Formation of molecules in interstellar clouds

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In collaboration with...

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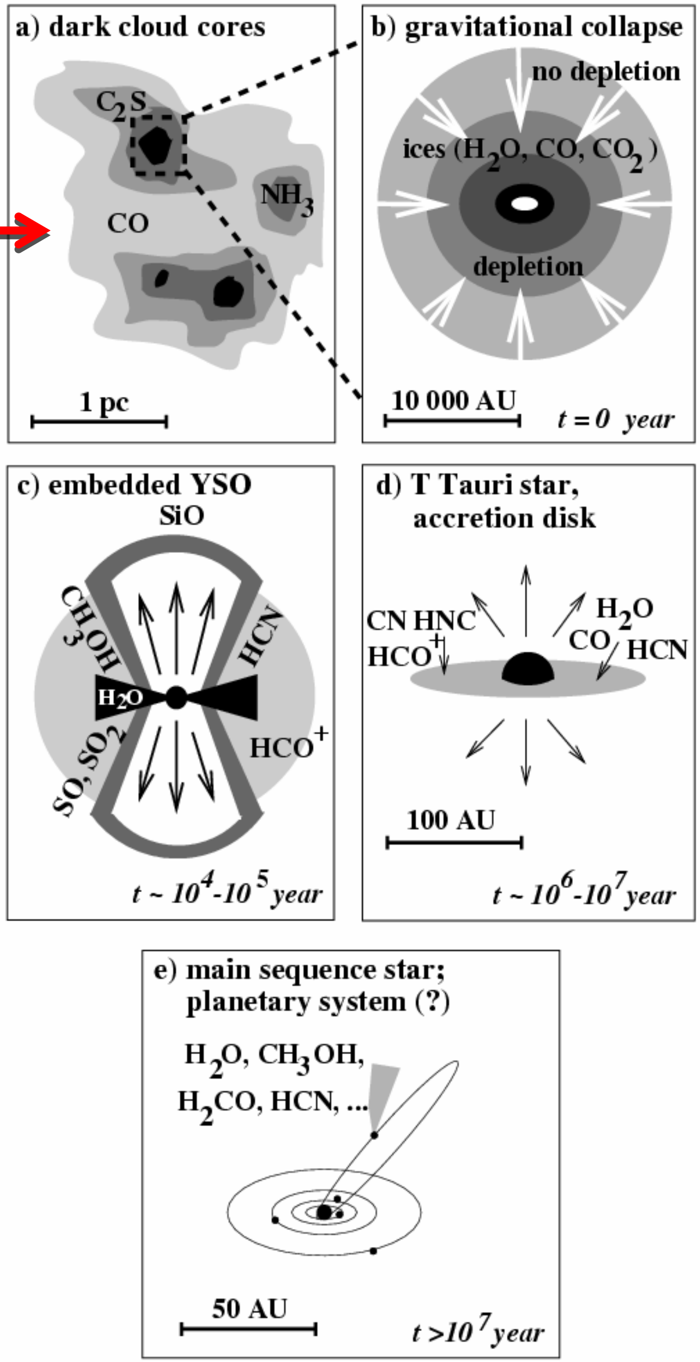
“Stars are among the most fundamental building blocks of the universe, and yet the processes by which they are formed are not understood.”

Derek Ward-Thompson
Science, January 4, 2002

Star formation flow chart

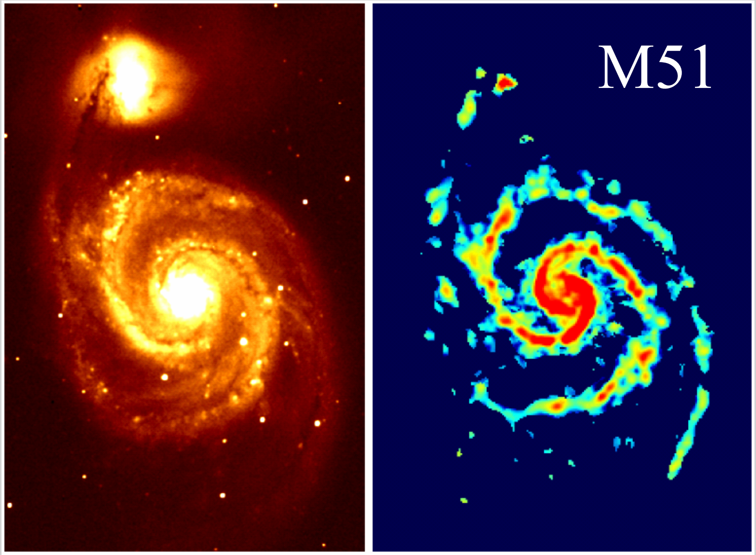
Initial conditions
for star formation?

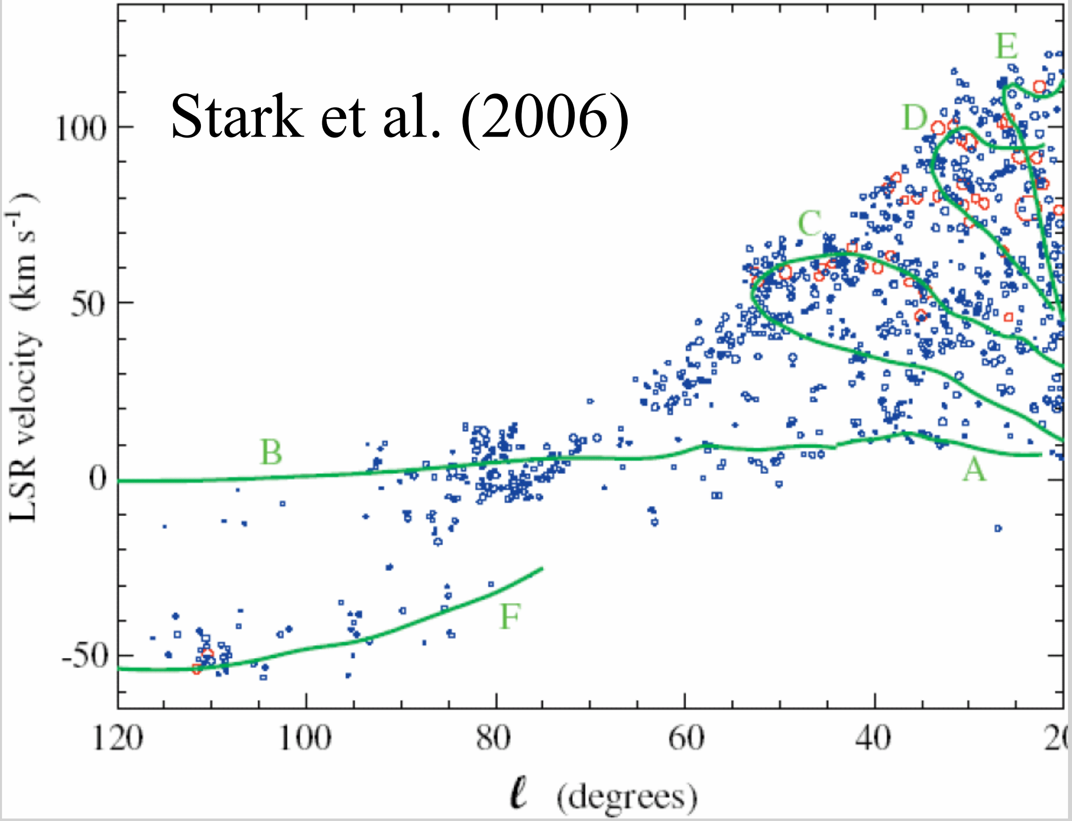


Molecular clouds

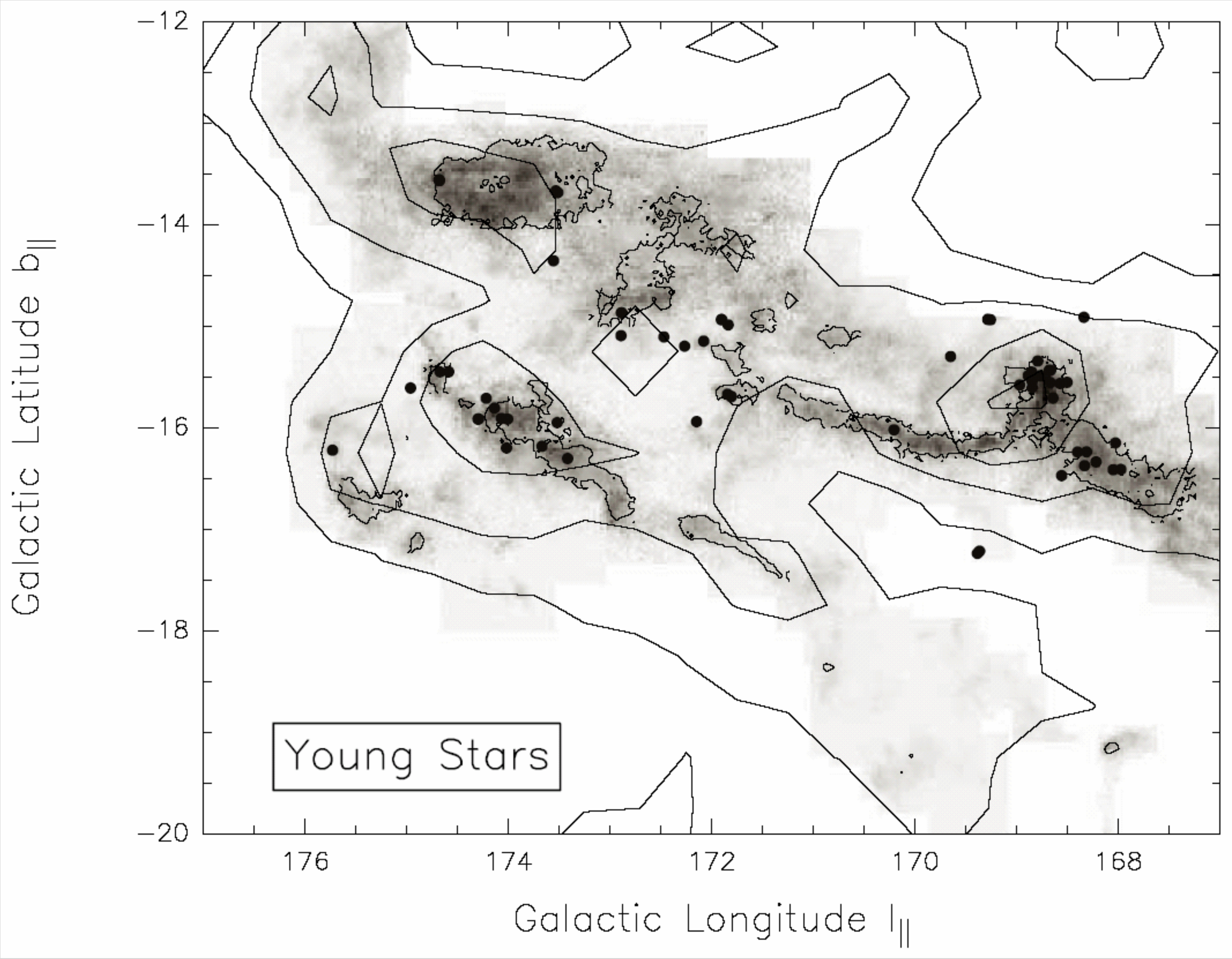
- Masses — up to $6 \cdot 10^6 \, M_\odot$
- Sizes — tens of pc
- Temperature — 10–50 K
- Density — > 200 cm^{-3}

Total mass — some $10^9 \, M_\odot$




Stark et al. (2006)

Palla & Stahler (2002)



Stars are forming too slow

- Molecular clouds are gravitationally (Jeans) unstable
- SFR in the Galaxy is 3 orders of magnitude lower than we would expect.

“Standard” model of star formation

- Molecular clouds are long-living entities
- They are supported by the magnetic field (turbulence dissipates too fast)
- Magnetic support is gradually lost due to ambipolar diffusion (Mestel & Spitzer 1956)

Stars are forming too fast

- We do not know molecular clouds without star formation (except for, may be, one)
- In star forming regions with molecular gas typical ages of young stars do not exceed 3 Myr

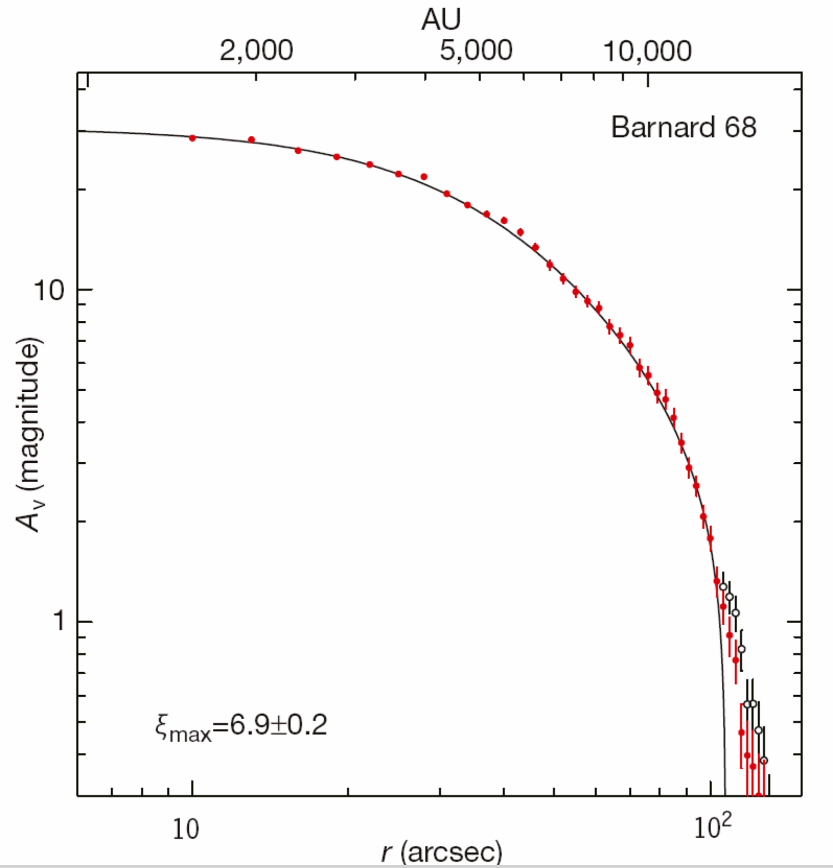
Gravoturbulent model of star formation

- Molecular clouds are transient entities
- Magnetic field either is not important or, at least, is not a major factor (Crutcher, Hakobian, & Troland 2008)
- Prestellar cores (and, may be, molecular clouds themselves) form due to convergence of turbulent flows

