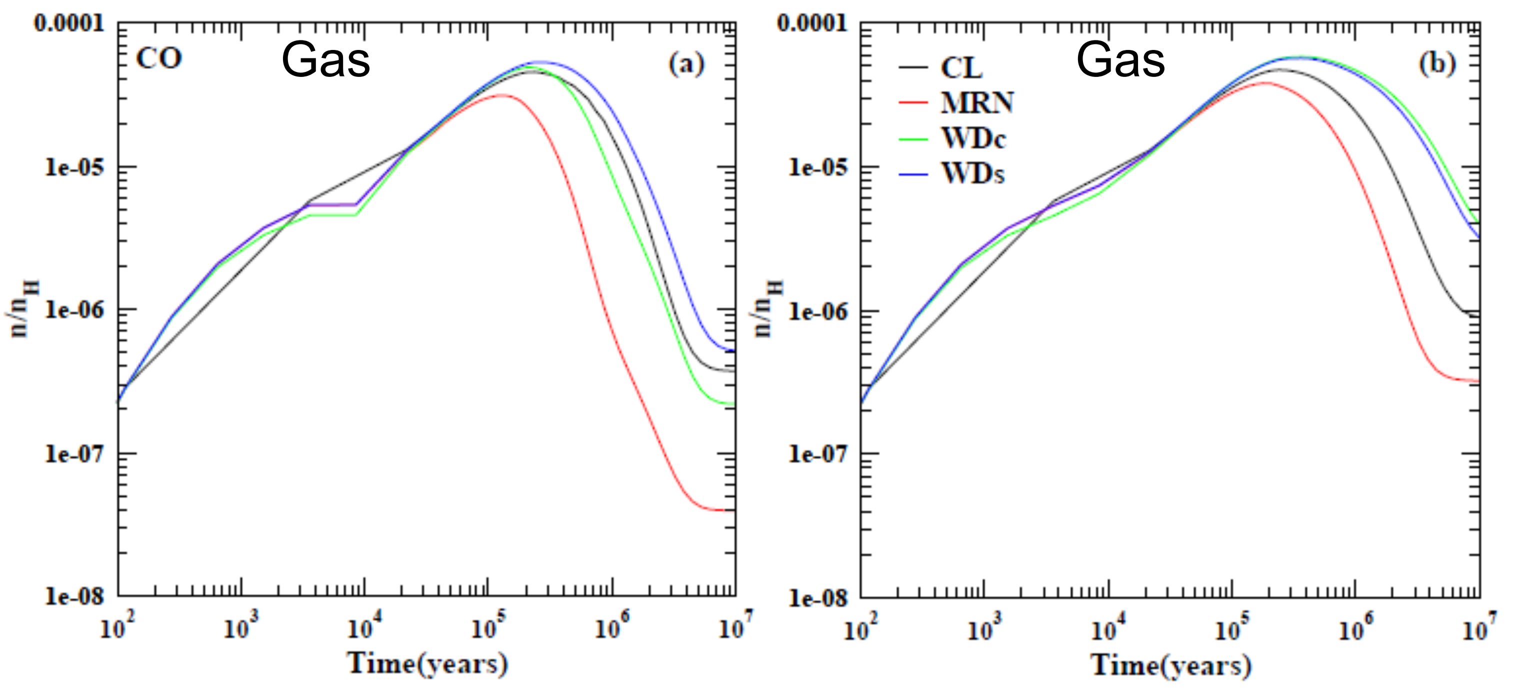


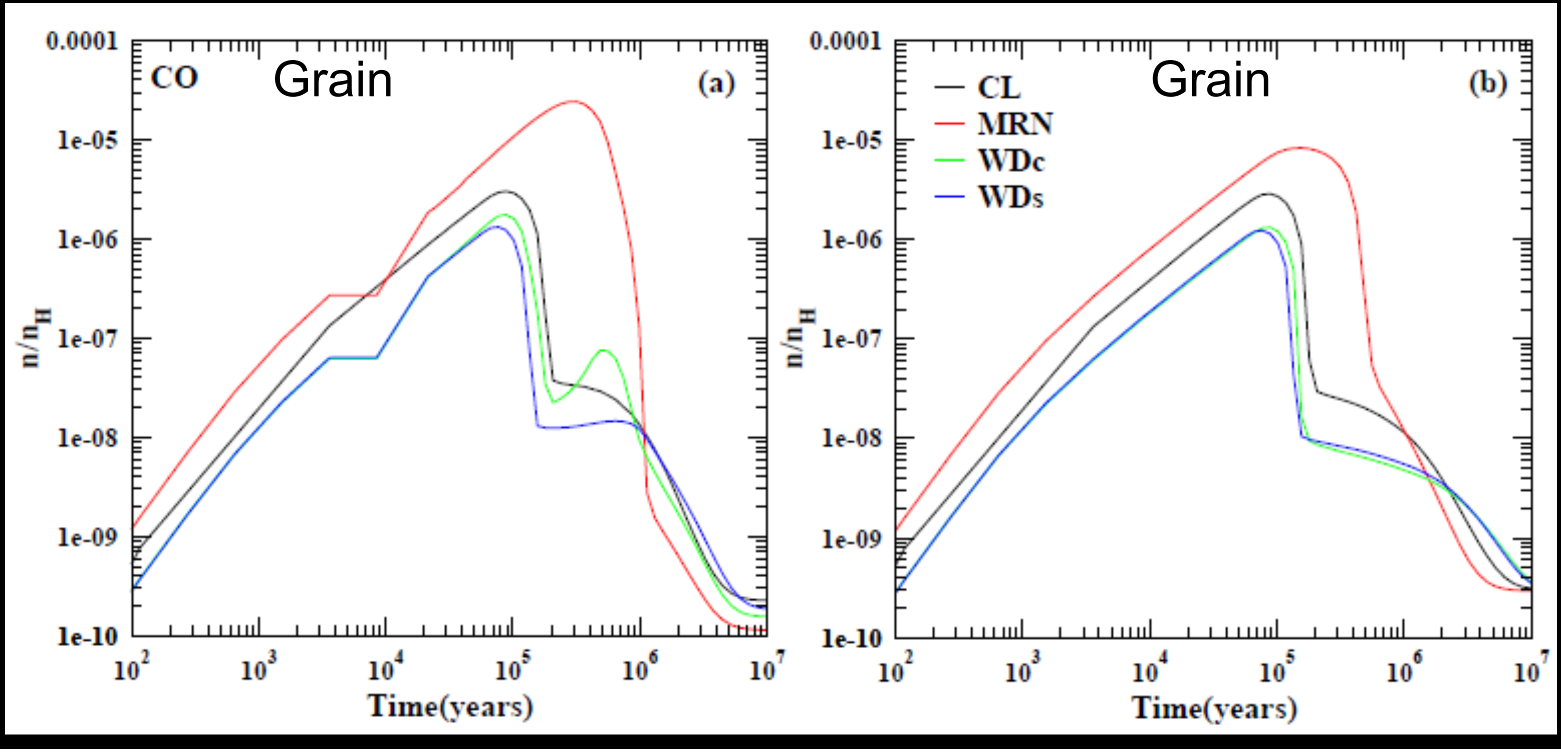
$$4\pi a^2 da.\rho_g = M_g$$

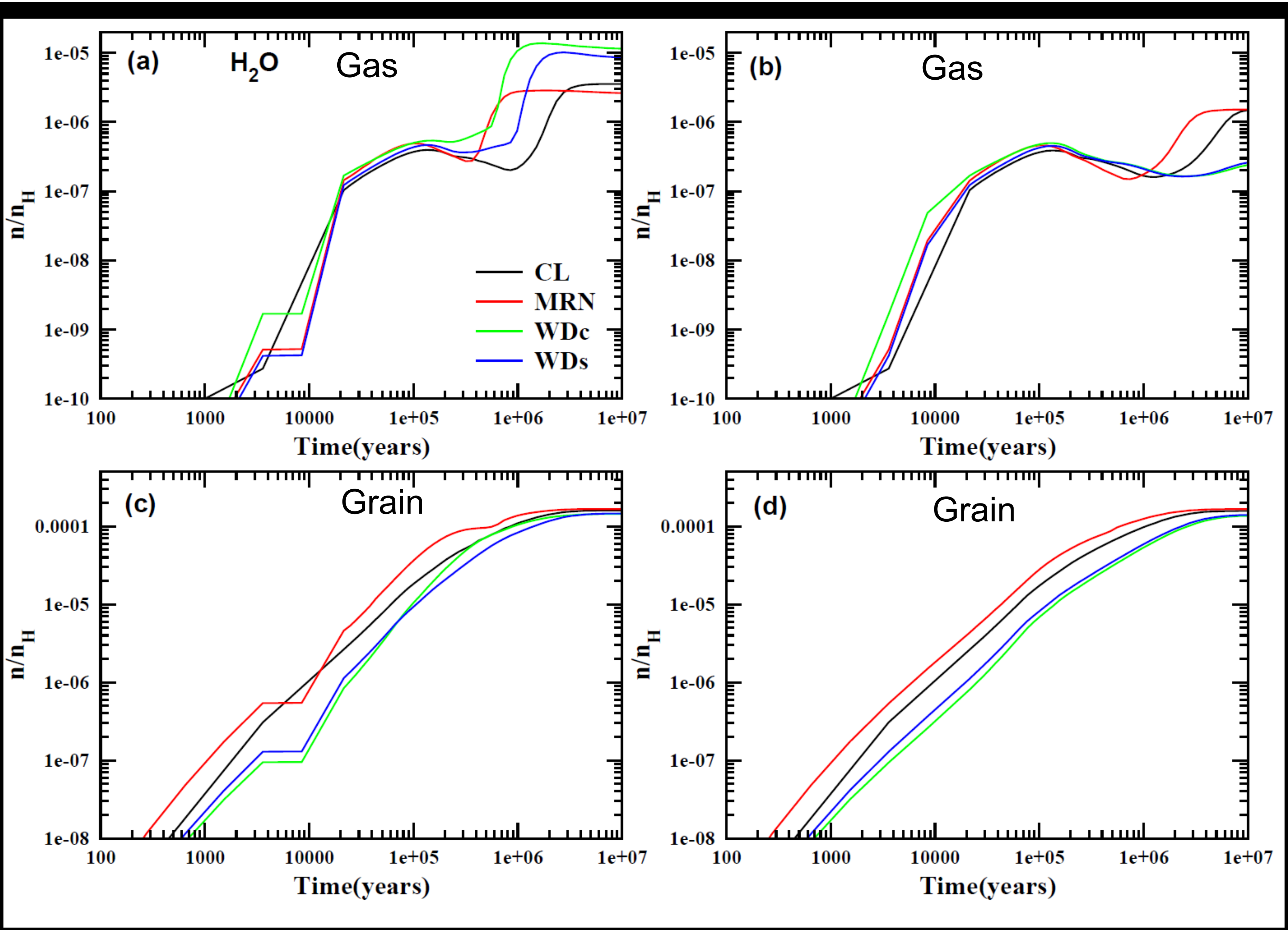
Classical grains, a = 0.1μm, $N_s = 10^6$, $n_d = 1.33 \times 10^{-12} n_H$

