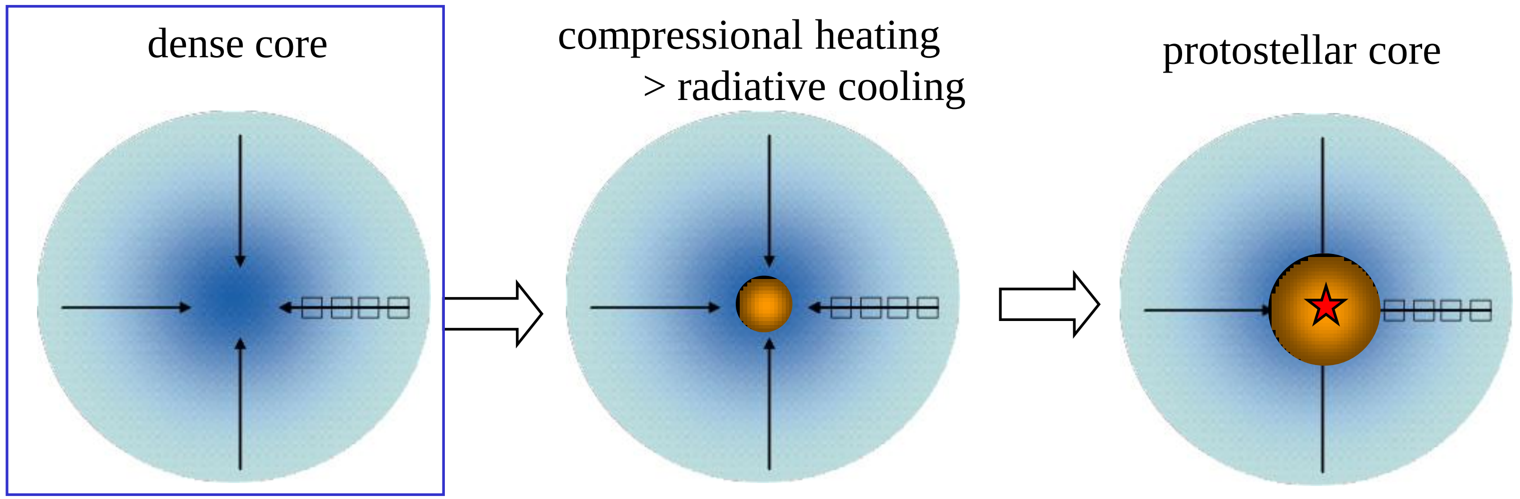
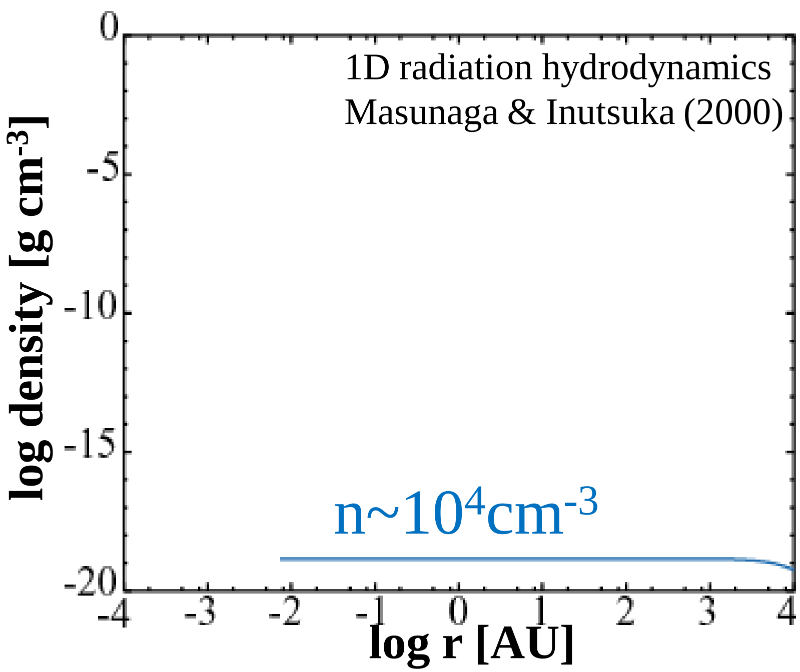
Hydrodynamical-chemical models from prestellar cores to protostellar cores

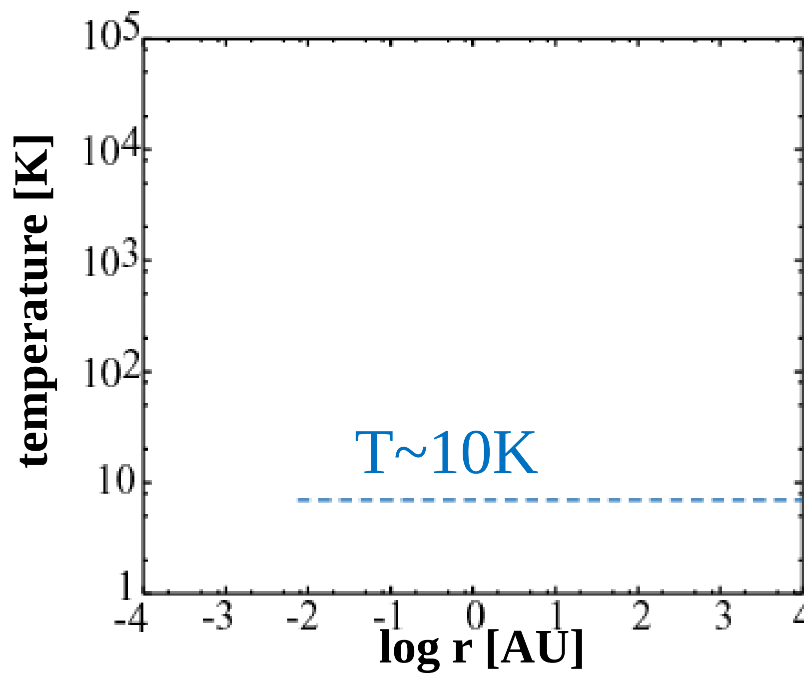
Yuri Aikawa (Kobe University)

Collaborators:
Kenji Furuya (Kobe Univ), Valentine Wakelam, Frank Hersant (Bordeaux)
Tomoaki Matsumoto (Housei Univ), Koji Tomisaka, Kengo Tomida (NAOJ),
Robin Garrod (Cornel), Eric Herbst (OSU)

From prestellar core to protostellar core







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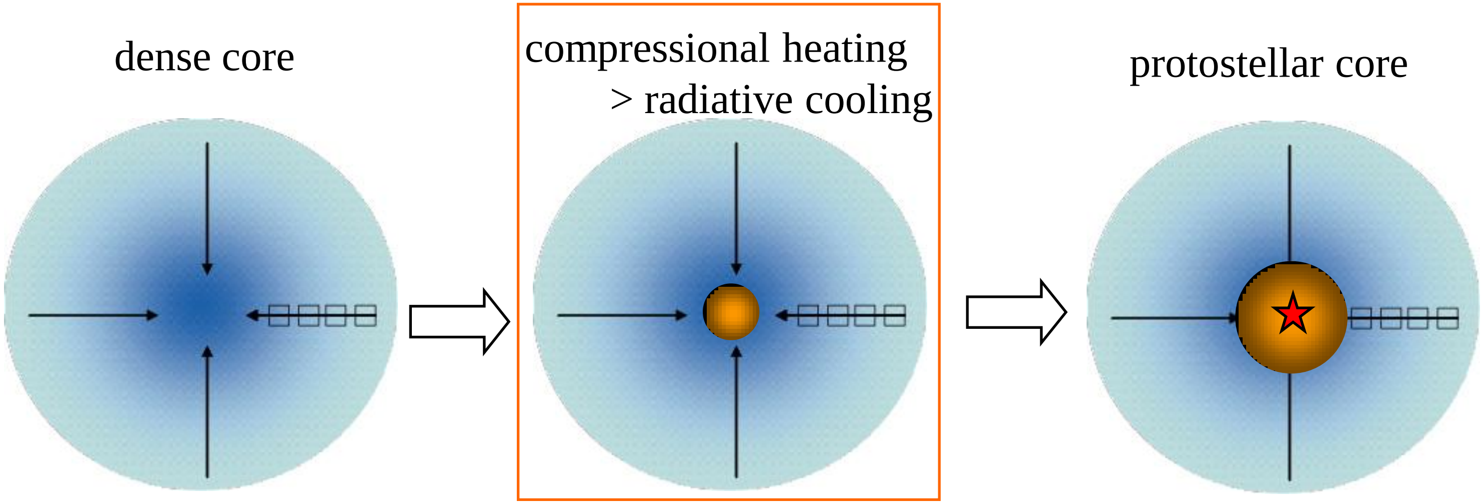

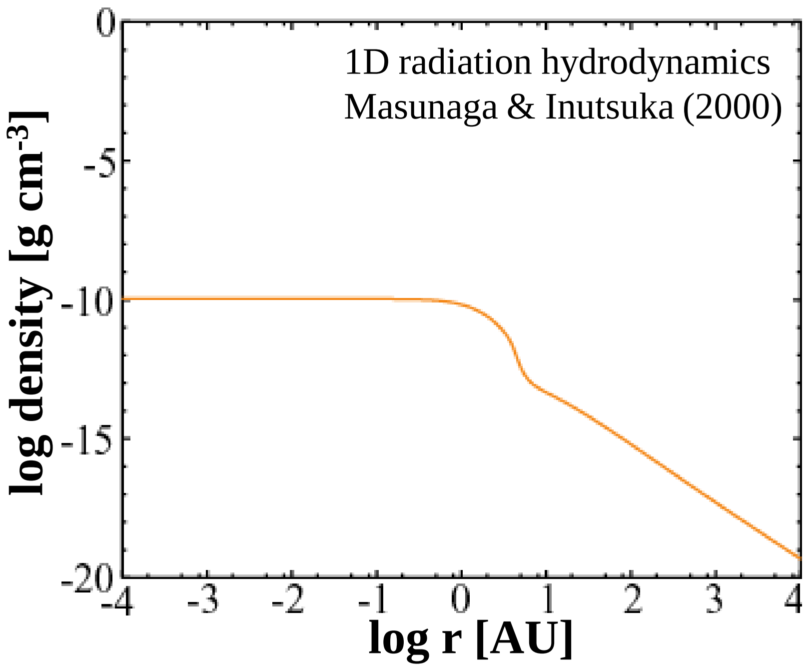

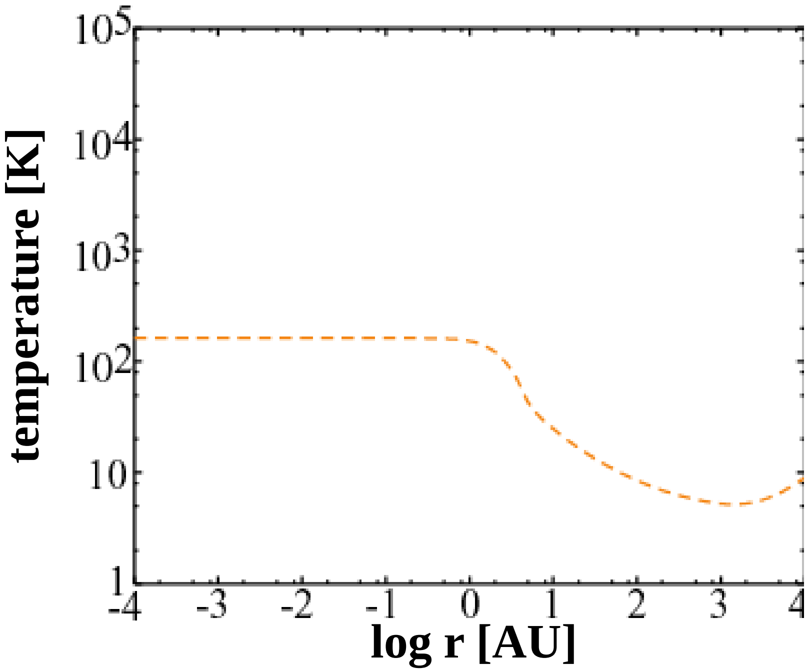

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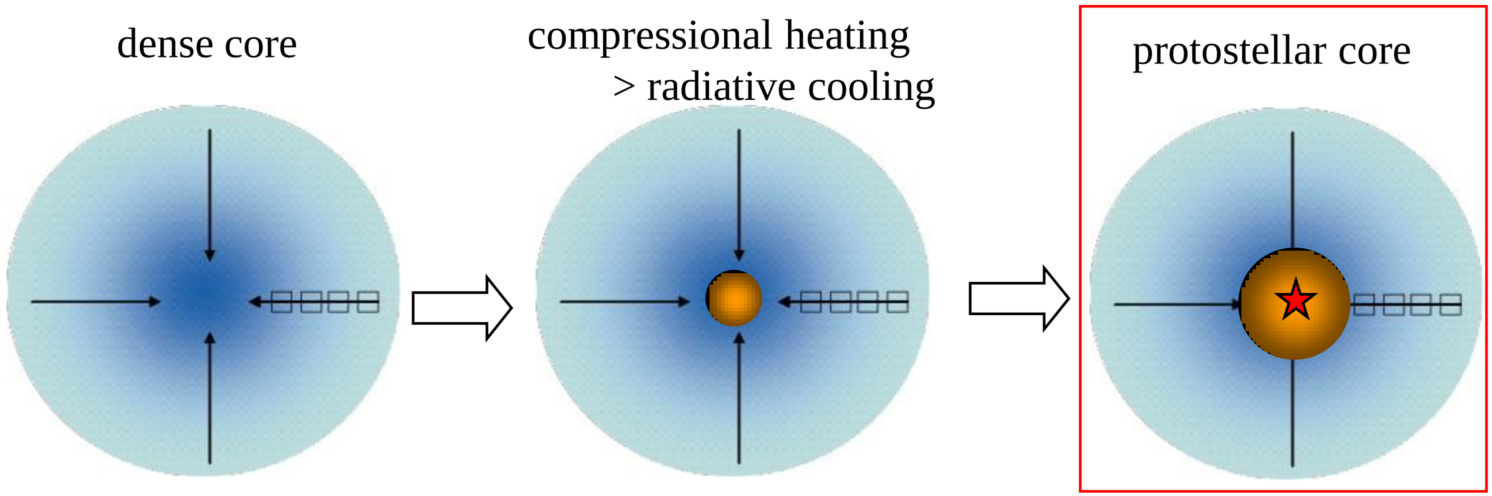
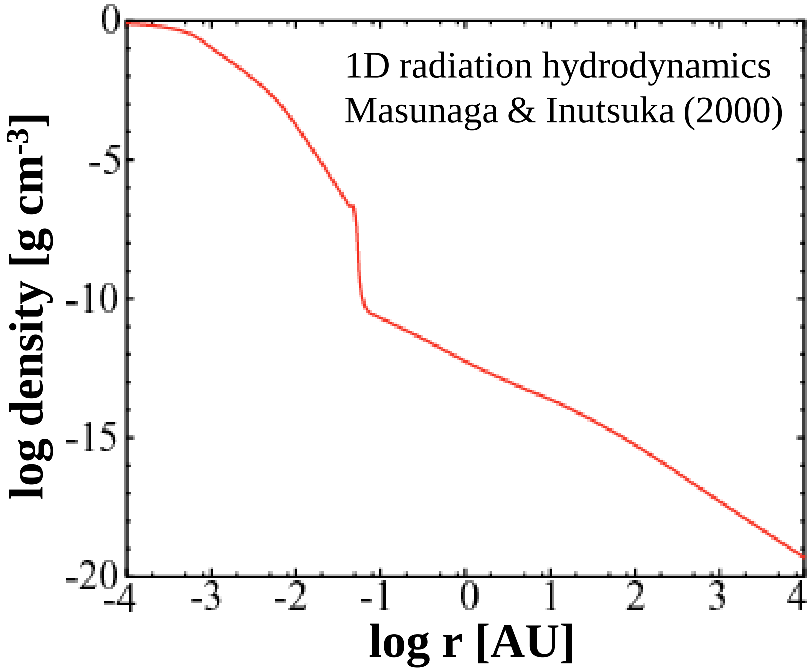
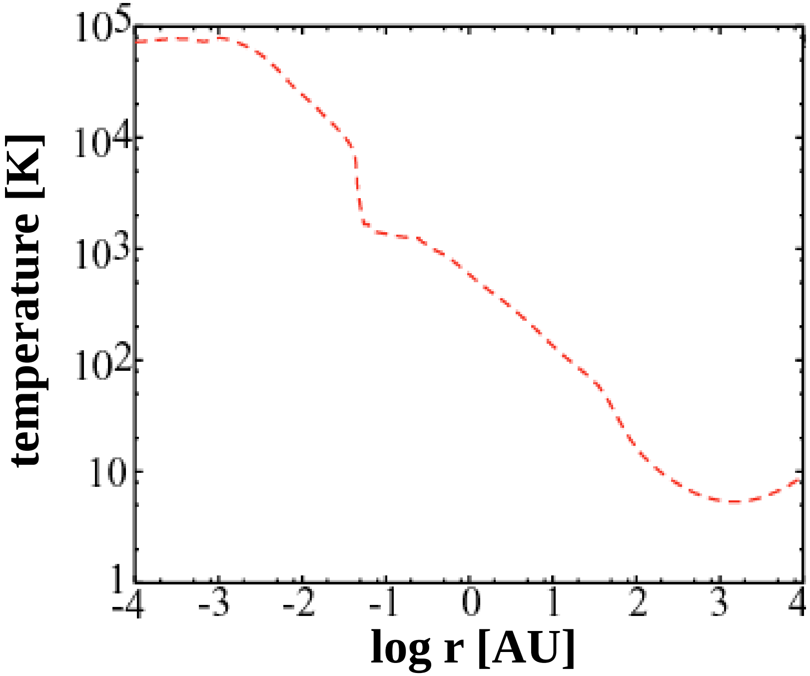
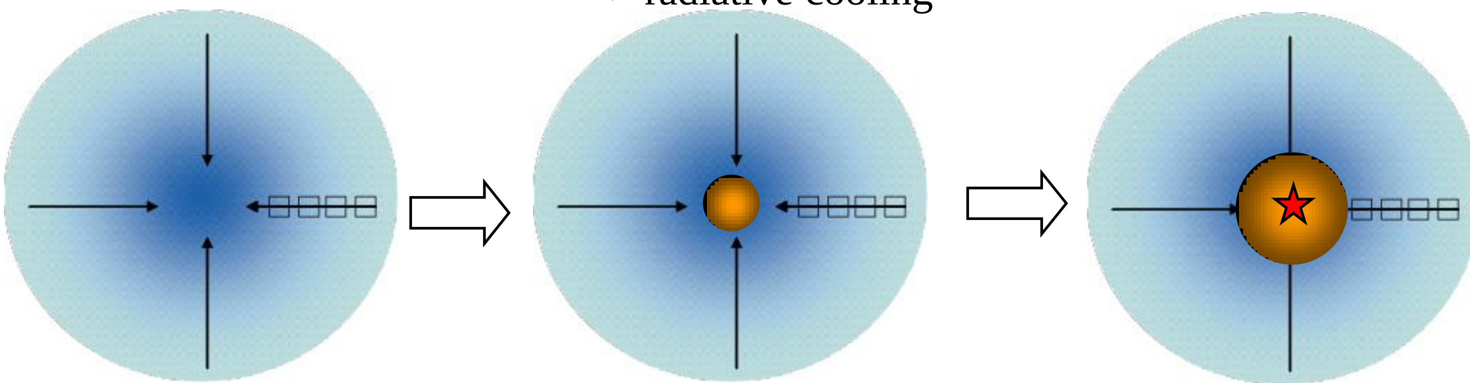






