Ugo Hincelin – University of Virginia – Eric Herbst group

Modeling of Astrochemistry during Star Formation

1/ Deuterium chemistry

2/ Grain surface processes

Interstellar matter is heterogeneous and active

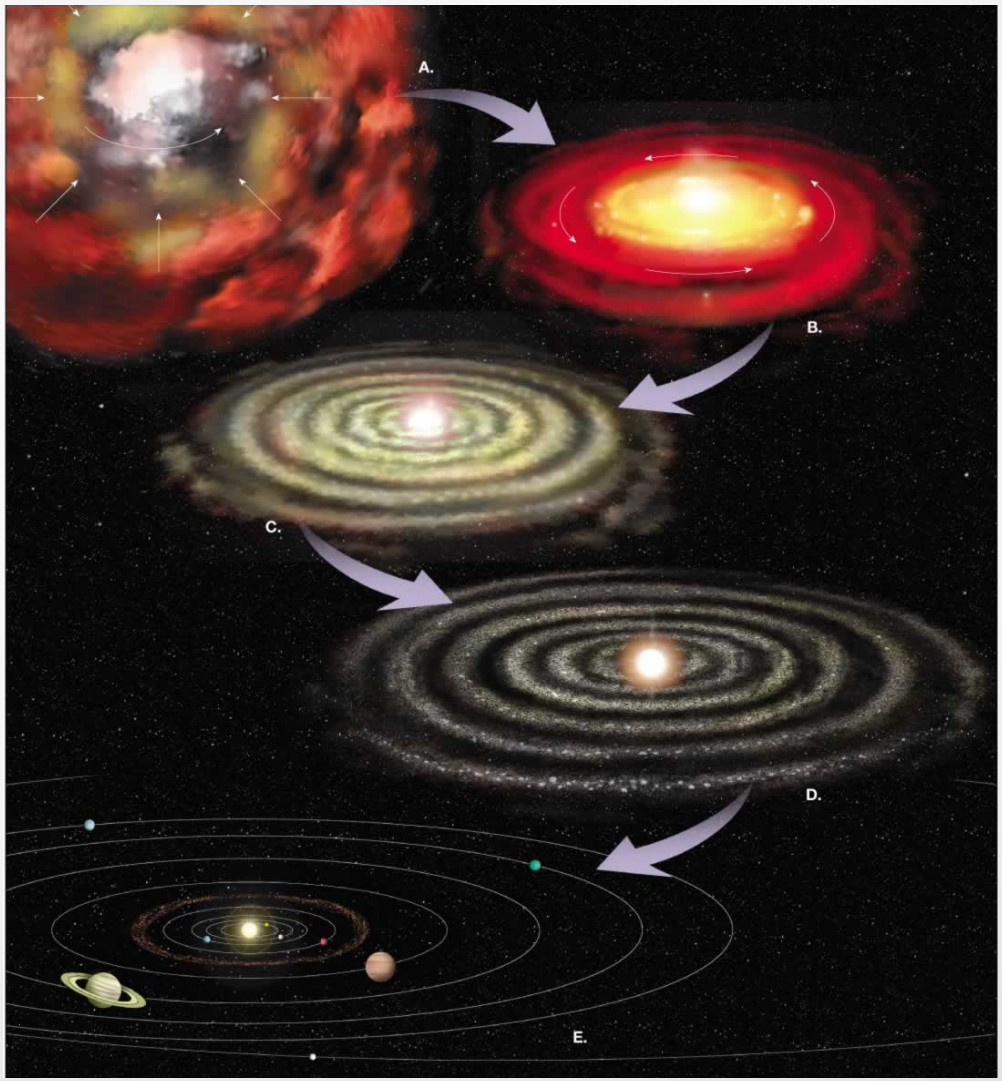
In interstellar cloud

By mass : 1 % grain
99 % gas

(by number :
grain/gas = 10^{-12})

Molecular cloud
~$10^{4\text{-}5}$ cm^{-3}, ~10 K

Prestellar core
~10^{16} cm^{-3}, ~1,000 K (inner core)



Diffuse cloud
~$10^{0\text{-}2}$ cm^{-3}
~50 K

Protostar
~10^{24} cm^{-3}
~10^{5} K
(inner core)

