Monte Carlo simulations versus rate coefficient methods

A.I. Vasyunin

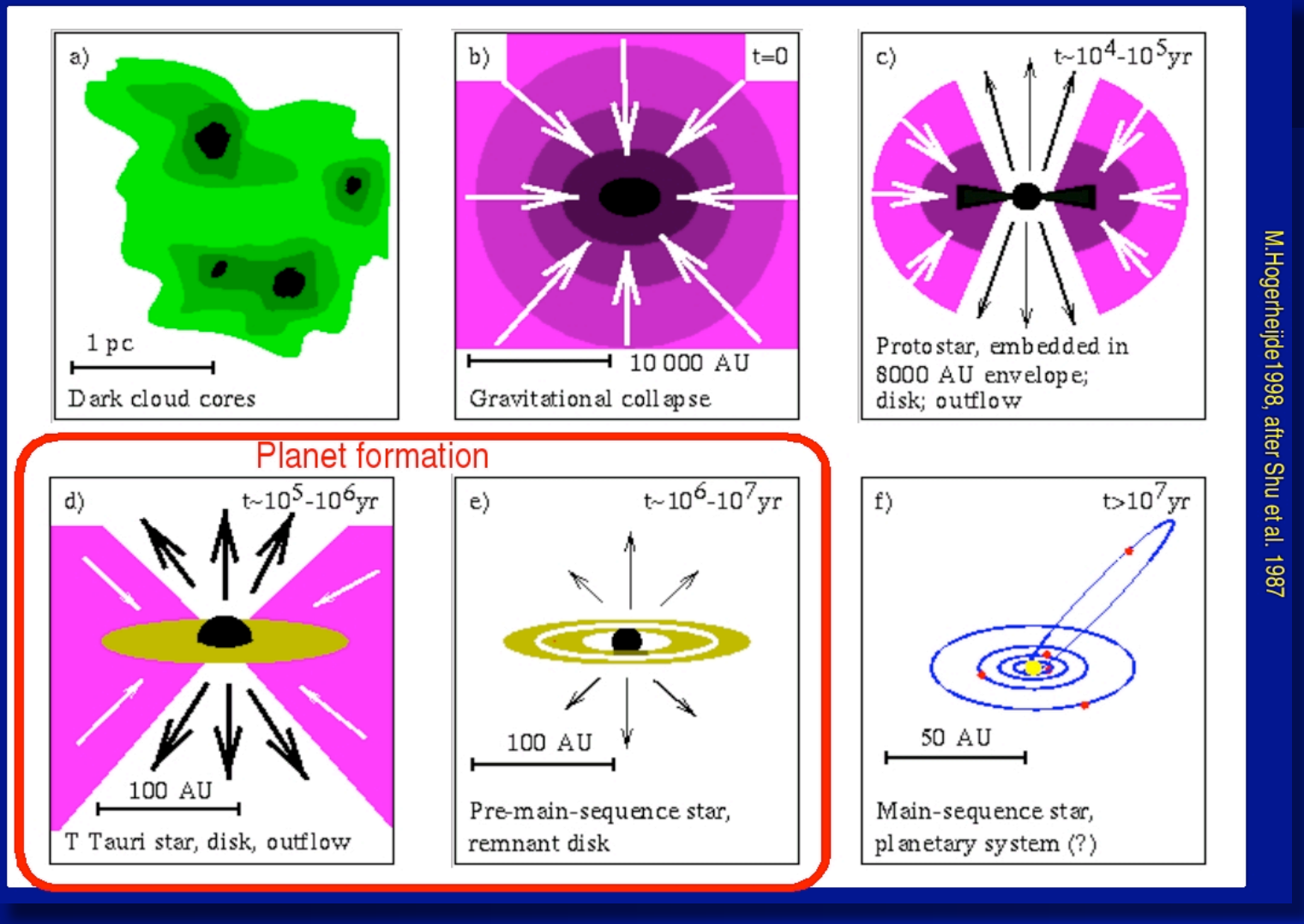
D.A. Semenov, Th. Henning, D.S. Wiebe, R. Garrod