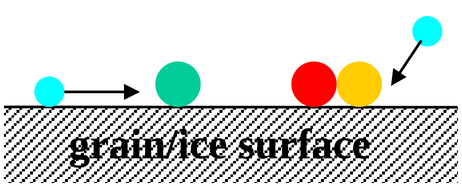
Chemical processes in star forming cores

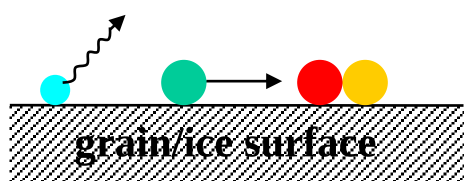


Low temperature: T < 20K
Increasing density
-Molecules freeze-out on grains
-hydrogenation on grain surface
e.g. $CO \rightarrow CH_3OH$

20K < T< 100K
- Grain-surface reactions of heavy species

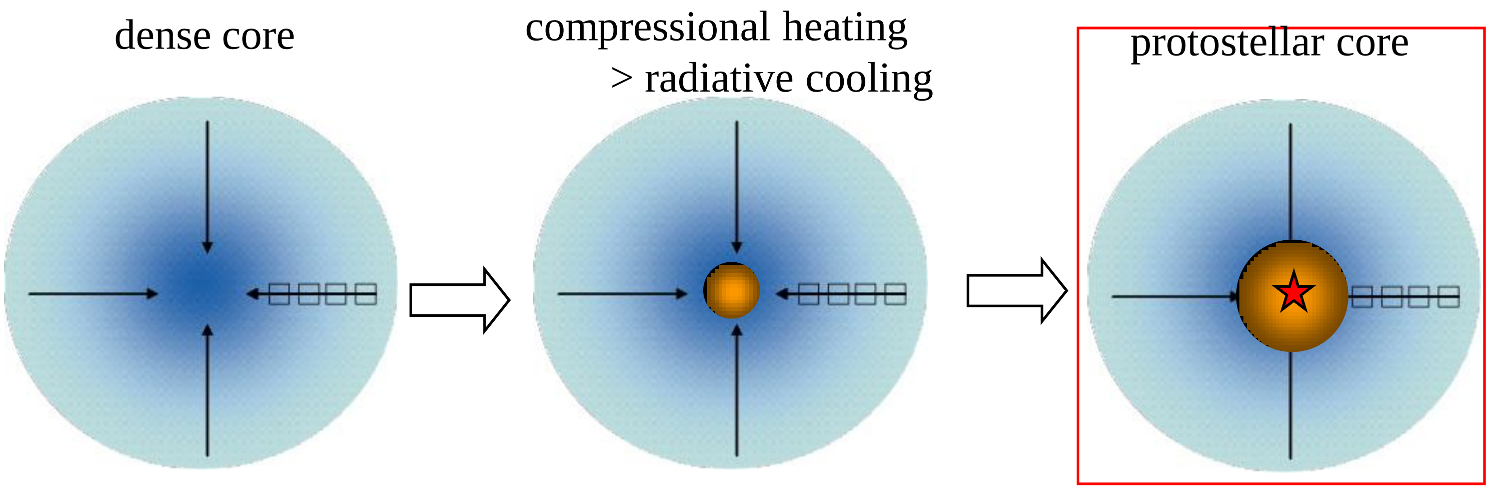
Gas-phase reactions of sublimates





Garrod & Herbst (2006)
van Dishoeck & Herbst (2009)

Hydrodynamical-chemical models



Chemistry is continuous and does not reach equilibrium
→ Hydrodynamical-chemical models

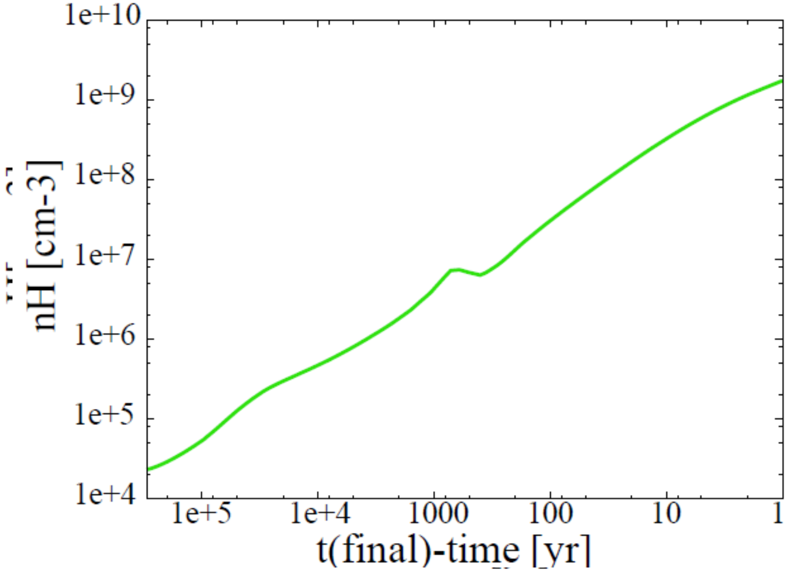
1D radiation hydrodynamics From prestellar to ptotostellar core (Masunaga & Inutsuka 2000)	+	Gas & grain-surface chemistry (Garrod & Herbst 2006) in infalling fluid parcels

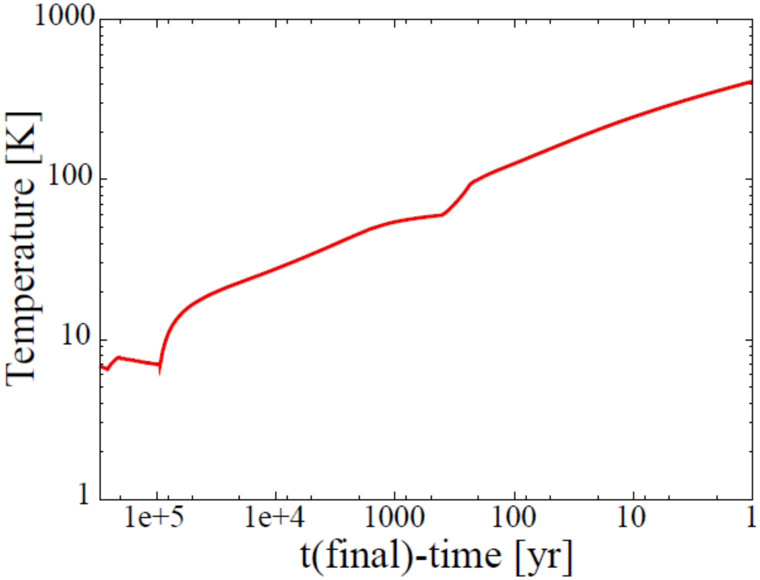
→Evolution of gas and ice (Aikawa et al. 2008)

Lee et al. (2004)
Visser's talk

Lagrangian view

Density & temperature in a fluid parcel falling from 10^4AU to 2.5AU





density & temperature rise accelerates at the latest moment

$\leftarrow t_{\mathrm{free-fall}} \propto n_{\mathrm{H}}^{-1/2}$

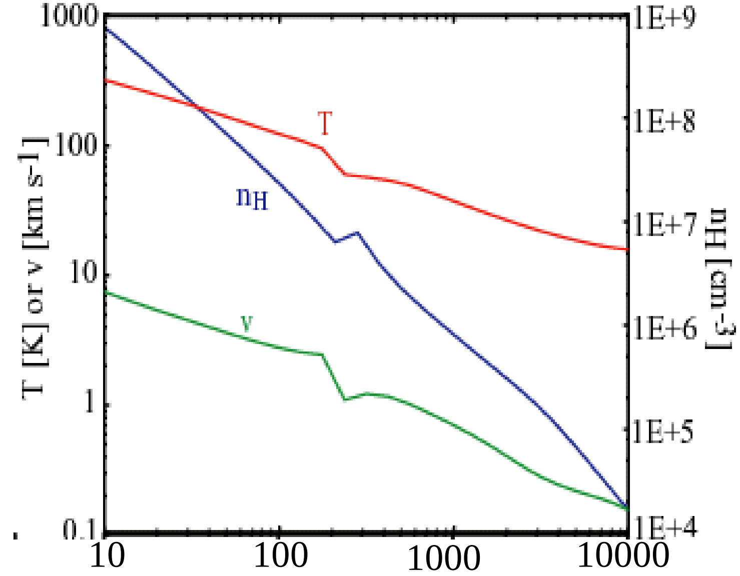
Duration of (Luke) warm chemistry ~ $r_{warm}/v_{free\text{-}fall}$

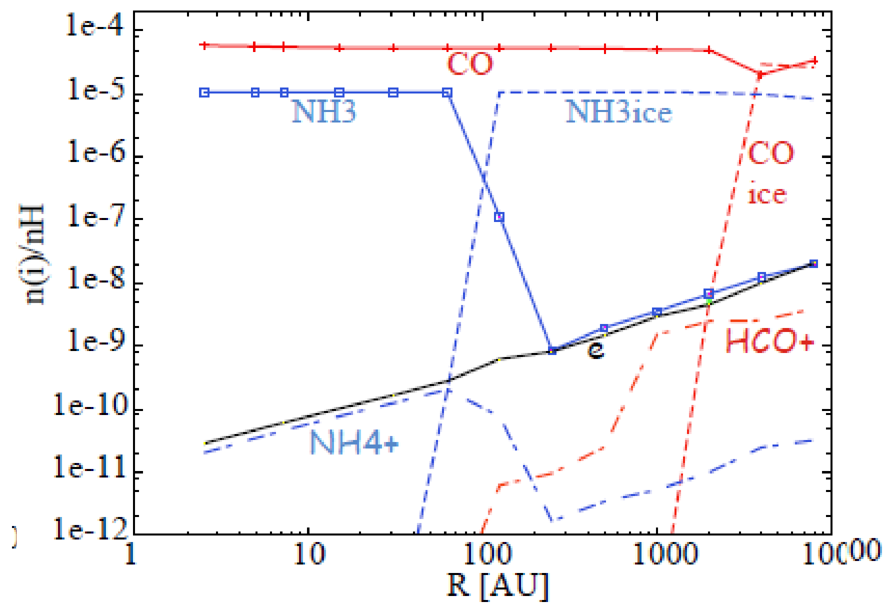
Distribution of Molecules in Protostellar Core

- Abundance jump at sublimation radii

-Dominant ion vary with rising temperature
  $HCO^+ \rightarrow HCO_2^+ \rightarrow NH_4^+$

~ 1 x 10^5yr after 2^{nd} collapse





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CH_3OH & H_2CO ice can form in ambient cloud
CH_3CHO, HCOOH gas/ice are abundant at T > 40K

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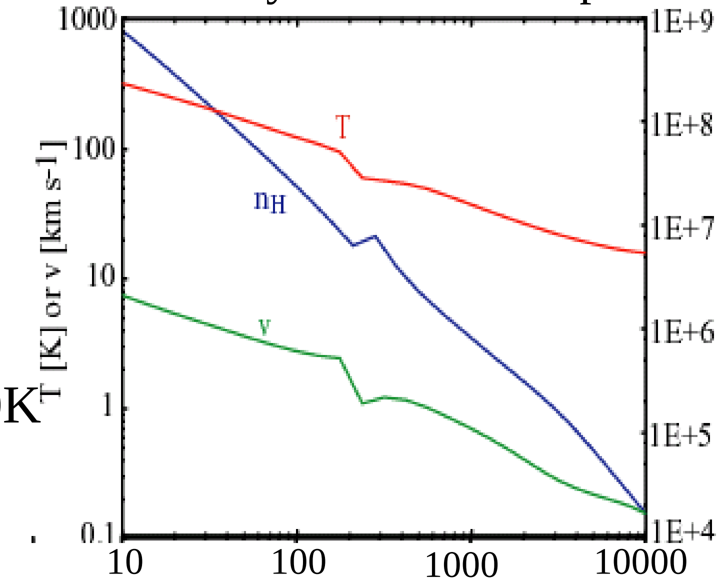

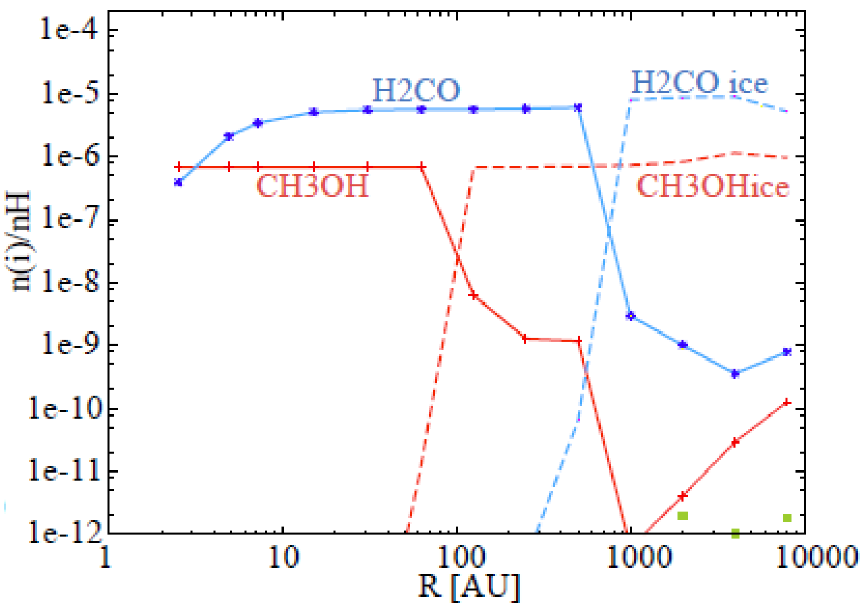

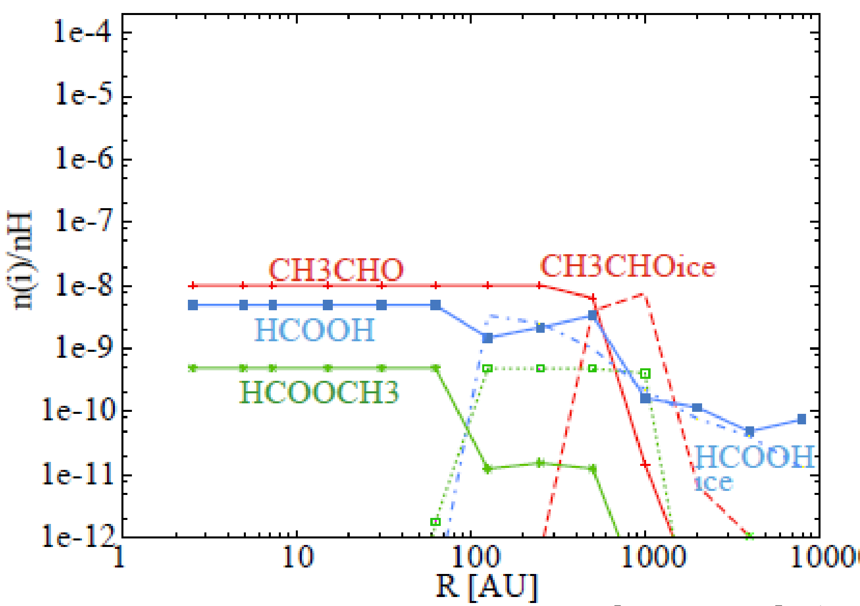

Aikawa et al. (2008)