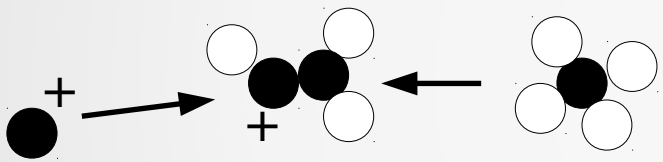
Protoplanetary disk
~$10^{9\text{-}12}$ cm^{-3}
~$10^{1\text{-}3}$ K

Stellar system

Modeling tool : gas grain chemical code

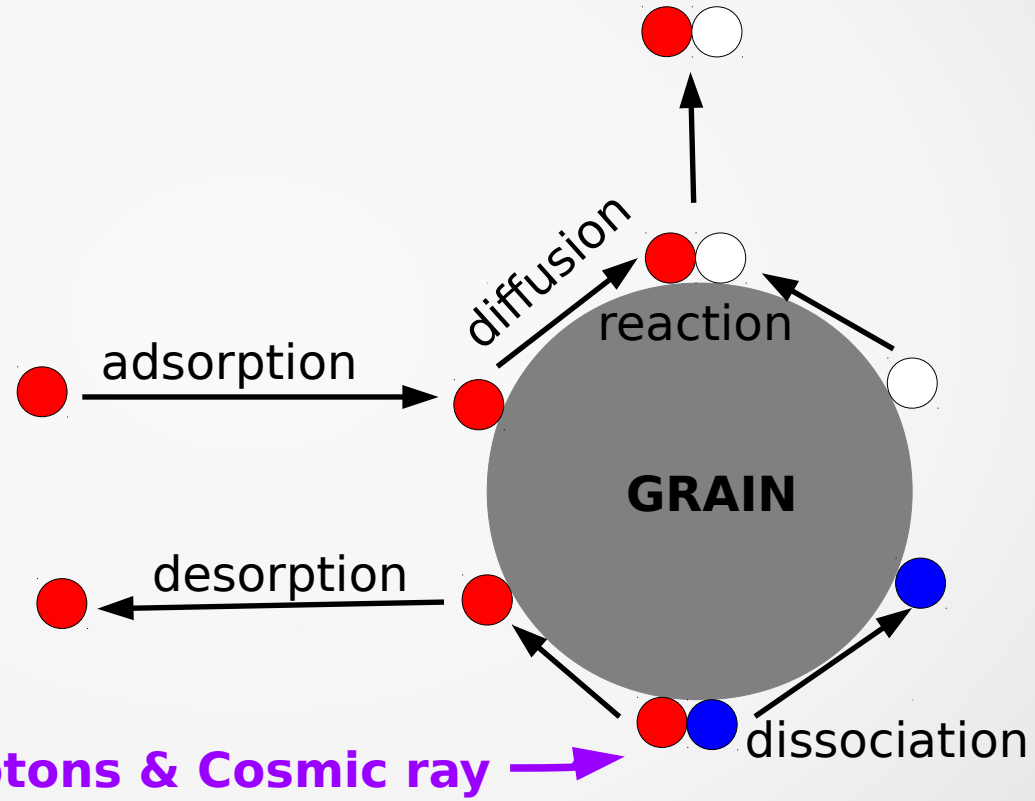
I - GAS PHASE

Main reactions : ion - neutral