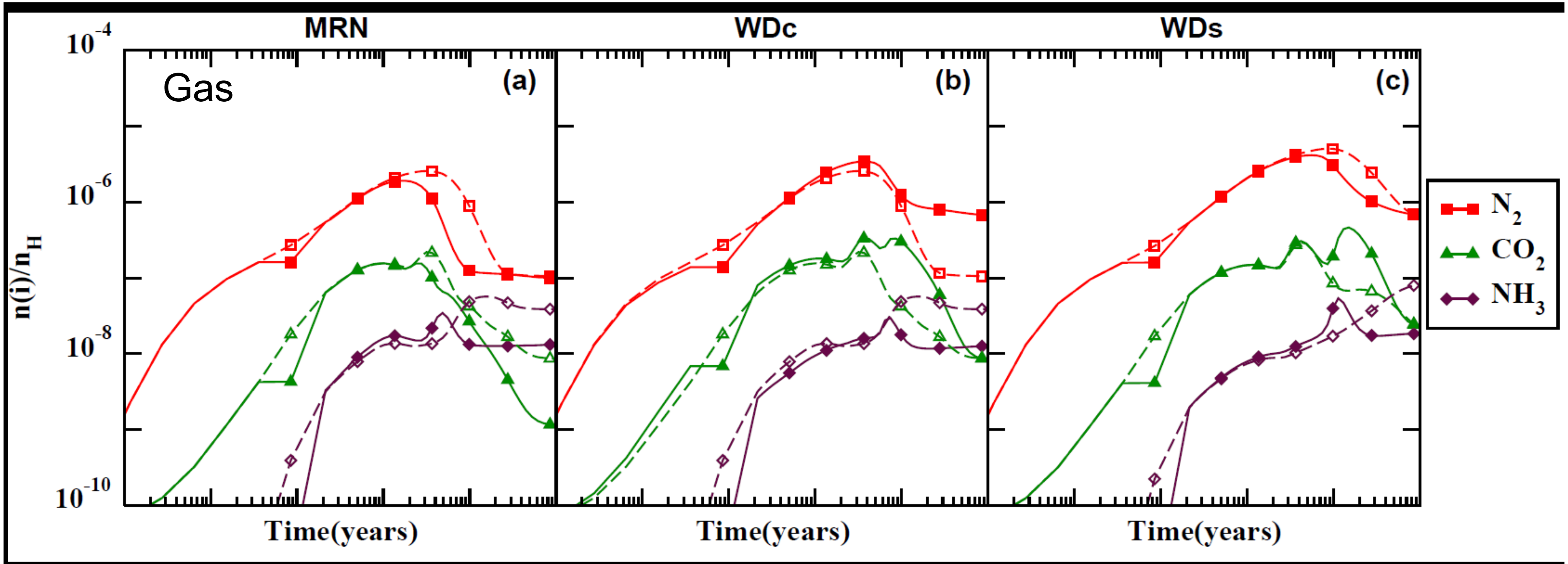


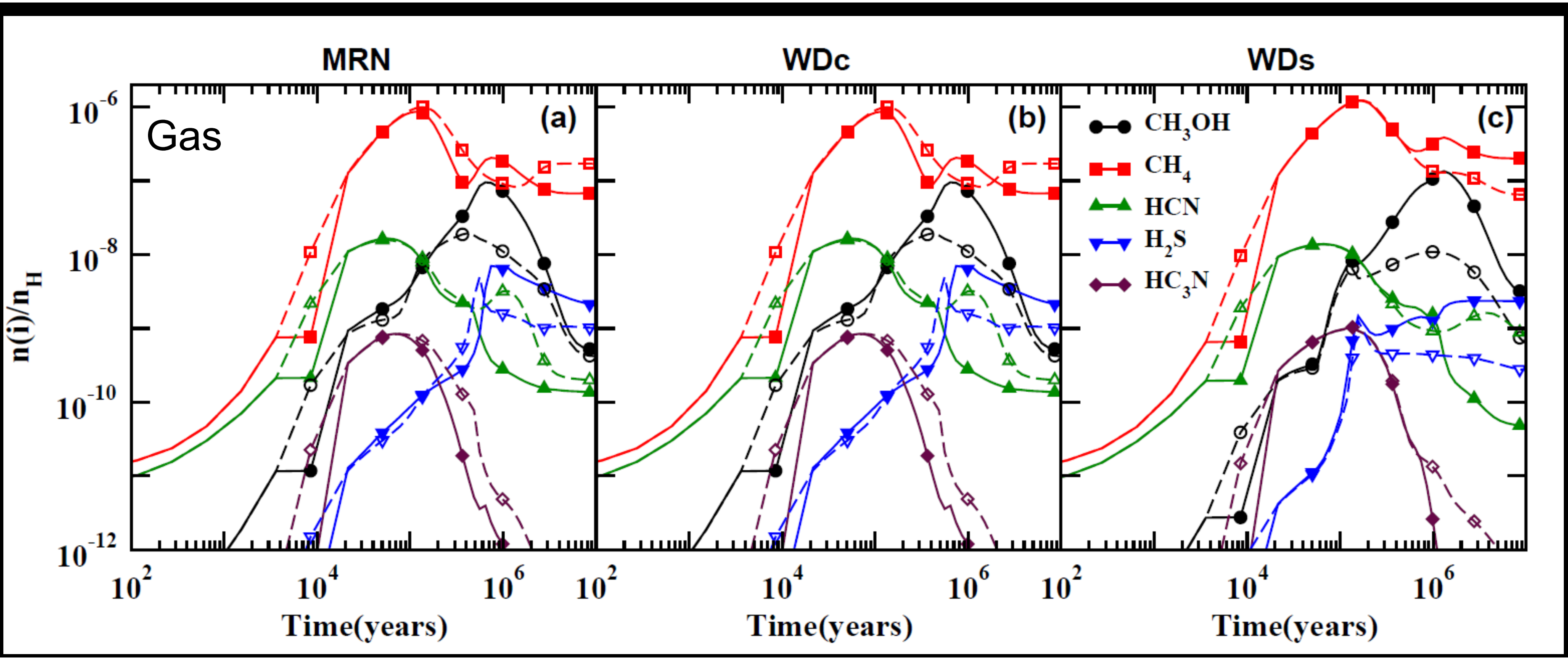

(a) Gas
(b) Gas
(c) Grain
(d) Grain
$n(i)/n_H$
Time (Years)
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
N_2
CO_2
H_2S
HC_3N
NH_3
CH_4
HCN

