

**Chemical Composition of the
interstellar grain mantle
under the effect of physical
parameters**

Dr. Ankan Das



**Indian Centre for Space
Physics**

Plan of my presentation

1. Introduction

2. Basic physical Process

3. Results

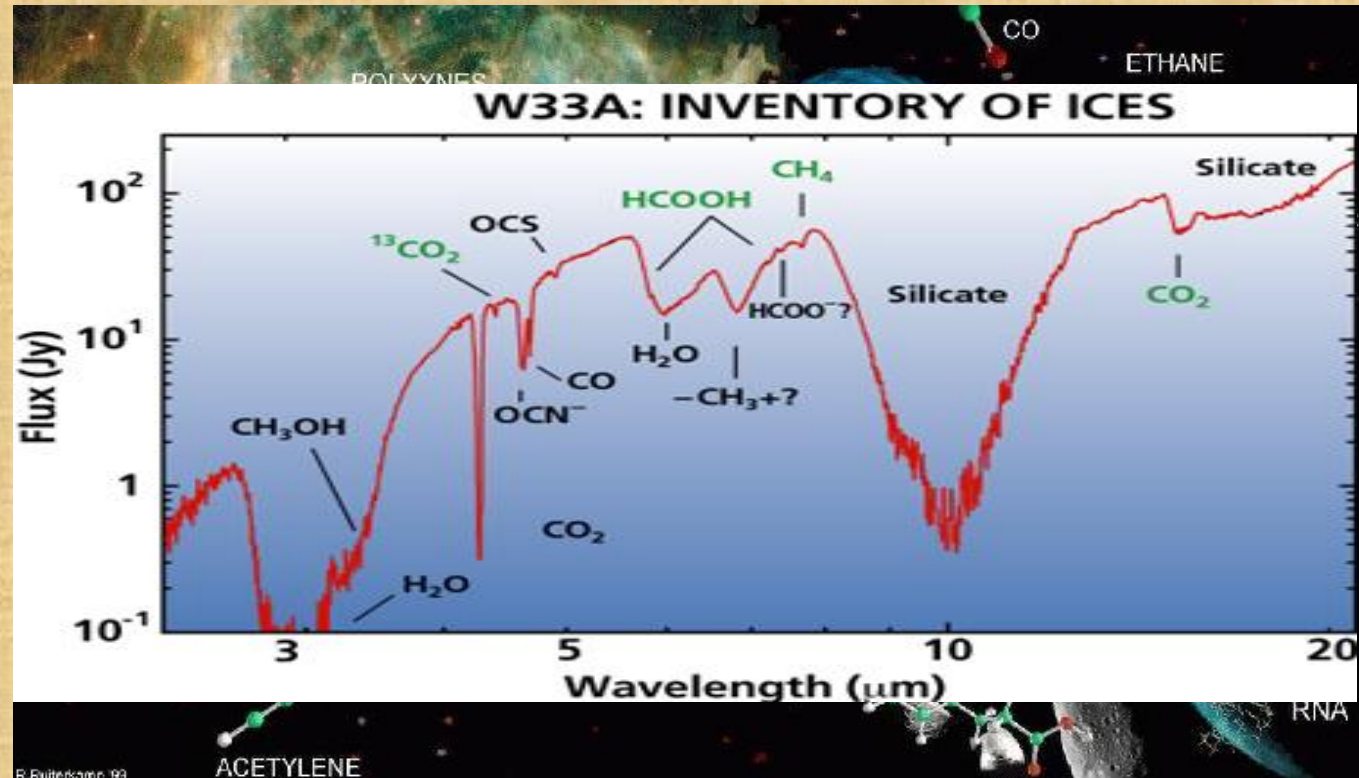
4. Summary

Interstellar Medium

ISM is the matter that exists in the space between the star systems in a galaxy .

Composition:

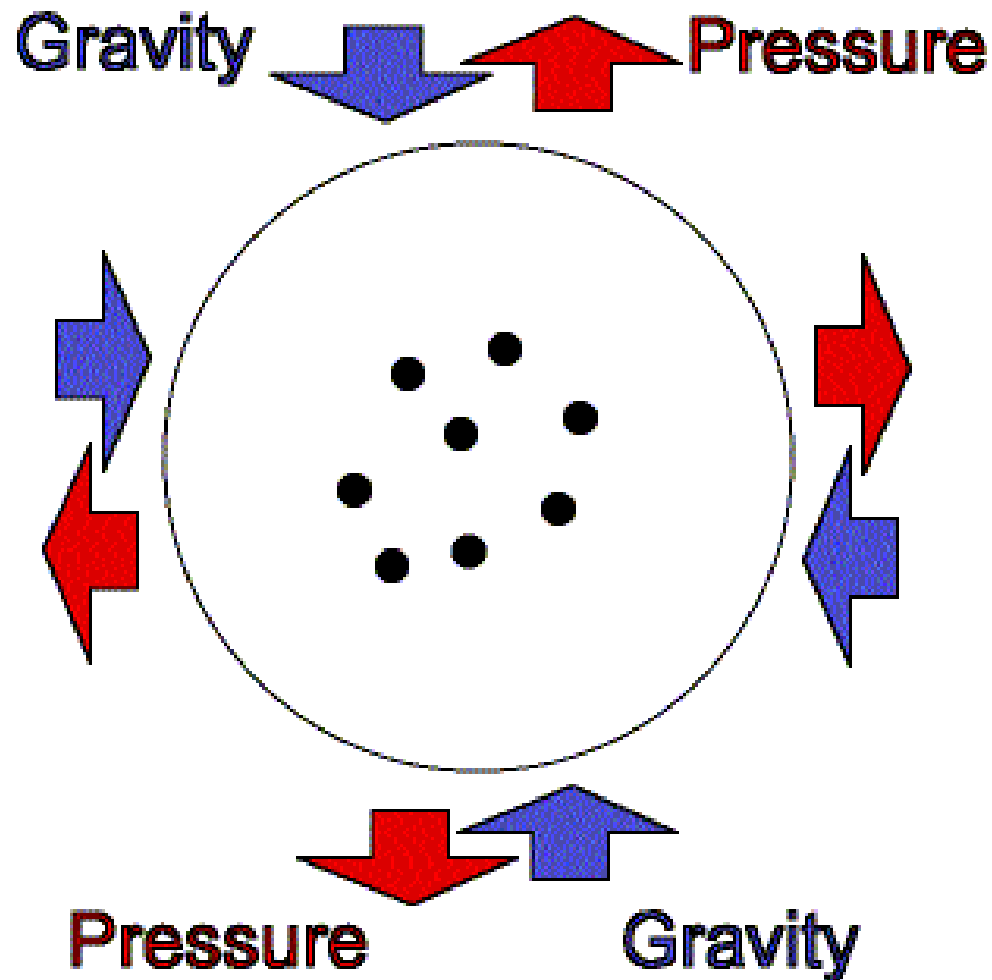
99% gas (89% hydrogen and 9% helium and 2% elements heavier than H or He) and 1% dust.