neutral - neutral



2 body reactions

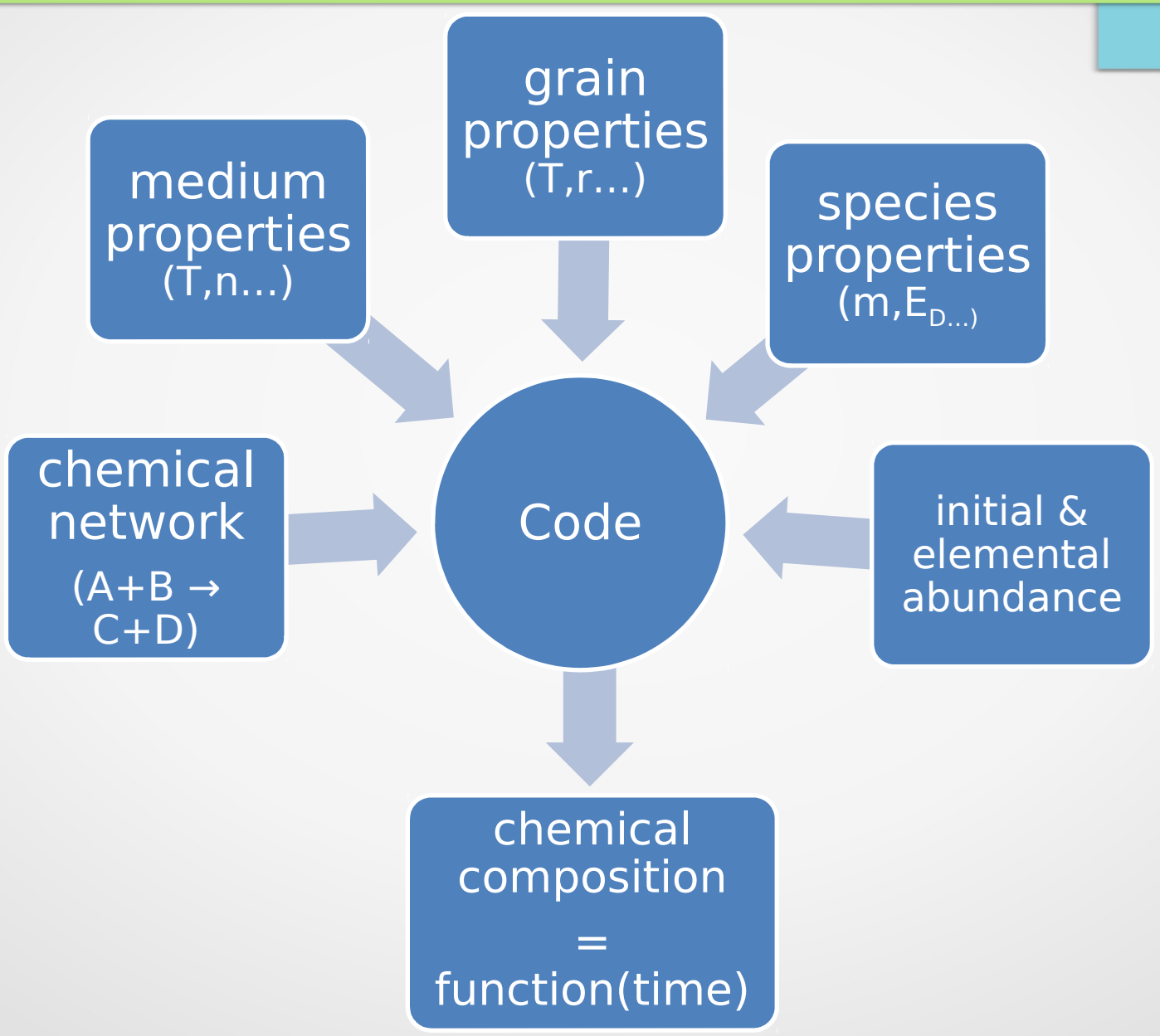
II - GRAIN SURFACE



~500 to ~1000 species
~4000 to ~110,000 reactions

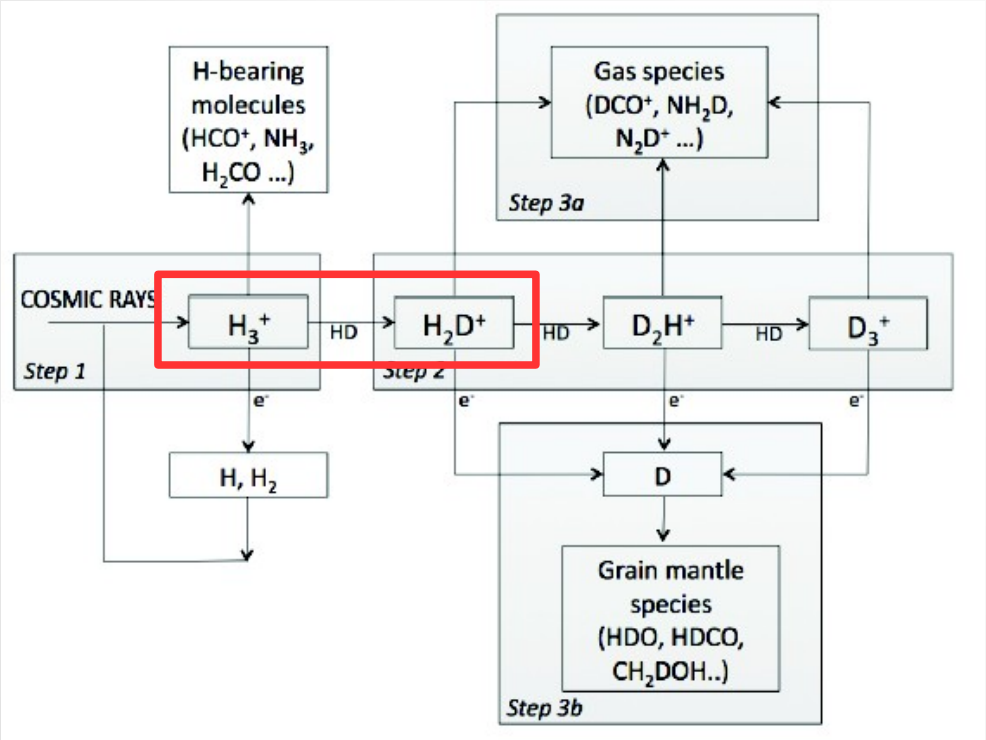
~200 to ~500 species
~2,000 to ~9,000 reactions