Prestellar cores

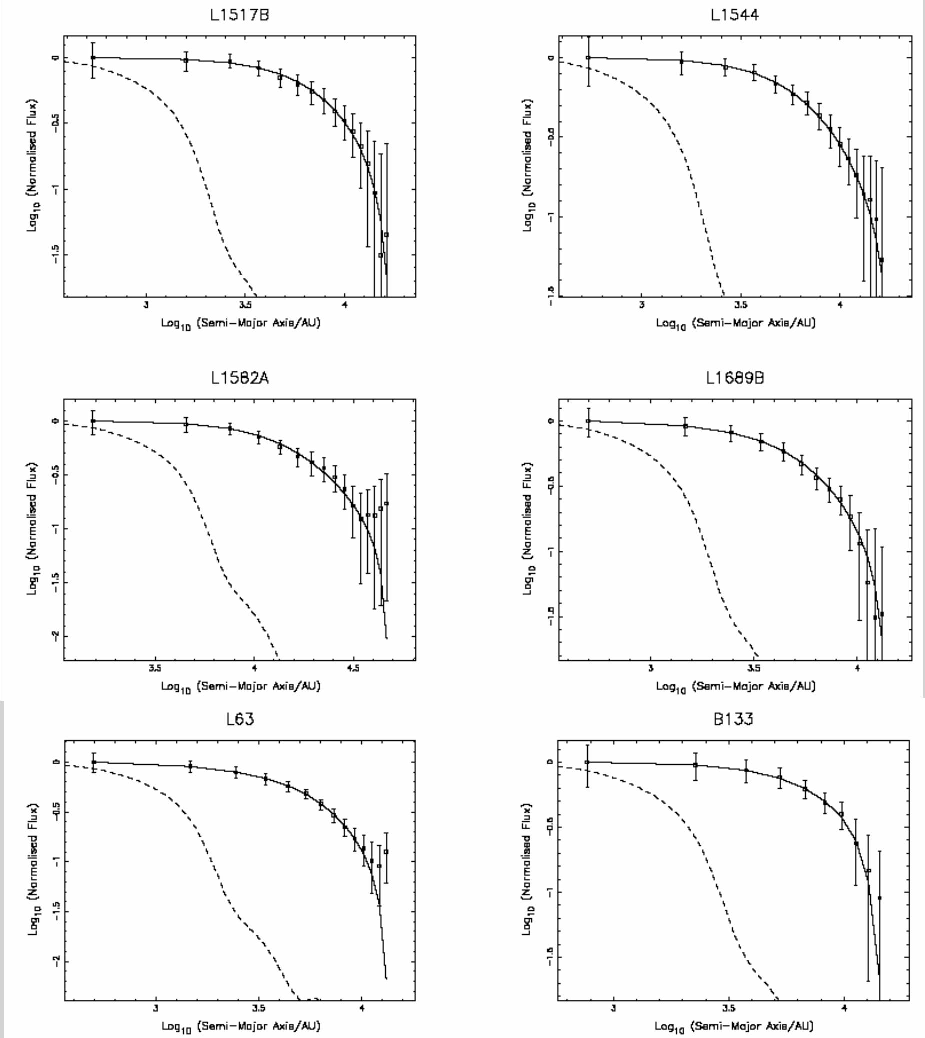
- ☐ Density profile
- ☐ Dust/gas temperature
- ☐ Magnetic field
- ☐ Velocity field
- ☐ Chemical composition (chemical clock)

Density distribution



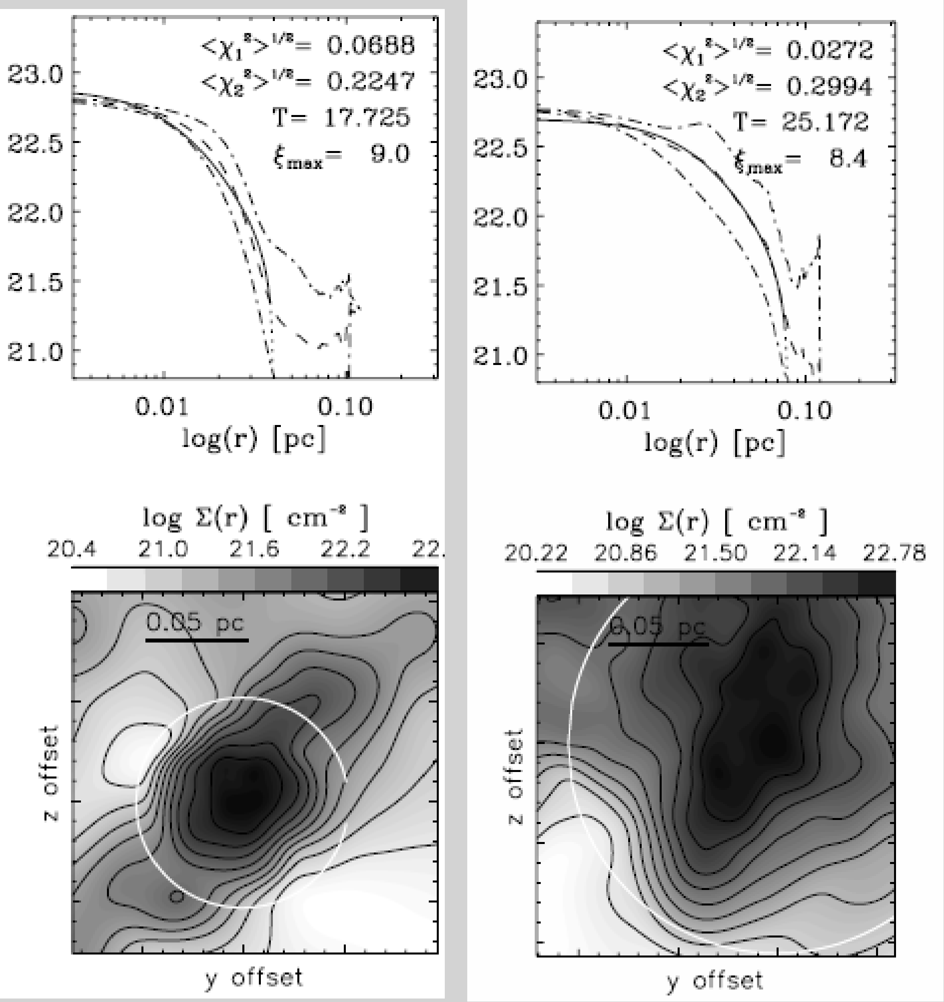
Alves et al. (2001)

Bonnor-Ebert profile



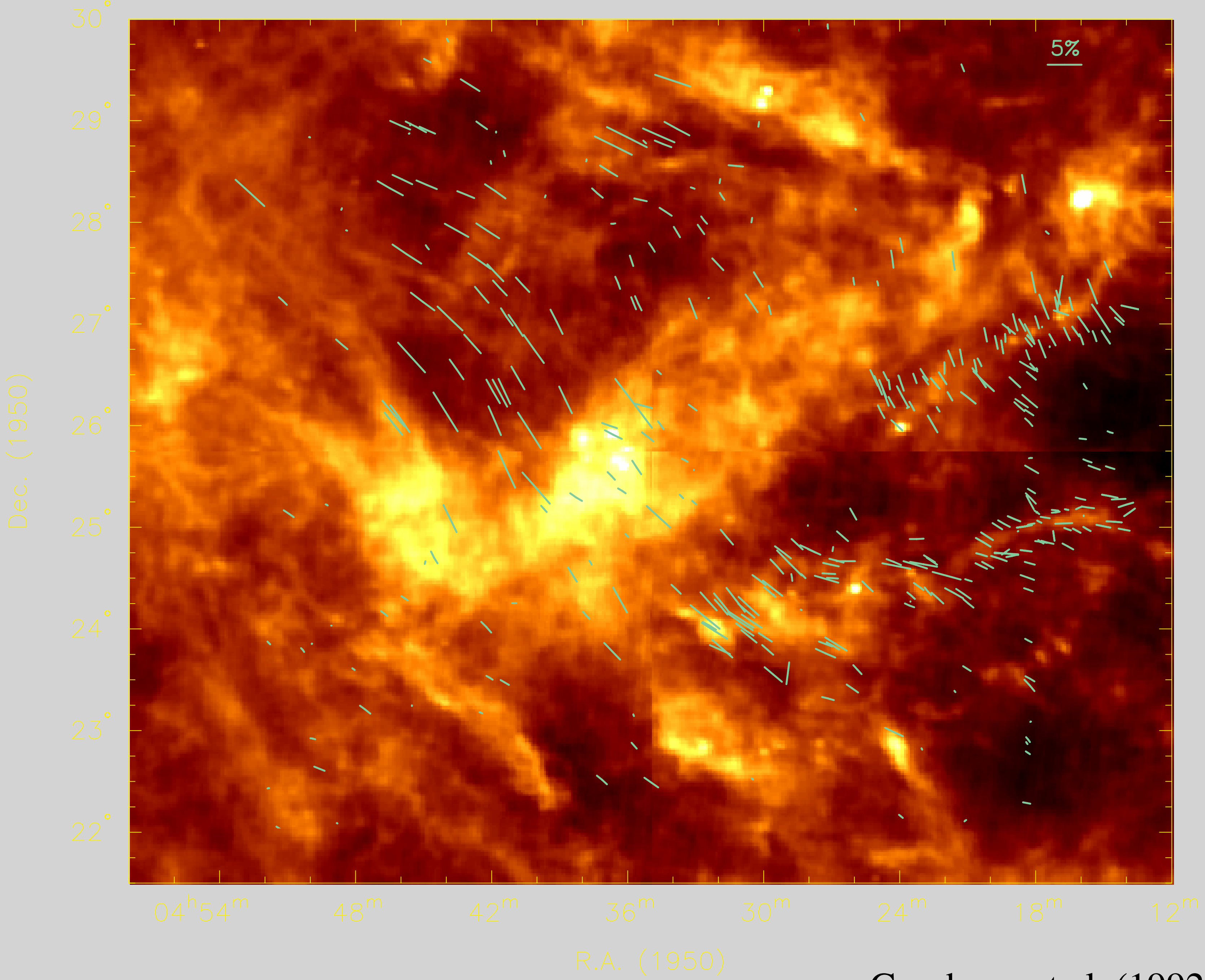
Kirk et al. (2005)

Dynamic cores in hydrostatic disguise



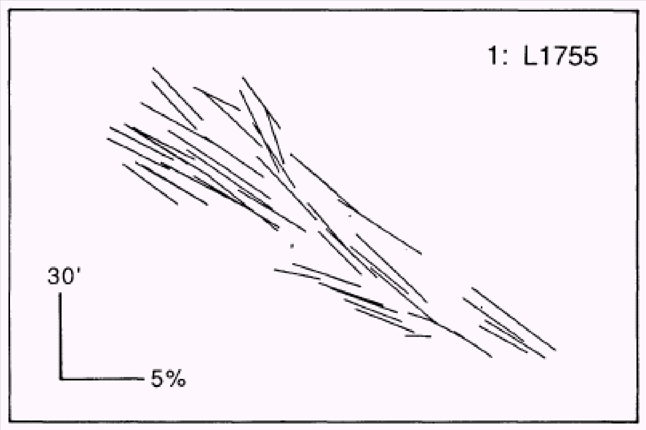
Ballesteros-Paredes et al. (2003)

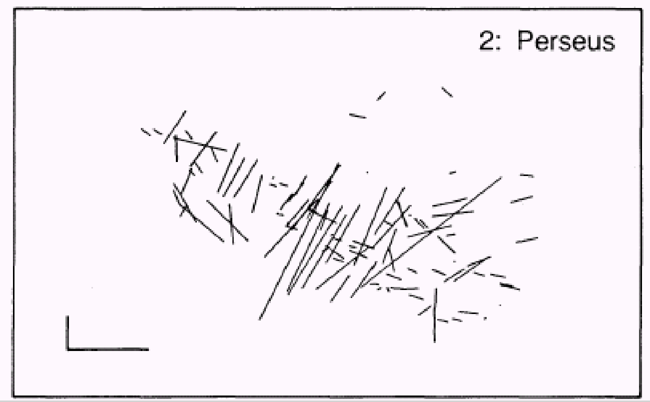
Of all artificial cores, about 65% have apparent BE profiles. Nearly half of these cores would be classified as gravitationally stable, even though in reality they are neither stable nor static.