Interstellar cloud

Number	Density (cm^{-3})	T(K)	Visual Extinction	Chemistry
Diffuse atomic cloud	10-100	30- 100	< 0.1	$f_{\text{H}_2}^n < 0.1$

Formation of proto-stars



Type of grains

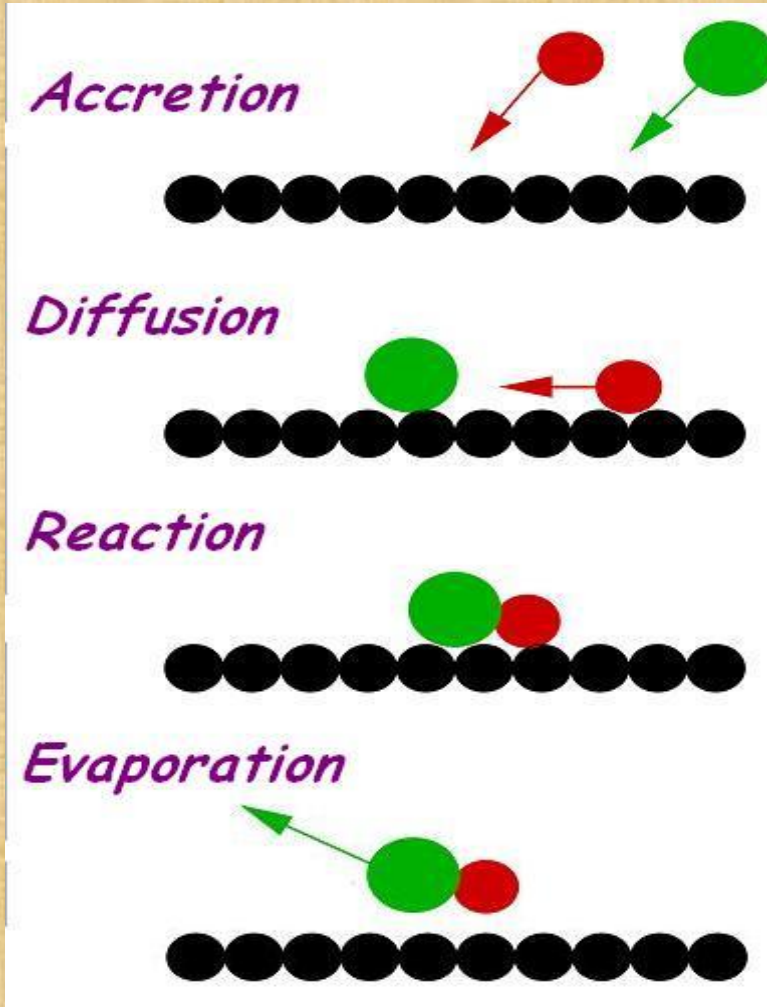


Olivine: $(\text{Mg,Fe})_2\text{SiO}_4$



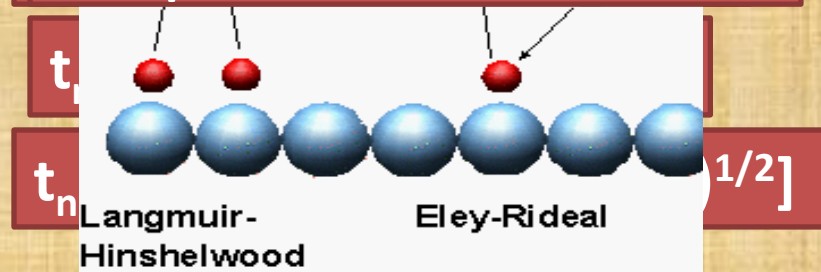
Amorphous Carbon

Basic Physical Process on Grain Surfaces



**Reaction
Evaporation**

$$t_{\text{evap}} = v_0^{-1} \exp(E_d / KT_d)$$



$$R_{i,j} = k_{i,j} (R_{\text{diff},i} + R_{\text{diff},j}) n_i n_j N_d$$

Different approaches to handle the Grain Chemistry

A. Deterministic Approach

B. Stochastic Approach

Surface Reactions considered in our H₂O & CO network

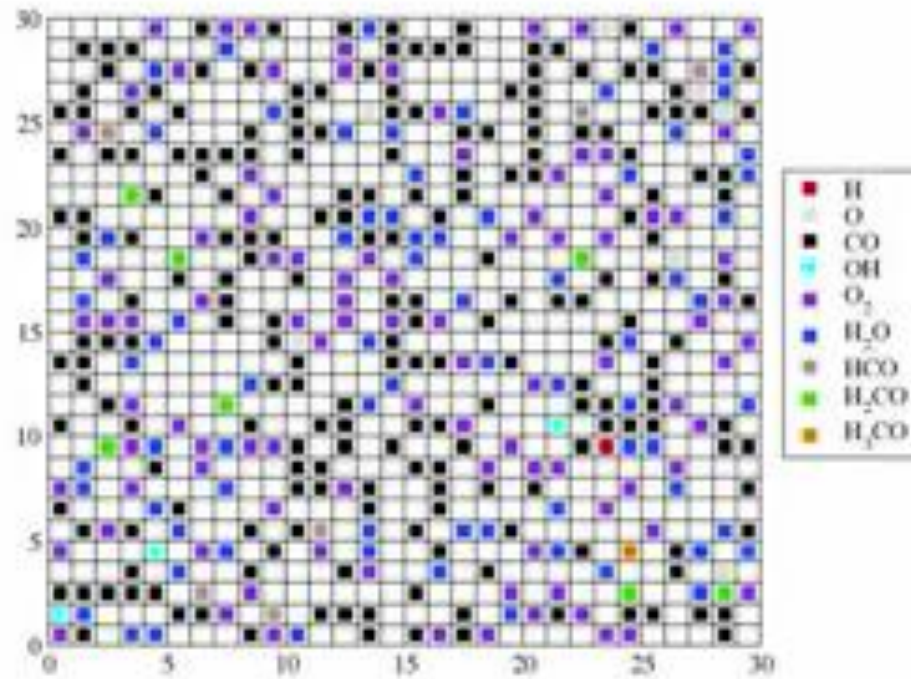
	Reactions	E _a (K)	Comments
1	H+H → H ₂		
2	H+O → OH		
3	H+OH → H ₂ O		
4	H+CO → HCO	2000	390K ± 40K at 12K (Fuchs et al., 2009)
5	H+HCO → H ₂ CO		
6	H+H ₂ CO → H ₃ CO	2000	415K ± 40K at 12K (Fuchs et al., 2009)
7	H+H ₃ CO → CH ₃ OH		
8	O+O → O ₂		
9	O+CO → CO ₂	1000	2970K (Talbi et al. 2002), 2500K (Goumans & Andersson 2010)
10	O+HCO → CO ₂ +H		
11	O+O ₂ → O ₃		
12	H+O ₂ → HO ₂	1200	barrier less (Ioppolo et al., 2008)
13	H+HO ₂ → H ₂ O ₂		
14	H+H ₂ O ₂ → H ₂ O+OH	1400	barrier less (Cazaux et al., 2010)
15	H+O ₃ → O ₂ +OH	450	
16	H ₂ +OH → H ₂ O+H	2600	