Modeling tool : gas grain chemical code



1/ Deuterium chemistry

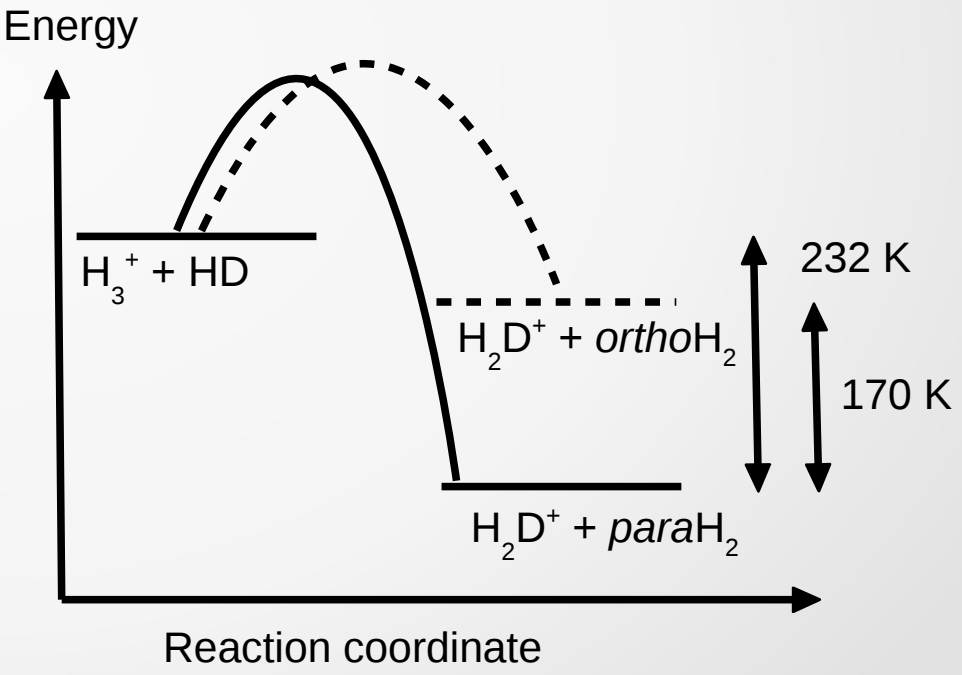
Deuterium fractionation



Ceccarelli et al. 2014 Protostar and Planets VI

Key Reaction & Spin states

$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2$

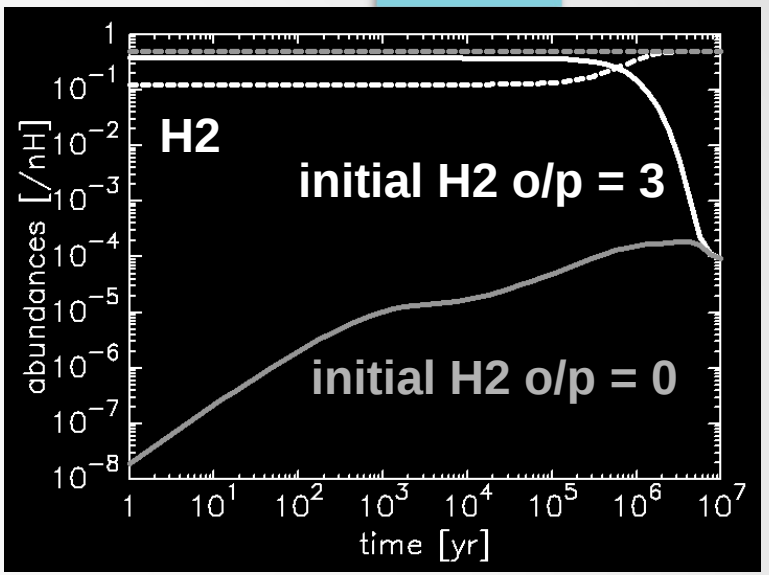


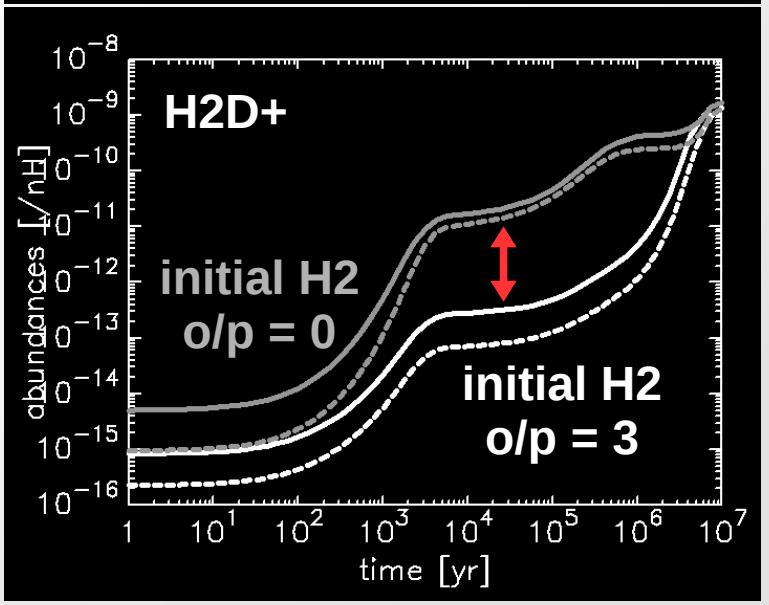
1/ Deuterium chemistry : new network