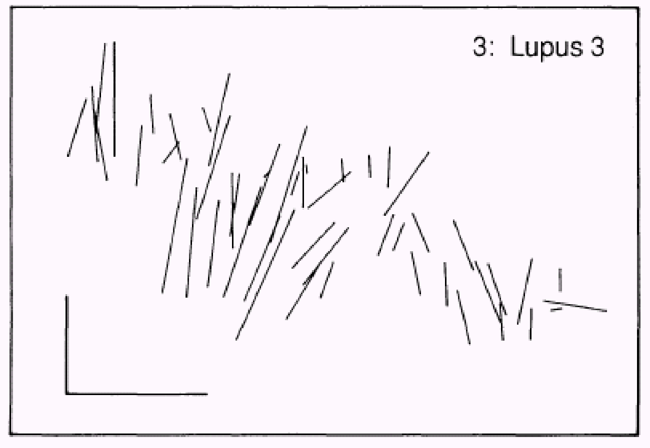


Goodman et al. (1992)

Magnetic field morphology



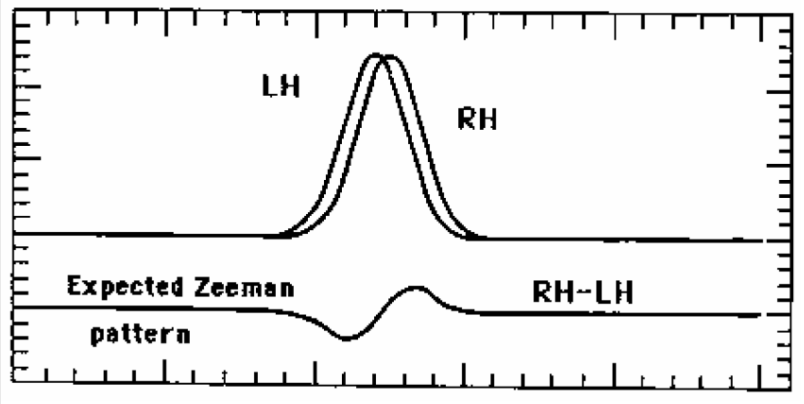


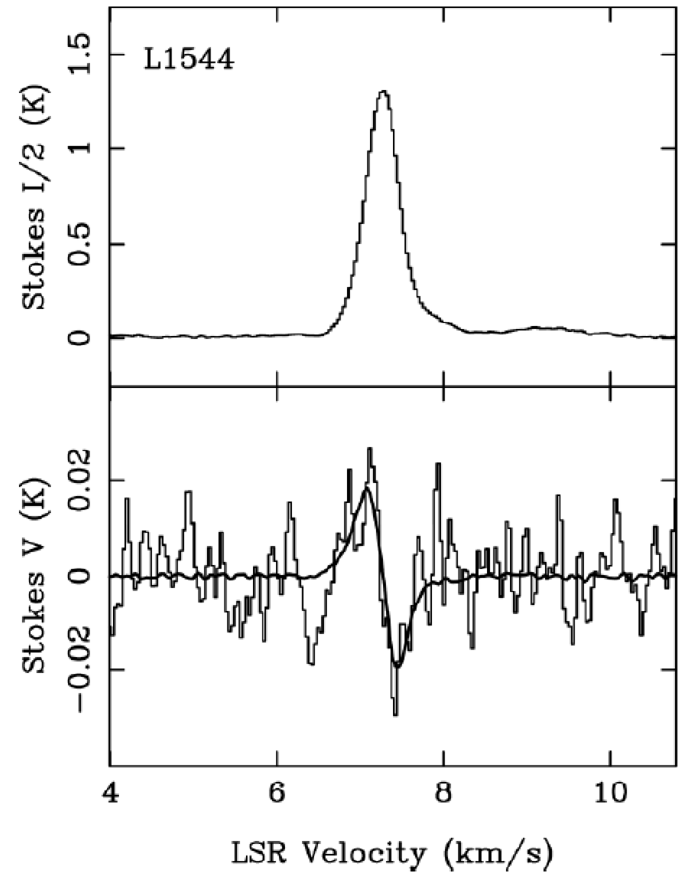


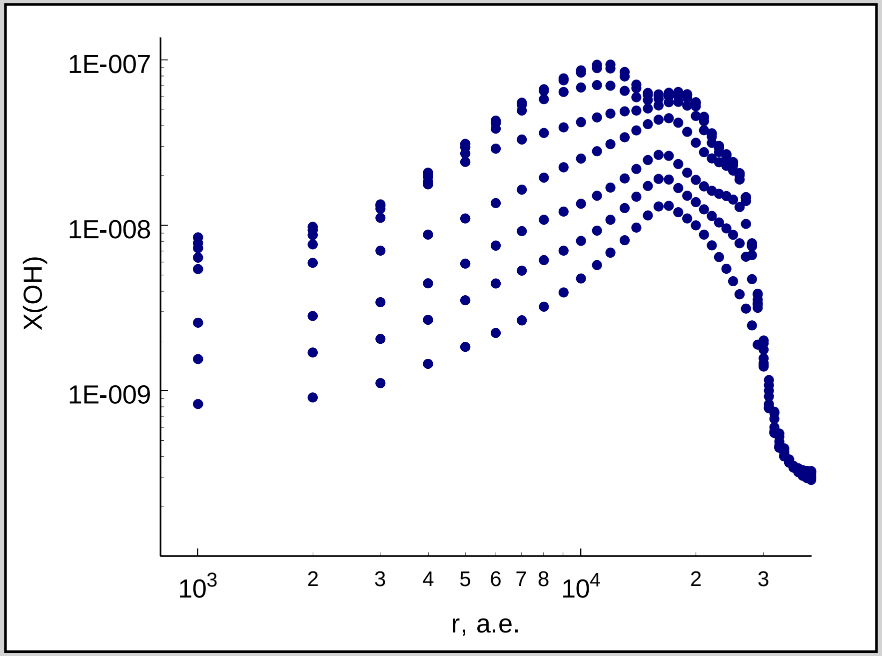
Myers & Goodman (1991)

Magnetic field strength

- Zeeman effect
- Chandrasekhar-Fermi relation



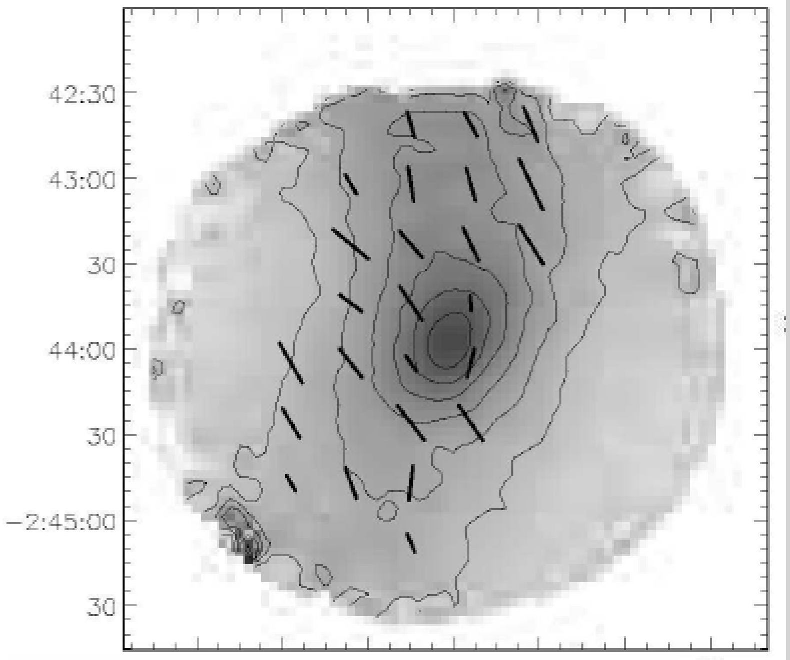


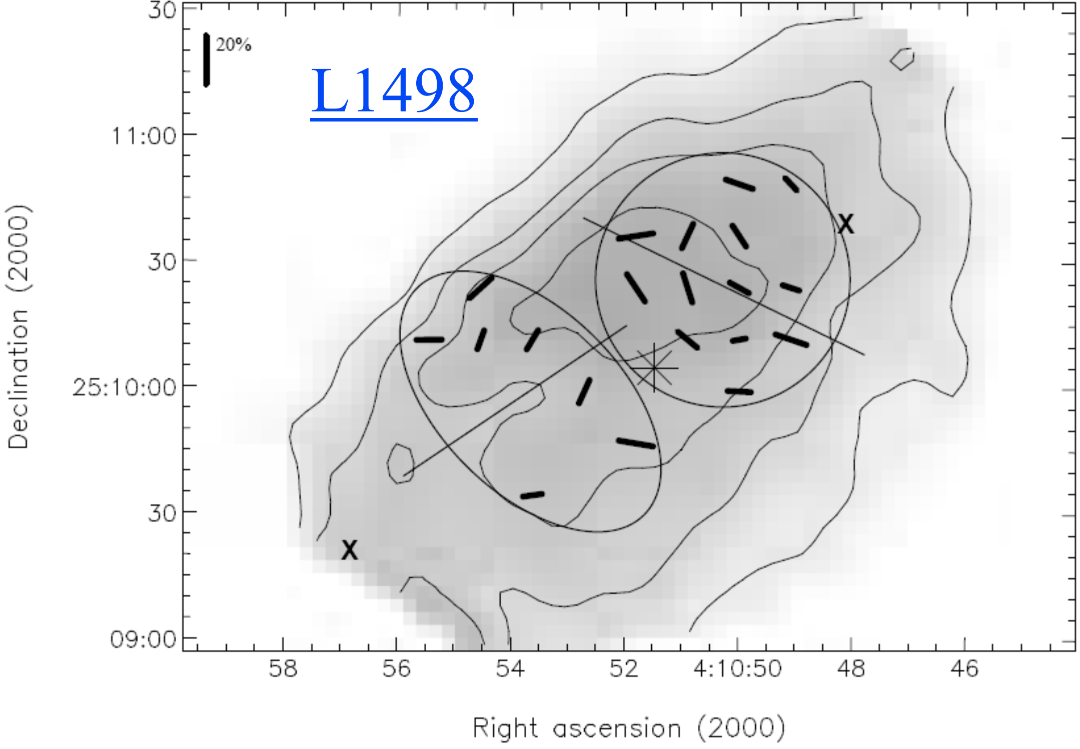


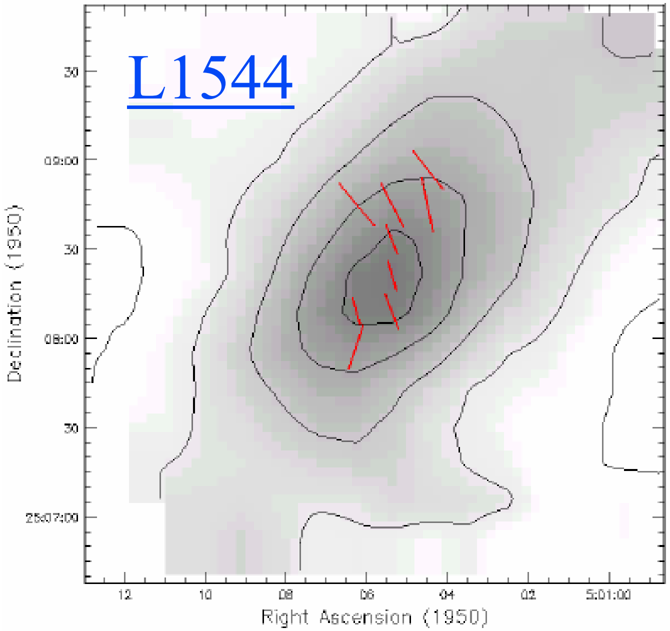
Crutcher & Troland (2000)

L183

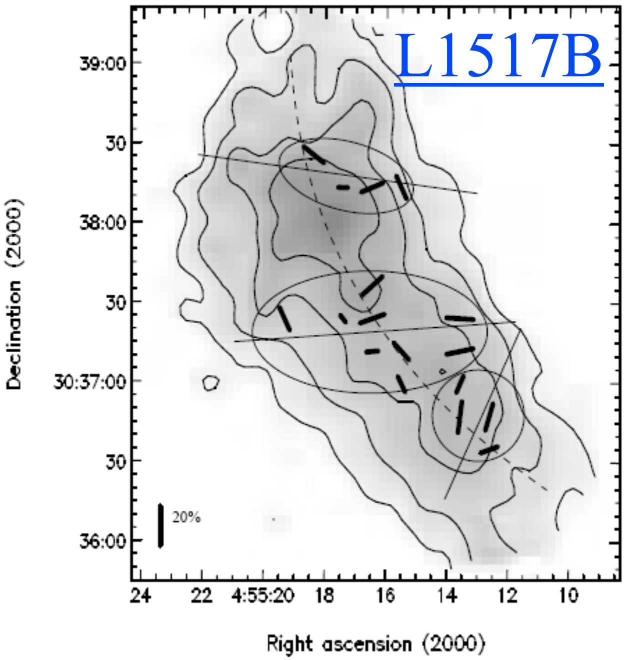
Crutcher et al. (2004)




L1498

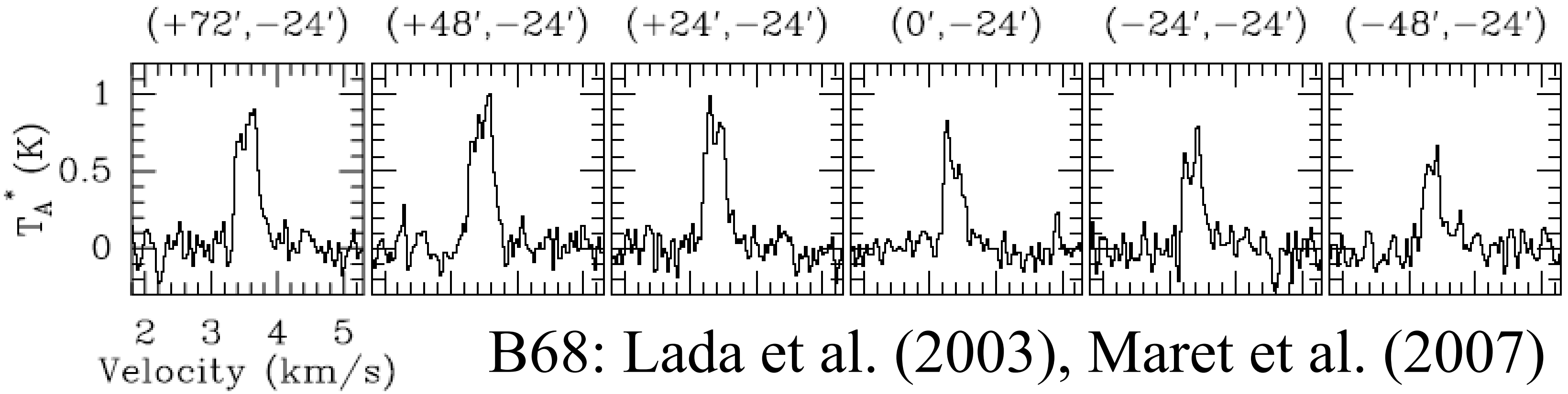

L1544

Ward-Thompson et al. (2000)