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-Carbon Chains
Abundant inside CH_4 sublimation radius
(Warm Carbon Chain Chemistry: Sakai et al. 2008
see also Hassel & Herbst 2008)

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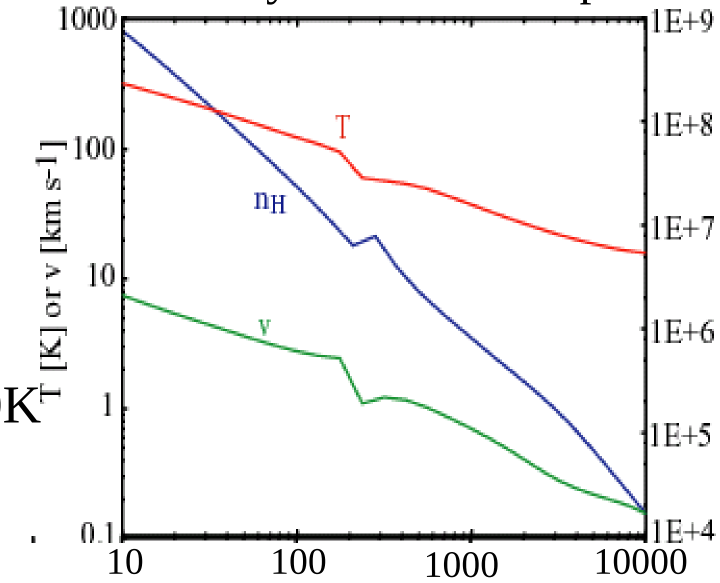
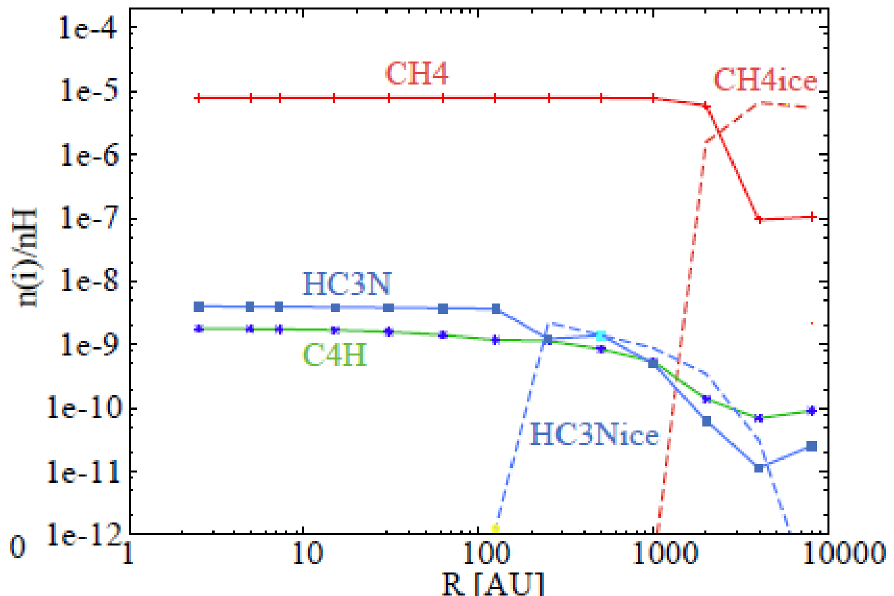




Aikawa et al. (2008)

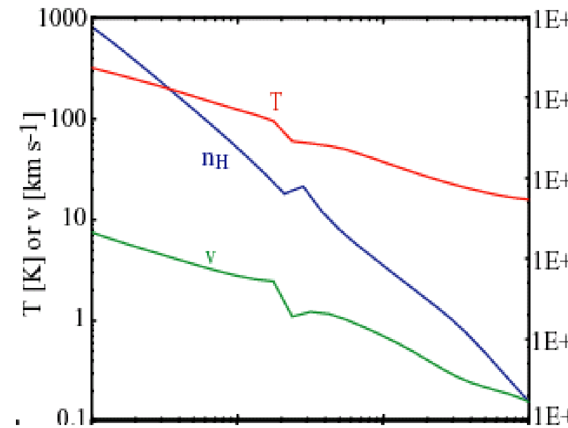
D/H ratio

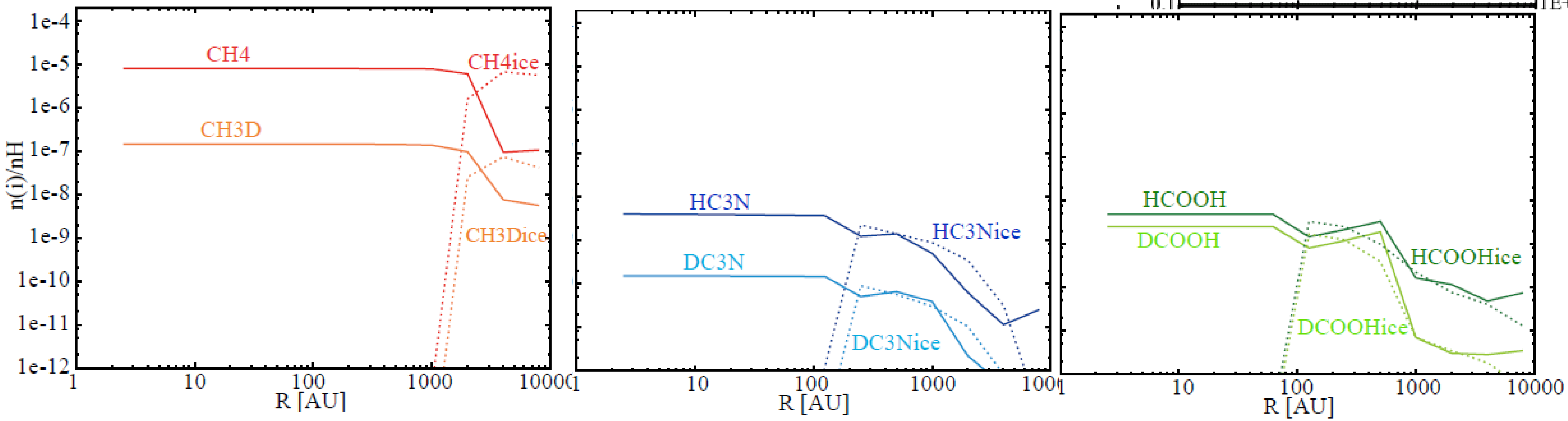
D/H in protostellar core ~ several %

- formation in low temperature era … neutral species survive > 10^4yr
- inherit high D/H of ingredients
- very high DCOOH/HCOOH

  $OH + D \rightarrow OD + H + 810K$

  $OD + H_2CO \rightarrow DCOOH + H$





Aikawa et al. in prep

Discussion 1: Hot Corino vs WCCC

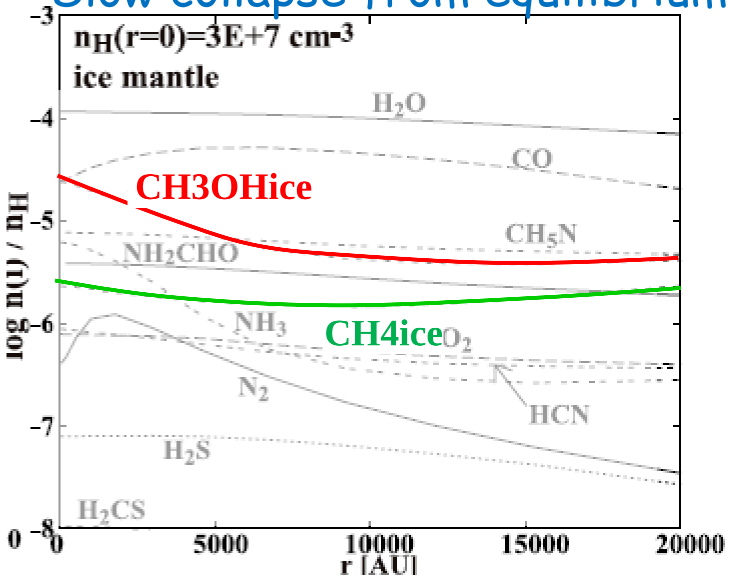
Both Hot Corino & WCCC are in the model

In observations

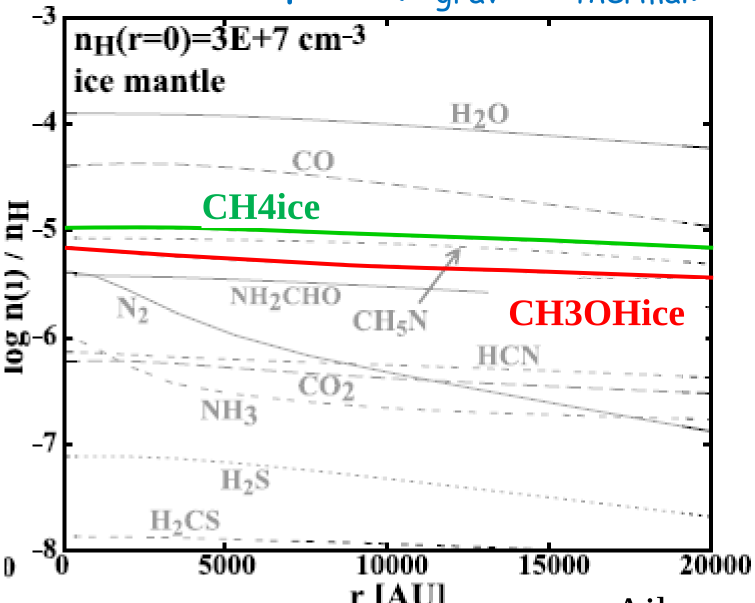
- carbon chains are *not abundant* in hot corinos
- hot corino species are *not abundnt* in WCCC
  - fast collapse → CH_4-rich ice → WCCC
  - slow collapse → CH_3OH-rich ice → Hot Corino

(Sakai et al. 2009)

Slow collapse from equilibrium



Fast collapse ($E_{grav} > E_{thermal}$)



Aikawa et al. (2005)

Discussion 2: abundance of Hot Corino species

Gas-phase molecular abundances in IRAS 16293-2422 and model results

Species	IRAS 16293-2422	model
H_2CO	1.0(-7)[b] , 1.1(-7)[c]	6 (-6)
CH_3OH	1.0(-7)[d] , 9.4(-8)[c]	7 (-7)
$HCOOCH_3$	2.5-5.5(-7)[e] , 2.6-4.3(-9)[f] , > 1.2(-8)[g]	5 (-10)
HCOOH	6.2(-8)[e] , 2.5(-9)[g]	5 (-9)
CH_3OCH_3	2.4(-7)[e] , 7.6(-8)[c]	2 (-11)
CH_3CN	1.0(-8)[e] , 7.5(-9)[h]	5 (-9)

Our model do not produce enough hot corino species?

\# improve grain-surface chemistry model

stochastic model, layered ice mantle…Vasyunin's talk

\# improve physical model

Star Formation is NOT spherical

- Spherical symmetry and free-fall are good approximation in envelope

- Flatted "disk" appears inside the centrifugal radius

$$r_{\rm cent} = \frac{(r^2\omega)^2_{\rm init}}{GM}$$

$r \sim 0.1$pc, $\omega \sim 10^{-14}$ s^{-1} → $r_{\rm cent} \sim 100$AU

- Fluid parcels could stay in the "disk" for $t > t_{\text{free-fall}}$

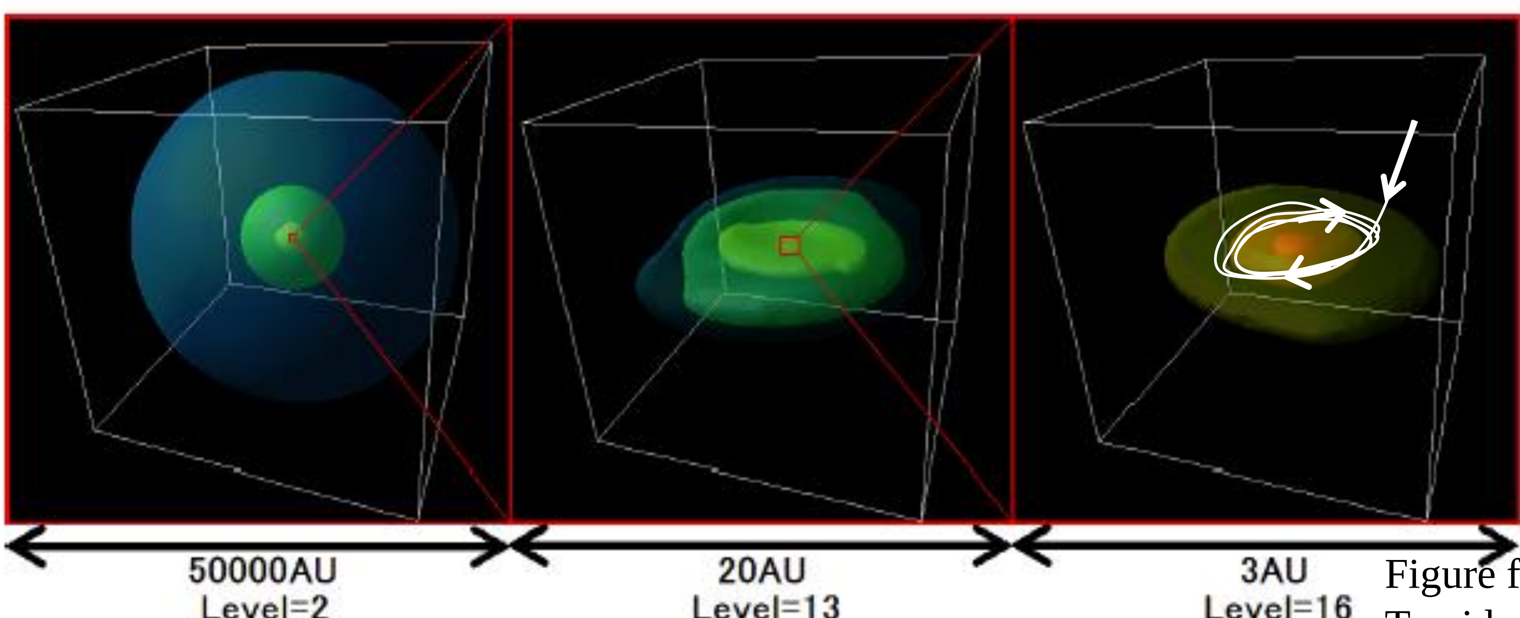
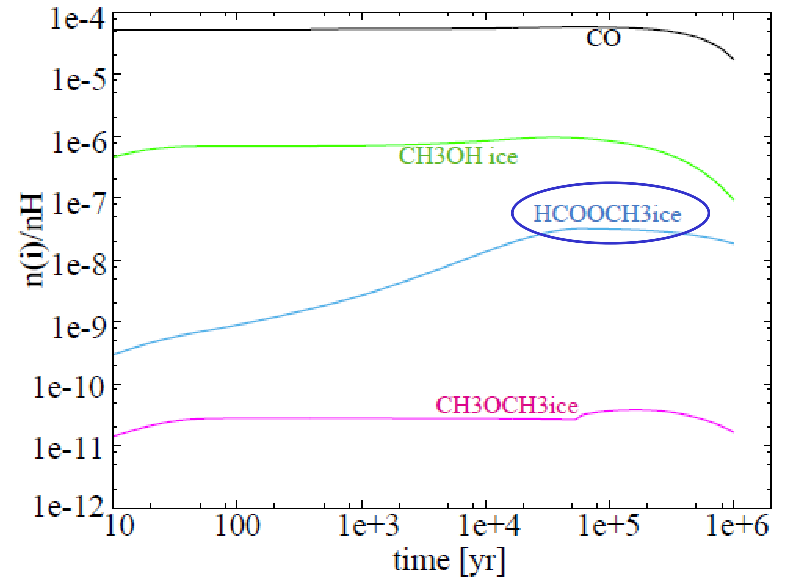


Figure from Tomida (Master thesis)

In the "disk"…

T=40K (n_H=4x10^8cm^{-3})