- Low & high Temperature chemistry
  10 to 800 K
- Low & high Density chemistry
  10^4 to 10^{12} cm^{-3}
- Up to triply deuterated species
- Ortho, para, and meta spin states of
  H2, D2, H3+, H2D+, D2H+, and D3+

~1,600 species linked by ~120,000 reactions

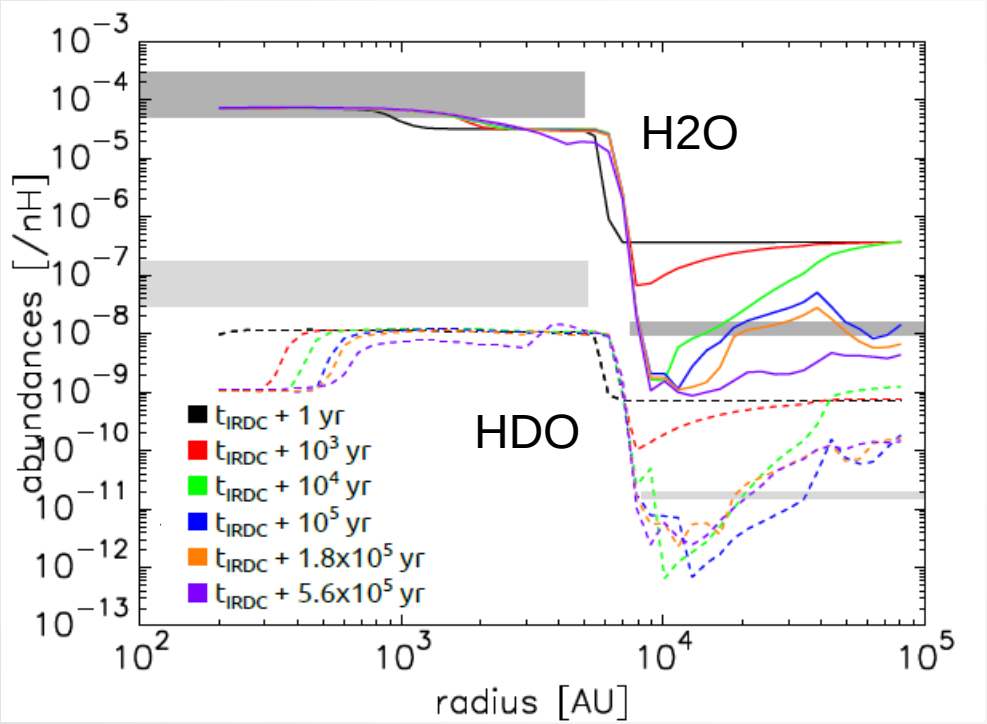
spin state effects : abundances can be reduced by several orders of magnitude (see ↕)