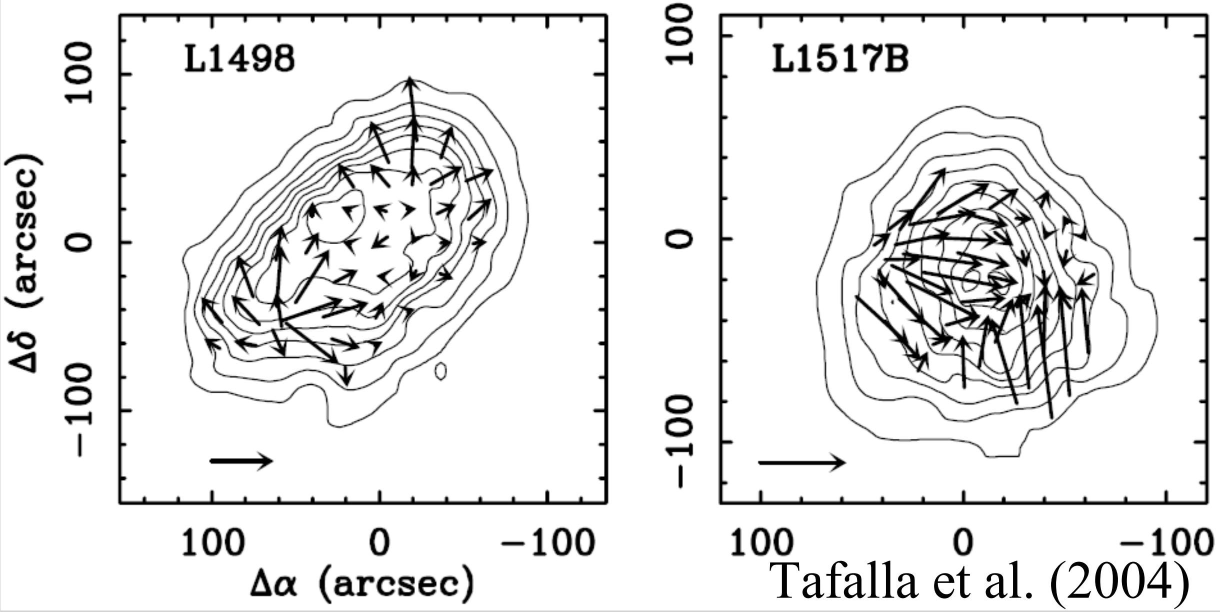

L1517B

Kirk et al. (2006)

Velocity field

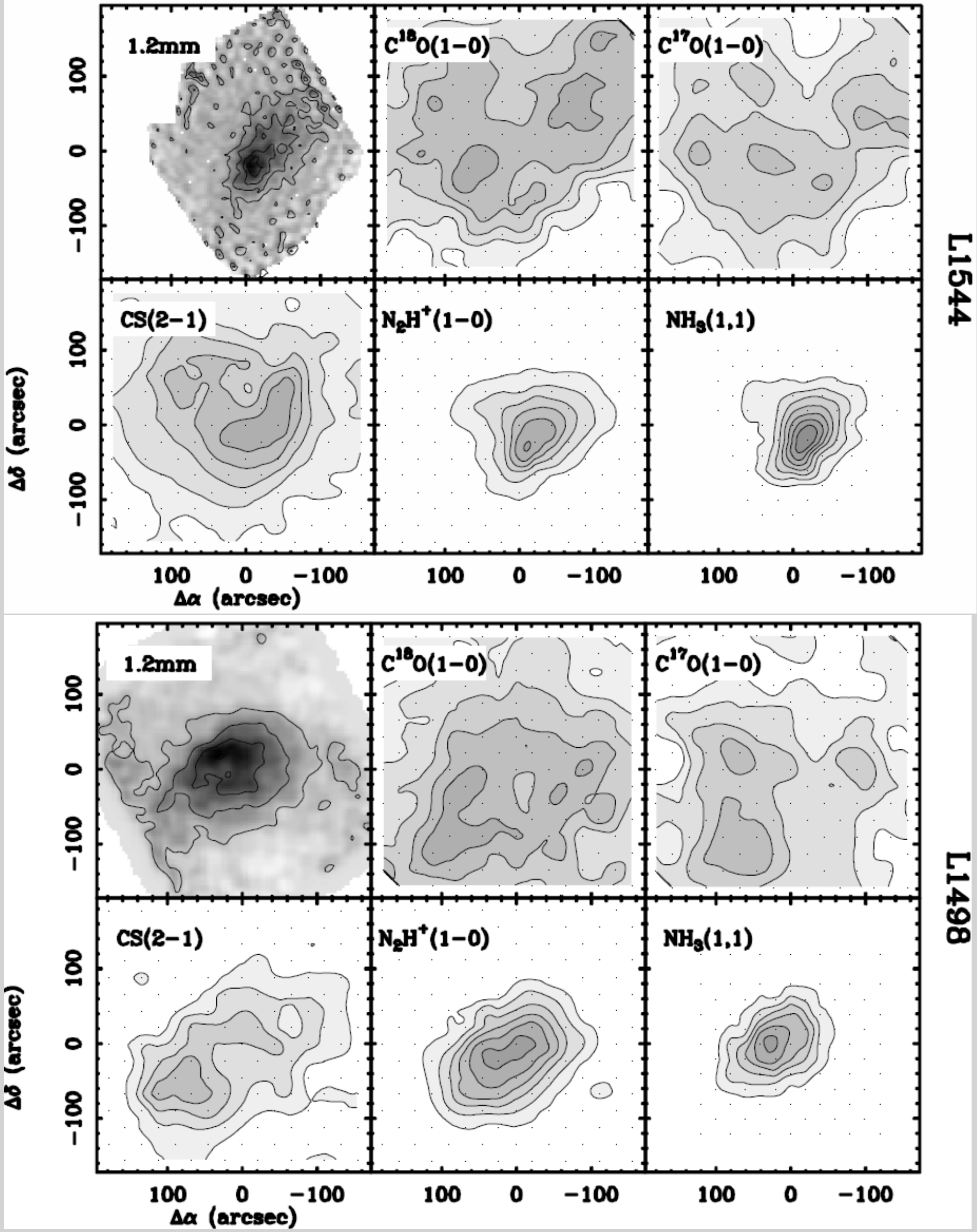


B68: Lada et al. (2003), Maret et al. (2007)



Tafalla et al. (2004)

Molecular composition



Tafalla et al. (2002)

Molecular lines as a discriminator for star formation models

Kinematics (quiescent vs transsonic)
Magnetic field (OH vs CN)
Age (short timescale vs long timescale)

Chemistry is important!

It is complicated, it has thousands of free parameters, but it cannot be avoided…

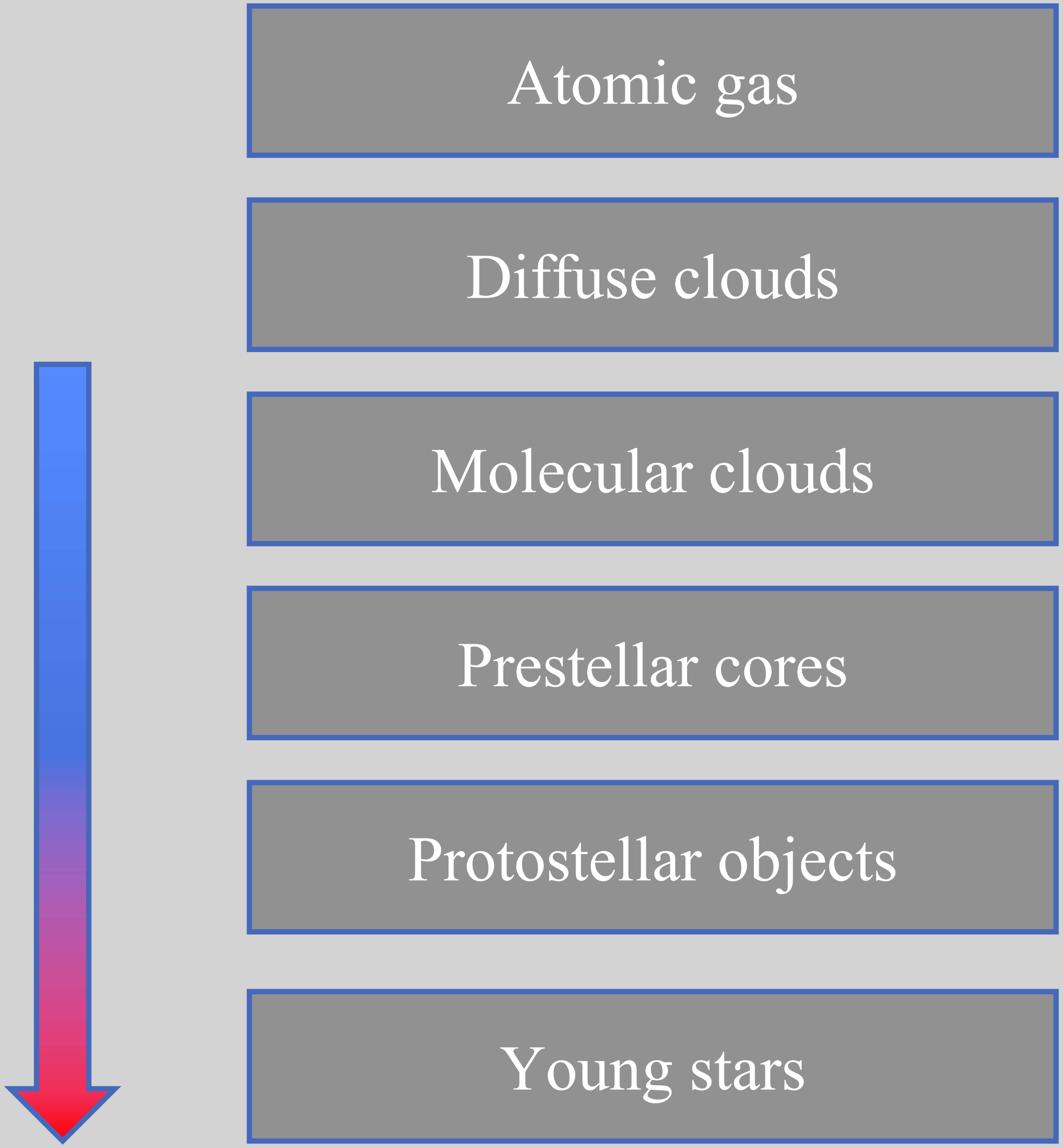
Equations of chemical kinetics

$$\frac{d}{dt} n_i^{\mathrm{g}}(r,t) = \sum_j \sum_l K_{lj}^{\mathrm{g}} n_l^{\mathrm{g}} n_j^{\mathrm{g}} - n_i^{\mathrm{g}} \sum_j K_{ij}^{\mathrm{g}} n_j^{\mathrm{g}} - k_j^{\mathrm{acc}} n_i^{\mathrm{g}} + k_i^{\mathrm{des}} n_i^{\mathrm{d}}$$

$$\frac{d}{dt} n_i^{\mathrm{d}}(r,t) = \sum_j \sum_l K_{lj}^{\mathrm{d}} n_l^{\mathrm{d}} n_j^{\mathrm{d}} - n_i^{\mathrm{d}} \sum_j K_{ij}^{\mathrm{d}} n_j^{\mathrm{d}} + k_j^{\mathrm{acc}} n_i^{\mathrm{g}} - k_i^{\mathrm{des}} n_i^{\mathrm{d}}$$

- Gas-Phase Chemistry
- Gas-Dust Interaction
- Surface Chemistry

Initial Conditions for Star Formation



Atomic gas

Diffuse clouds

Molecular clouds

Prestellar cores

Protostellar objects

Young stars

Initial conditions are especially important for chemistry

What is a diffuse cloud?

$H^+ \longrightarrow H \longrightarrow H_2$ $C^+ \longrightarrow C \longrightarrow CO$

	Diffuse atomic	**Diffuse molecular**	**Translucent**	**Dense molecular**
Property	$f(H_2) < 0.1$	$f(H_2) > 0.1$ $f(C^+) > 0.5$	$f(C^+) < 0.5$ $f(CO) < 0.9$	$f(CO) > 0.9$
A_v	0	0.2	1–2	5–10
n_H (cm^{-3})	10–100	100–500	500–5000	> 5000
T (K)	30–100	30–100	15–50	10–50
Observational techniques	UV, visible, 21 cm	UV, visible, IR, mm (abs)	UV, visible, IR, mm (abs) & mm (emis)	IR (abs), mm (emis)

$A_V = 0^m - 1^m$ $A_V = 1^m - 5^m$

Snow & McCall (2006)

Molecules in diffuse clouds

Weight	Species	Method	Target	N(X)/NH
2	H_2	UV	ζ Oph	0.56
3	HD	UV	ζ Oph	4.5 (−7)
3	H_3^+	IR	ζ Per	5.1 (−8)
13	CH	Optical	ζ Oph	1.5 (−9)
13	CH^+	Optical	ζ Oph	2.4 (−8)
14	$^{13}CH^+$	Optical	ζ Oph	3.5 (−10)
15	NH	Optical	ζ Oph	6.2 (−10)
17	OH	UV	ζ Oph	3.3 (−8)
24	C_2	Optical	ζ Oph	1.3 (−8)
25	C_2H	mm abs.	BL Lac	1.8 (−8)
26	CN	Optical	ζ Oph	1.9 (−9)
27	HCN	mm abs.	BL Lac	2.6 (−9)
27	HNC	mm abs.	BL Lac	4.4 (−10)
28	N_2	UV	HD 124314	3.1 (−8)
28	CO	UV	X Per	6.4 (−6)
29	HCO^+	mm abs.	BL Lac	1.5 (−9)
29	HOC^+	mm abs.	BL Lac	2.2 (−11)
29	^{13}CO	UV	X Per	8.9 (−8)
29	$C^{17}O$	UV	X Per	7.4 (−10):
30	$C^{18}O$	UV	X Per	2.1 (−9):
30	H_2CO	mm abs.	BL Lac	3.7 (−9)
36	C_3	Optical	ζ Oph	1.1 (−9)
36	HCl	UV	ζ Oph	1.9 (−10)
38	C_3H_2	mm abs.	BL Lac	6.4 (−10)
44	CS	mm abs.	BL Lac	1.6 (−9)
64	SO_2	mm abs.	BL Lac	≤8.2 (−10)

Snow & McCall (2006)

+ H_2S, HCS^+ (Lucas & Liszt 2002), NH_3 (Liszt et al. 2006), HOC^+ (Liszt et al. 2004)

Molecular composition of diffuse clouds

1. Physical conditions in diffuse clouds
2. Dynamical evolution of molecular clouds
3. Initial conditions for chemical evolution in prestellar cores

Hydrogen is not entirely molecular

Other molecules are abundant

What is used?