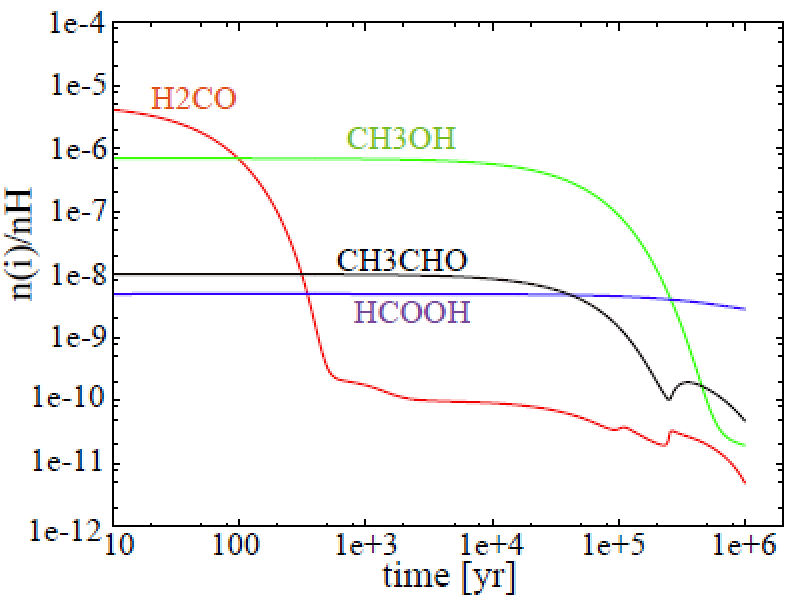
- **HCOOCH$_3$** are formed on the grain surface

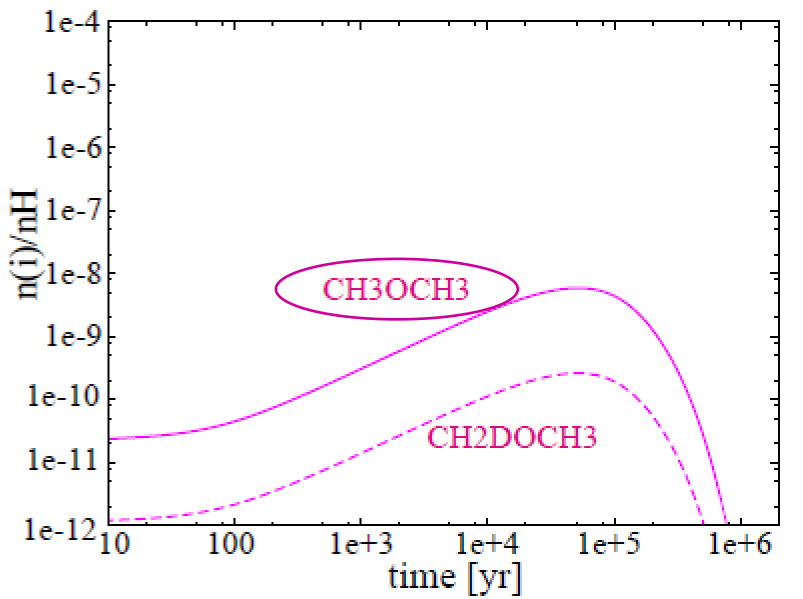


T=260K (n_H=4x10^8cm^{-3})

- CH$_3$OH and CH$_3$CHO decrease in ~10^5yr
  … time scale vary among species

- **CH$_3$OCH$_3$** are formed… high D/H ratio





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improve grain-surface chemistry model

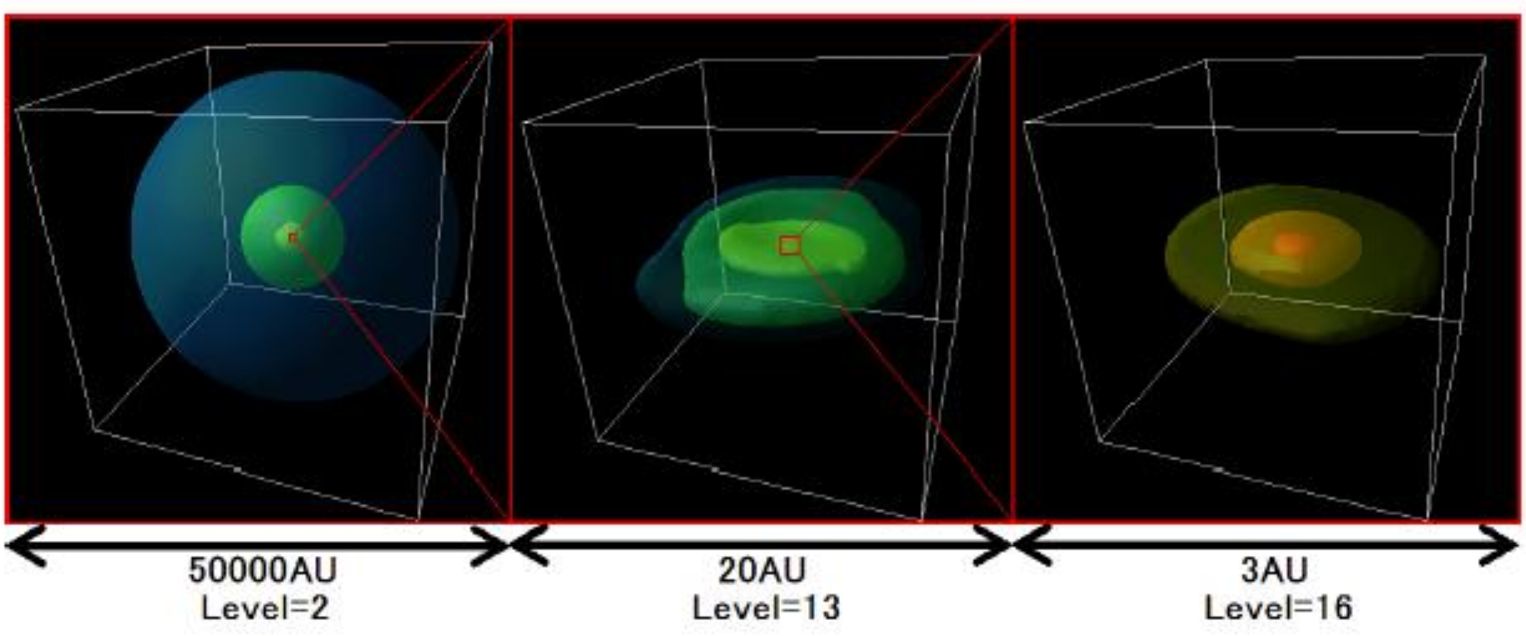
stochastic model, layered ice mantle…Vasyunin's talk

improve physical model

Chemistry in the 3-D Model of the First Core Formation

Furuya et al. poster

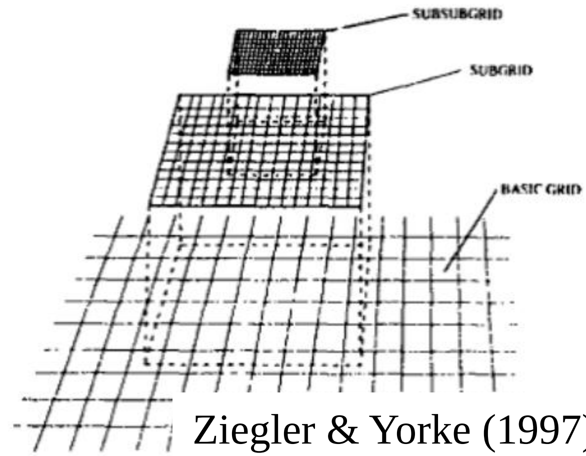
First Core
- First hydrostatic core of H_2
- Fragment to form binary?
- Outflow
- Evolves to the protoplanetary disk (Machida & Matsumoto 2010)



Model

Hydrodynamic model

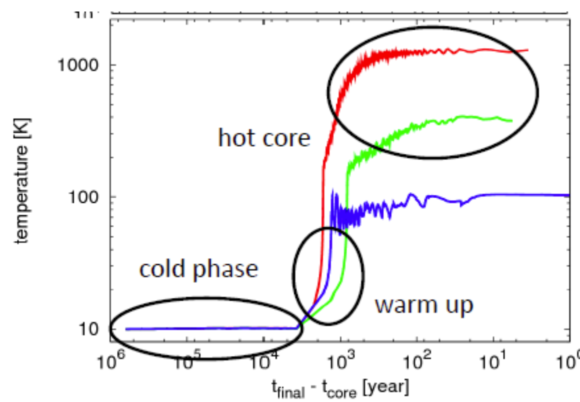
- 3D nested grid: 32^3 x 16 level
  (Matsumoto & Hanawa 2003; Tomida et al 2011)
- from ~0.1 pc to 0.08 AU
- flow particle trajectories at each time step
  → temporal variation of physical conditions in the particles

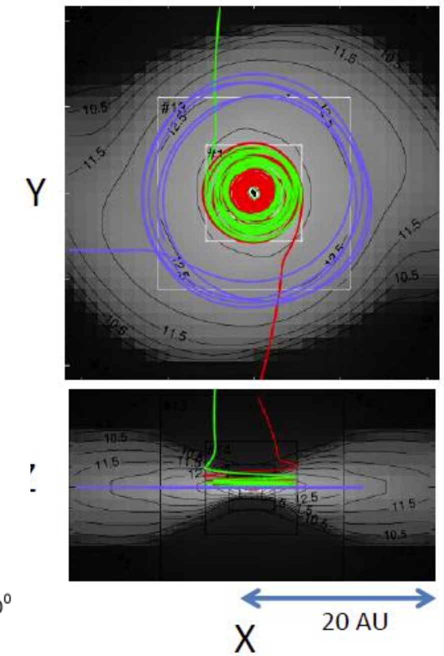


Ziegler & Yorke (1997)

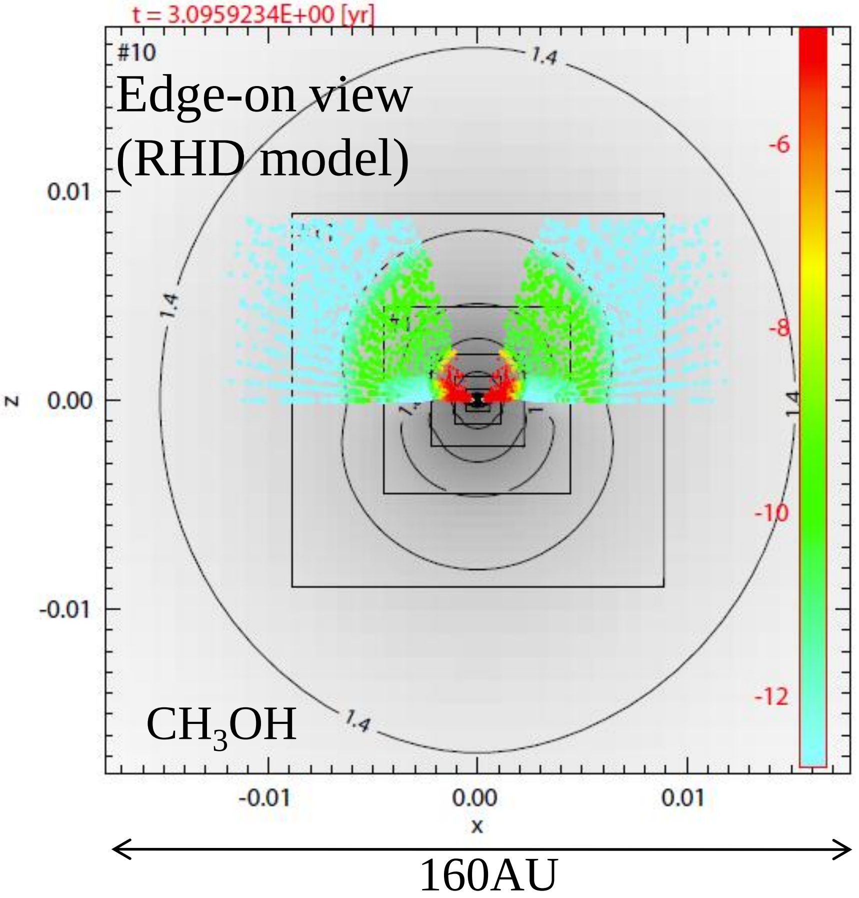
Chemical model

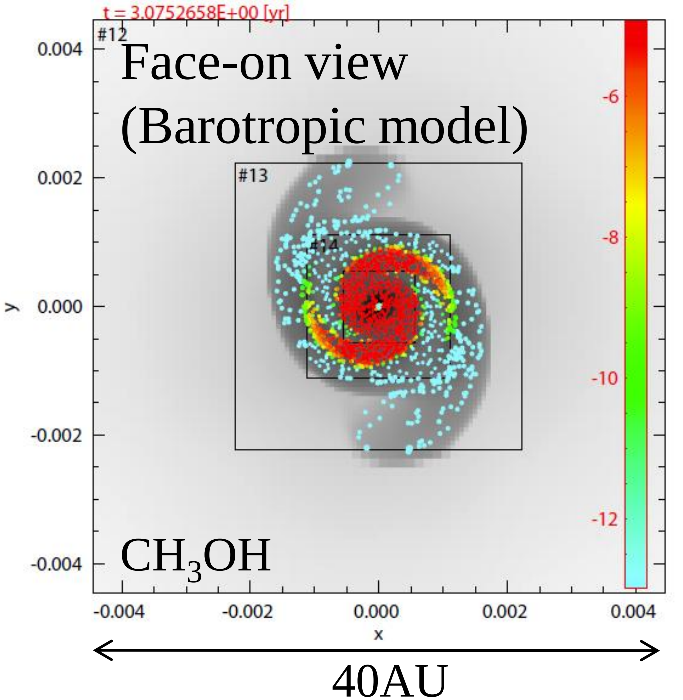
- T< 100 K: Garrod & Herbst (2006)
- T > 100K: Harada et al. (2010)
- collisional dissociations, 3-body reactions: Willacy et al. (1998) +α
- grain charge balance: Umebayashi (1980)





Result





- Abundance is determined mainly by sublimation & local temperature
  - ice region
  - sublimated region
  - central region (R<1AU) … destruction of CH_3OH

Summary

10K | several 10 K | >100K

freeze-out & hydrogenation

Hot corino species on grains

Warm Carbon Chain Chemistry

Gas-phase reactions of sublimates

$t_{\mathrm{collapse}} \sim 10^6$yr

$R_{\mathrm{warm}}/v_{\mathrm{ff}} \sim 10^4$yr

$R_{\mathrm{hot}}/v_{\mathrm{ff}} \sim 10^2$yr

longer in the "disk"

- Some Hot corino species are more abundant in the "disk" ?
  → need spatial resolution

-high D/H ratios ... originates in cold phase
  → high D/H does not necessarily mean low-T formation of the molecule itself

- Chemistry in 3D model of the first core
  abundances mostly determined by sublimation & local temperature
  ← due to the mass accretion & short lifetime of the first core