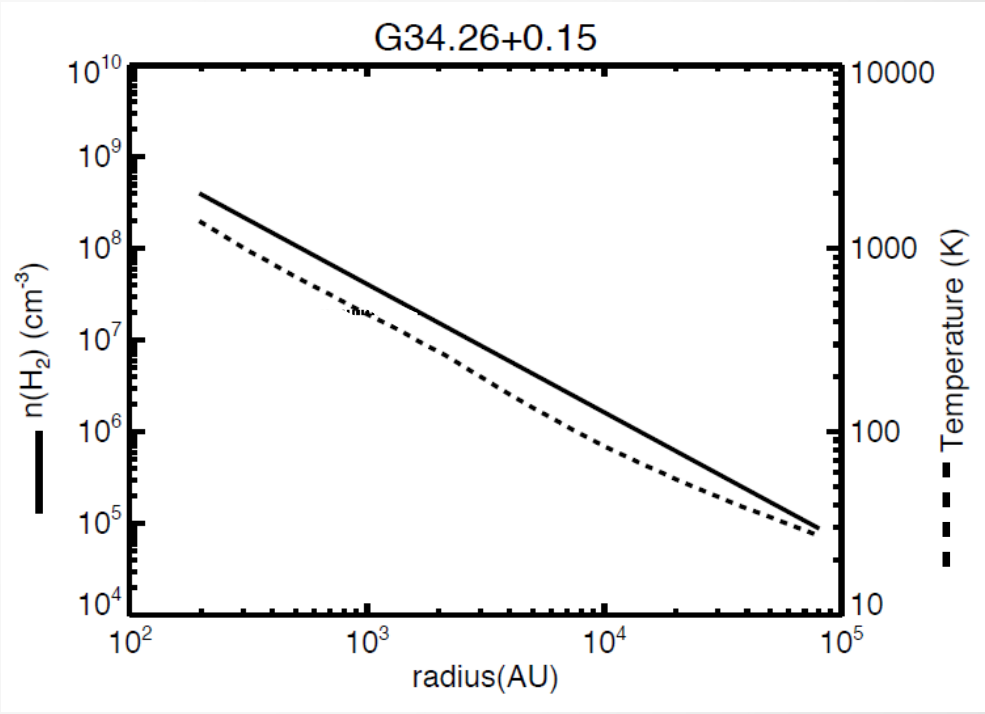


1/ Deuterium chemistry : HDO/H2O in high mass star forming region

Source : hot molecular core G34.26+0.15
Modeling : Molecular cloud condition followed by a 1D static physical structure of the core