Study	Initial density	Initial abundances
Bergin & Langer (1997)	$3 \cdot 10^3$	**Hydrogen is totally molecular**; other elements are atoms or ions
Aikawa et al. (2001)	$3 \cdot 10^4$	**Hydrogen is totally molecular**; other elements are atoms or ions
Shematovich et al. (2003)	10^3	**Hydrogen is totally molecular**; other elements are atoms or ions; some C and O are converted to CO
Lee at al. (2004)	10^3	**Hydrogen is totally molecular**; other elements are atoms or ions
Pavlyuchenkov et al. (2006)	$5 \cdot 10^3$	**Hydrogen is totally molecular**; other elements are atoms
Tsamis et al. (2008)	10^3	Chemical equilibrium

Role of molecular hydrogen

$$C^+ + H_2 \xrightarrow{4500K} CH^+ + H$$

$$CH^+ + e^- \rightarrow C + H$$

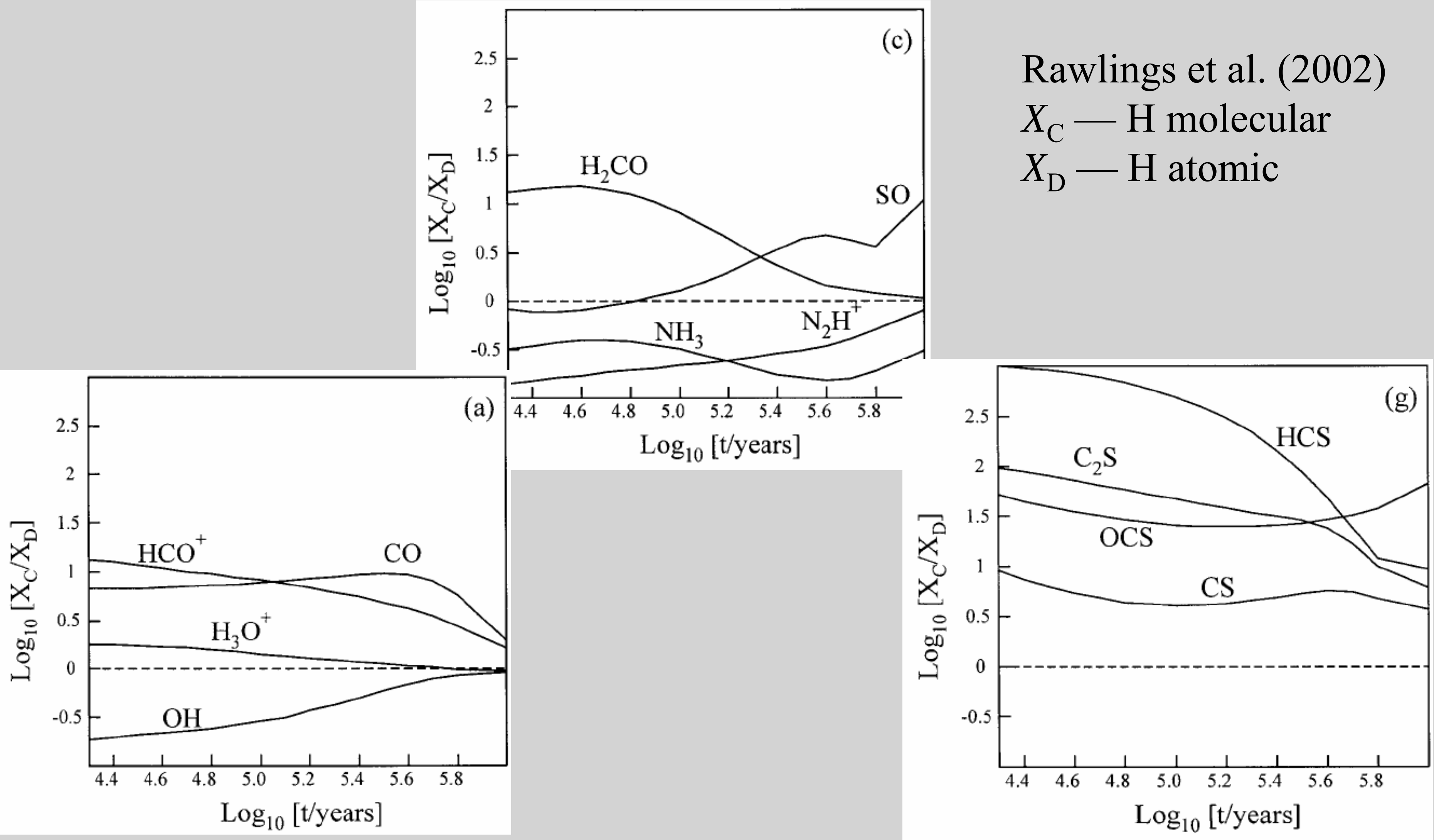
$$CH^+ + H \rightarrow C^+ + H_2$$

$$CH^+ + H_2 \rightarrow CH_2{}^+ + H$$

The oldest unsolved astrophysical problem (Liszt 2006):

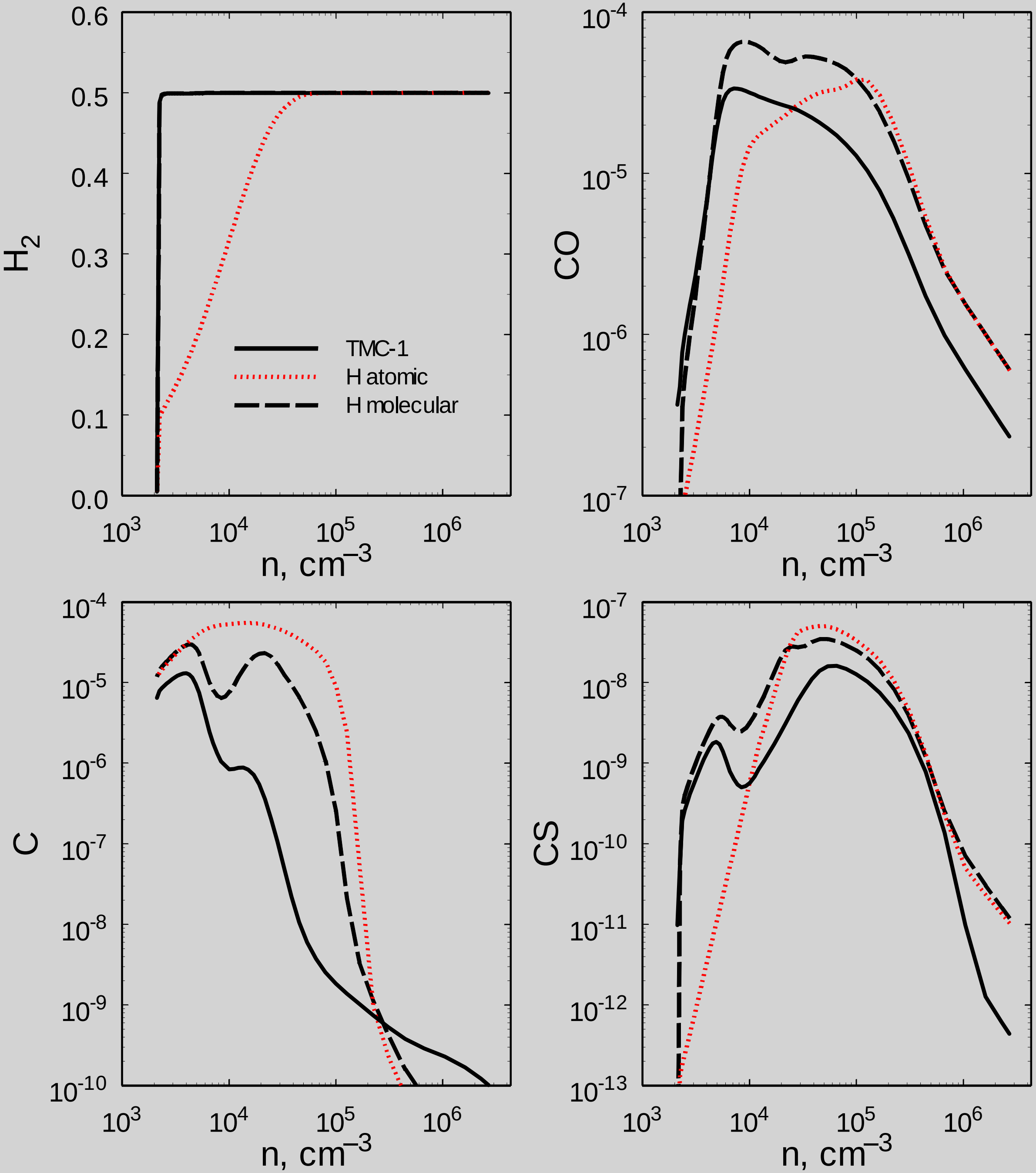
C-shocks?
Diffusion?
Turbulent dissipation?

Dark cloud chemistry in initially H-rich regions



Rawlings et al. (2002)
X_C — H molecular
X_D — H atomic

Model	**Initial abundances**
H-atomic	Hydrogen is totally atomic; other elements are atoms
H-molecular	Hydrogen is totally molecular; other elements are atoms
TMC-1	Complex molecular composition, but hydrogen is still totally molecular



$$\frac{\partial \zeta}{\partial m} = \frac{1}{\rho \zeta^2}$$

$$\frac{\partial u}{\partial \tau} = -\frac{m}{\zeta^2} - \zeta^2 \frac{\partial}{\partial m}\left(\frac{\rho}{2\alpha_c} + \frac{b^2}{2}\right)$$

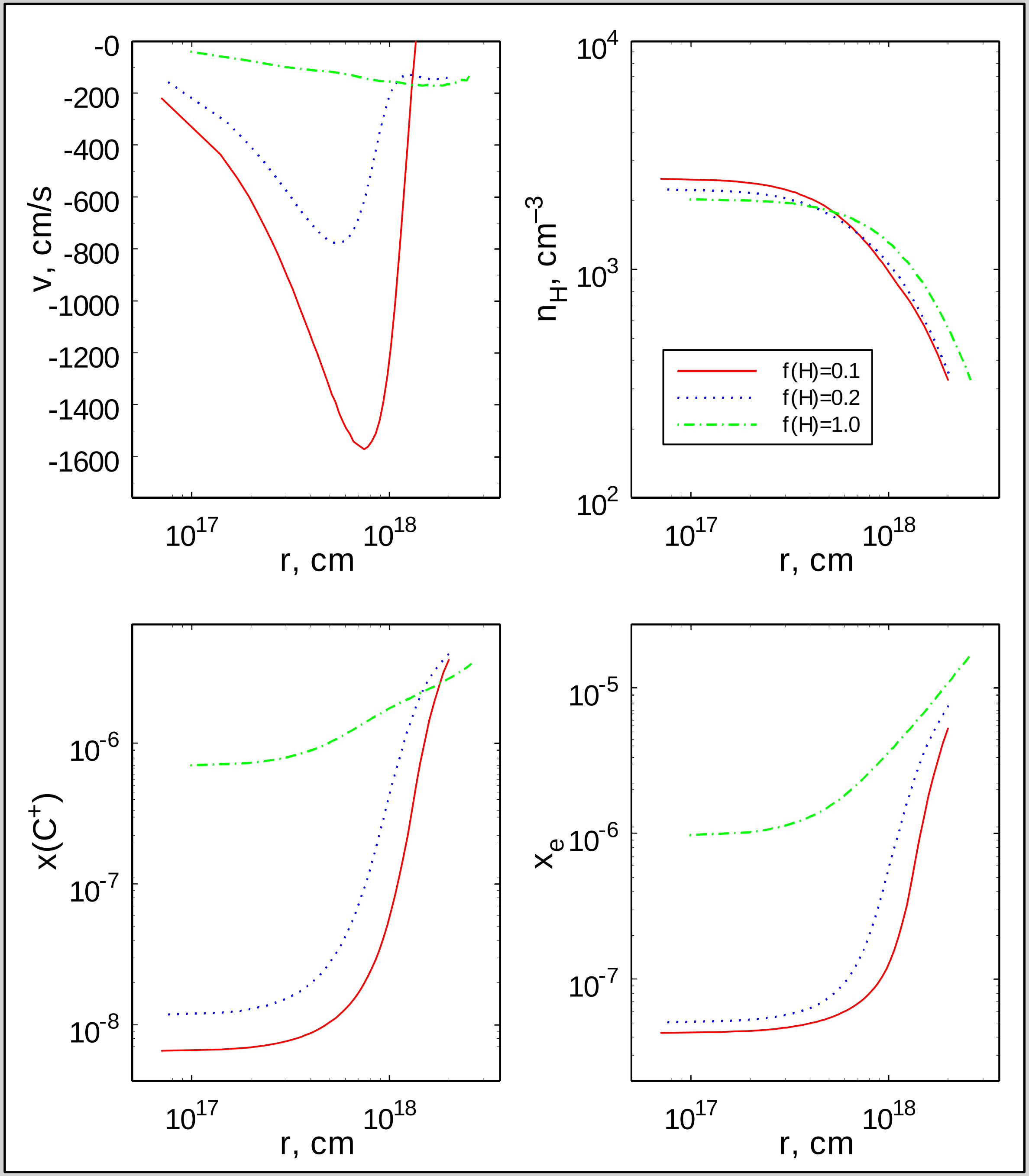
$$\frac{\partial}{\partial \tau}\left(\frac{b}{\rho \zeta}\right) = \frac{\partial}{\partial m}\left(\frac{1.4}{\nu_{\rm ff}} \frac{b^2 \zeta^2}{\sqrt{\rho}} \frac{\partial b}{\partial m}\right)$$

$$u = \frac{\partial \zeta}{\partial \tau}$$

$$\alpha_c = \frac{B_c}{8\pi\rho_c a^2}$$

$$\nu_{ff} = \frac{t_{ff}}{\tau_{ni}} = \frac{\gamma \rho_i}{\sqrt{4\pi G \rho}}$$

Shematovich et al. (2003)



Why do we take wrong initial conditions?