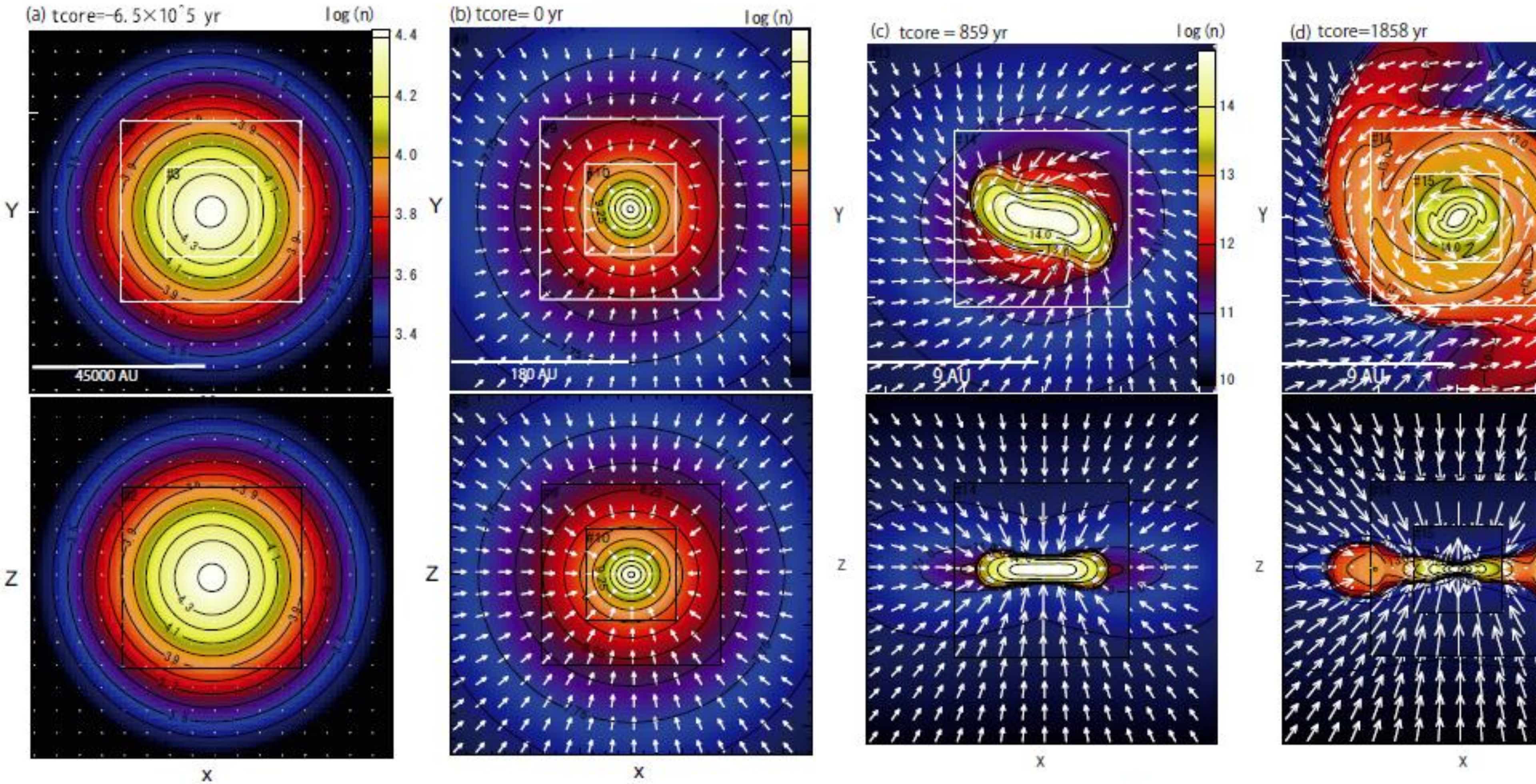


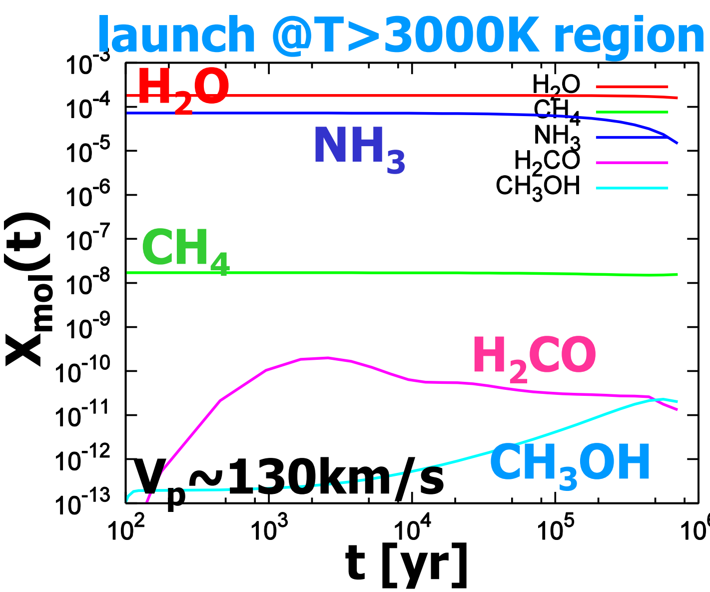
Figure.3.2 continue.

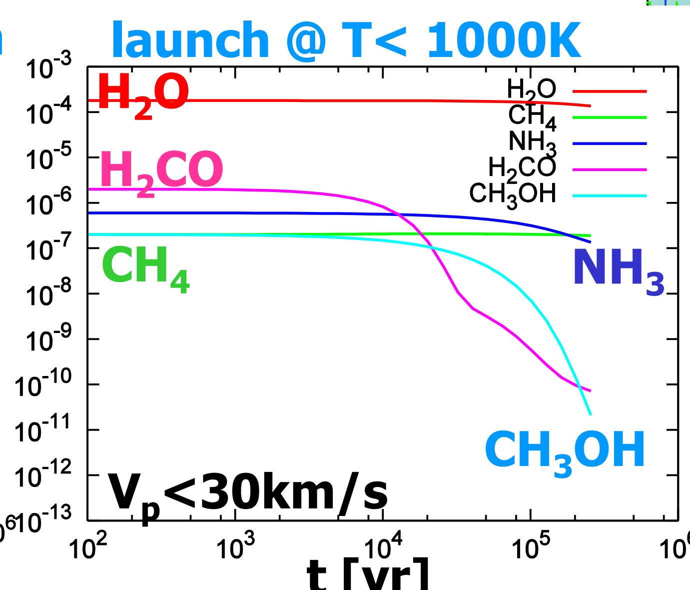
with ALMA's high spatial resolution

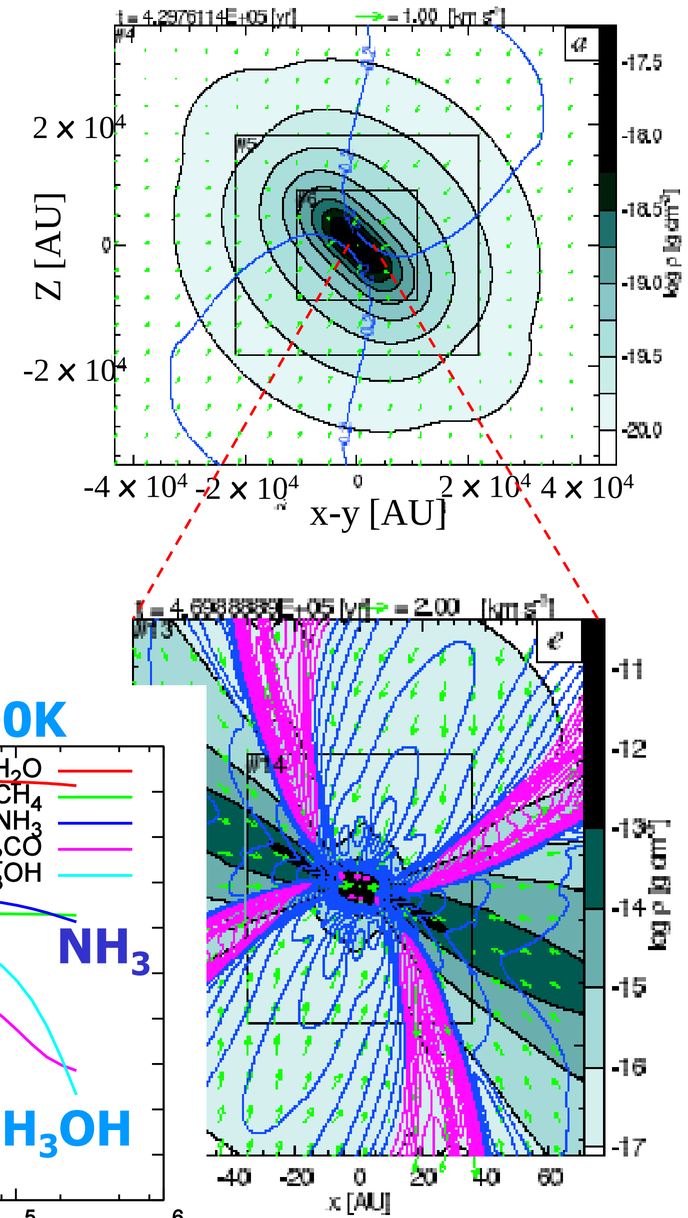
- Derive molecular abundance without beam dilution

- Spatial distribution
  → formation mechanism: gas-phase or grain surface ?
    - Outflow : Nomura (Poster J3)

    - forming disk
      sublimation of H_2O ice by accretion shock
      >90% at r < 30AU → re-condense
      (Lunine et al 1991; Visser et al 2009)



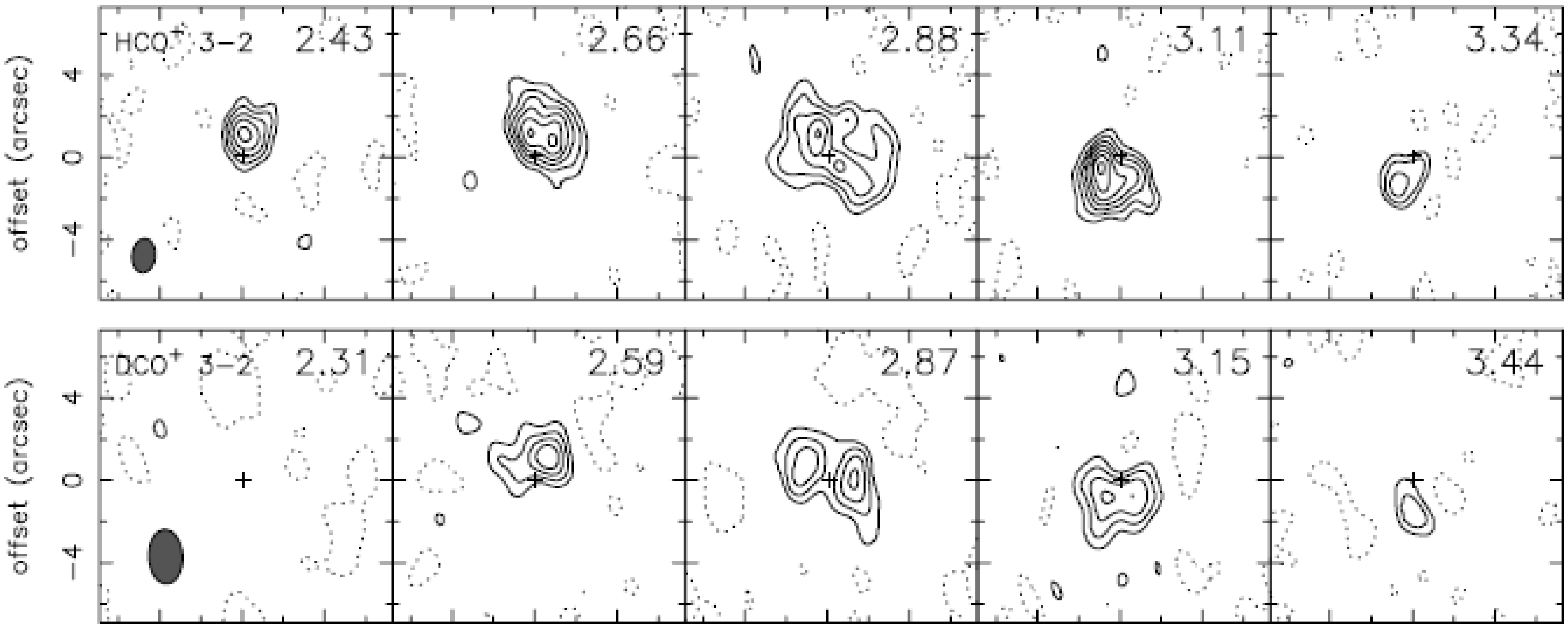




umoto & Tomisaka (2004)

DCO$^+$: Deuterium Chemistry

TW Hya   Qi et al. (2008)



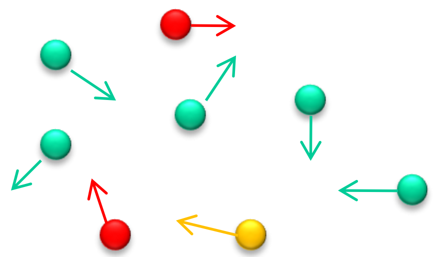
- DCO+/HCO+ ratio increases outwards
  0.01 at < 30 AU to 0.1at > 70AU

- ionization degree of HCO+ layer: [e] ~ 10^{-7}

$$\frac{n(\mathrm{DCO}^+)}{n(\mathrm{HCO}^+)} = \frac{1}{3}\frac{n(\mathrm{H_2D}^+)}{n(\mathrm{H_3^+})} = \frac{1}{3}\frac{k_1 n(\mathrm{HD})}{k_3 n(\mathrm{CO}) + \beta_5 n(e)}.$$

- Upper limit to H_2D^+: 1.7 x 10^{12}cm^{-2}

Chemical Processes in Cloud Cores



Gas-phase reactions

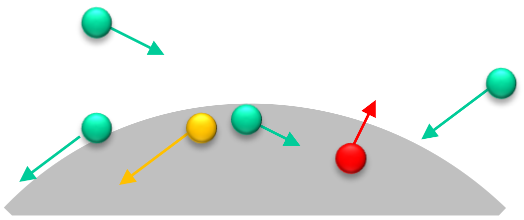
- Cosmic-ray ionization
- Ion-molecule reactions
- Neutral-Neutral reactions
- Photolysis etc…

cf. AB + C → A + BC

Adsorption

Desorption

- thermal
- non-thermal
  - cosmic-ray
  - UV
  - reaction heat



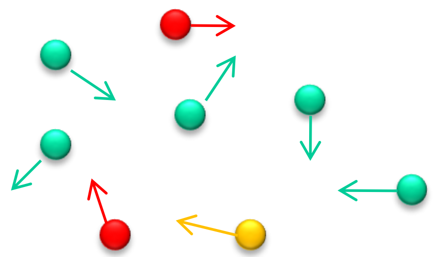
Grain-surface reactions

- Hydrogenation: A +H → AH
- Reaction among heavy-element species

☺ AB + C → ABC

☺ Concentration of heavy-element species

Chemical Processes in Cloud Cores



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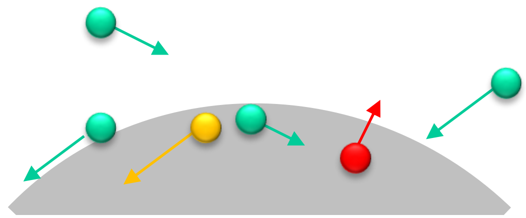

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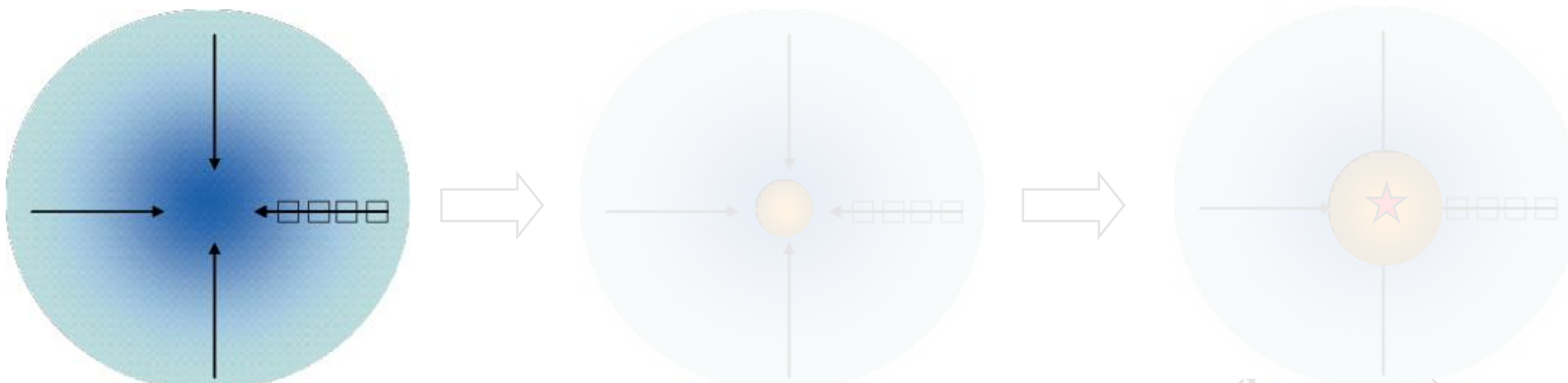
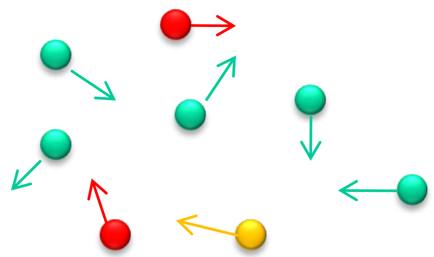


prestellar core

(low-mass) protostellar core

Chemical Processes in Cloud Cores



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Reaction among sublimates

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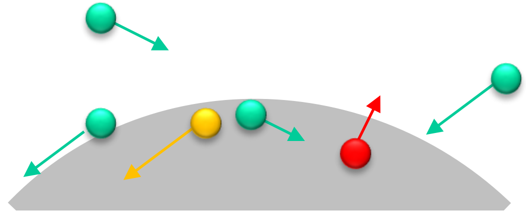

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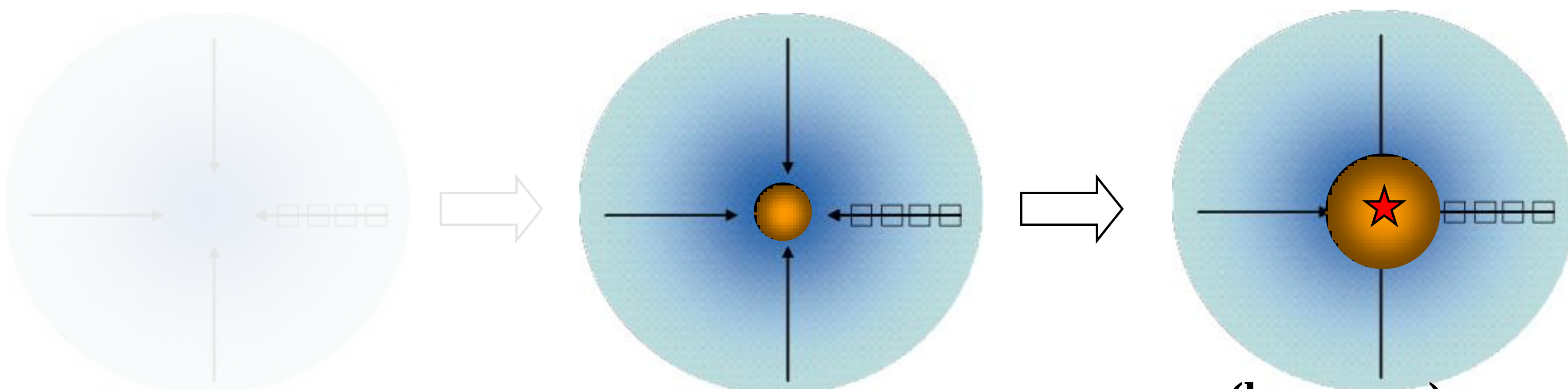
- Hydrogenation
- Reaction among heavy-element species