Coutens, Vastel, Hincelin, Herbst et al 2014

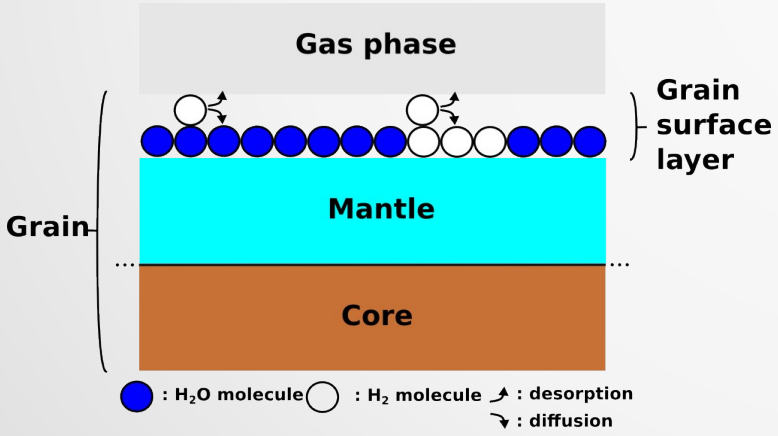


van der Tak et al 2013

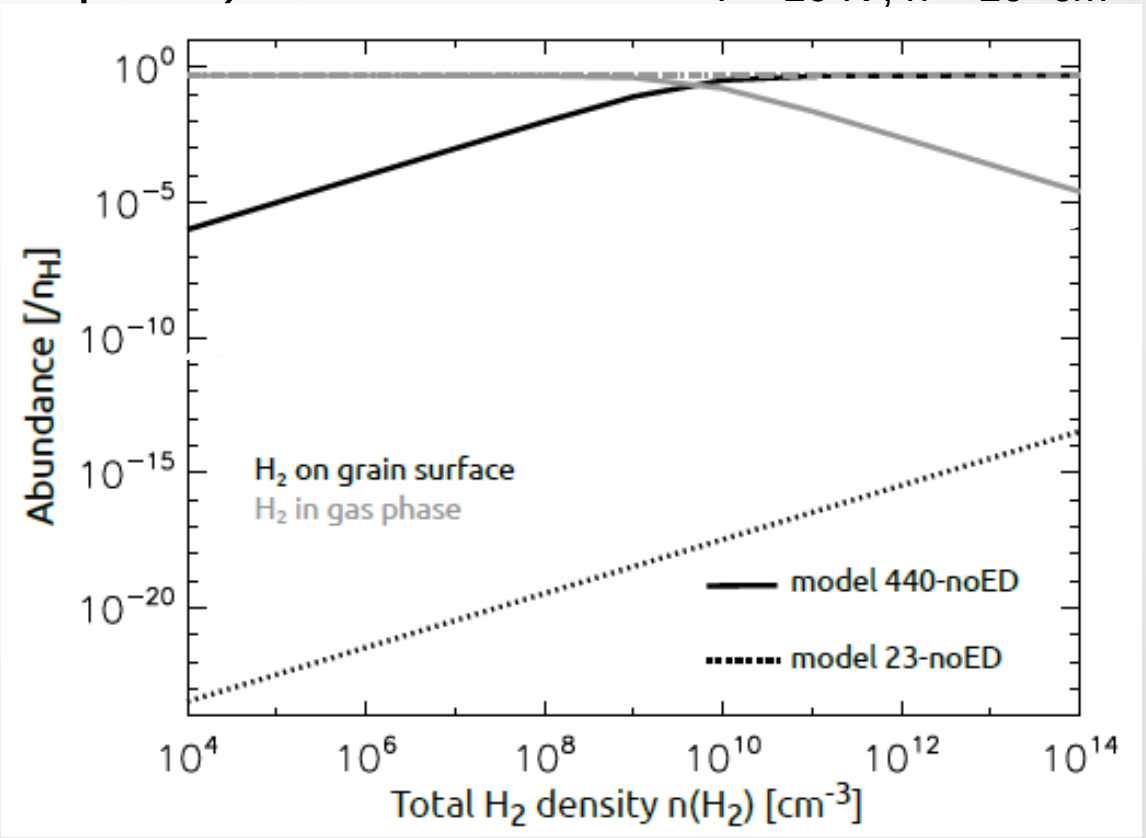
- Observations reproduced. Lower abundance of HDO in the inner core (o/p effect?)
- Important reactions with H, HCO+ (destruction), H3O+, H2DO+ (formation)
- Chemical simulations gives constraints on the source age : ~10^5 yrs

2/ Grain surface processes : Desorption due to H2 coverage

- Desorption energy of H2 on a water substrate : 440 K [1]
- Desorption energy of H2 on a H2 substrate : 23 K [1]
  → Desorption of H2 when on top of H2 substrate (called “encounter desorption”)