MPIA, Heidelberg, Germany

INASAN, Moscow, Russia

Cornell University, USA

Scheme of low-mass star formation:

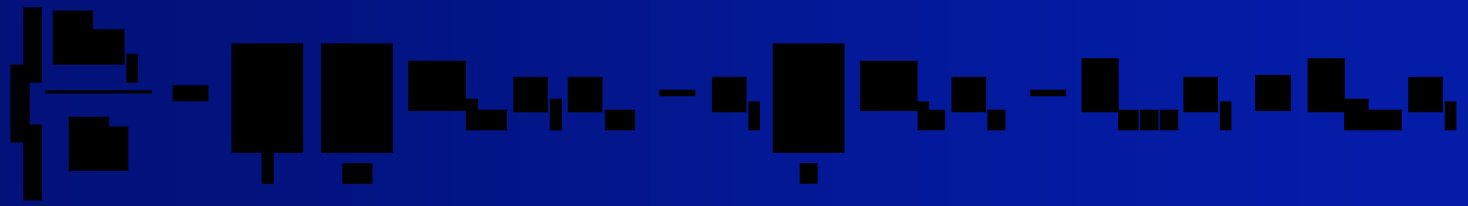


Sketch taken from M.Hogerheijde 1998, after the model of Shu et al. 1987

Chemical master equation:

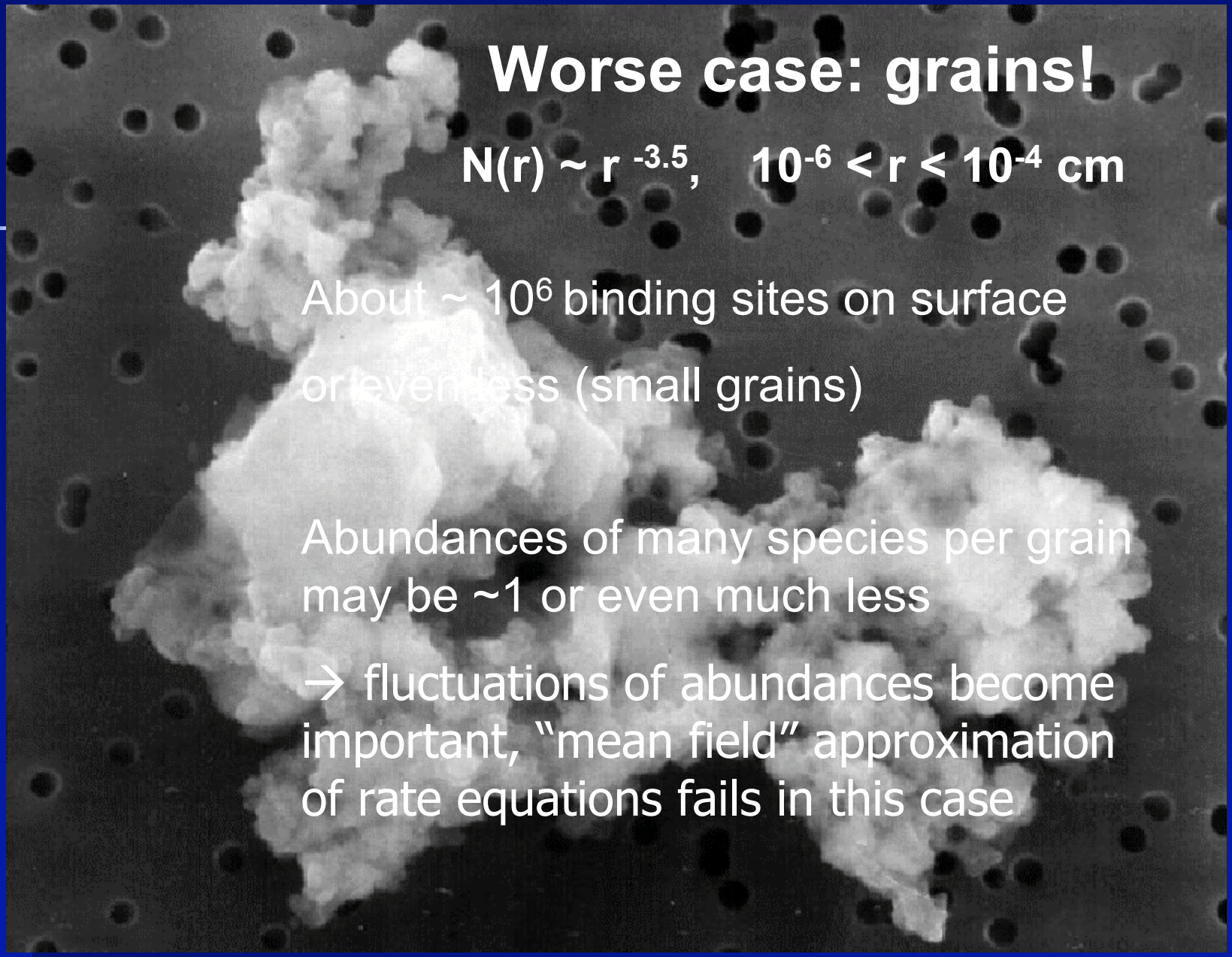
A kind of Boltzmann's equation, describes evolution of any chemically reacting system (living cells, gas-phase reactions in ISM, gas-grain ISM etc.)