Gas-phase H_2 formation

Three-body reaction:

$$H + H + H \rightarrow H_2 + H$$

Very slow reaction:

$$H^+ + H \rightarrow H_2^+ + h\nu$$

$$H_2^+ + H \rightarrow H_2 + H^+$$

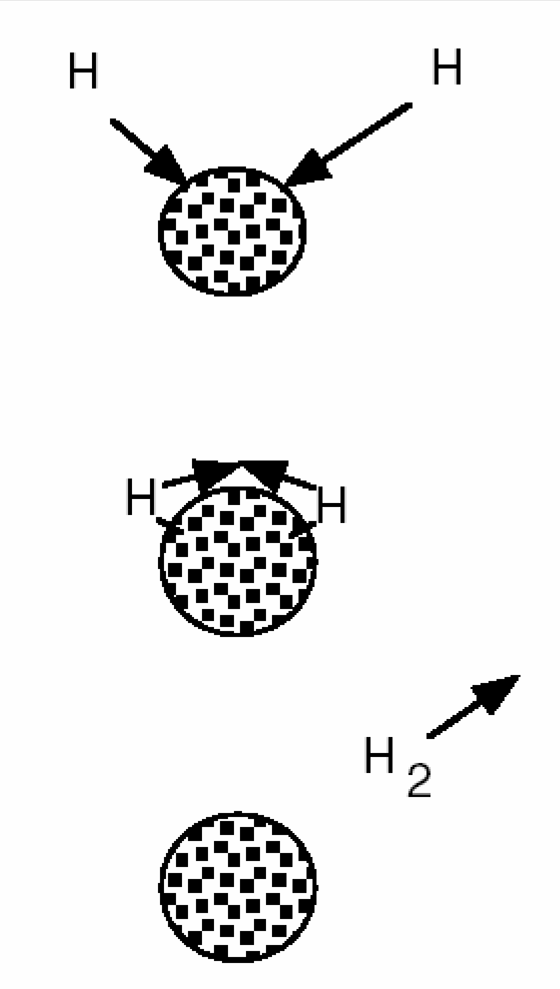
Very slow reaction:

$$H + e^- \rightarrow H^- + h\nu$$

$$H^+ + H^- \rightarrow H_2$$

$$H_2^+ + H^- \rightarrow H_2 + H$$

Dust surface H_2 formation



1. H atoms stick to a grain.

2. They migrate over its surface, collide, and form H_2 molecule.

3. Newly formed H_2 desorbs into the gas-phase.

It is necessary to include surface chemistry in the model

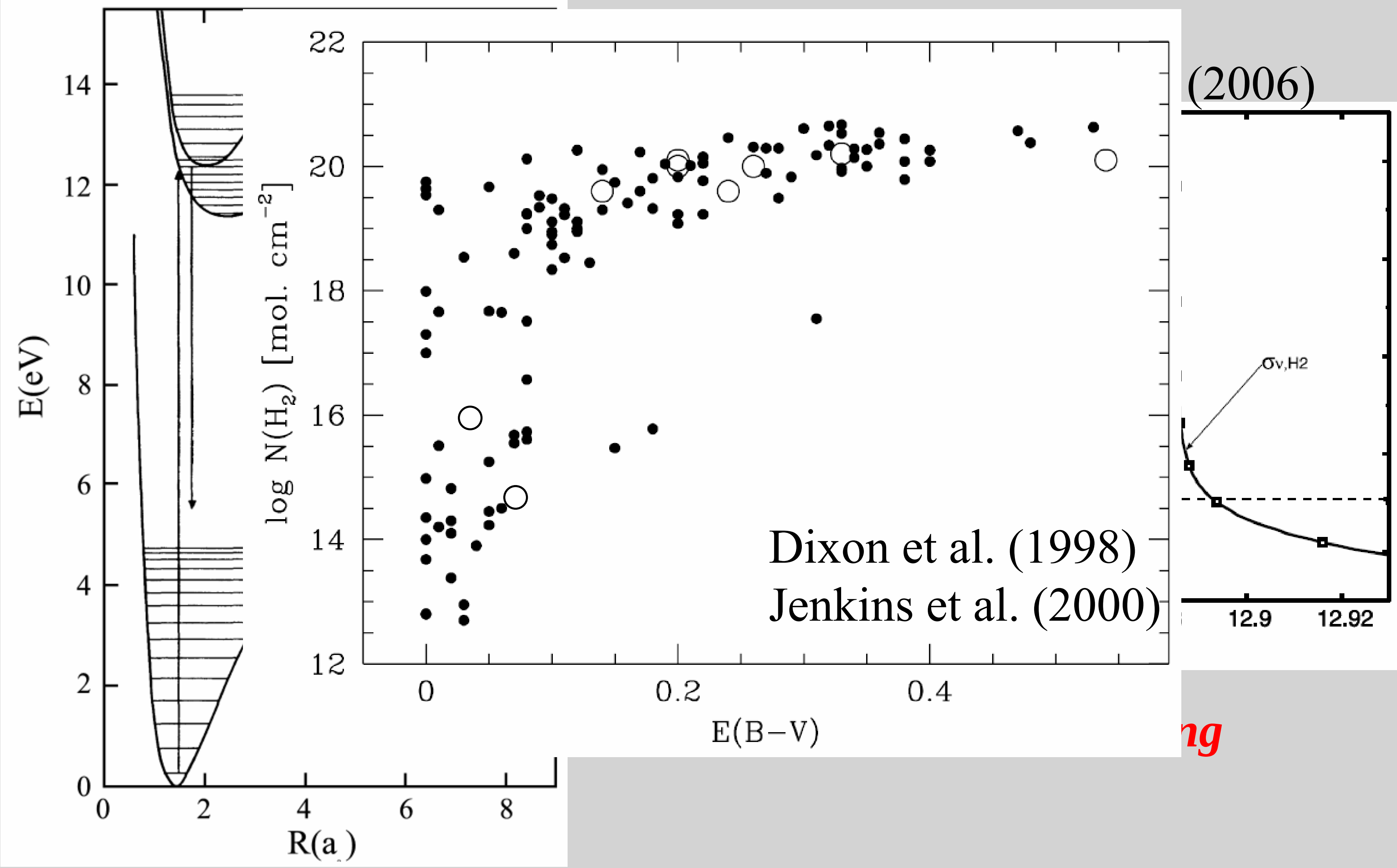
Dust surface H_2 formation

Even on surfaces it is a very slow process

Effective only at dust temperatures between 10K and 20K

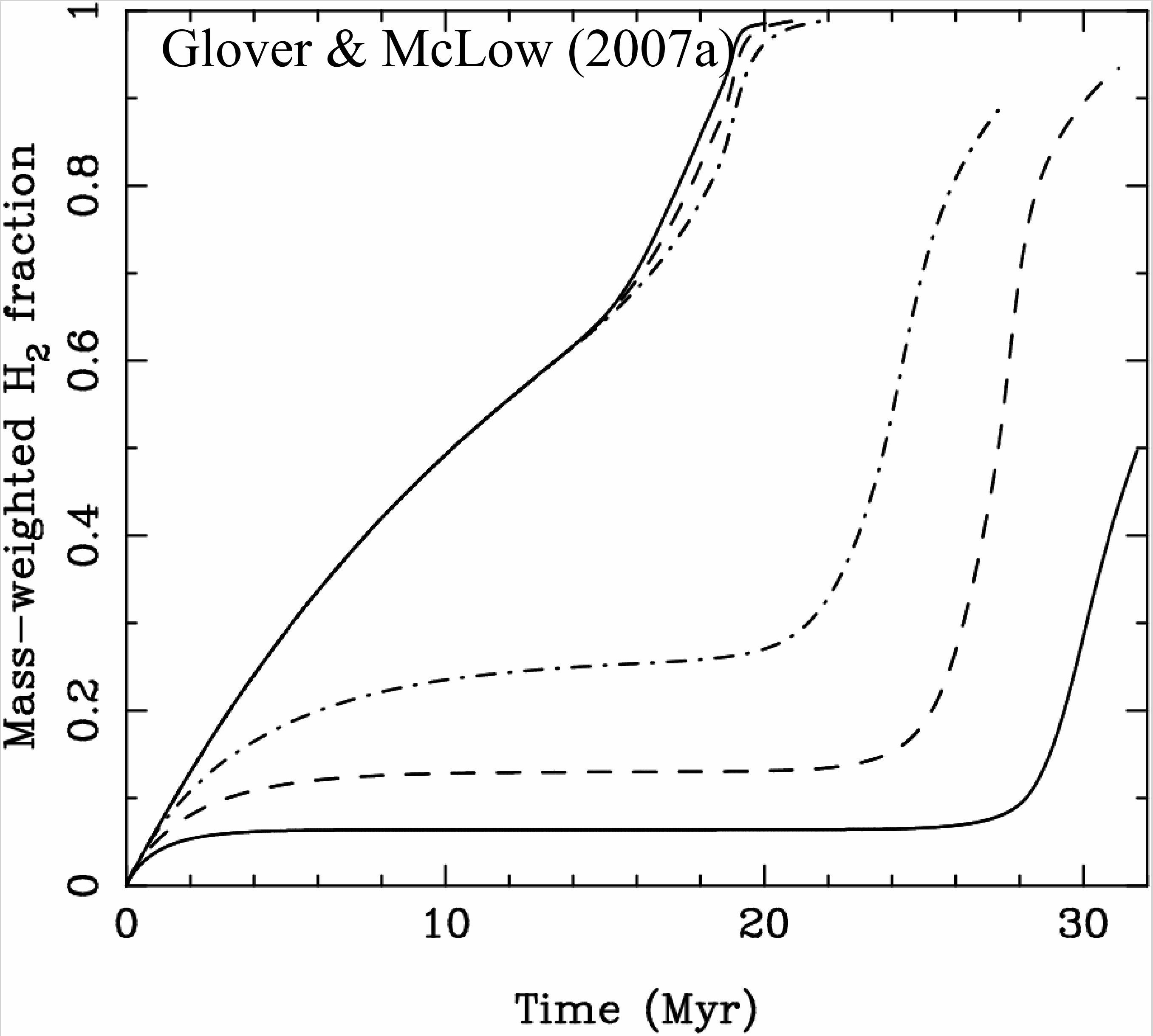
Newly formed H_2 is dissociated by UV photons

Dissociation H_2

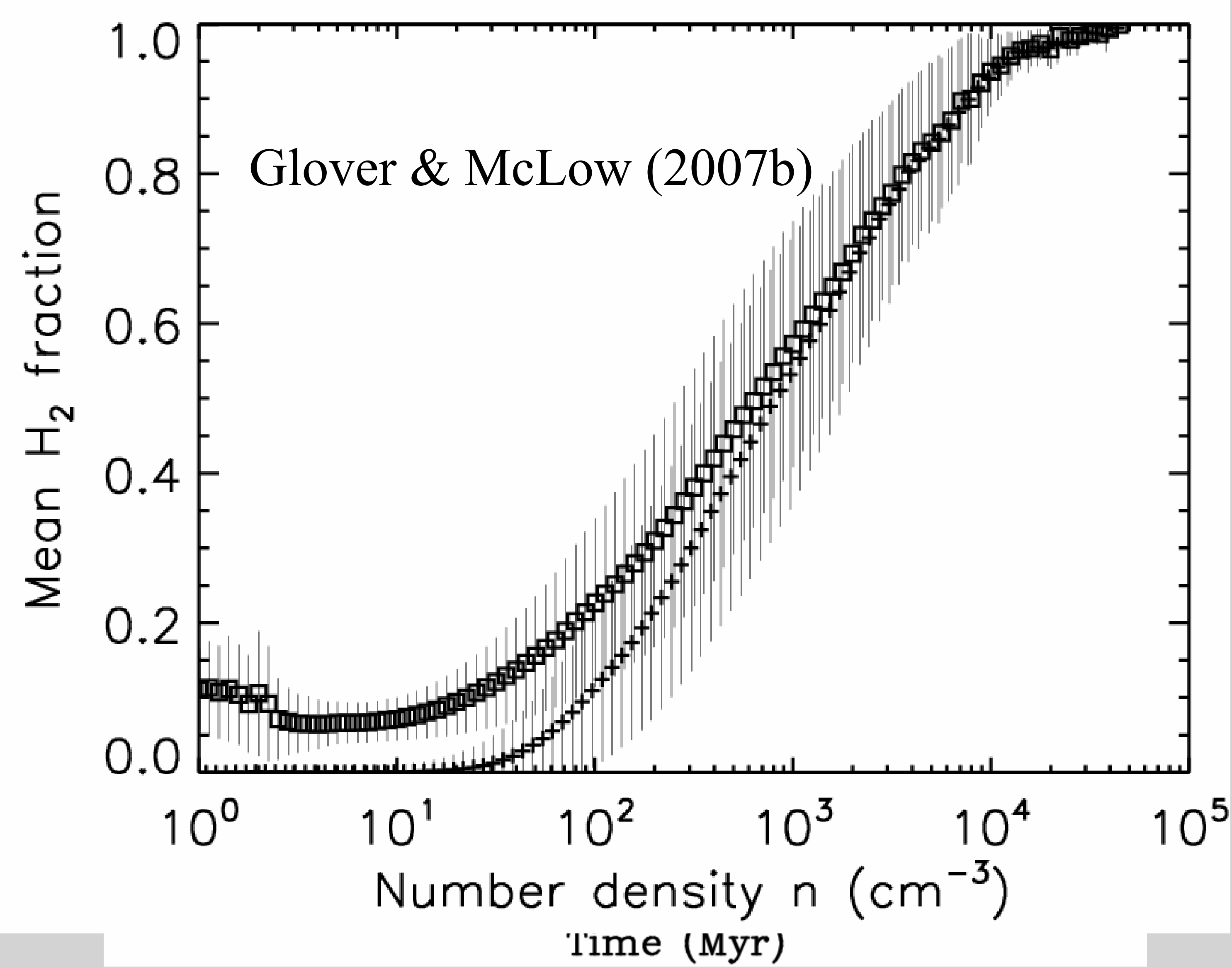


Dixon et al. (1998)
Jenkins et al. (2000)

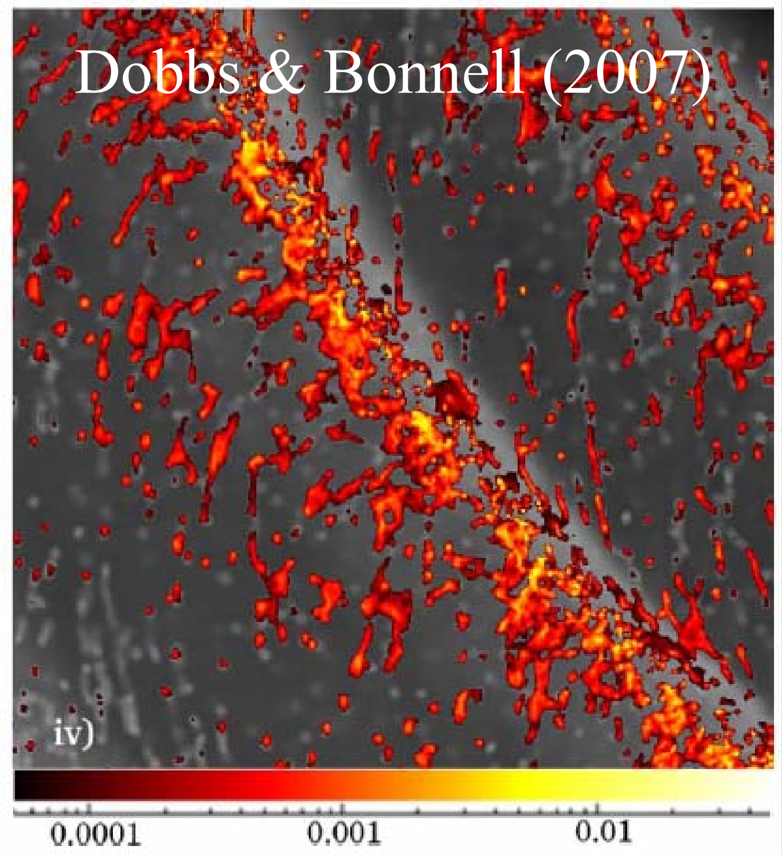
H_2 accumulation in quiescent molecular clouds