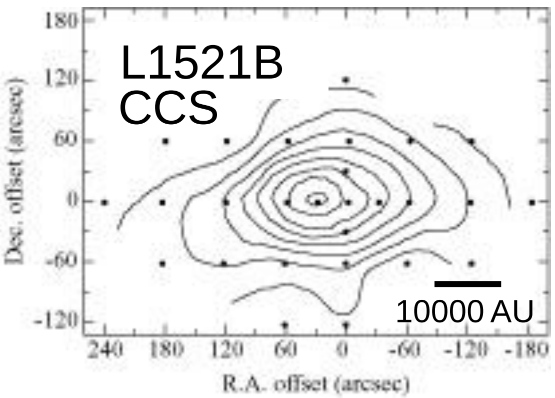


prestellar core

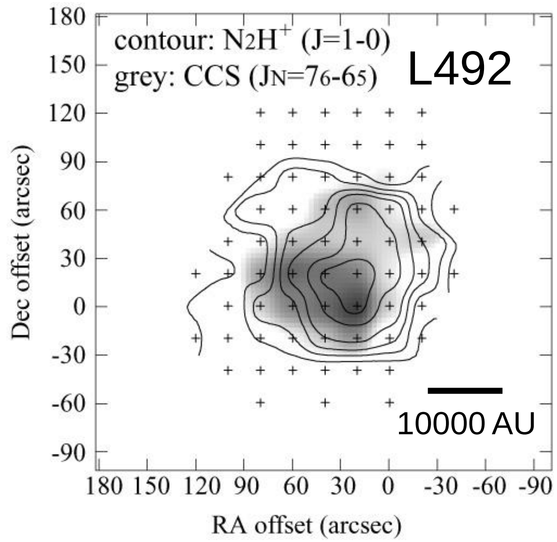
(low-mass) protostellar core

Variation among Cores

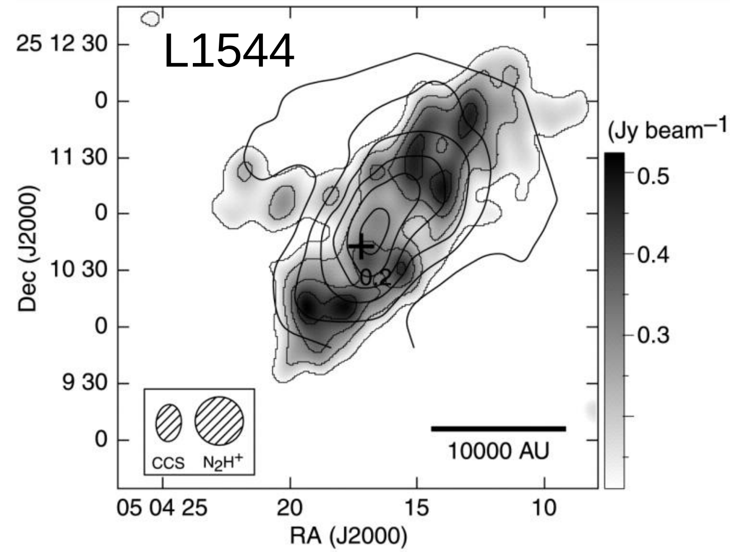
Low D/H ratio
No depletion
No infall



Low D/H ratio
Small depletion?
Infall



High D/H ratio
Significant depletion
Infall



Chemical & Dynamical Evolution?

(fast) Accumulation/collapse speed? (slow)

Thermally Subcritical/Supercritical ?

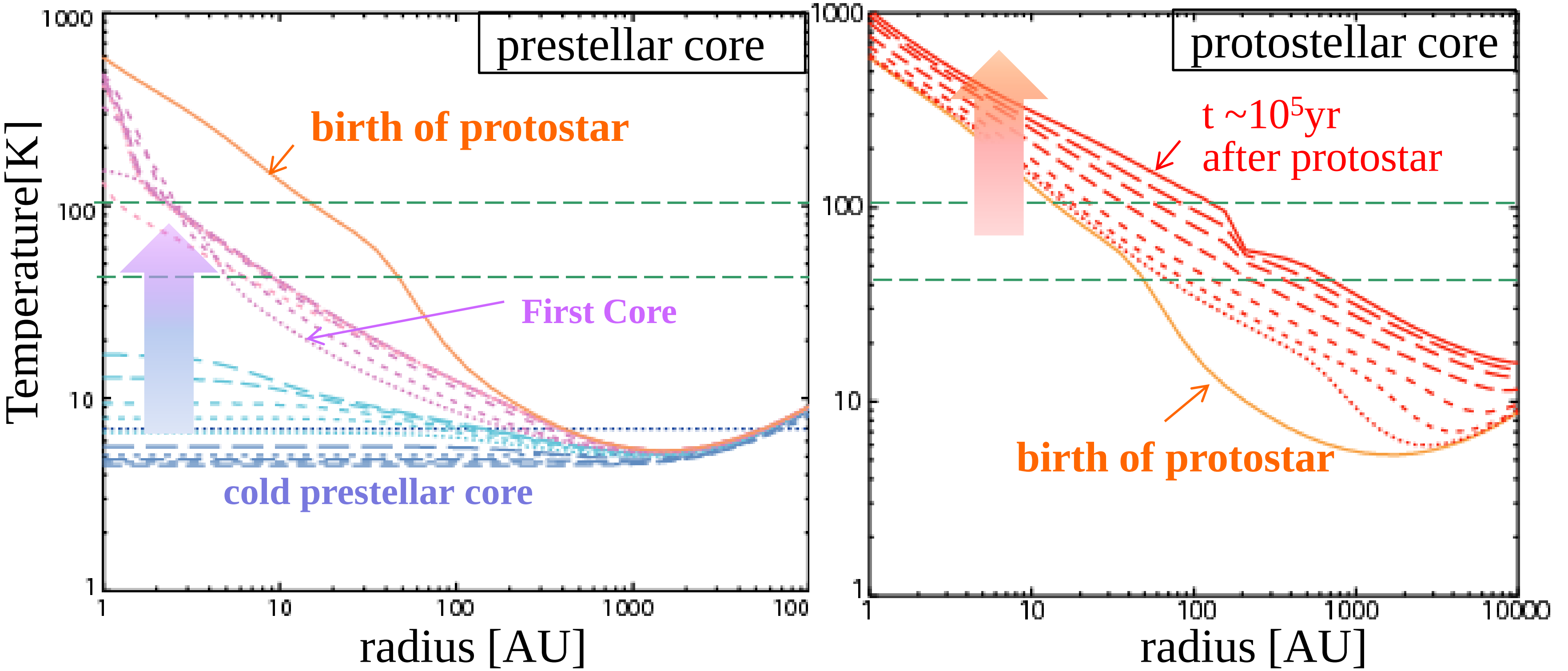
(Aikawa et al. 2001, Tafalla & Santiago 2004 , Hirota & Yamamoto 2006, Keto & Caselli 2008)

From prestellar core to protostellar core

Gravitational collapse → density & temperature increase

T=20K: CO sublimation
T~100K: large organics

Resolution of 10 AU → CO towards the first core
large organics towards new-born protostar



1D radiation-hydrodynamic model (Masunaga & Inutsuka 2000)

D/H

- Chemical Fractionation

C- species … depleted at core center

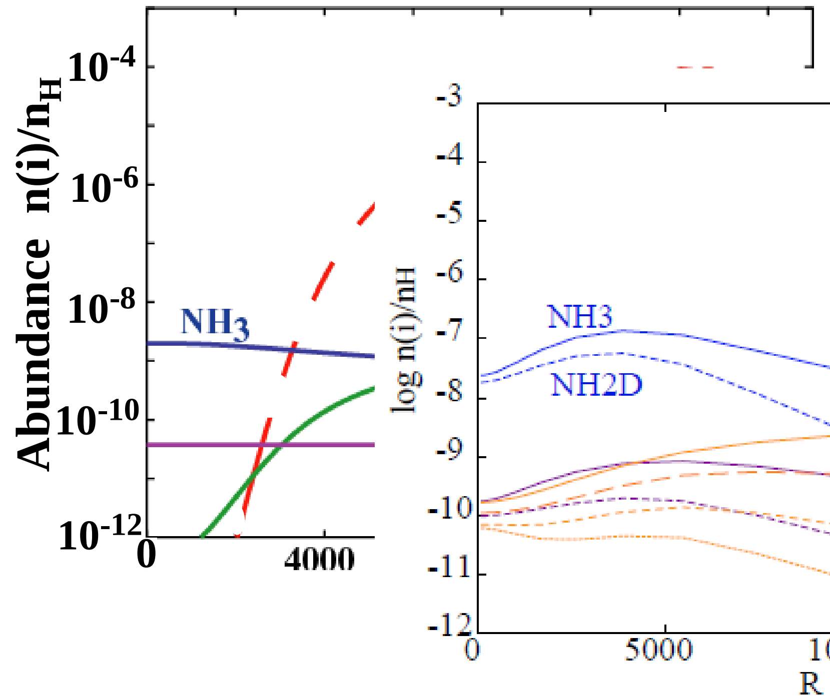
$t_{collapse} \sim 10^6 \, (10^4 \, cm^{-3}/n_H)^{1/2} yr$

$t_{freeze\text{-}out} \sim 10^6 \, (10^4 \, cm^{-3}/n_H) \, yr$

N- species… constant or centrally-peaked

$t_{C \rightarrow CO} \sim$ several 10^5 yr (@$10^4 cm^{-3}$)

$t_{N \rightarrow N2} \sim 10^6$ yr (@$10^4 cm^{-3}$) ← slow !



- Deuterium Enrichment

Exothermic exchange reaction

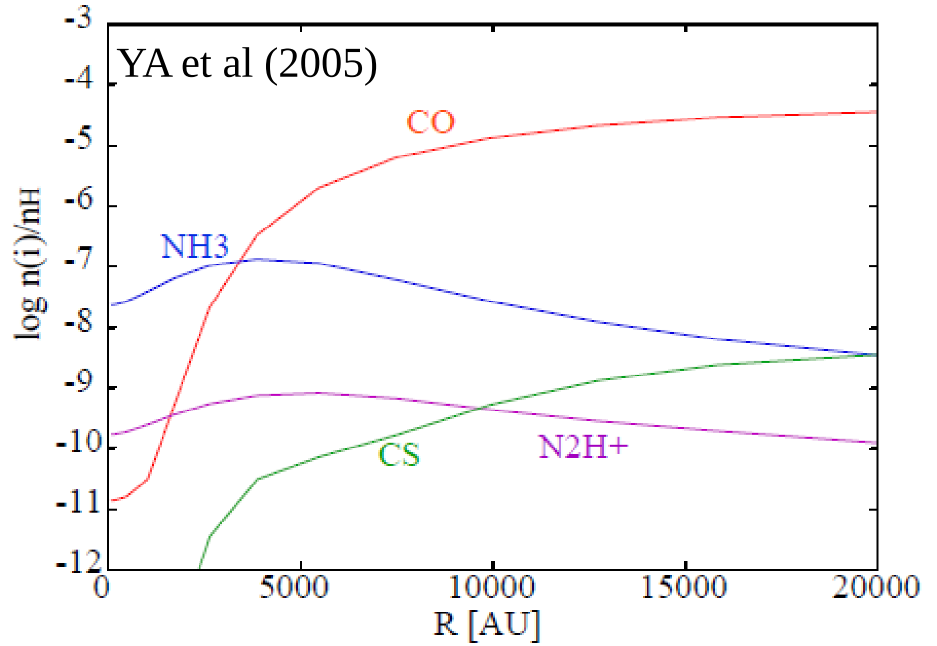
$H_3^+ + HD \rightarrow H_2D^+ + H_2 + \Delta E_1$

Enhancement by CO depletion

$$\frac{n(H_2D^+)}{n(H_3^+)} = \frac{k_1 n(HD)}{k_2 n(e) + k_3 n(CO)}$$

High D/H ratio of H_3^+ and H atoms

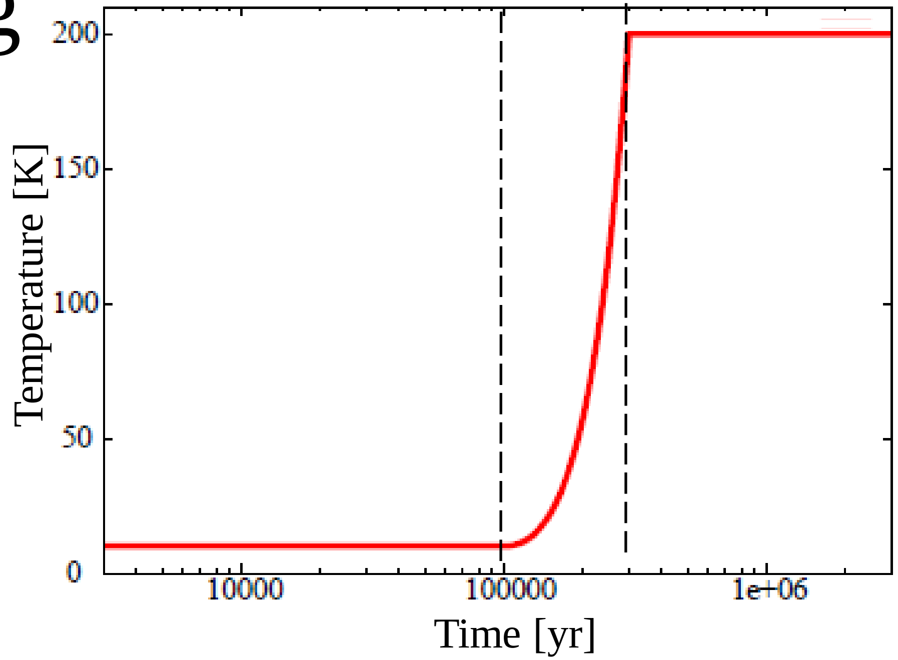
→ D/H enrichment of other species

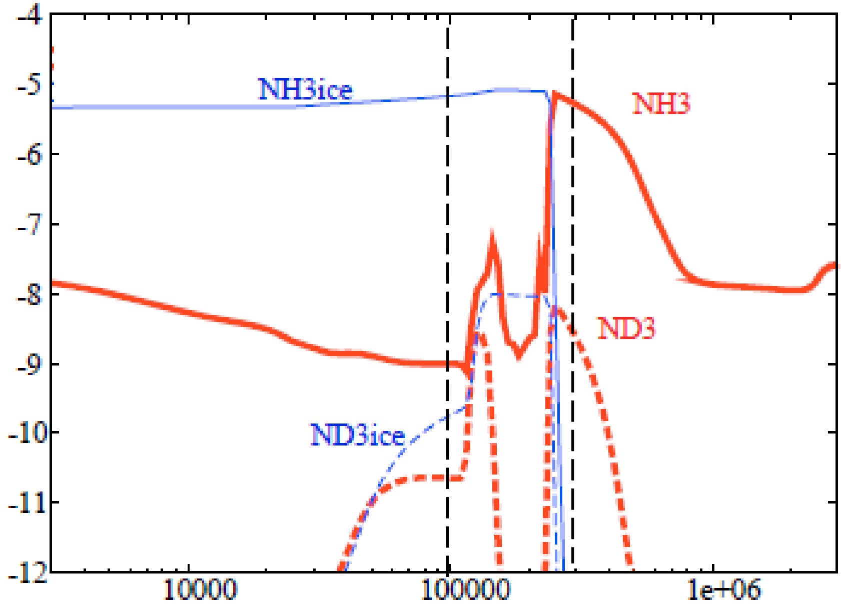


D/H ratios upon heating

- H_2D^+ decreases rapidly when T > 20K (so do DCO^+ and N_2D^+)

- D/H ratio is "diluted" as ice sublimates (NH_3, CH_4 and carbon chains)