Initial gas phase abundance

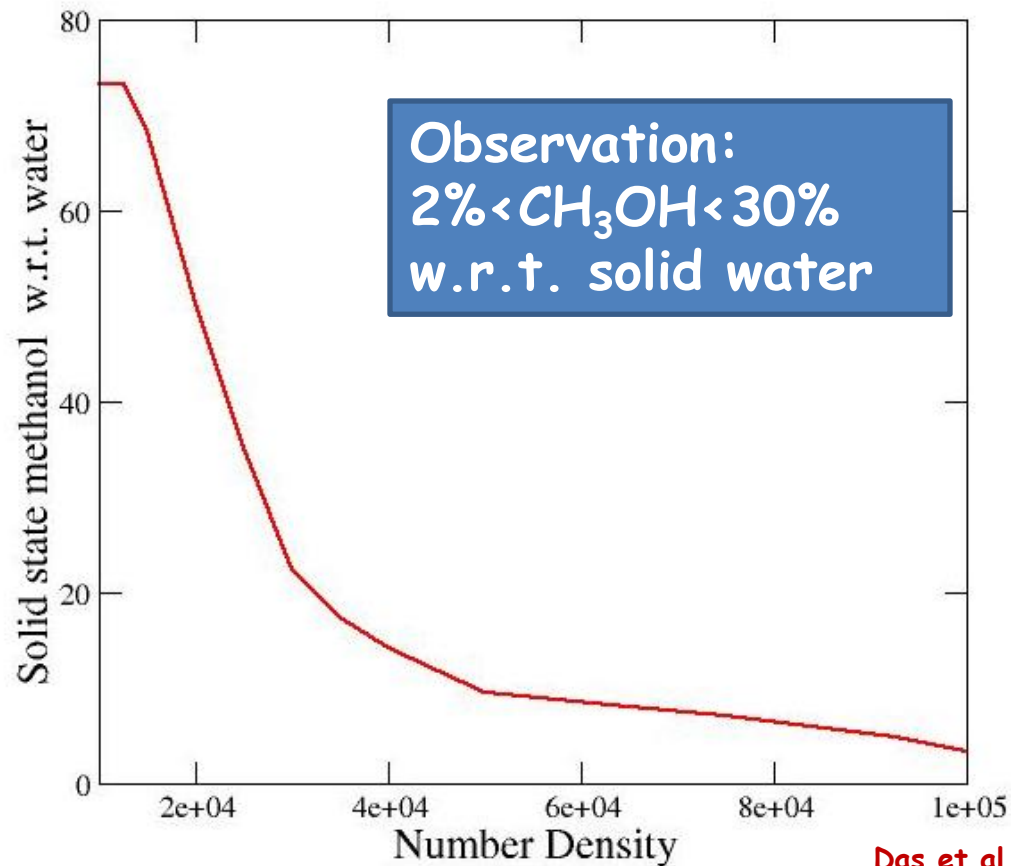
Species	High density (10^5 cm^{-3})	Intermediate density (10^4 cm^{-3})	Low density (10^3 cm^{-3})
H	1.10	1.15	1.15
O	7.0	0.75	0.09
CO	7.5	0.75	0.075

Stantcheva et al., 2002

Methanol formation in Mono-layer regime

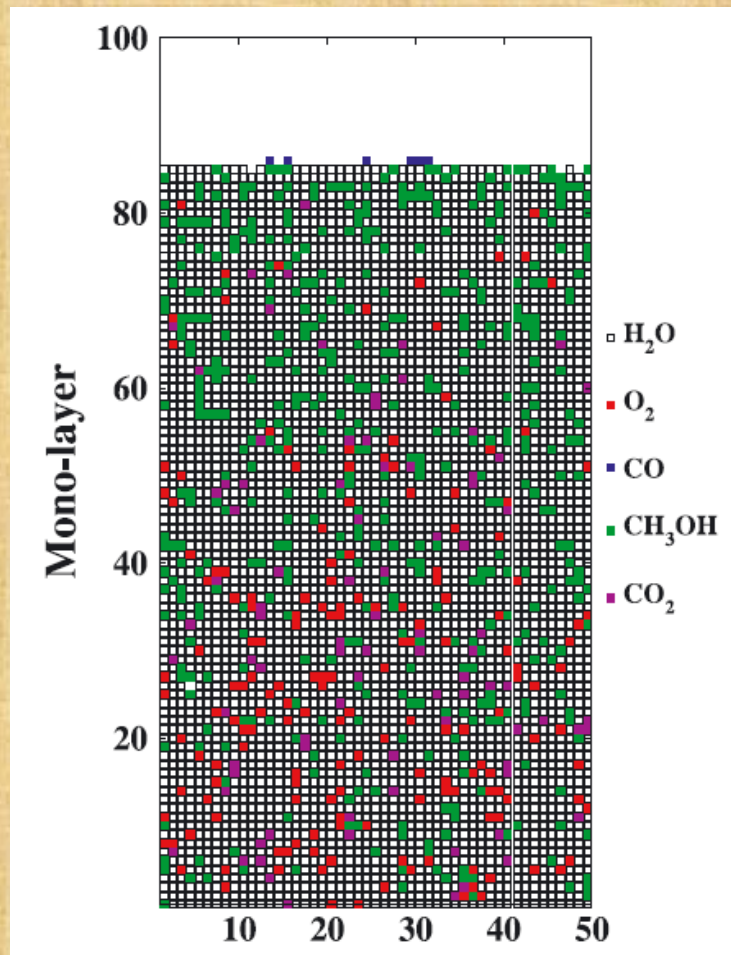


Methanol formation in mono-layer regime



Das et al., 2008, A&A

Typical structure of the grain mantle



Das et al., 2010, MNRAS

Dominated by,
H₂O, CH₃OH
and CO₂

Observation

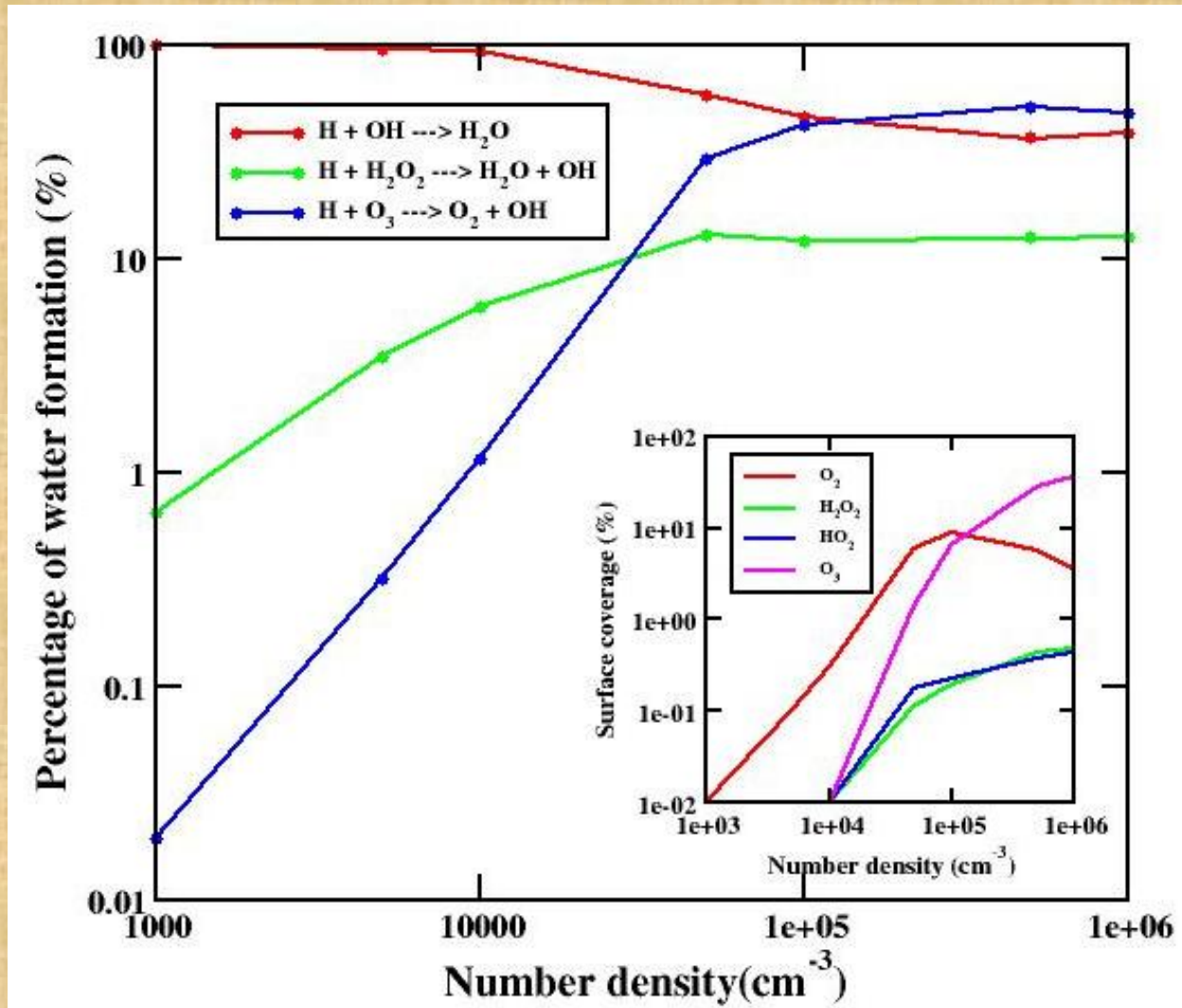
No. of layers ~ 100

Surface coverage of
H₂O > 60% (~10⁻⁴)