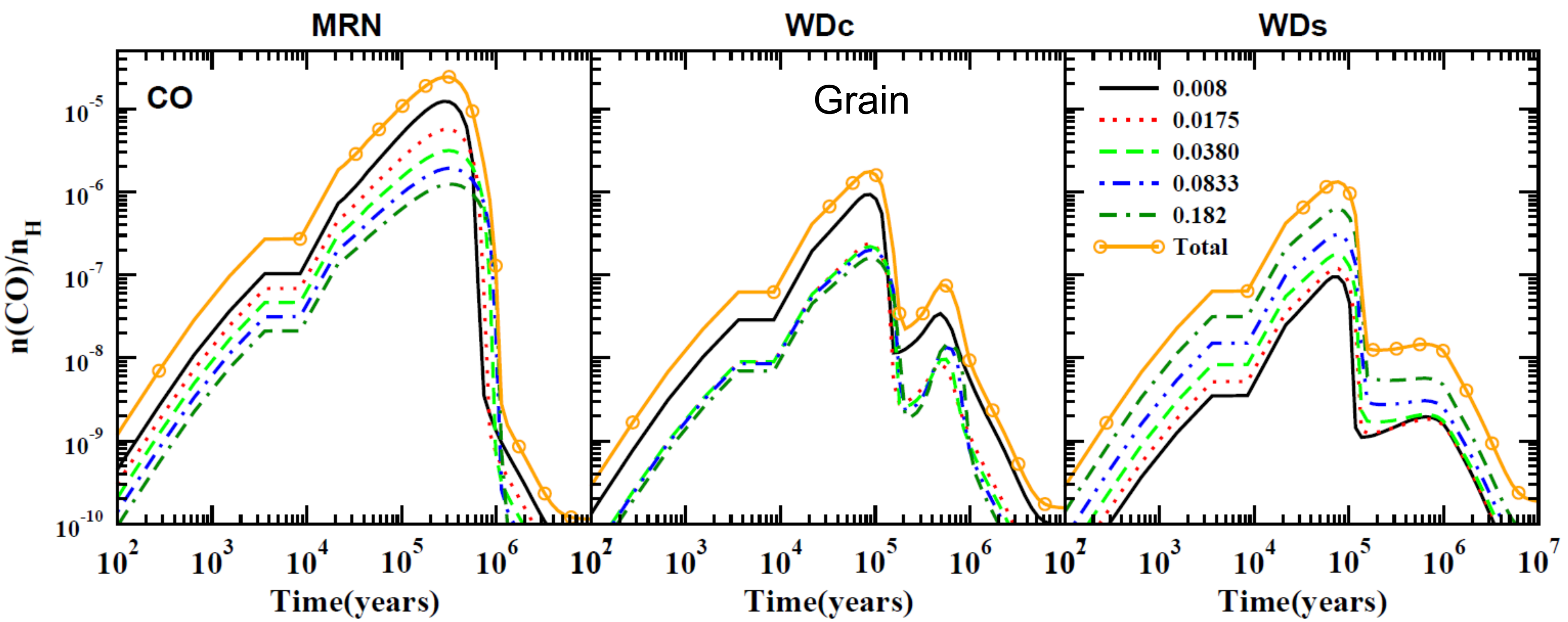

CO
Gas
(a)
Gas
(b)
— CL
— MRN
— WDc
— WDs
n/n$_H$
0.0001
1e-05
1e-06
1e-07
1e-08
10^2
10^3
10^4
10^5
10^6
10^7
Time(years)


CO
Grain
(a)
Grain
(b)
— CL
— MRN
— WDc
— WDs
n/n$_H$
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
10^2
10^3
10^4
10^5
10^6
10^7
Time(years)

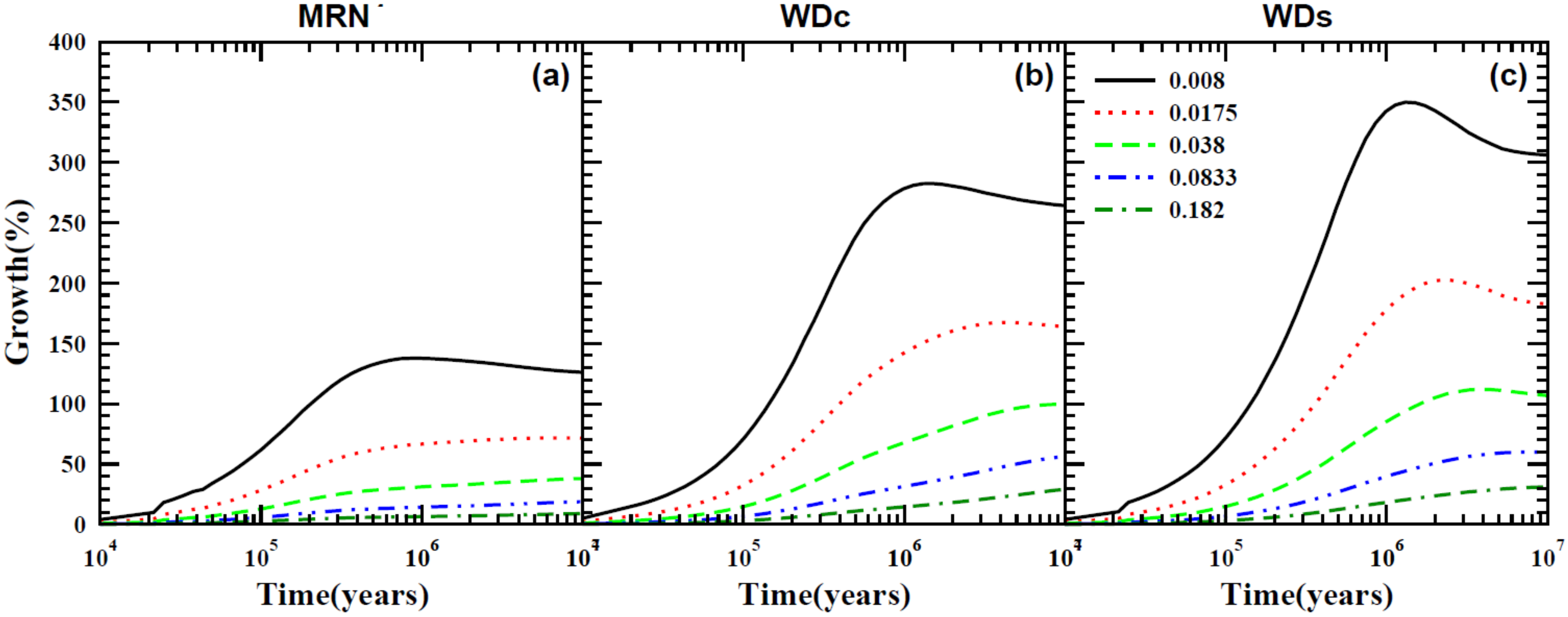

(a)
H_2O
Gas
(b)
Gas
(c)
Grain
(d)
Grain
CL
MRN
WDc
WDs
n/n_H
Time(years)
1e-10
1e-09
1e-08
1e-07
1e-06
1e-05
1e-08
1e-07
1e-06
1e-05
0.0001
100
1000
10000
1e+05
1e+06
1e+07


MRN
WDc
WDs
Gas
(a)
(b)
(c)
10^{-4}
10^{-6}
10^{-8}
10^{-10}
n(i)/n$_H$
Time(years)
N_2
CO_2
NH_3

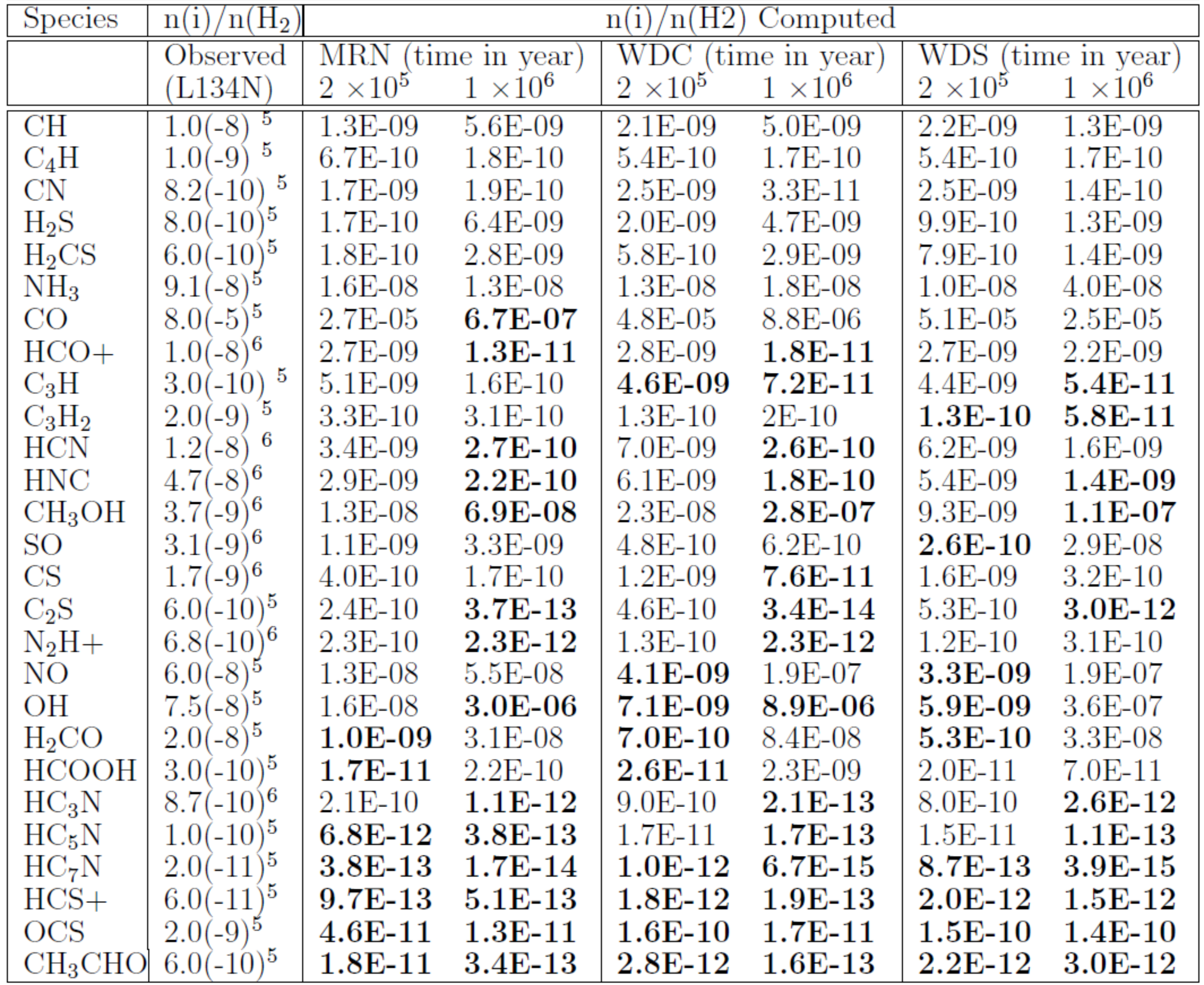

MRN
WDc
WDs
Gas
(a)
(b)
(c)
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{2}
10^{4}
10^{6}
n(i)/n$_H$
Time(years)
CH_3OH
CH_4
HCN
H_2S
HC_3N



Grain surface abundance of CO for different grain size distribution with grain growth taken into account. Grain radius is in μm.