T = 10 K ; n = 10^4 cm^{-3}



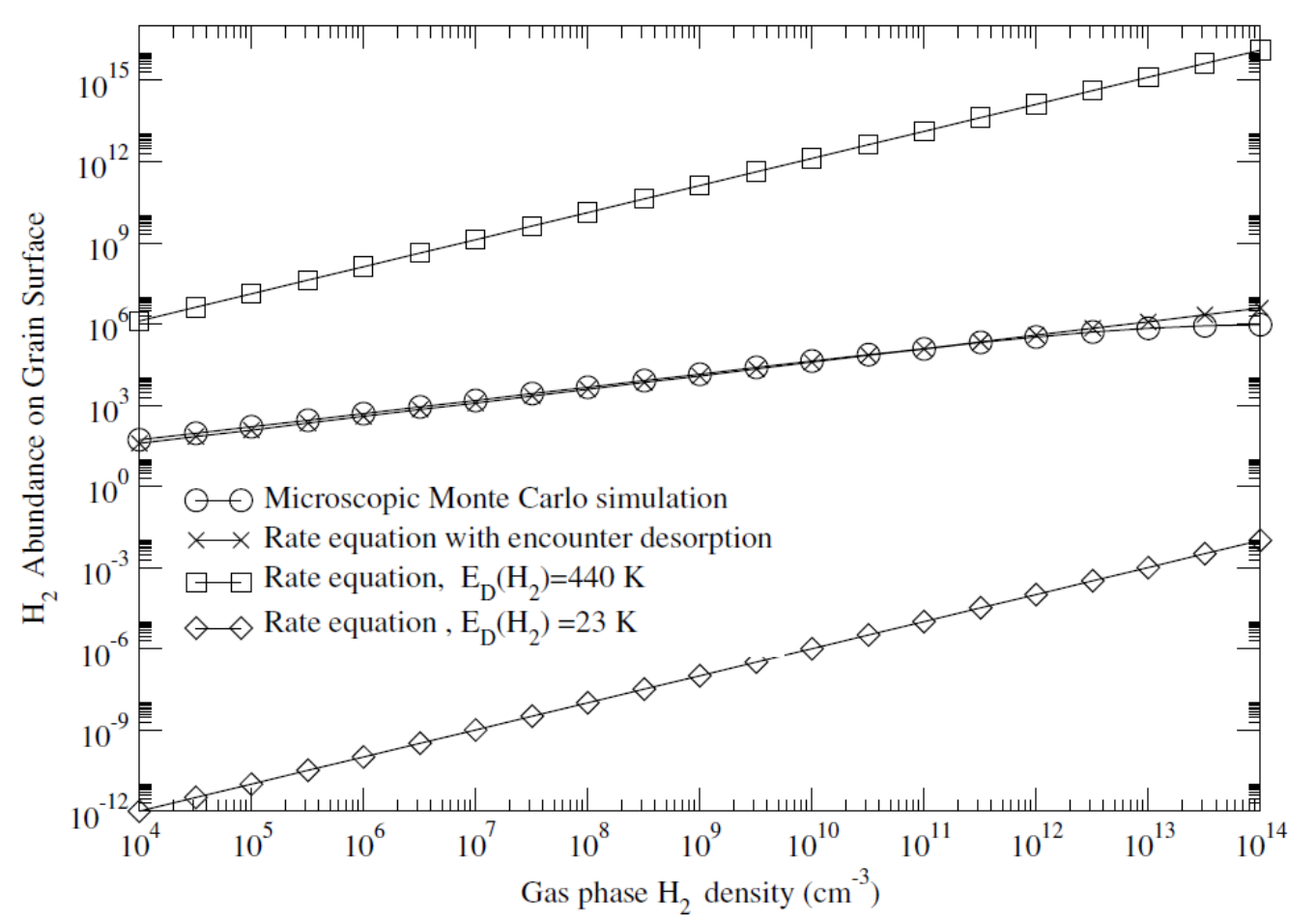
[1] : Cuppen & Herbst 2007

2/ Grain surface processes : Desorption due to H2 coverage

Basic idea : Microscopic Monte-Carlo models can reproduce this effect, but are still very time consuming → How to apply for complex star formation modeling?
One solution : Use rate equation model

Method :
1/ Add g-H2 + g-H2 → g-H2 + H2(gas) in rate equation models
2/ Use a formalism for diffusion and reaction on grain surface [2]
3/ Give a correct rate to this "reaction" that depends on :
- surface abundance of H2
- competition between desorption & diffusion
- desorption energy from H2 substrate

Results : Good reproduction of Microscopic Monte-Carlo models
Very low CPU time consuming



[2] Hasegawa & Herbst 1992

Summary

- New chemical network for deuterium chemistry
  (Hincelin et al 2014 in prep.)
- HDO/H2O in high mass star forming region
  (Coutens, Vastel, Hincelin, Herbst, et al 2014 submitted)
- Grain surface processes : desorption due to H2 coverage
  (Hincelin, Chang, Herbst 2014 in prep.)

- Perspective :

  - Coupling of deuterium chemistry and encounter desorption with complex 3D physical structure of star in formation
  (3 Dimensional Radiative Magneto Hydrodynamics, see Hincelin et al. 2013)
  - Application to Low and High mass star formation

Thank you for your attention :-)
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