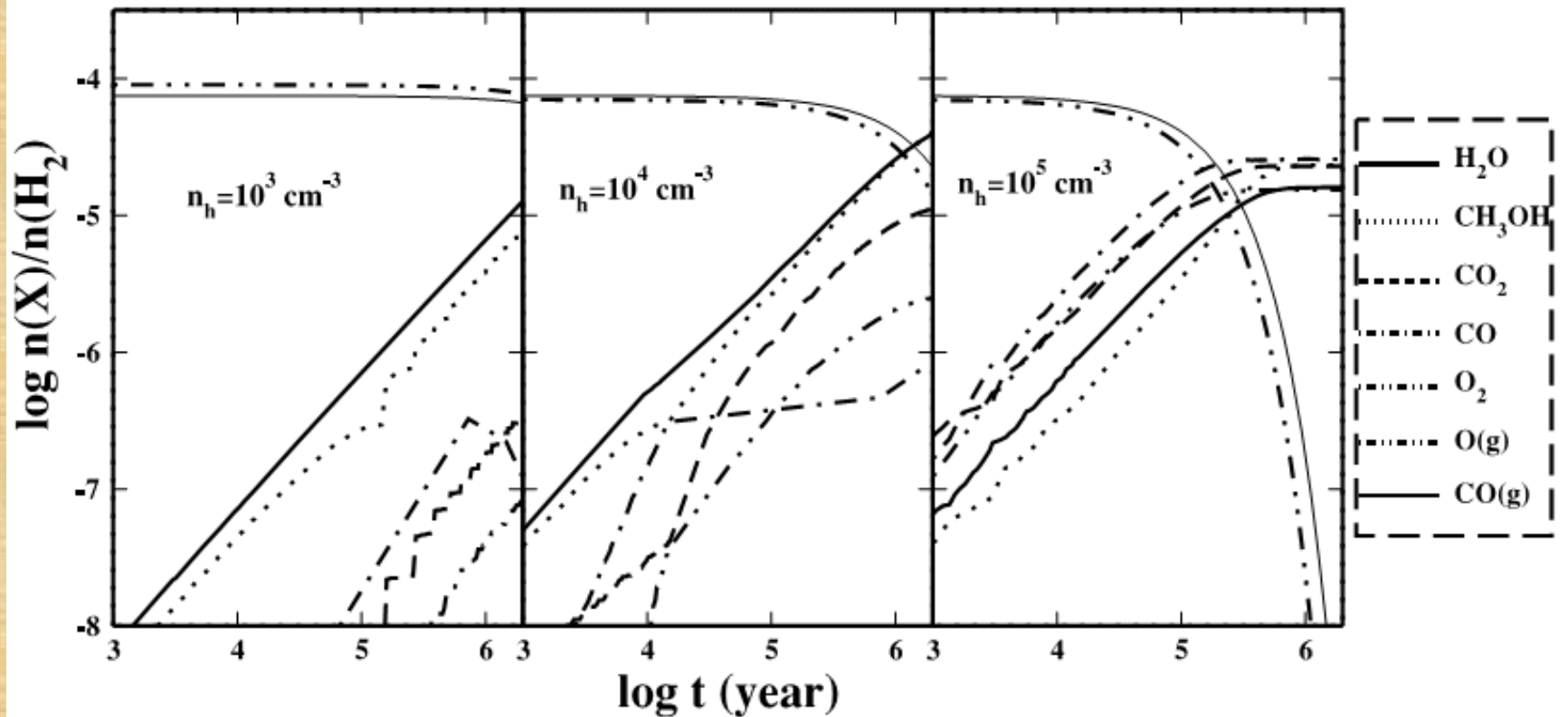
2% < CH₃OH < 30%
w.r.t. solid water

2% < CO₂ < 20%
w.r.t solid water

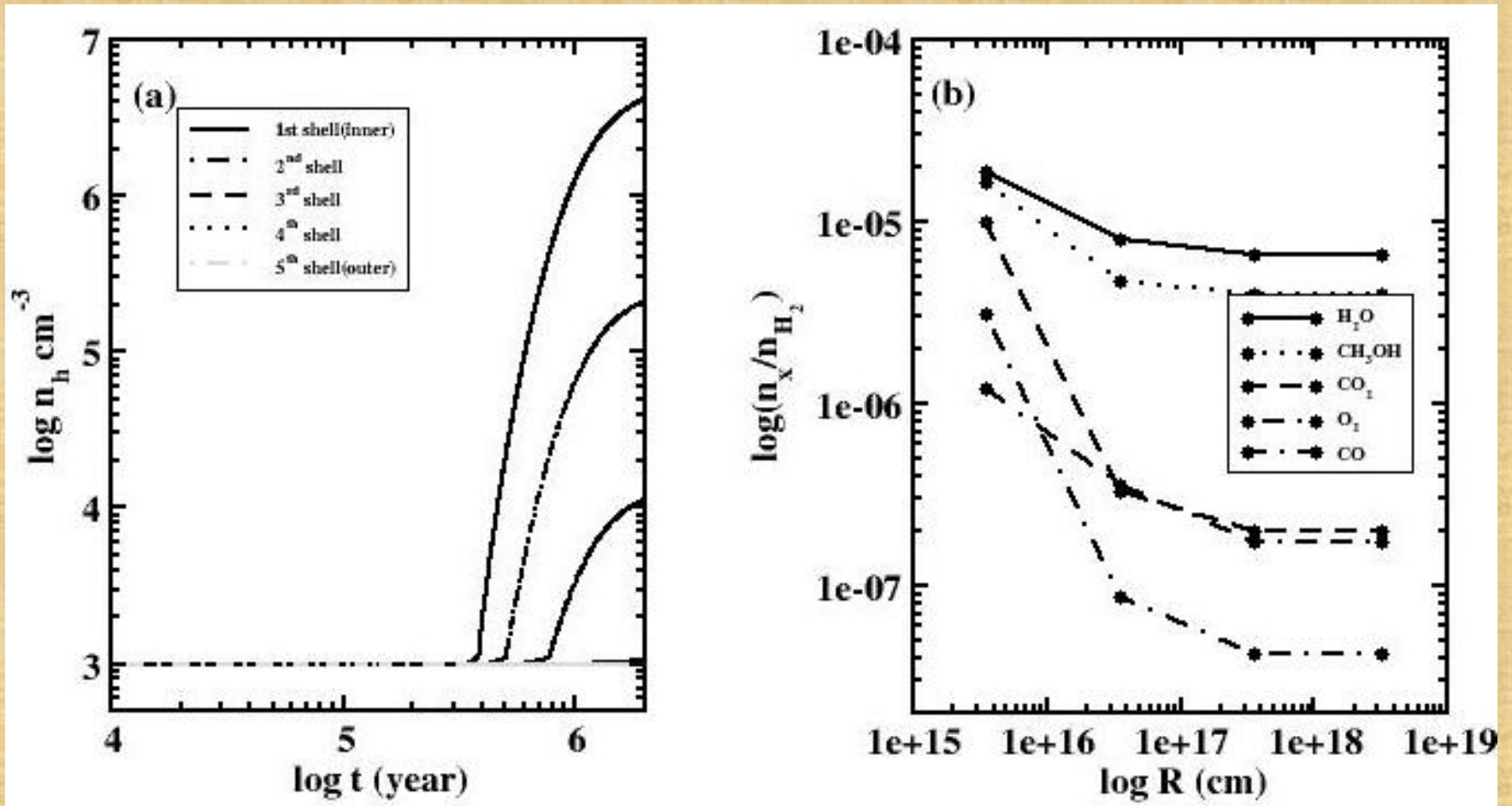
Different routes to the formation of Water