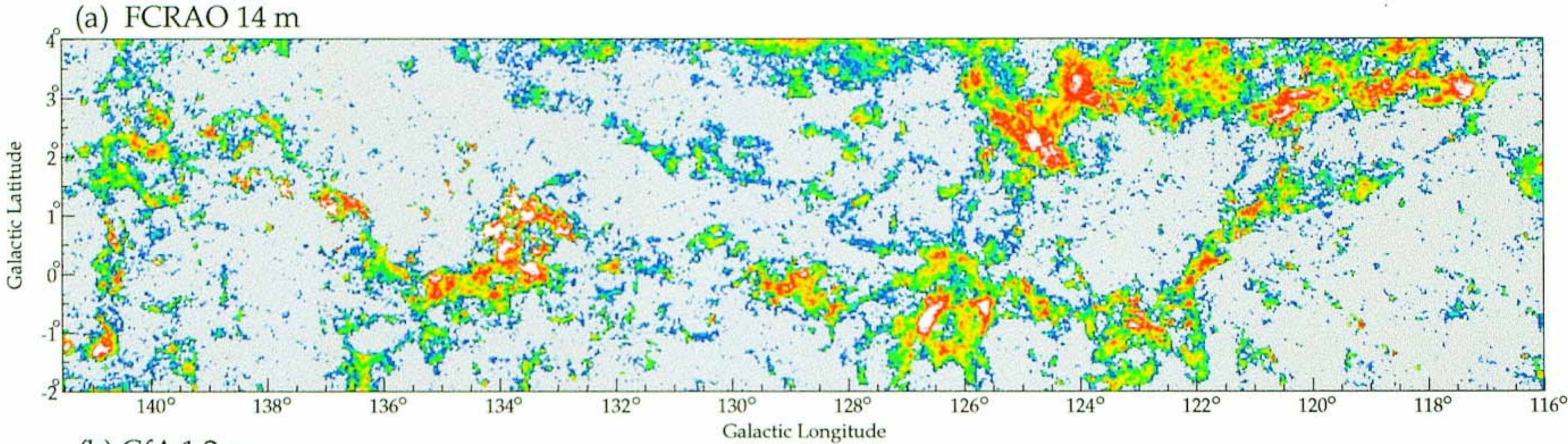
H_2 accumulation in turbulent molecular clouds



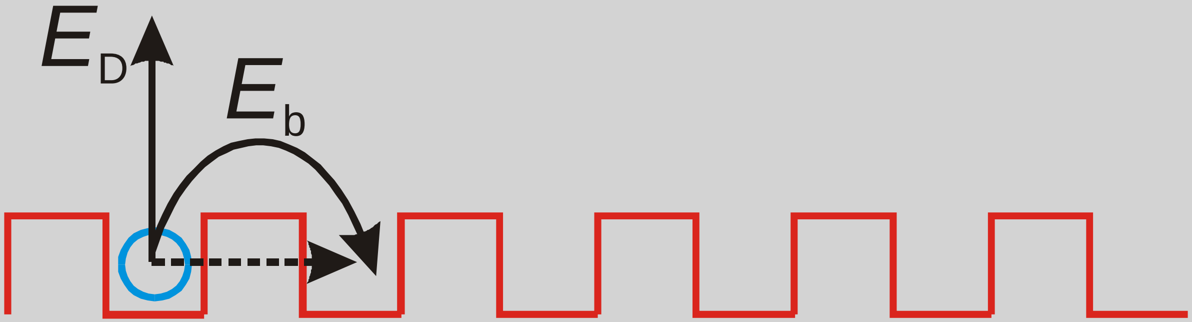
Other molecules (in particular, CO)

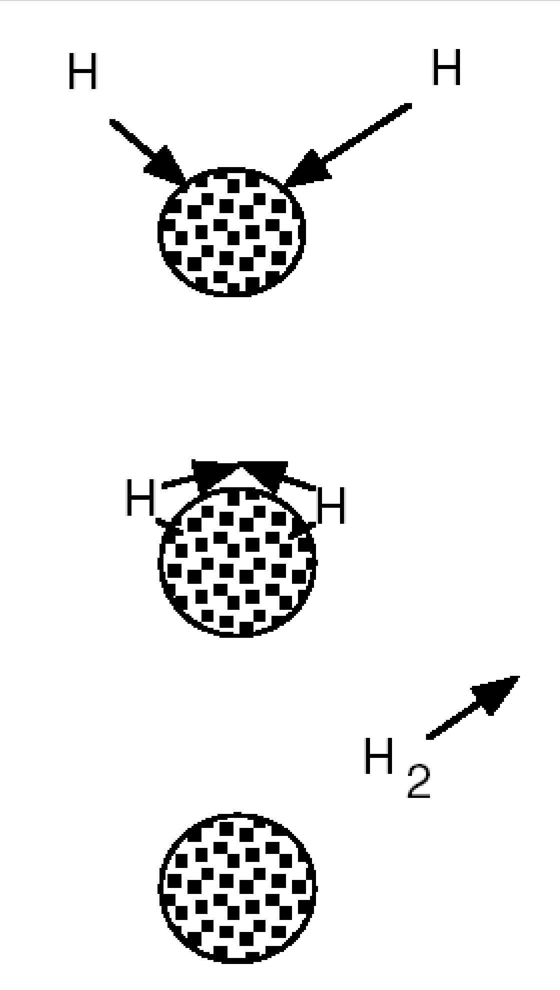


- Tracers
- Heating & cooling
- Fractional ionization



Other molecules: role of surface chemistry





Hasegawa, Herbst, Leung (1992)
Rate equation approach to surface chemistry

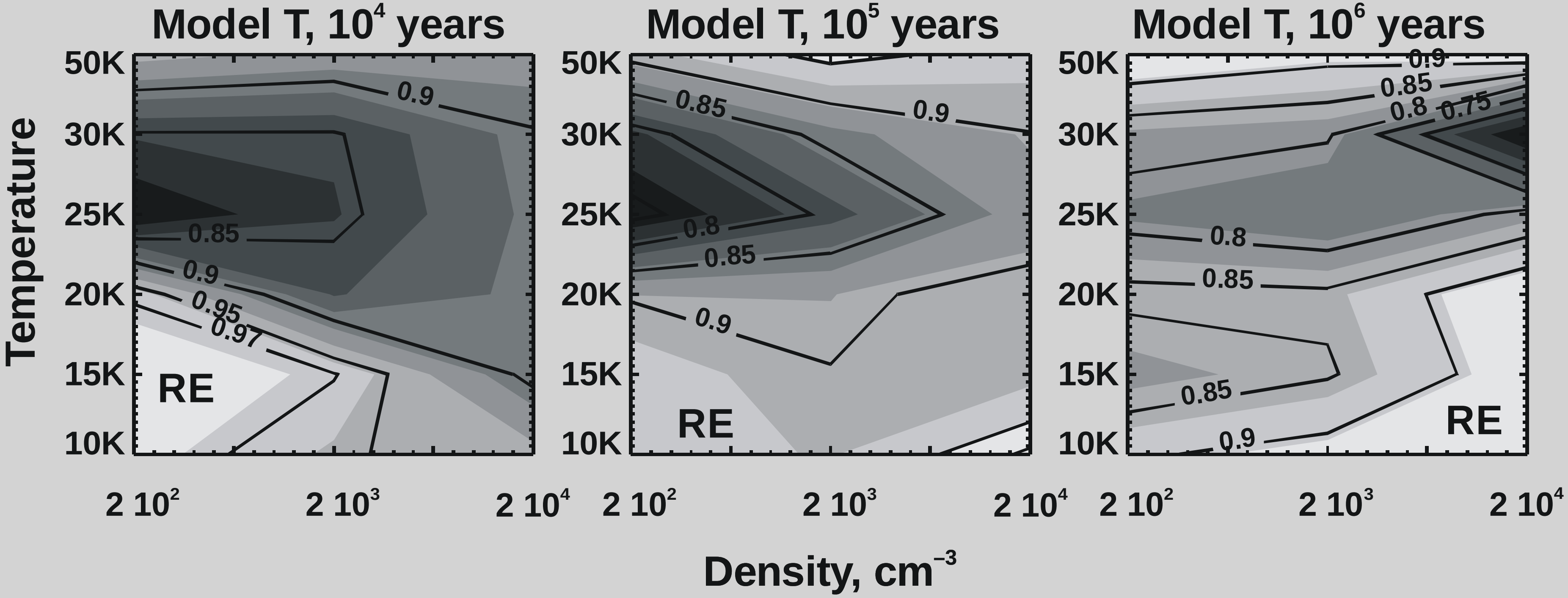
Unified Monte Carlo treatment of gas-grain chemistry

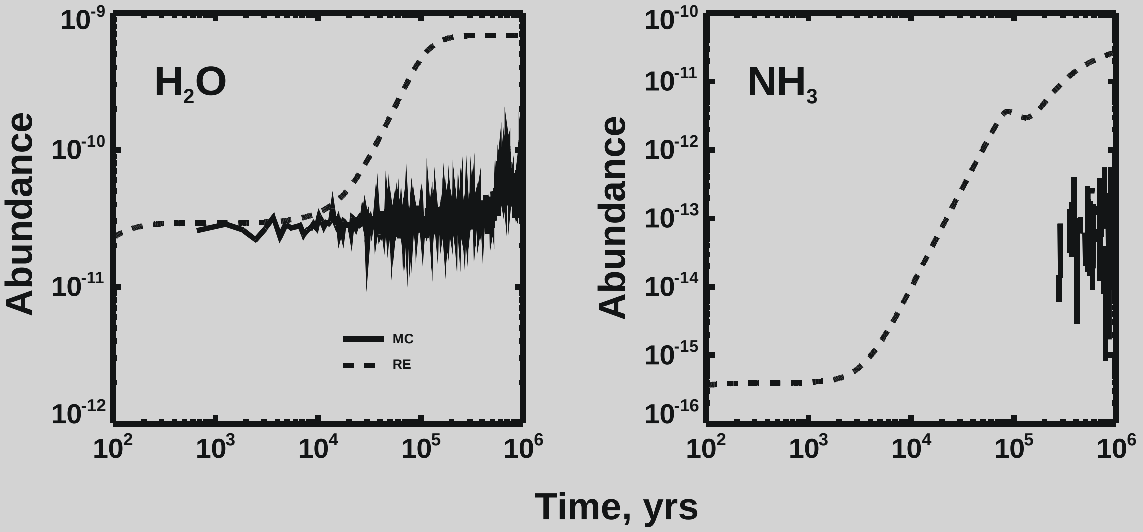
1. The Chemical Master Equation, universal and very slow

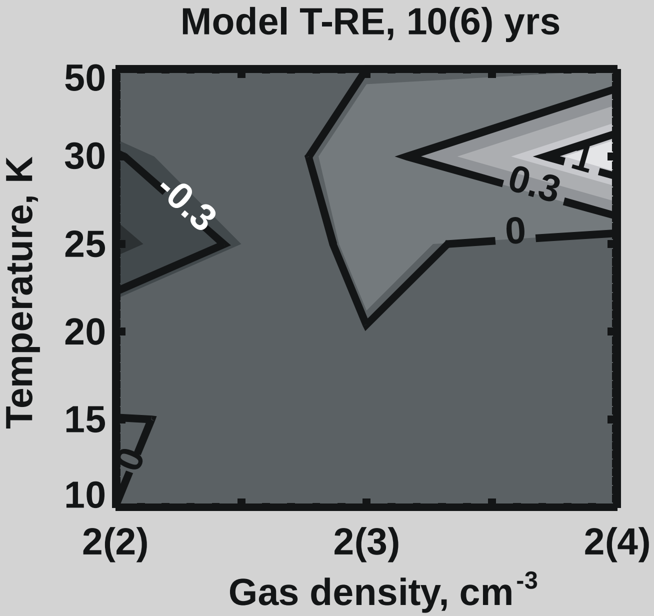
$$\frac{\partial P(\vec{X},t \mid \vec{X}_0,t_0)}{\partial t} = \sum_{j=1}^{M}[a_j(\vec{X}-\vec{\nu}_j)P(\vec{X}-\vec{\nu}_j,t \mid \vec{X}_0,t_0) - a_j(\vec{X})P(\vec{X},t \mid \vec{X}_0,t_0)]$$

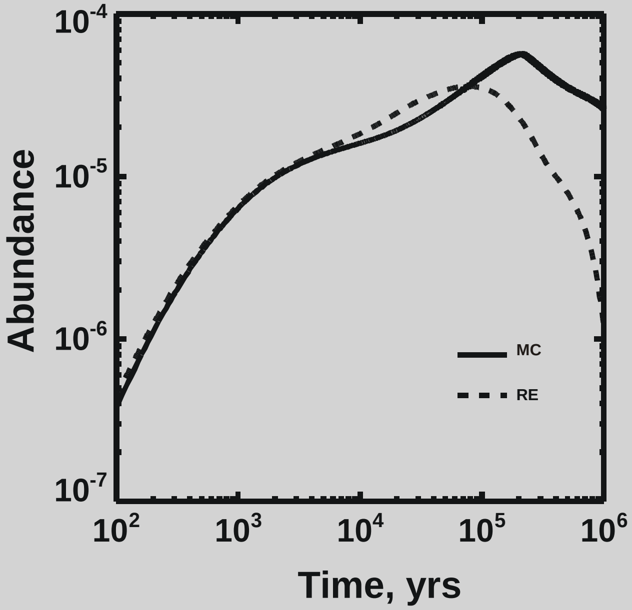
2. Rate Equations, very fast, but not universal