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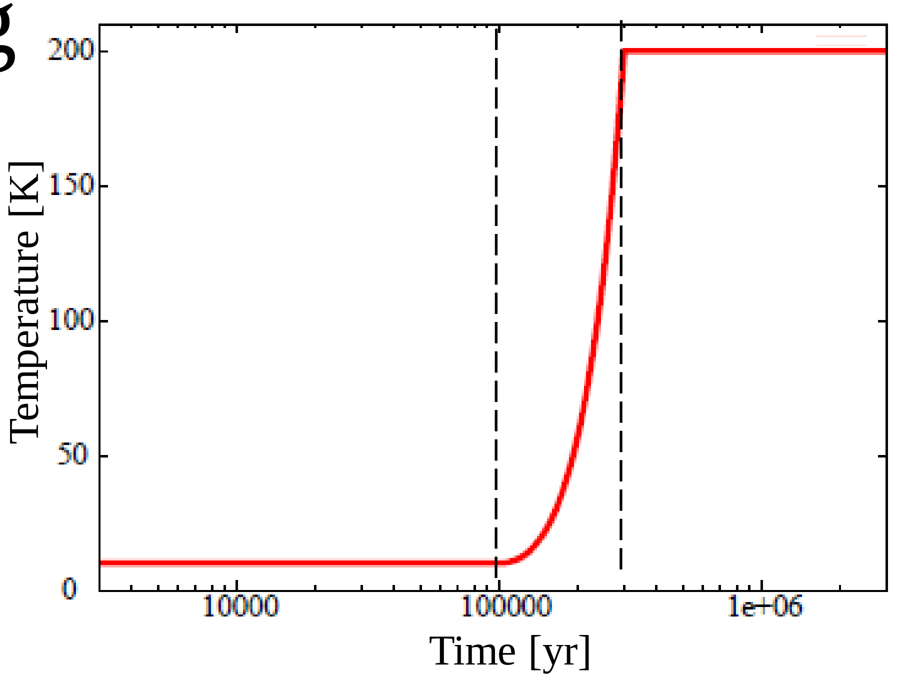

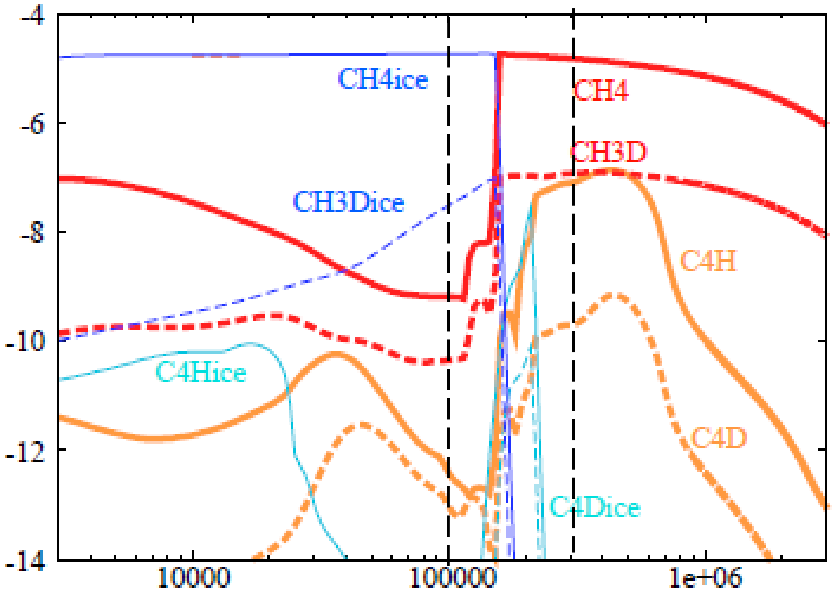

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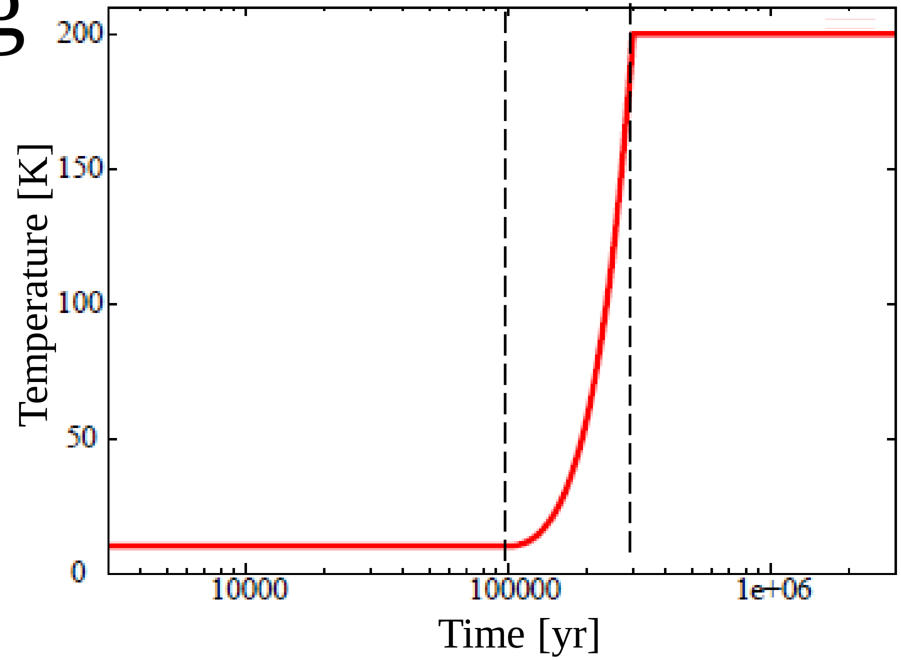
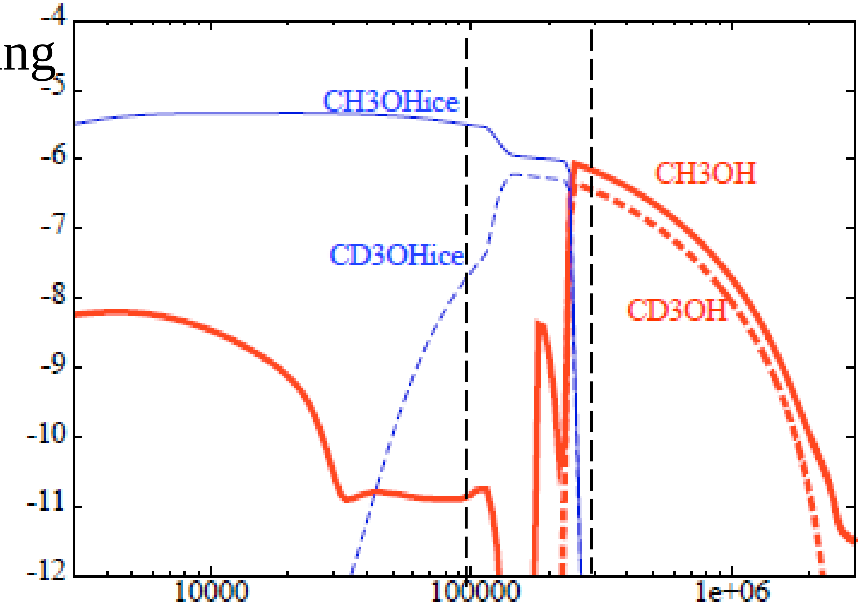
- high D/H ratio in CH_3OH ice due to
  $CH_3OH + D \rightarrow CH_2DOH + H$
  (Nagaoka et al 2005)
  → gaseous D/H ratio of CH_3OH upon heating





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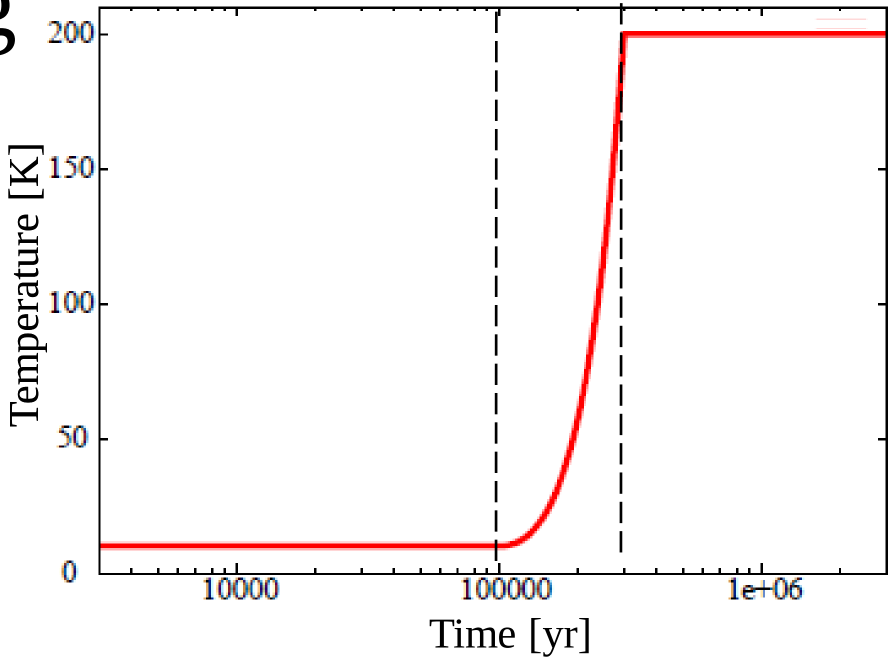
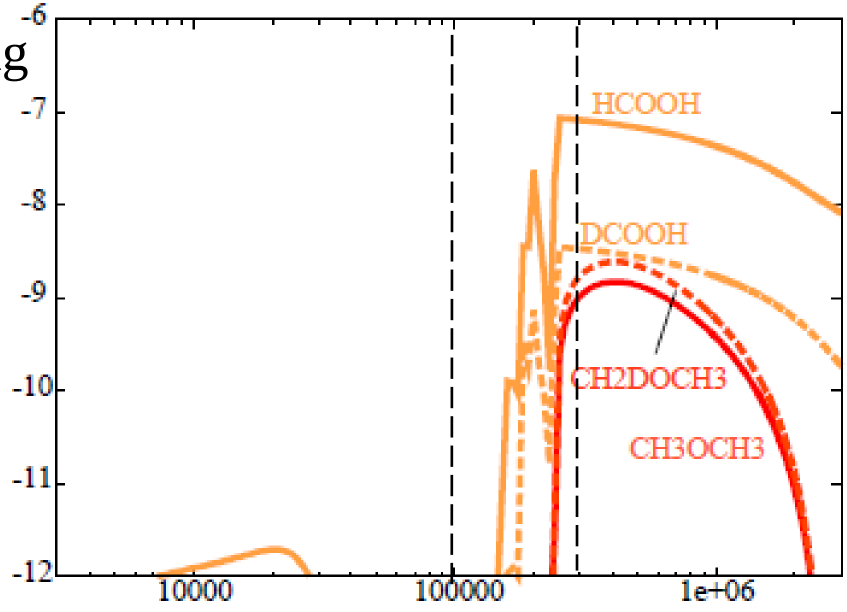
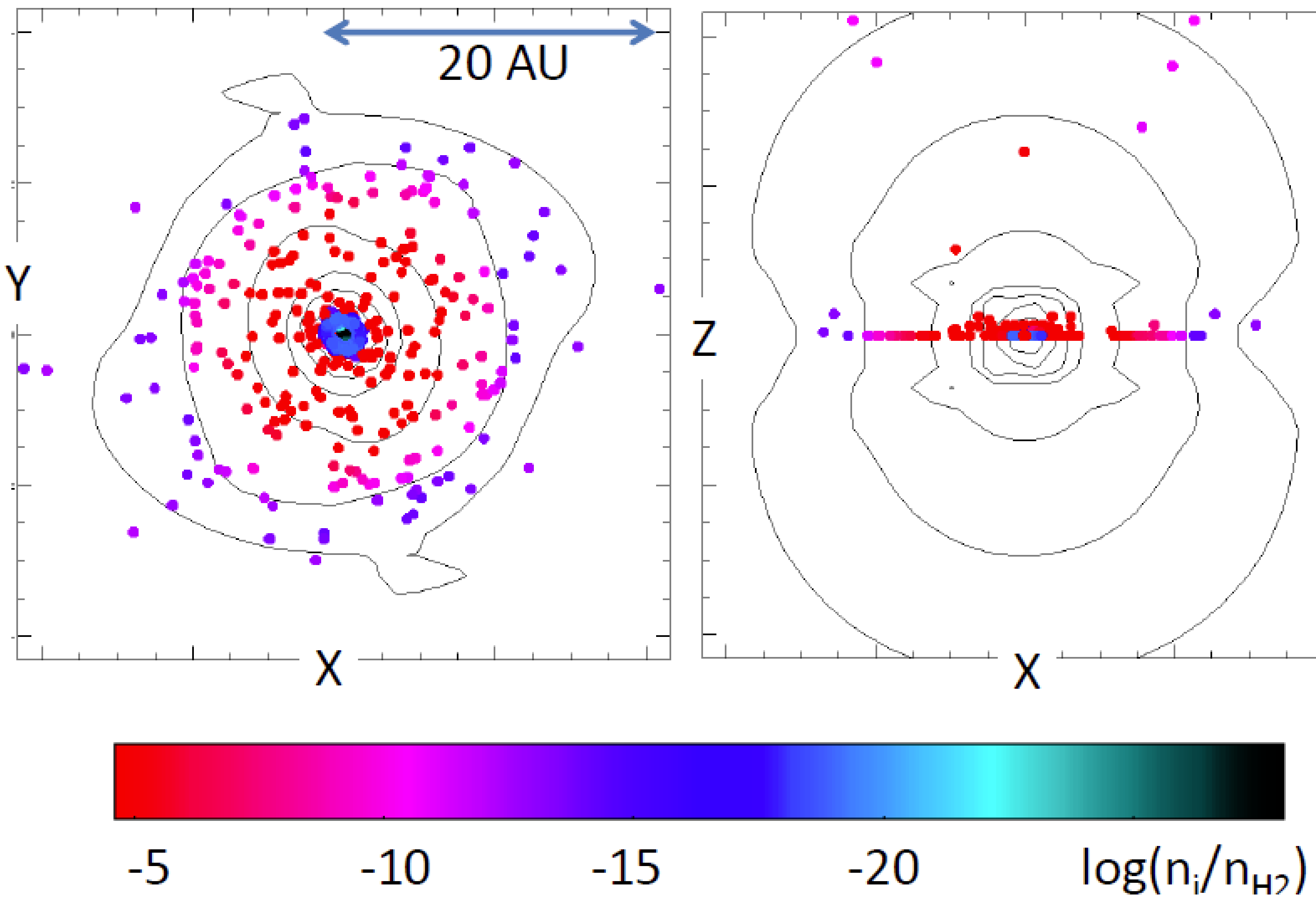
  $\rightarrow$ gaseous D/H ratio of CH_3OH upon heating

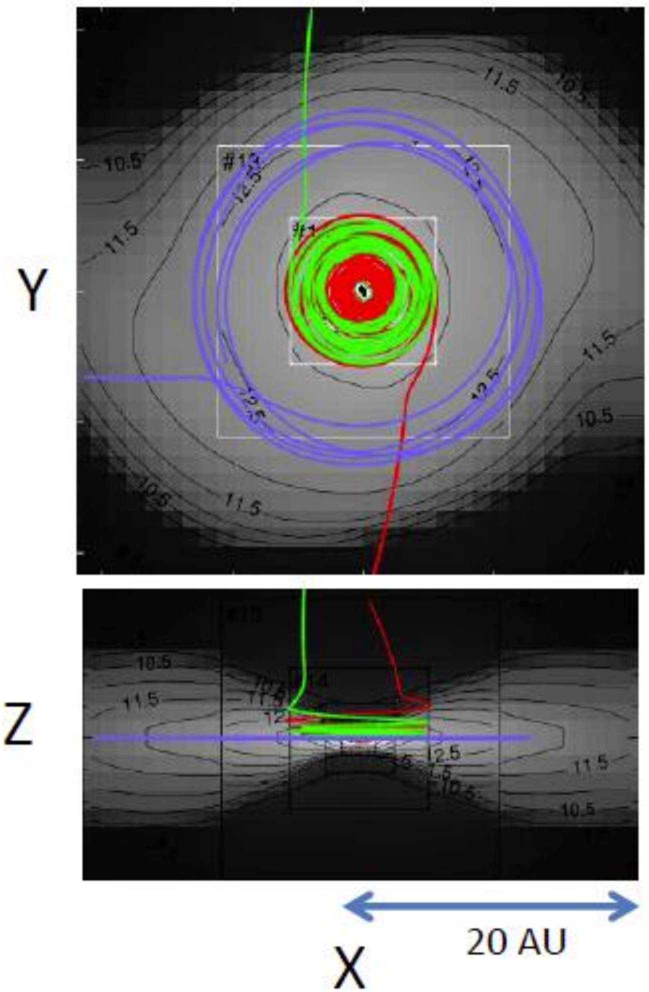
- Organics formed from CH_3OH carry high D/H ratio