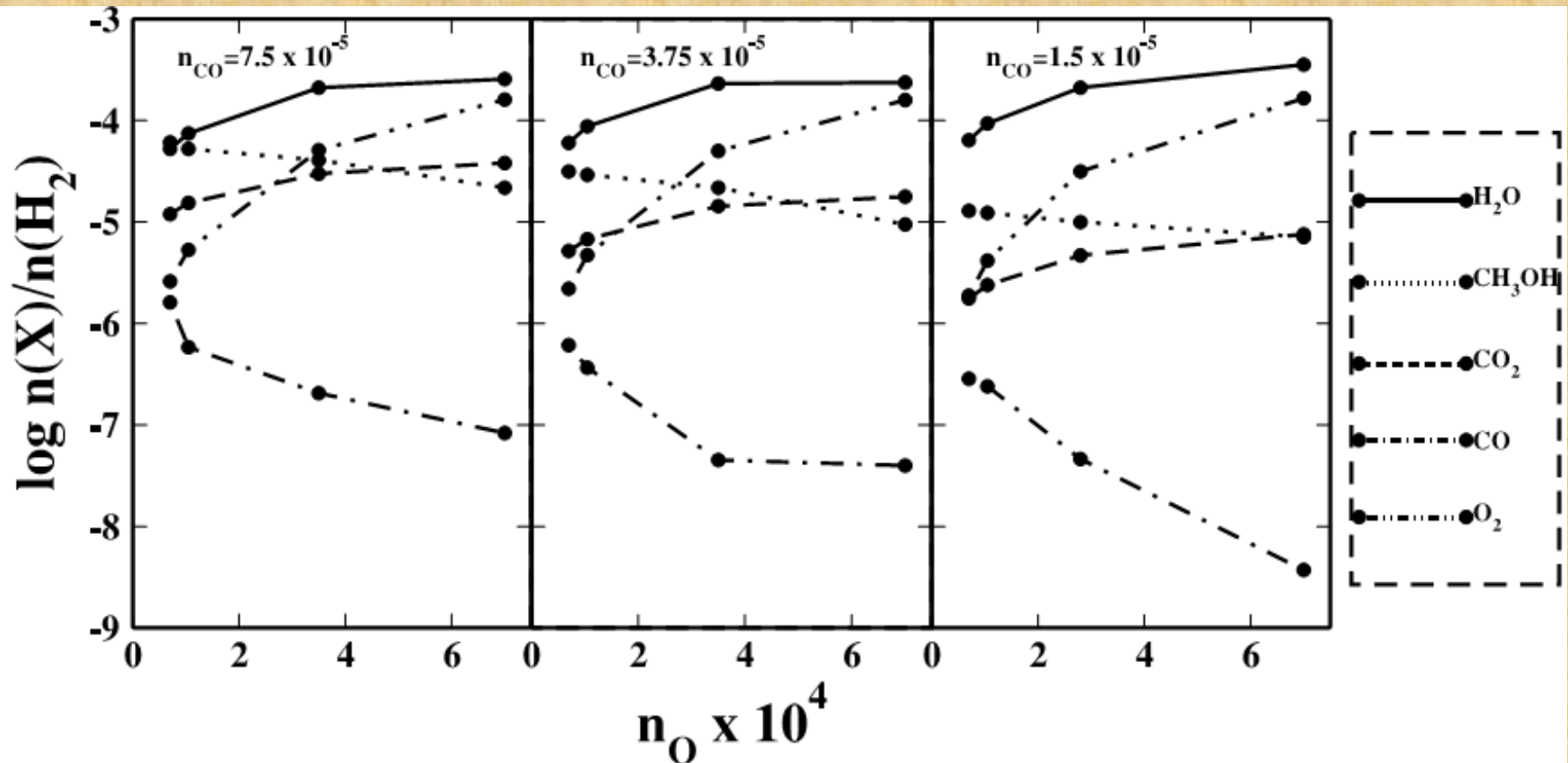
Time evolution of some selected gas-grain species