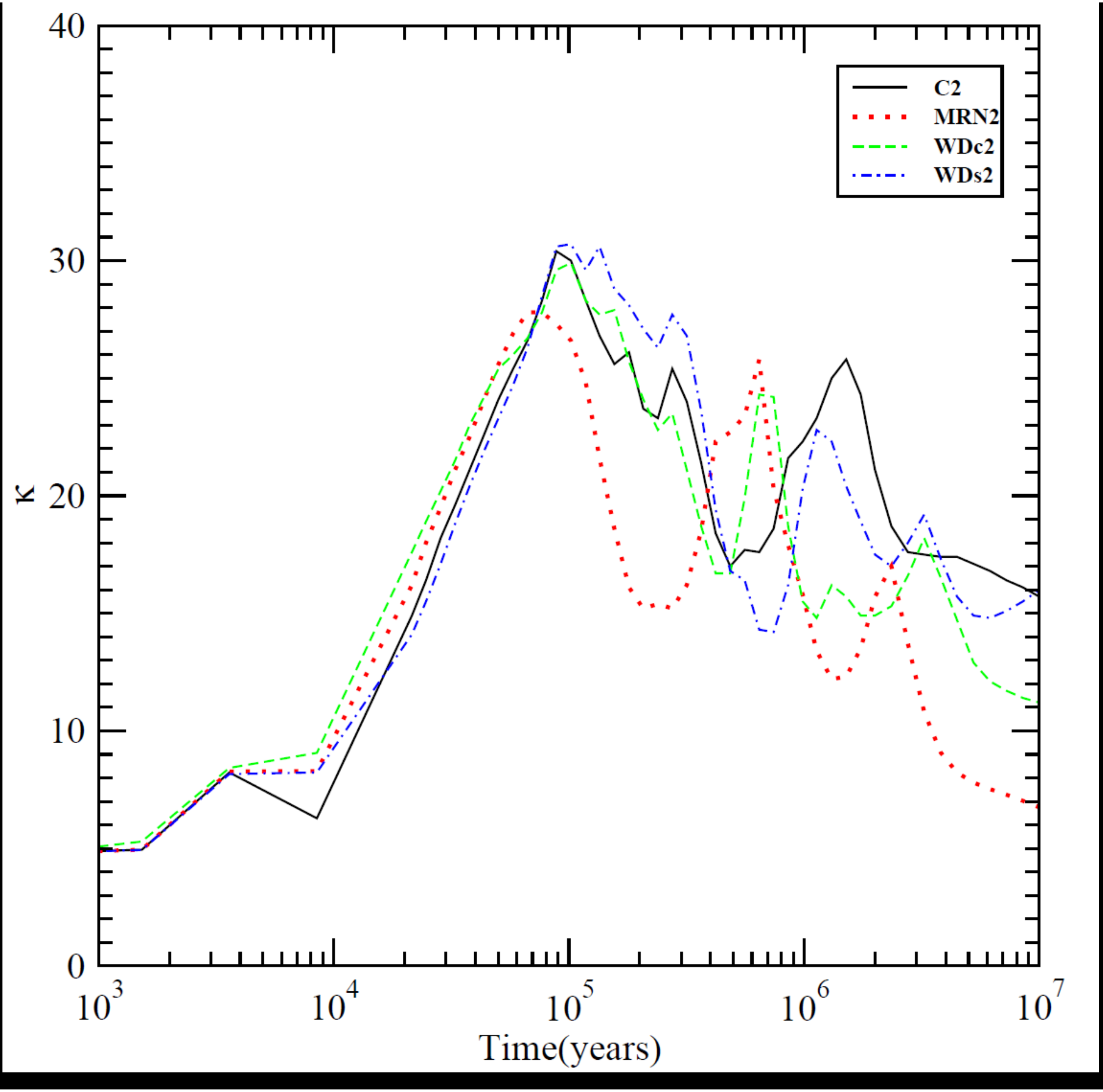


Percentage change in radius due to grain growth for different size distributions.