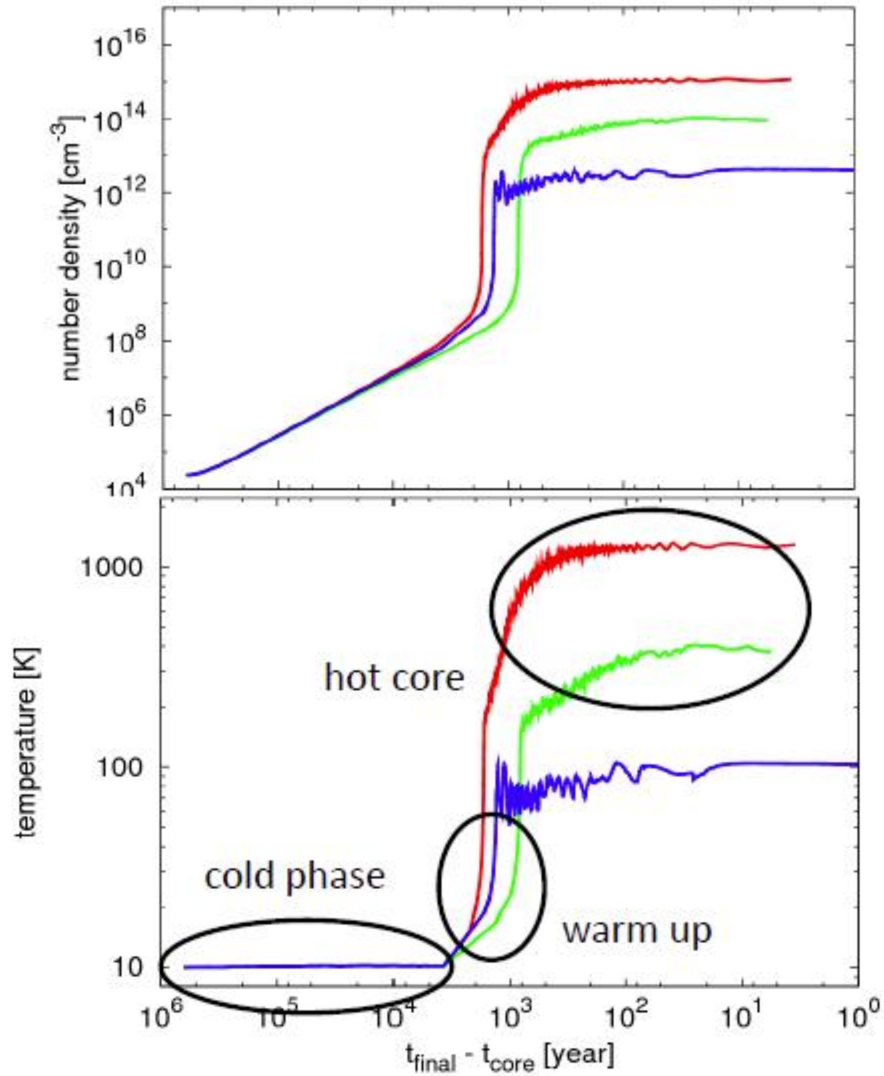


組成の3次元分布 (CH_3OH)





Y
Z
X
20 AU
10.5
11.5
12.5



number density [cm^{-3}]
10^{16}
10^{14}
10^{12}
10^{10}
10^{8}
10^{6}
10^{4}
temperature [K]
1000
100
10
hot core
cold phase
warm up
10^{6} 10^{5} 10^{4} 10^{3} 10^{2} 10^{1} 10^{0}
t_{final} - t_{core} [year]

D/H ratio

Deuterium Enrichment at low T

- Exothermic exchange reaction

  $H_3^+ + HD \rightarrow H_2D^+ + H_2 + \Delta E_1$

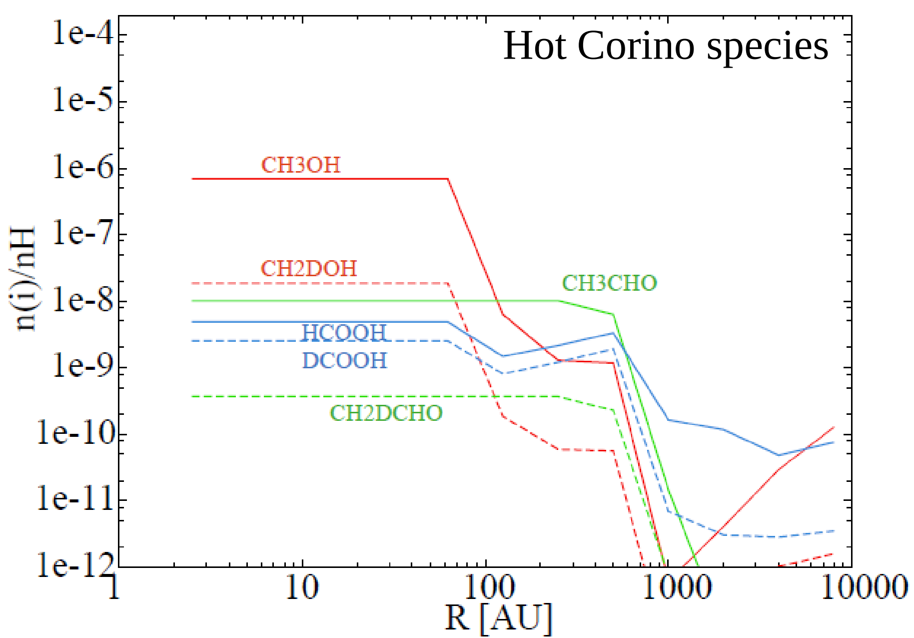
- Enhancement by CO depletion

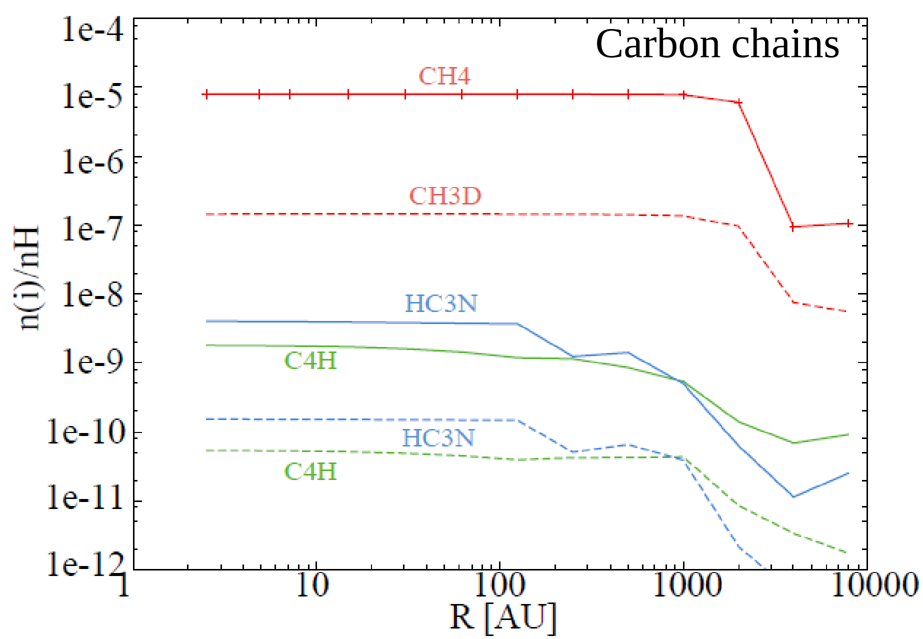
$$\frac{n(H_2D^+)}{n(H_3^+)} = \frac{k_1 n(HD)}{k_2 n(e) + k_3 n(CO)}$$

D/H in protostellar core ~ several %

- formation in low temperature era … neutral species survive > 10^4yr
- inherit high D/H from "raw material" … lesson for comet arguments!!
- very high DCOOH/HCOOH

  $OH + D \rightarrow OD + H$, $OD + H_2CO \rightarrow DCOOH + H$





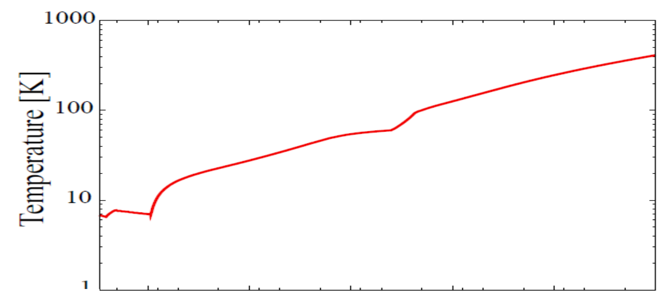
D/H ratio

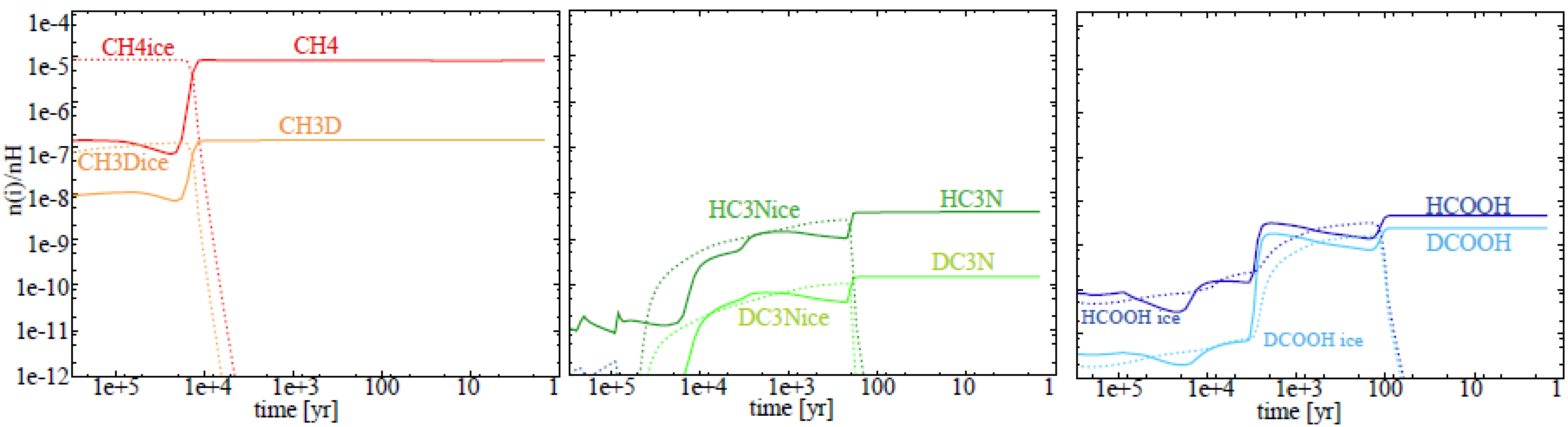
 # D/H in protostellar core ~ several %

- formation in low temperature era … neutral species survive > 10^4yr
- inherit high D/H of ingredients
- very high DCOOH/HCOOH

$OH + D \rightarrow OD + H + 810K$

$OD + H_2CO \rightarrow DCOOH + H$





Aikawa et al. in prep

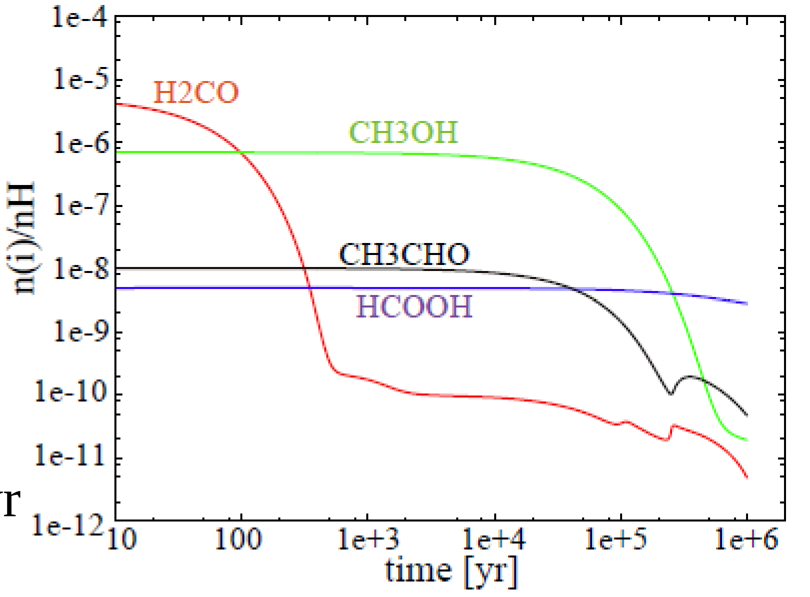
In the "disk"…

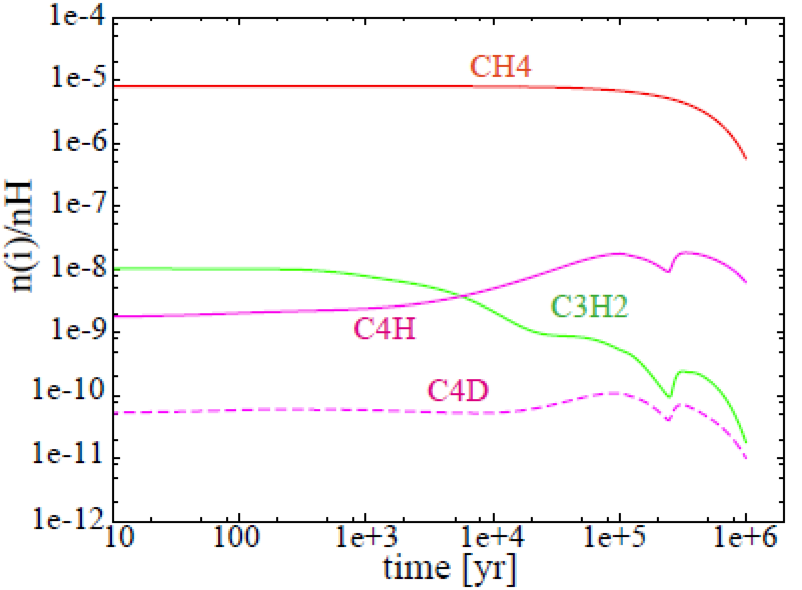
T=260K, n_H=4x10^8cm^{-3}

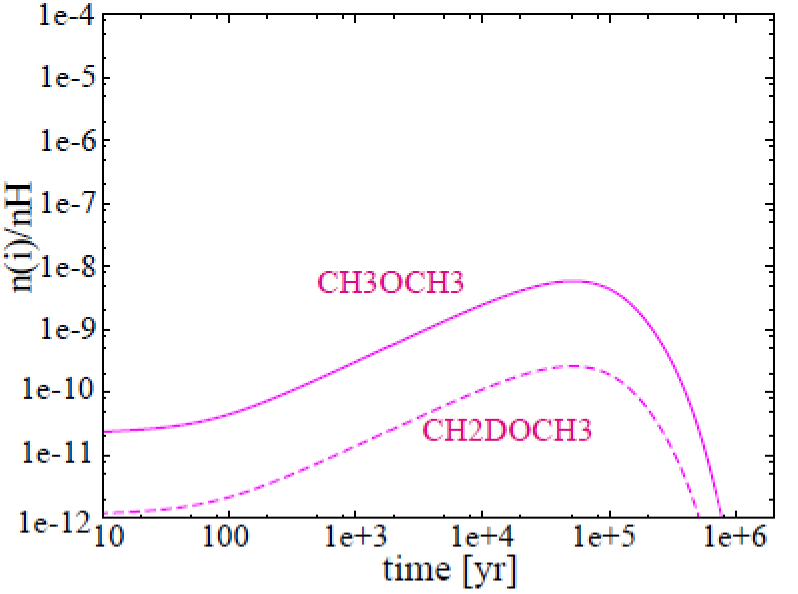
- hot corino species decrease in ~10^5yr
  … time scale vary among species

- CH_3OCH_3 are formed
  … high D/H ratio

-CH_4 and WCCC species survive ~ several 10^5yr
  (see also Hassel & Herbst 2008)







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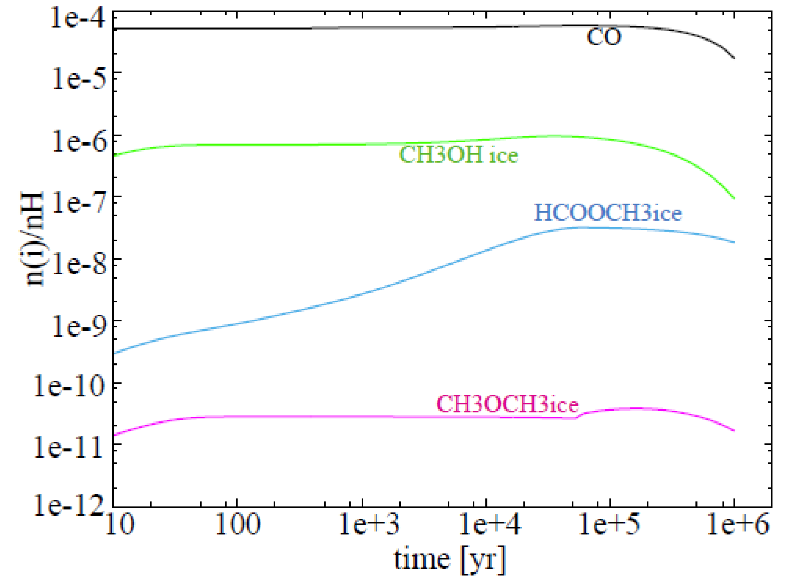

T=40K, n_H=4x10^{8}cm^{-3}

- $HCOOCH_3$ are formed on the grain surface

- Conversion of CO → CO_2
  CH_4 → C_2H_6
  ← sink effect