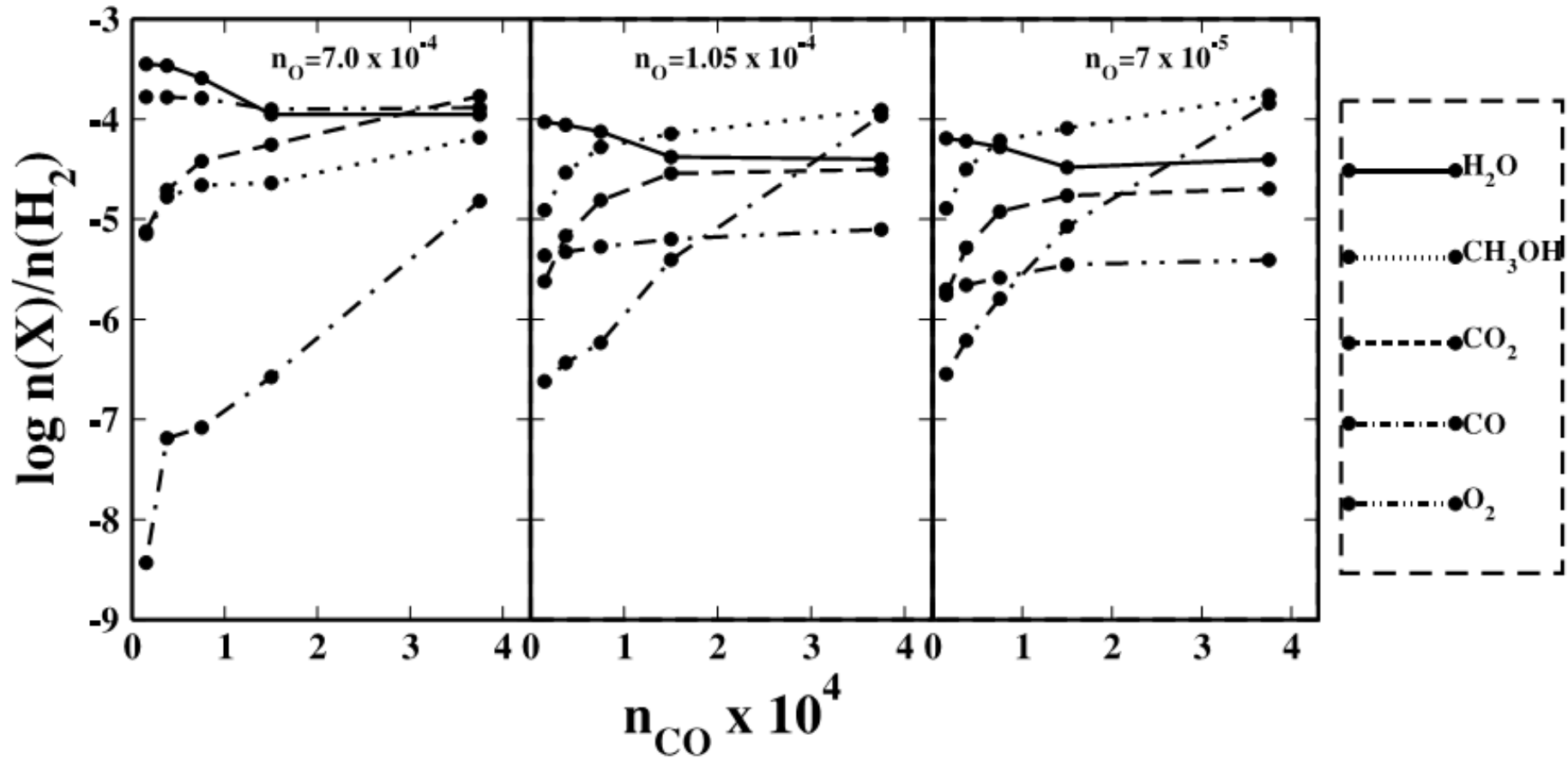
Time dependent study



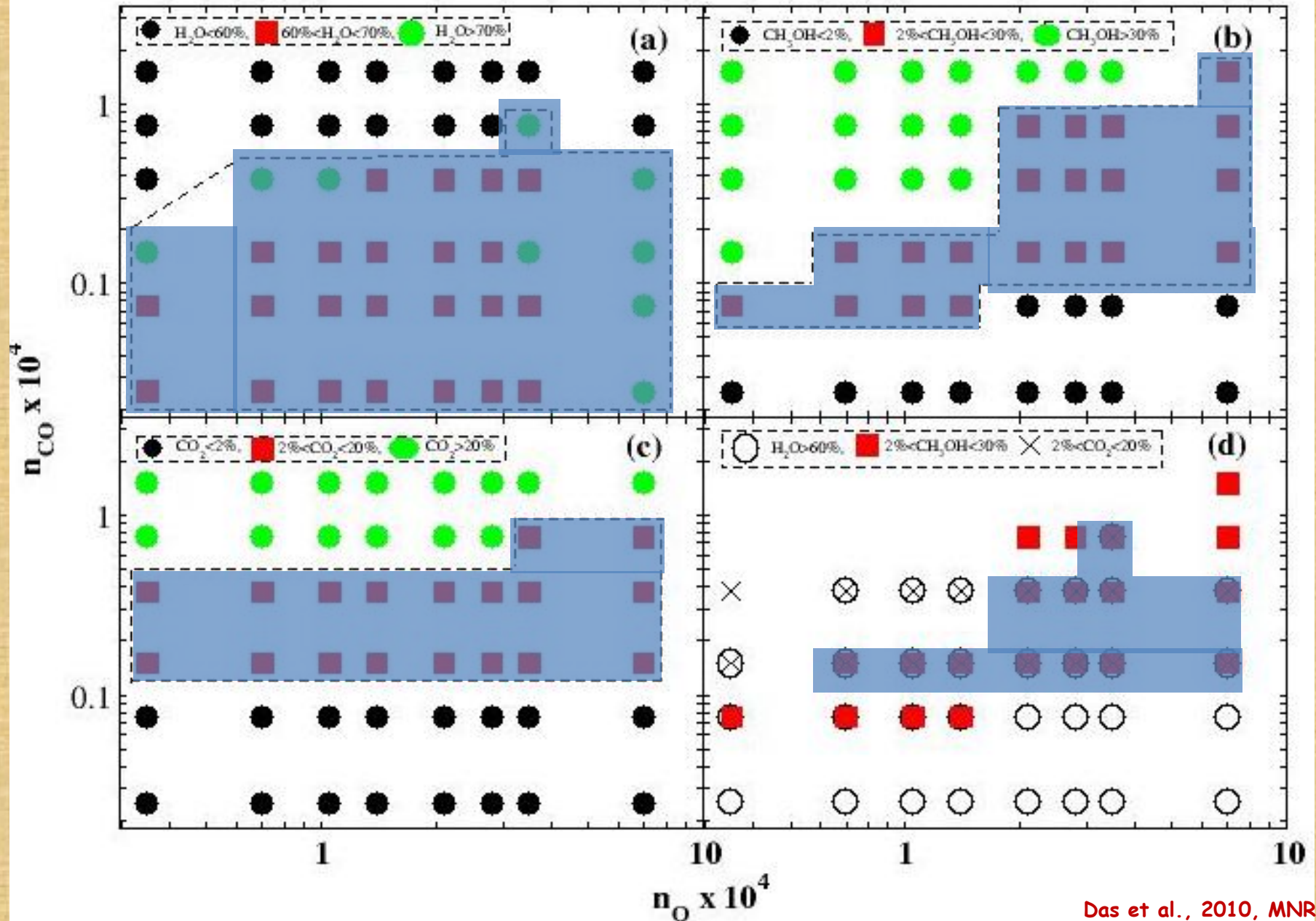
Variation of final abundance as a function of initial gas phase O



Variation of final abundance as a function of initial gas phase CO



Favourable zone for $T=10\text{K}$, $A_V=10$, and $n_H=10^4\text{ cm}^{-3}$



Effect of Photo-dissociation

Cosmic Ray induced Photoreaction rates:

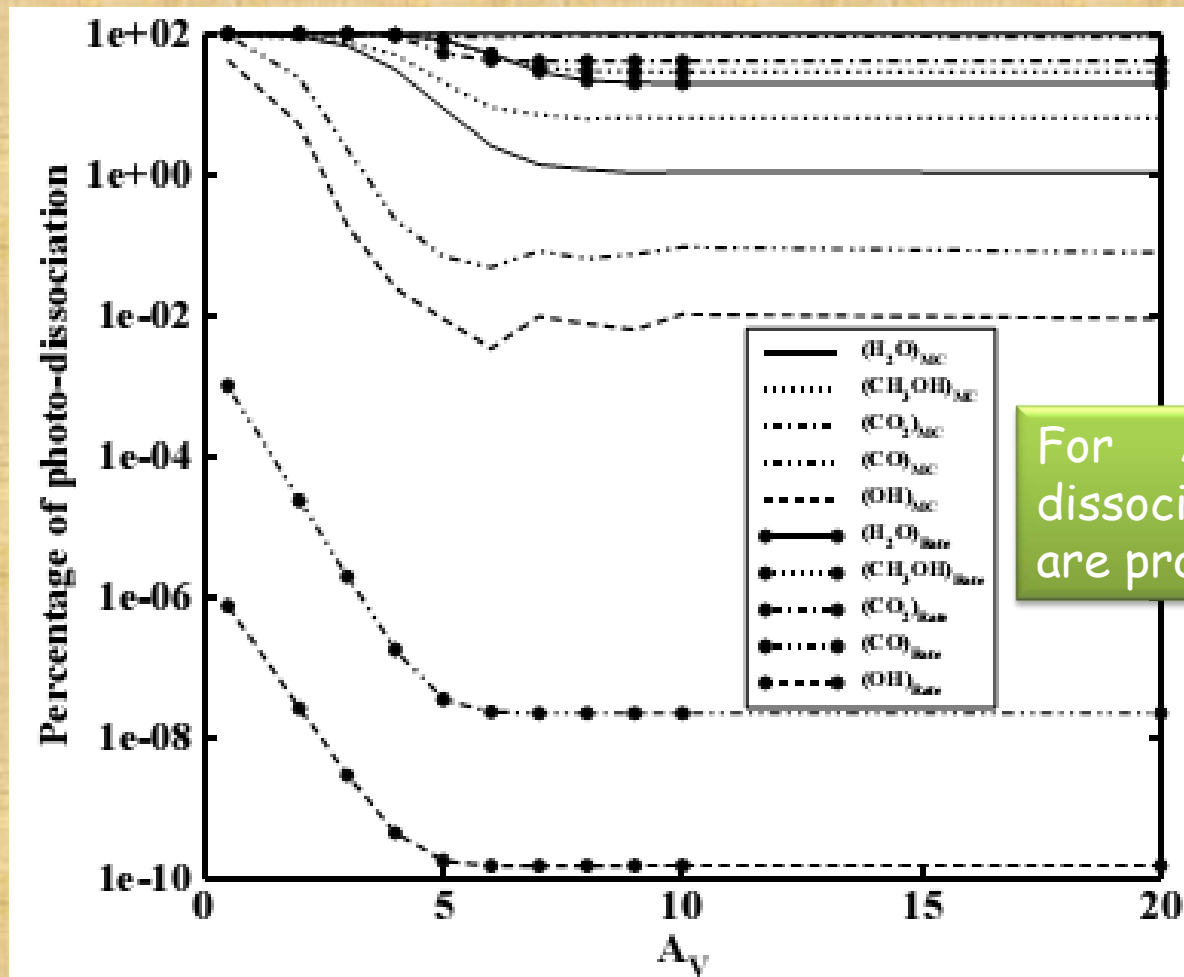
$$R_i = \alpha \left(\frac{T}{300} \right)^\beta \frac{\gamma}{1 - \omega} \text{ s}^{-1},$$