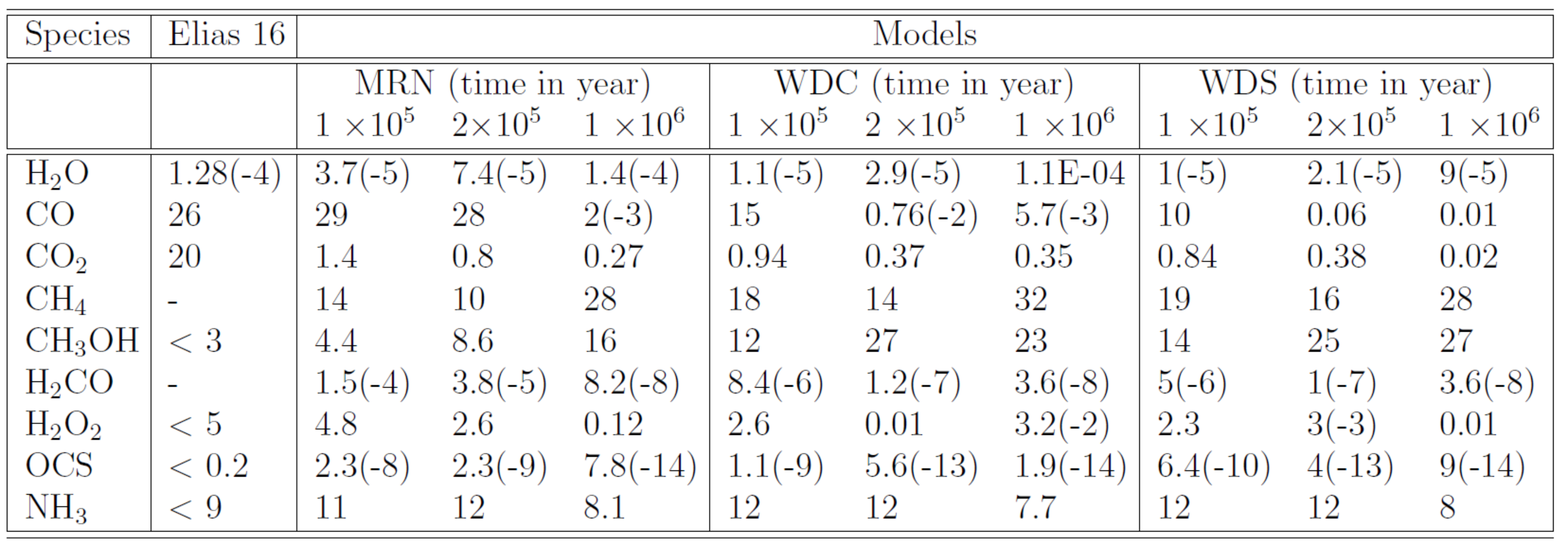


Species	$n(i)/n(H_2)$	$n(i)/n(H2)$ Computed					
	Observed (L134N)	MRN (time in year) 2×10^5	1×10^6	WDC (time in year) 2×10^5	1×10^6	WDS (time in year) 2×10^5	1×10^6
CH	1.0(-8)[5]	1.3E-09	5.6E-09	2.1E-09	5.0E-09	2.2E-09	1.3E-09
C_4H	1.0(-9)[5]	6.7E-10	1.8E-10	5.4E-10	1.7E-10	5.4E-10	1.7E-10
CN	8.2(-10)[5]	1.7E-09	1.9E-10	2.5E-09	3.3E-11	2.5E-09	1.4E-10
H_2S	8.0(-10)[5]	1.7E-10	6.4E-09	2.0E-09	4.7E-09	9.9E-10	1.3E-09
H_2CS	6.0(-10)[5]	1.8E-10	2.8E-09	5.8E-10	2.9E-09	7.9E-10	1.4E-09
NH_3	9.1(-8)[5]	1.6E-08	1.3E-08	1.3E-08	1.8E-08	1.0E-08	4.0E-08
CO	8.0(-5)[5]	2.7E-05	**6.7E-07**	4.8E-05	8.8E-06	5.1E-05	2.5E-05
HCO+	1.0(-8)[6]	2.7E-09	**1.3E-11**	2.8E-09	**1.8E-11**	2.7E-09	2.2E-09
C_3H	3.0(-10)[5]	5.1E-09	1.6E-10	**4.6E-09**	**7.2E-11**	4.4E-09	**5.4E-11**
C_3H_2	2.0(-9)[5]	3.3E-10	3.1E-10	1.3E-10	2E-10	**1.3E-10**	**5.8E-11**
HCN	1.2(-8)[6]	3.4E-09	**2.7E-10**	7.0E-09	**2.6E-10**	6.2E-09	1.6E-09
HNC	4.7(-8)[6]	2.9E-09	**2.2E-10**	6.1E-09	**1.8E-10**	5.4E-09	**1.4E-09**
CH_3OH	3.7(-9)[6]	1.3E-08	**6.9E-08**	2.3E-08	**2.8E-07**	9.3E-09	**1.1E-07**
SO	3.1(-9)[6]	1.1E-09	3.3E-09	4.8E-10	6.2E-10	**2.6E-10**	2.9E-08
CS	1.7(-9)[6]	4.0E-10	1.7E-10	1.2E-09	**7.6E-11**	1.6E-09	3.2E-10
C_2S	6.0(-10)[5]	2.4E-10	**3.7E-13**	4.6E-10	**3.4E-14**	5.3E-10	**3.0E-12**
N_2H+	6.8(-10)[6]	2.3E-10	**2.3E-12**	1.3E-10	**2.3E-12**	1.2E-10	3.1E-10
NO	6.0(-8)[5]	1.3E-08	5.5E-08	**4.1E-09**	1.9E-07	**3.3E-09**	1.9E-07
OH	7.5(-8)[5]	1.6E-08	**3.0E-06**	**7.1E-09**	**8.9E-06**	**5.9E-09**	3.6E-07
H_2CO	2.0(-8)[5]	**1.0E-09**	3.1E-08	**7.0E-10**	8.4E-08	**5.3E-10**	3.3E-08
HCOOH	3.0(-10)[5]	**1.7E-11**	2.2E-10	**2.6E-11**	2.3E-09	2.0E-11	7.0E-11
HC_3N	8.7(-10)[6]	2.1E-10	**1.1E-12**	9.0E-10	**2.1E-13**	8.0E-10	**2.6E-12**
HC_5N	1.0(-10)[5]	**6.8E-12**	**3.8E-13**	1.7E-11	**1.7E-13**	1.5E-11	**1.1E-13**
HC_7N	2.0(-11)[5]	**3.8E-13**	**1.7E-14**	**1.0E-12**	**6.7E-15**	**8.7E-13**	**3.9E-15**
HCS+	6.0(-11)[5]	**9.7E-13**	**5.1E-13**	**1.8E-12**	**1.9E-13**	**2.0E-12**	**1.5E-12**
OCS	2.0(-9)[5]	**4.6E-11**	**1.3E-11**	**1.6E-10**	**1.7E-11**	**1.5E-10**	**1.4E-10**
CH_3CHO	6.0(-10)[5]	**1.8E-11**	**3.4E-13**	**2.8E-12**	**1.6E-13**	**2.2E-12**	**3.0E-12**

(5) Ohishi et al, 1992, and (6) Dickens et al., 2000



Variation of overall confidence (multiplied by 100) with time for different models of L134N with observations excluding molecules with observed upper or lower limits.



Species	Elias 16	Models								
		MRN (time in year)			WDC (time in year)			WDS (time in year)		
		1×10^5	2×10^5	1×10^6	1×10^5	2×10^5	1×10^6	1×10^5	2×10^5	1×10^6
H_2O	1.28(-4)	3.7(-5)	7.4(-5)	1.4(-4)	1.1(-5)	2.9(-5)	1.1E-04	1(-5)	2.1(-5)	9(-5)
CO	26	29	28	2(-3)	15	0.76(-2)	5.7(-3)	10	0.06	0.01
CO_2	20	1.4	0.8	0.27	0.94	0.37	0.35	0.84	0.38	0.02
CH_4	-	14	10	28	18	14	32	19	16	28
CH_3OH	< 3	4.4	8.6	16	12	27	23	14	25	27
H_2CO	-	1.5(-4)	3.8(-5)	8.2(-8)	8.4(-6)	1.2(-7)	3.6(-8)	5(-6)	1(-7)	3.6(-8)
H_2O_2	< 5	4.8	2.6	0.12	2.6	0.01	3.2(-2)	2.3	3(-3)	0.01
OCS	< 0.2	2.3(-8)	2.3(-9)	7.8(-14)	1.1(-9)	5.6(-13)	1.9(-14)	6.4(-10)	4(-13)	9(-14)
NH_3	< 9	11	12	8.1	12	12	7.7	12	12	8

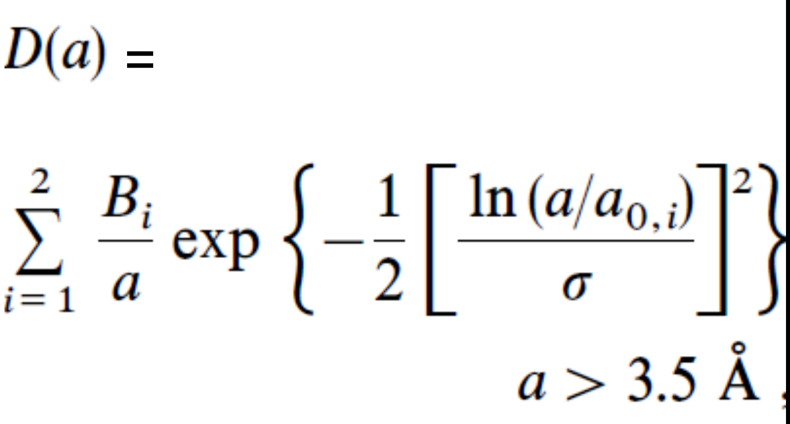
Summary

1. I have shown how complex molecules can from in star forming regions.
2. Formation of molecular hydrogen requires grain surface. Master equation and rate equation methods can be coupled.
3. H_2 formation efficiency is strongly dependent on temperature.
4. Then we discussed formation water and methanol and showed that when the number density of accreting O is less than three times that of CO, methanol is always overproduced.
5. Using the available reaction pathways it appears to be difficult to match the exact observed abundances of all three molecules simultaneously.
6. Only in a narrow region of parameter space are all three molecules produced within the observed limits.

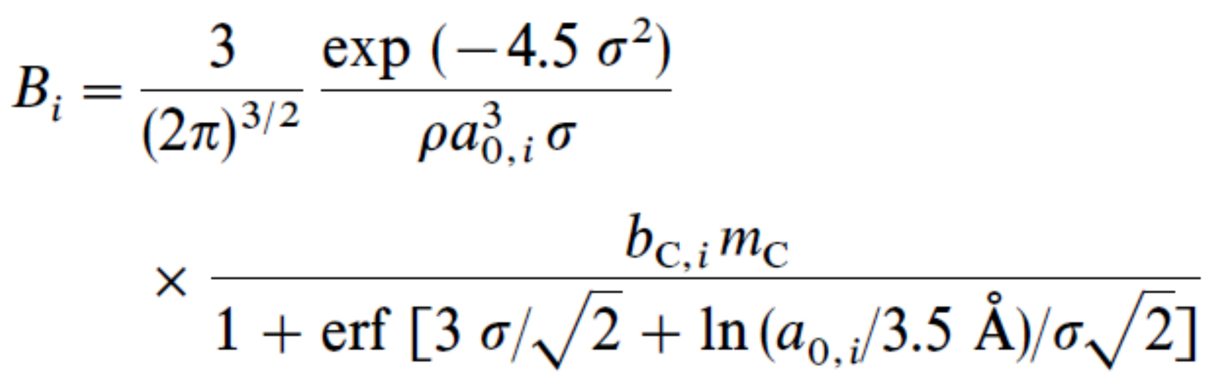
6. We have investigated the formation of complex molecules in star forming clouds using three different grain size distributions and also found out the effect of grain growth on the molecular abundances.
7. We found grains of different sizes have different contributions to the final gas phase and grain surface molecular abundances.
8. Species like H_2O, NH_3, CH_4 etc which are efficiently forms on the grain surface has higher gas phase abundance due to non thermal desorption mechanisms.
9. Species like CO, which are produced efficiently in the gas phase has lower gas phase abundance due to depletion.
10. Larger is the effective surface area shorter is the time scale.

Thank You

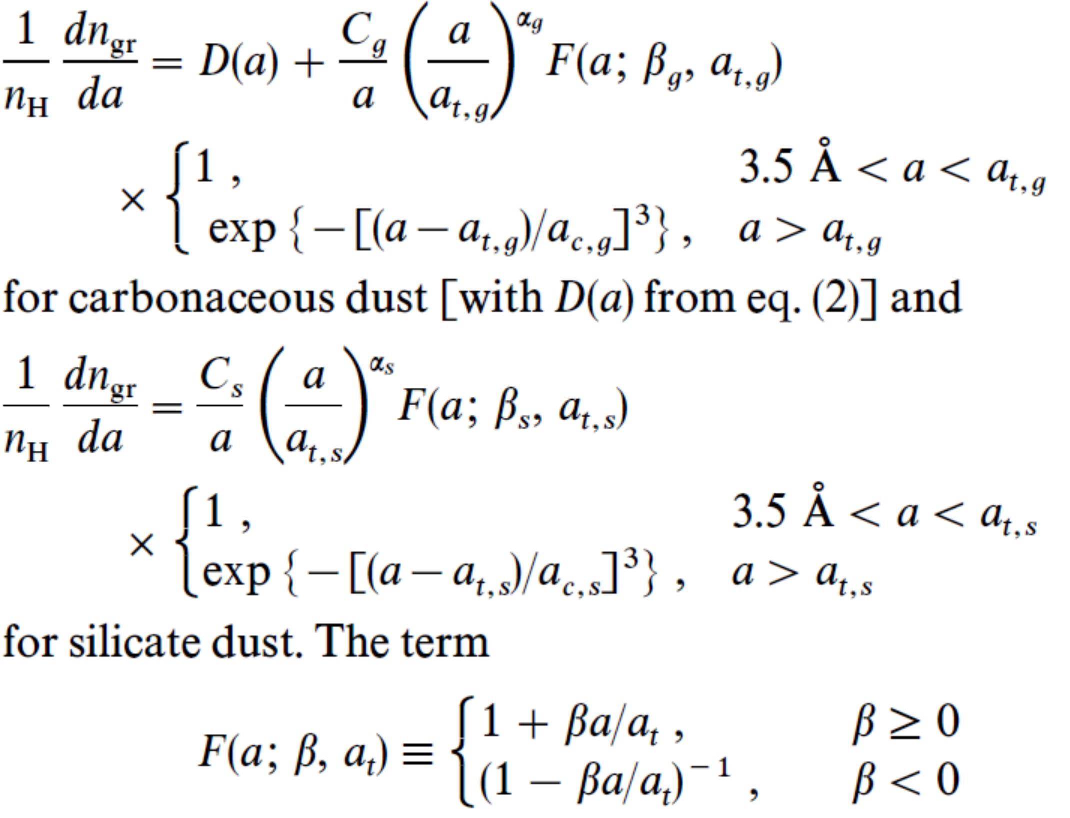
WD Size Distribution



$$D(a) = \sum_{i=1}^{2} \frac{B_i}{a} \exp\left\{-\frac{1}{2}\left[\frac{\ln(a/a_{0,i})}{\sigma}\right]^2\right\} \qquad a > 3.5\ \text{Å}$$