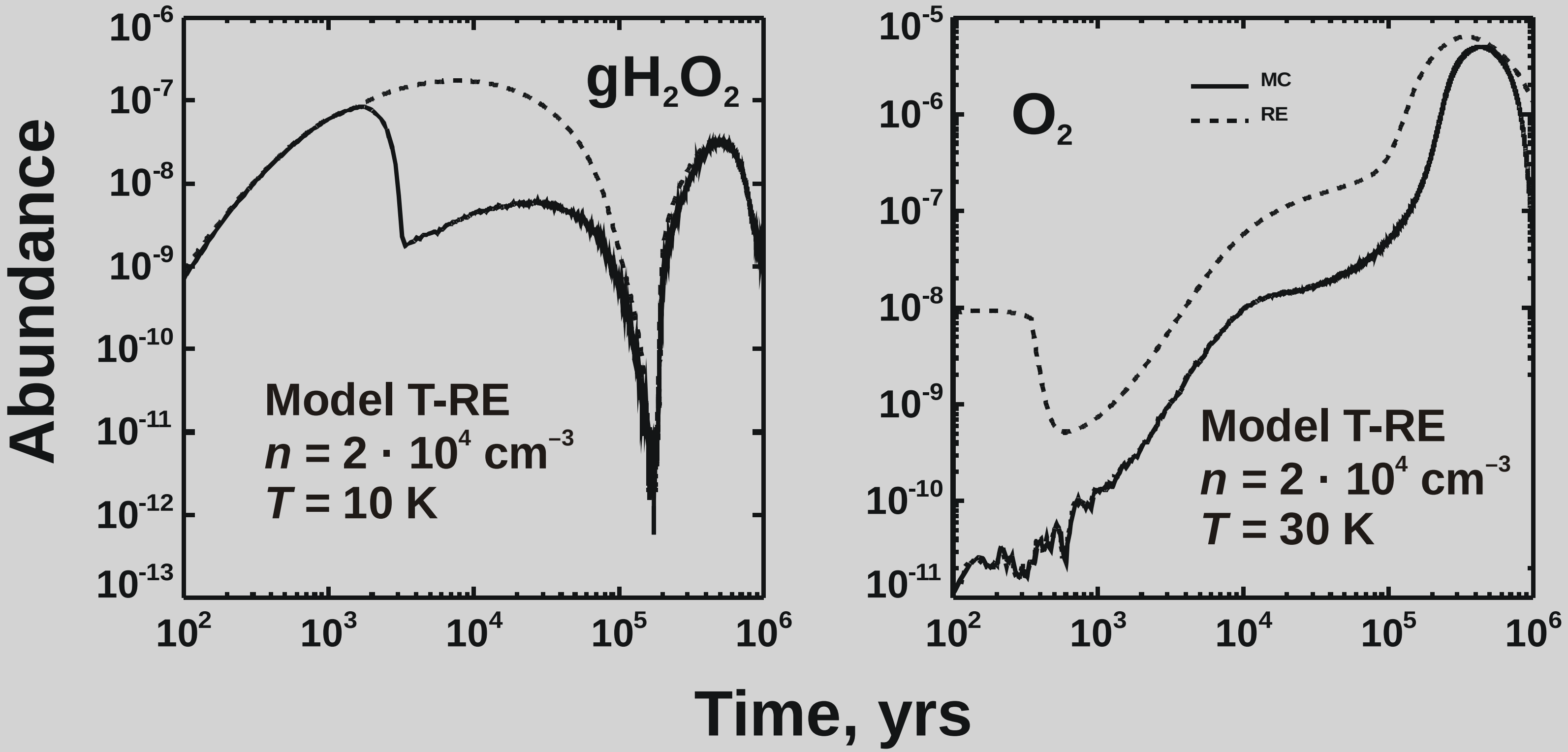
Unified treatment of gas-phase and surface chemistry in large chemical networks — Vasyunin et al. (submitted)


Model T, 10^4 years
Model T, 10^5 years
Model T, 10^6 years
Temperature
50K
30K
25K
20K
15K
10K
0.9
0.85
0.95
0.97
0.8
0.75
RE
2 10^2
2 10^3
2 10^4
Density, cm^{-3}


H_2O
NH_3
Abundance
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
10^{-16}
MC
RE
10^2
10^3
10^4
10^5
10^6
Time, yrs


Model T-RE, 10(6) yrs
Temperature, K
50
30
25
20
15
10
-0.3
1
0.3
0
0
2(2)
2(3)
2(4)
Gas density, cm^{-3}

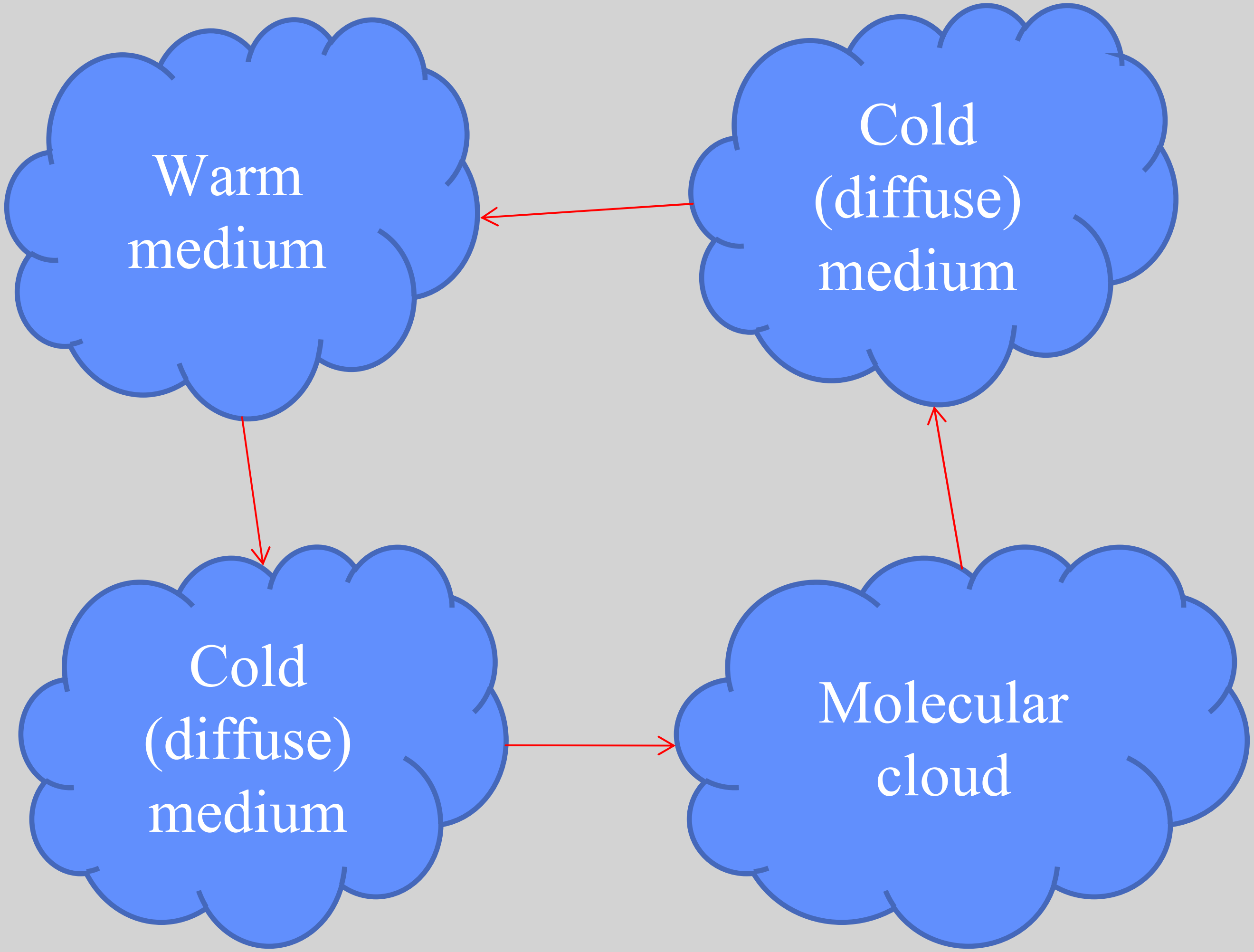

Abundance
10^{-4}
10^{-5}
10^{-6}
10^{-7}
MC
RE
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
Time, yrs



Incorrect treatment of surface reaction leads to significant errors in computed abundances of important molecules at densities and temperatures typical of translucent clouds.

Grain size, composition, structure…

Evolutionary status of diffuse clouds



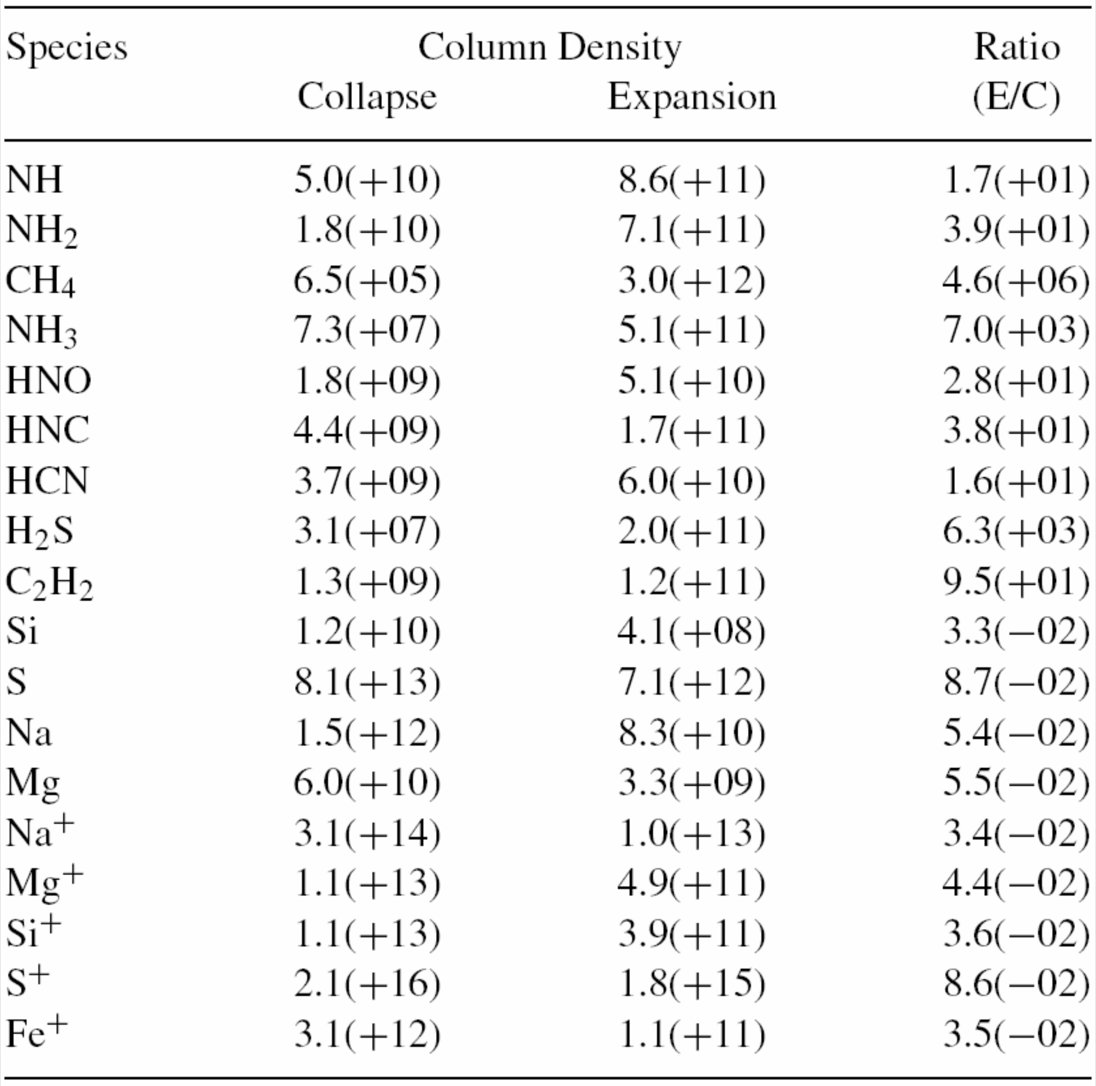
Warm medium

Cold (diffuse) medium

Cold (diffuse) medium

Molecular cloud

Collapse vs expansion



Species	Column Density		Ratio
	Collapse	Expansion	(E/C)
NH	5.0(+10)	8.6(+11)	1.7(+01)
NH_2	1.8(+10)	7.1(+11)	3.9(+01)
CH_4	6.5(+05)	3.0(+12)	4.6(+06)
NH_3	7.3(+07)	5.1(+11)	7.0(+03)
HNO	1.8(+09)	5.1(+10)	2.8(+01)
HNC	4.4(+09)	1.7(+11)	3.8(+01)
HCN	3.7(+09)	6.0(+10)	1.6(+01)
H_2S	3.1(+07)	2.0(+11)	6.3(+03)
C_2H_2	1.3(+09)	1.2(+11)	9.5(+01)
Si	1.2(+10)	4.1(+08)	3.3(−02)
S	8.1(+13)	7.1(+12)	8.7(−02)
Na	1.5(+12)	8.3(+10)	5.4(−02)
Mg	6.0(+10)	3.3(+09)	5.5(−02)
Na^+	3.1(+14)	1.0(+13)	3.4(−02)
Mg^+	1.1(+13)	4.9(+11)	4.4(−02)
Si^+	1.1(+13)	3.9(+11)	3.6(−02)
S^+	2.1(+16)	1.8(+15)	8.6(−02)
Fe^+	3.1(+12)	1.1(+11)	3.5(−02)

Price et al. (2003)

Conclusions

1. Diffuse and translucent clouds represent truly initial conditions for prestellar cores.

2. Abundances in prestellar cores (and conclusions which are based on these abundances) sensitively depend on the initial fraction of molecular hydrogen.

3. Incorrect treatment of surface reaction leads to significant errors in computed abundances of important molecules at densities and temperatures typical of translucent clouds.