Direct cosmic ray rates:

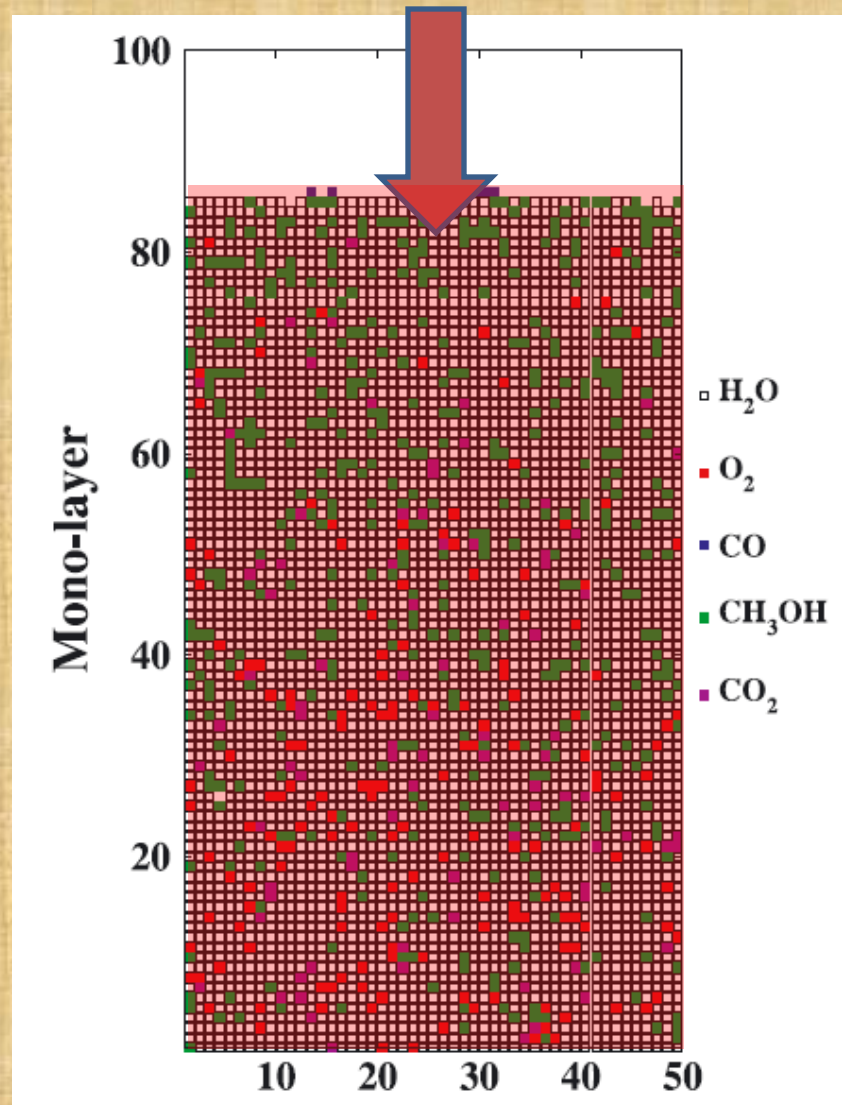
$$R_d = \alpha \exp(-\gamma A_v) \text{ s}^{-1}$$

Reactions	Cosmic ray induced rates (R_i)			Direct cosmic ray rates (R_d)		
	α	β	γ	α	β	γ
1 $^a\text{O}_2 \rightarrow \text{O} + \text{O}$	1.0(-16)	0(0)	3.755(2)	1.90(-9)	0(0)	1.85(0)
2 $^a\text{OH} \rightarrow \text{O} + \text{H}$	1.0(-16)	0(0)	2.545(2)	3.90(-10)	0(0)	2.24(0)
3 $\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	1.3(-17)	0(0)	4.855(2)	5.90(-10)	0(0)	1.70(0)
4 $\text{CO} \rightarrow \text{C} + \text{O}$	1.3(-17)	0(0)	1.050(2)	2.00(-10)	0(0)	2.50(0)
5 $\text{HCO} \rightarrow \text{H} + \text{CO}$	1.3(-17)	0(0)	2.105(2)	1.10(-9)	0(0)	8.0(-1)
6 $\text{H}_2\text{CO} \rightarrow \text{H}_2 + \text{CO}$	1.3(-17)	0(0)	1.329(3)	7.00(-10)	0(0)	1.7(0)
7 $\text{CH}_3\text{OH} \rightarrow \text{CH}_3 + \text{OH}$	1.3(-17)	0(0)	7.520(2)	6.00(-10)	0(0)	1.8(0)
8 $\text{CO}_2 \rightarrow \text{CO} + \text{O}$	1.3(-17)	0(0)	8.540(2)	1.40(-9)	0(0)	2.50(0)
9 $\text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{OH}$	1.3(-17)	0(0)	7.500(2)	5.90(-10)	0(0)	1.7(0)
10 $^a\text{O}_3 \rightarrow \text{O}_2 + \text{O}$	1.0(-16)	0(0)	3.755(2)	1.95(-9)	0(0)	1.85(0)
11 $^a\text{HO}_2 \rightarrow \text{OH} + \text{O}$	1.0(-16)	0(0)	3.750(2)	6.70(-9)	0(0)	2.12(0)