$$B_i = \frac{3}{(2\pi)^{3/2}} \frac{\exp(-4.5\,\sigma^2)}{\rho a_{0,i}^3 \sigma} \times \frac{b_{\mathrm{C},i} m_{\mathrm{C}}}{1 + \mathrm{erf}\left[3\,\sigma/\sqrt{2} + \ln(a_{0,i}/3.5\ \text{Å})/\sigma\sqrt{2}\right]}$$



$$\frac{1}{n_{\mathrm{H}}} \frac{dn_{\mathrm{gr}}}{da} = D(a) + \frac{C_g}{a}\left(\frac{a}{a_{t,g}}\right)^{\alpha_g} F(a;\, \beta_g,\, a_{t,g}) \times \begin{cases} 1\,, & 3.5\ \text{Å} < a < a_{t,g} \\ \exp\{-[(a - a_{t,g})/a_{c,g}]^3\}\,, & a > a_{t,g} \end{cases}$$

for carbonaceous dust [with $D(a)$ from eq. (2)] and

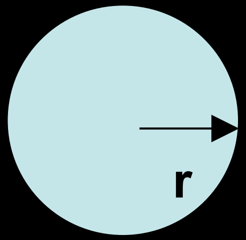
$$\frac{1}{n_{\mathrm{H}}} \frac{dn_{\mathrm{gr}}}{da} = \frac{C_s}{a}\left(\frac{a}{a_{t,s}}\right)^{\alpha_s} F(a;\, \beta_s,\, a_{t,s}) \times \begin{cases} 1\,, & 3.5\ \text{Å} < a < a_{t,s} \\ \exp\{-[(a - a_{t,s})/a_{c,s}]^3\}\,, & a > a_{t,s} \end{cases}$$

for silicate dust. The term

$$F(a;\, \beta,\, a_t) \equiv \begin{cases} 1 + \beta a/a_t\,, & \beta \geq 0 \\ (1 - \beta a/a_t)^{-1}\,, & \beta < 0 \end{cases}$$

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

Accretion



Velocity (v), cross section (σ) and number density of grain (n_d)

$$F_h = S\,\pi\,r^2\,v\,n_x\,n_d$$

S= sticking coefficients

r = Radius of the grain,

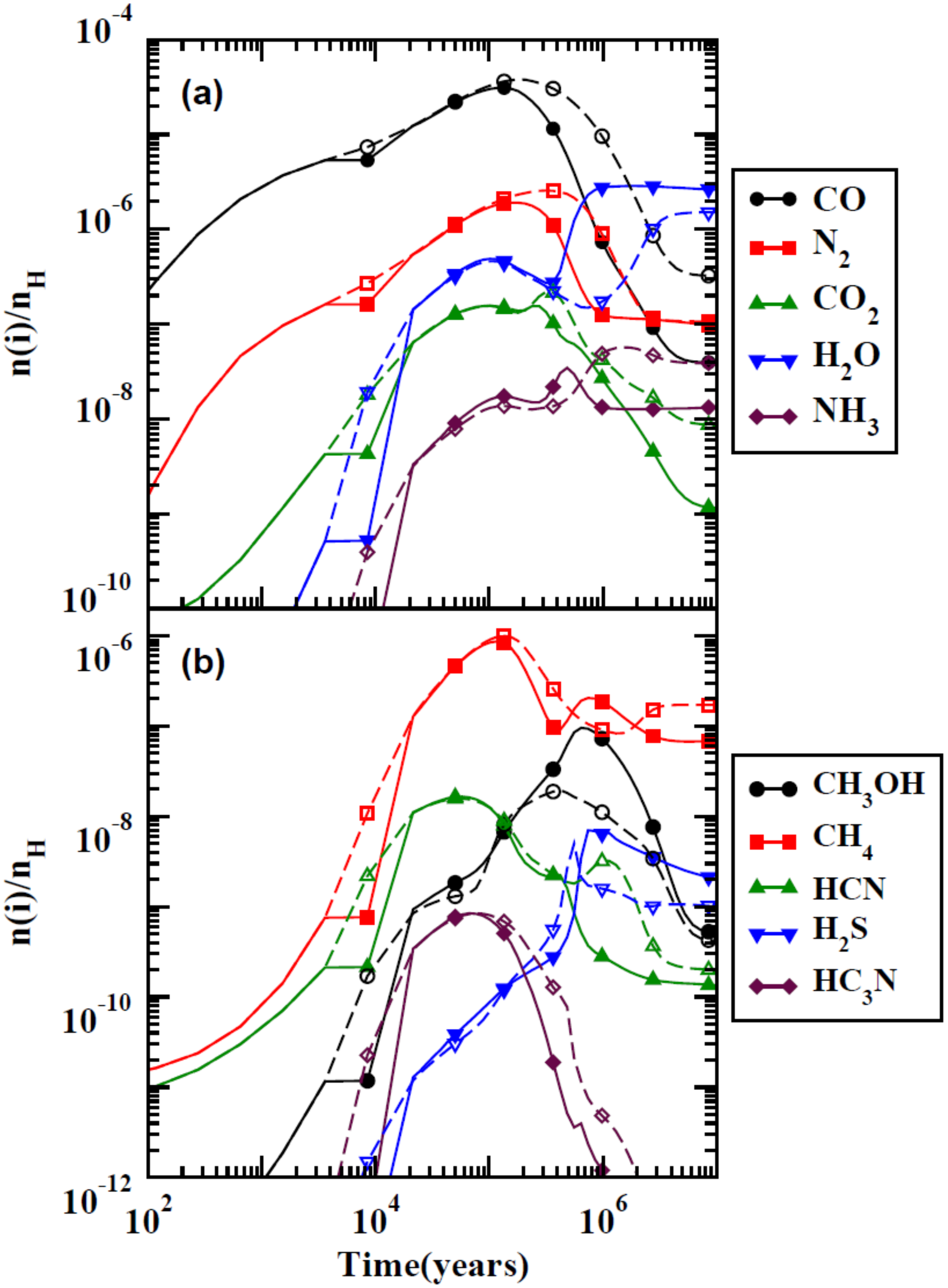
$v = (8KT/\pi m_x)^{1/2}$ = The thermal velocity,

n_x = the number density of any species 'x' and

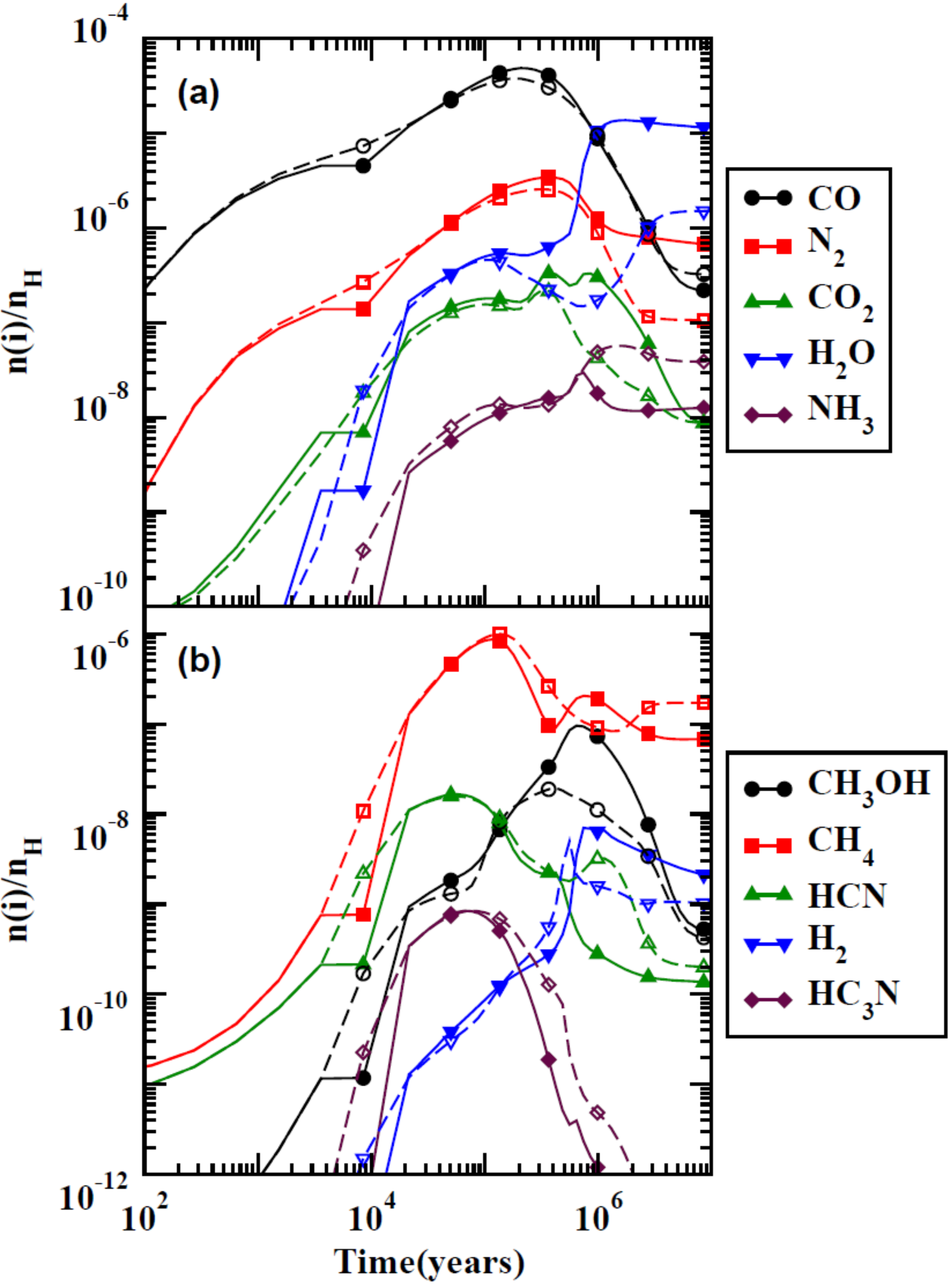
[redacted]