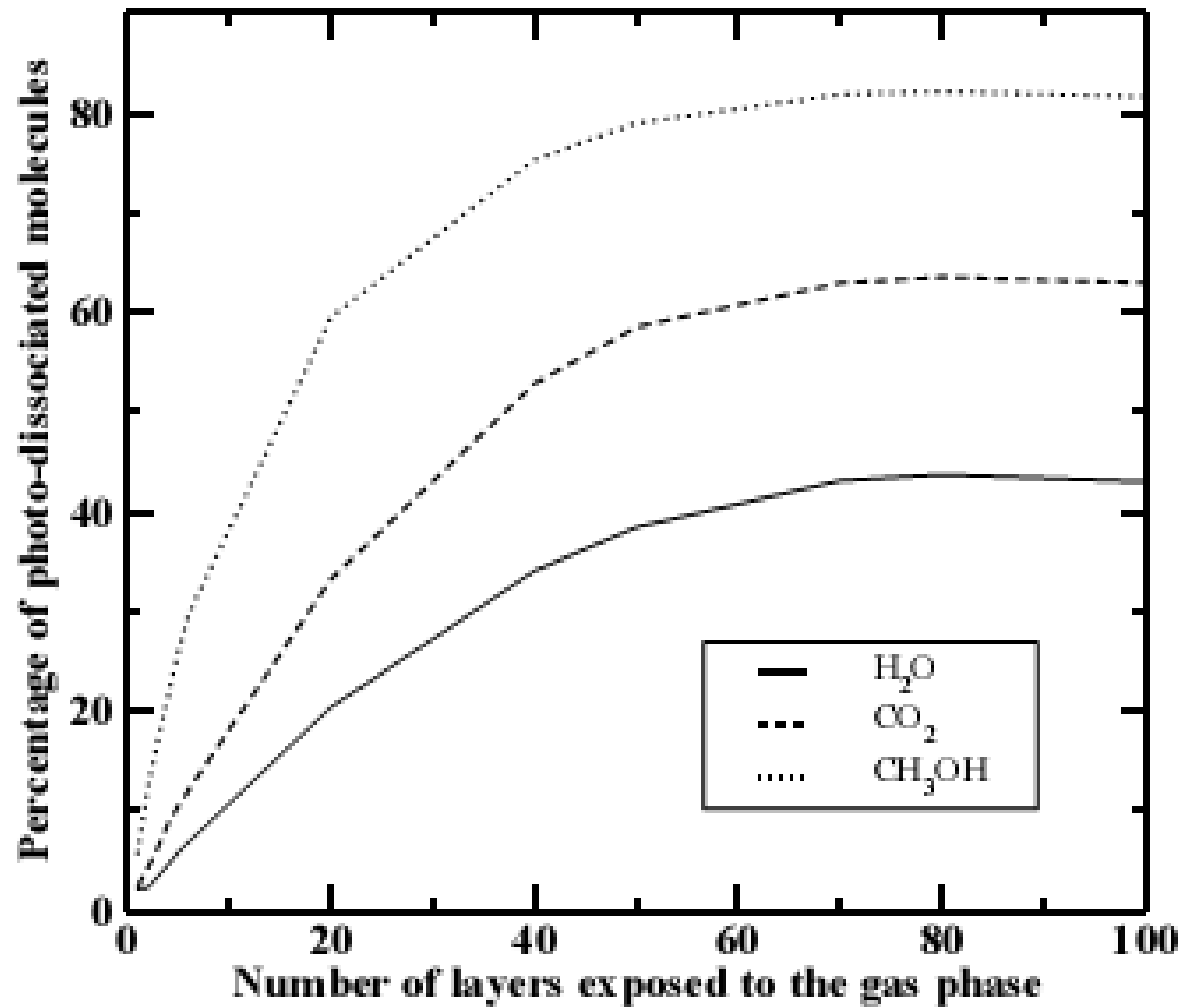
Percentage of Photo-dissociation as a function of extinction parameter



Effect of Photo-dissociation



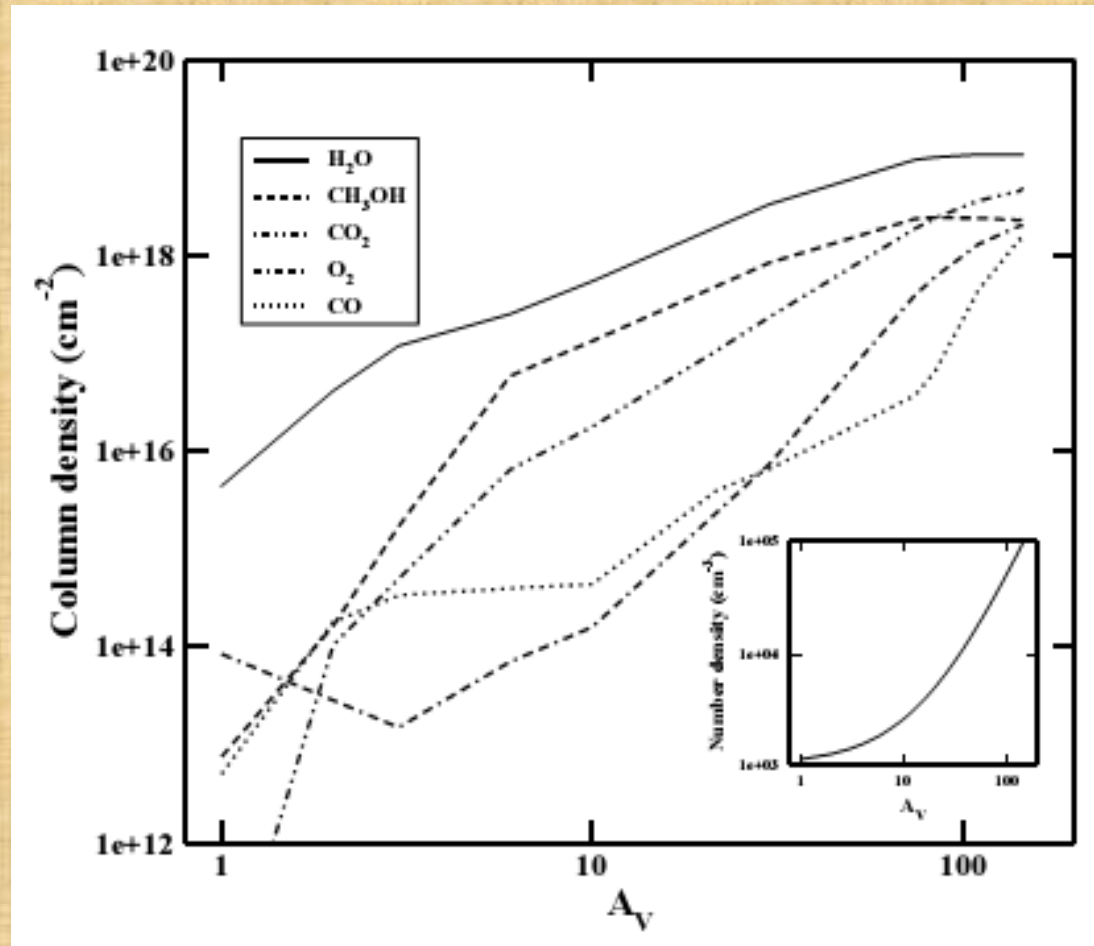
Effect of Photo-dissociation



Variation of Column density with the extinction parameter

Following Lee et al., 1996 the relationship between hydrogen number density and visual extinction is given by,

$$n_H = n_{H0} \left[1 + \left[\left(\frac{n_{H \max}}{n_{H0}} \right)^{1/2} - 1 \right] \frac{A_v}{A_{v \max}} \right]^2$$



Summary

Monte Carlo method should be used to have an exact information about the interstellar grain mantle

Formation of H_2O via H_2O_2 and O_3 also contributes significantly around the high density region

In a narrow region of parameter space the observed abundances of H_2O , CH_3OH , and CO_2 could be reproduced

For the lower value of $A_V (< 6)$ photo-dissociation dominates

Stable species like H_2O , CH_3OH , and CO_2 photo-dissociating more strongly in the Rate equation method

Thank
You