Species	$n(i)/n(H_2)$	n(i)/n(H2) Computed					
	Observed	MRN (time in year)		WDC (time in year)		WDS (time in year)	
	(L134N)	2×10^5	1×10^6	2×10^5	1×10^6	2×10^5	1×10^6
C_3H_4	$\leq$1.2(-9)[5]	2.2E-10	2.4E-09	**7.5E-11**	1.4E-09	**4.5E-11**	6.5E-10
C_2H	$\leq$5.0(-8)[5]	5E-09	**2.8E-10**	6.2E-09	**2.3E-11**	6.0E-09	**4.3E-11**
C	$\geq$1.0(-6)[4]	1.0E-07	**2.3E-09**	2.3E-06	**8.9E-10**	2.9E-06	**6.5E-10**
CH_2CN	$\leq$1.0(-9)[5]	1.3E-10	**4.6E-12**	1.4E-10	**8.4E-12**	1.1E-10	**2.5E-11**
C_3N	$\leq$2.0(-10)[5]	2.3E-10	**6.6E-13**	2.6E-10	**1.0E-13**	2.5E-10	**1.4E-12**
CH_2CO	$\leq$7.0(-10)[5]	1.5E-09	**1.8E-13**	3.1E-09	**5.0E-14**	3.0E-09	1.3E-11
C_3O	$\leq$5.0(-11)[5]	1.8E-10	4.4E-11	2.2E-10	5.9E-11	1.9E-10	**3.7E-12**
C_3S	$\leq$2.0(-10)[5]	3.9E-11	**8.8E-14**	1.1E-10	**1.0E-14**	1.0E-10	**4.8E-13**
H_2O	$\leq$3.0(-7)[7]	3.7E-07	2.8E-06	5.2E-07	**1.1E-05**	4.2E-07	7.4E-07
O_2	$\leq$1.7(-7)[8]	1.5E-06	6.1E-07	2.8E-07	**5.9E-06**	2.1E-07	**2.0E-05**
SO_2	$\leq$1.6(-9)[6]	**3.8E-11**	**3.3E-08**	**1.2E-11**	**5.5E-08**	**6.3E-12**	1.5E-08
C_3H_3N	$\leq$1.0(-10)[5]	**2.4E-12**	**3.3E-12**	**2.4E-12**	**1.3E-13**	**4.1E-13**	**3.1E-14**
CH_3CN	$\leq$1.0(-9)[5]	**7.5E-12**	**6.4E-13**	**6.6E-11**	**3.8E-13**	**5.9E-11**	**3.7E-12**
H_2CN+	$\leq$3.1(-9)[5]	**5.3E-11**	**3.6E-12**	**8.8E-11**	**2.6E-12**	**7.4E-11**	**2.5E-11**

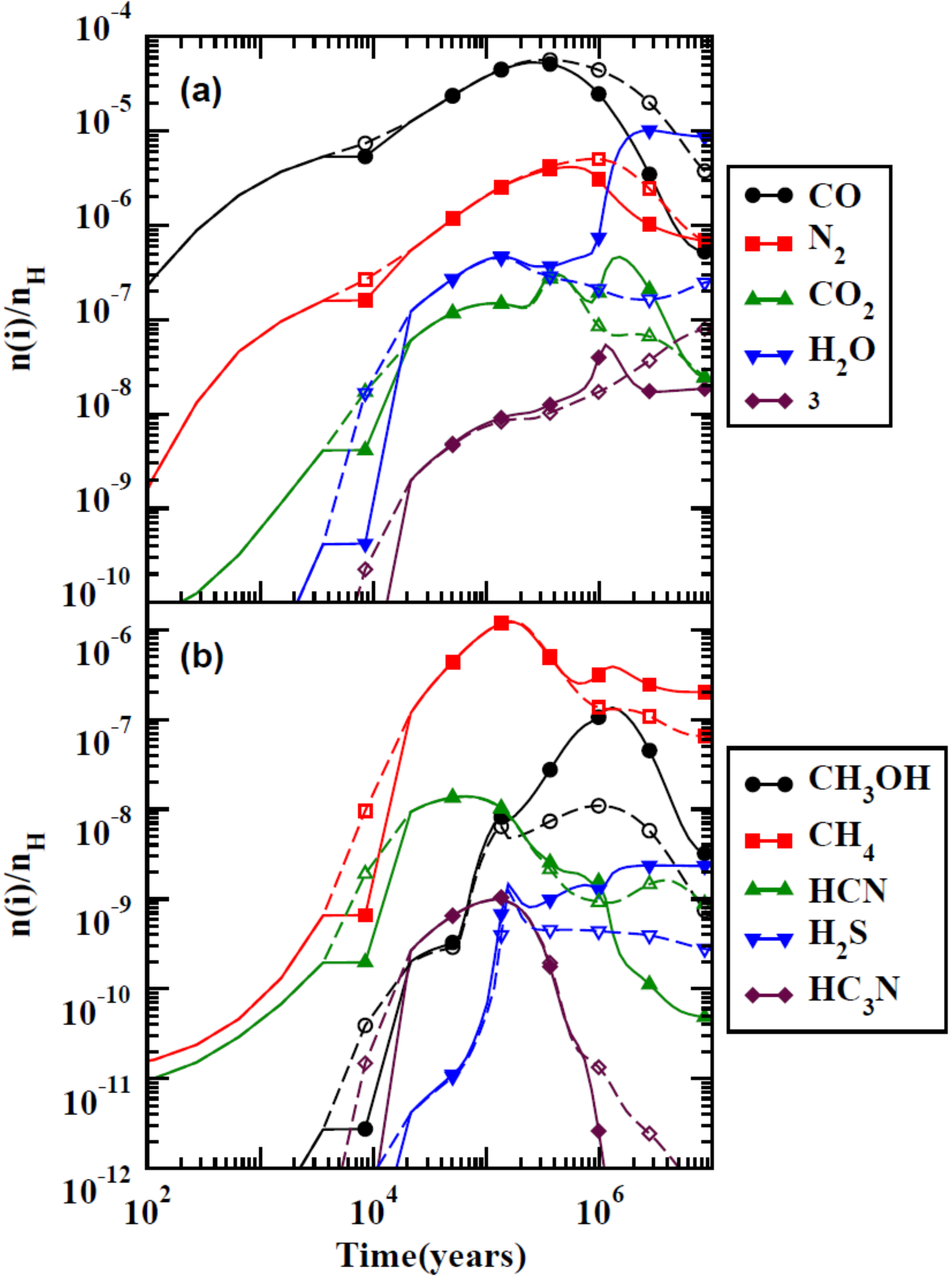
[redacted]



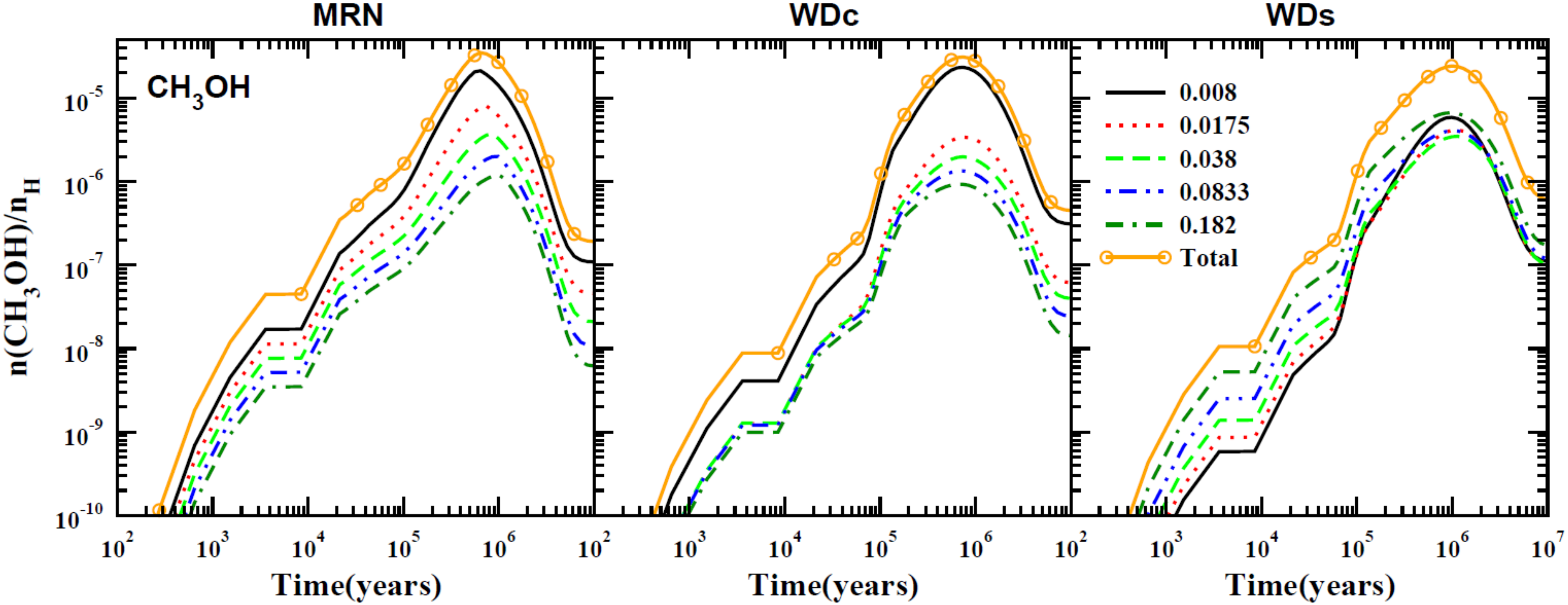
Gas phase abundances for few selected species with grain growth (solid line and with solid symbol) and without grain growth (dash line and hollow symbol) for MRN model

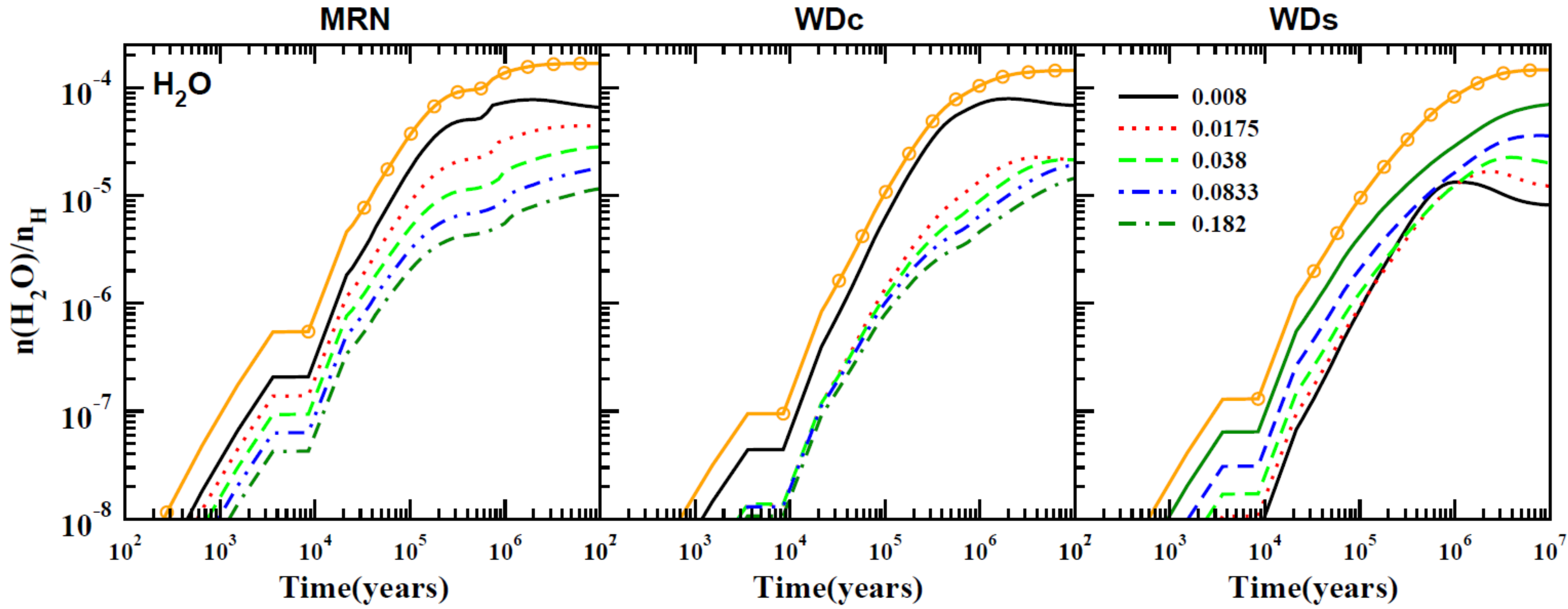


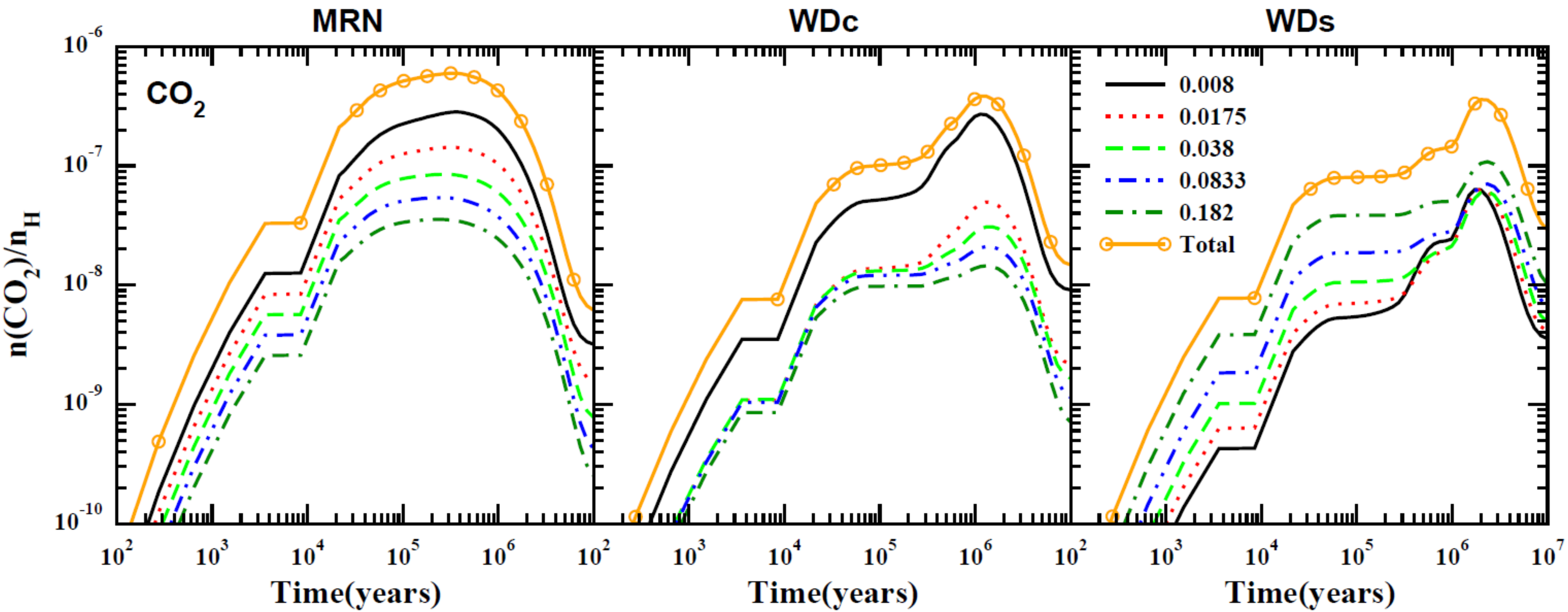
Gas phase abundances for few selected species with grain growth (solid line and with solid symbol) and without grain growth (dash line and hollow symbol) for WDc model



Gas phase abundances for few selected species with grain growth (solid line and with solid symbol) and without grain growth (dash line and hollow symbol) for WDs model


MRN
WDc
WDs
CH$_3$OH
$n(CH_3OH)/n_H$
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
Time(years)
0.008
0.0175
0.038
0.0833
0.182
Total


MRN
WDc
WDs
H$_2$O
n(H$_2$O)/n$_H$
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^2
10^3
10^4
10^5
10^6
10^7
Time(years)
0.008
0.0175
0.038
0.0833
0.182


MRN
WDc
WDs
CO$_2$
n(CO$_2$)/n$_H$
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^2
10^3
10^4
10^5
10^6
10^7
Time(years)
0.008
0.0175
0.038
0.0833
0.182
Total

✓Chemical Composition

The principal molecular ingredients of the interstellar dust are deduced from the way they absorb or emit infrared radiation.

Fortunately, the so-called fingerprint region of the infrared spectrum from 2.5 to 25 μm, where most vibrations of the molecular groups containing C, N, O and H occur, is accessible with modern telescopes.