Rate equations:



Valid approximation of the Master equation in the limit of infinite number of reacting atoms/molecules

→ Good approximation for gas-phase chemistry



Worse case: grains!

$N(r) \sim r^{-3.5}, \quad 10^{-6} < r < 10^{-4}$ cm

About ~ 10^6 binding sites on surface

or even less (small grains)

Abundances of many species per grain may be ~1 or even much less

→ fluctuations of abundances become important, "mean field" approximation of rate equations fails in this case

Previous works:

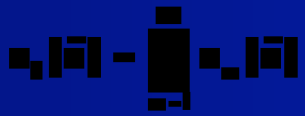
- Tielens & Hagen (1982)
- Charnley (1997, 2001)
- Stantcheva & Herbst (2001 – 2004)
- Group of O.Biham
- Cuppen et al. (2005 – 2008)

Our aims

- To develop a “full-scale” model of chemical evolution of the ISM with proper account for stochastic effects
- To investigate the validity of (modified) rate equations over a set of physical conditions typical for early phases of star formation

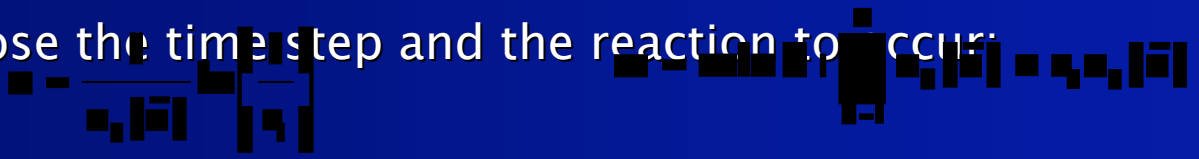
Stochastic simulation algorithm – SSA (D. Gillespie, 1976)

- Calculate the sum of all reaction rates at current time moment:

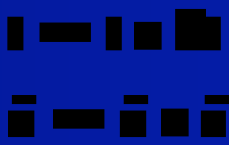


- Select two random numbers r_1 & r_2 uniformly distributed over [0,1]

- Choose the time step and the reaction to occur:



- Update abundances:



- If final time is not reached repeat the steps above

Main drawback: in SSA each reaction event is simulated, therefore, may be very slow and computationally demanding

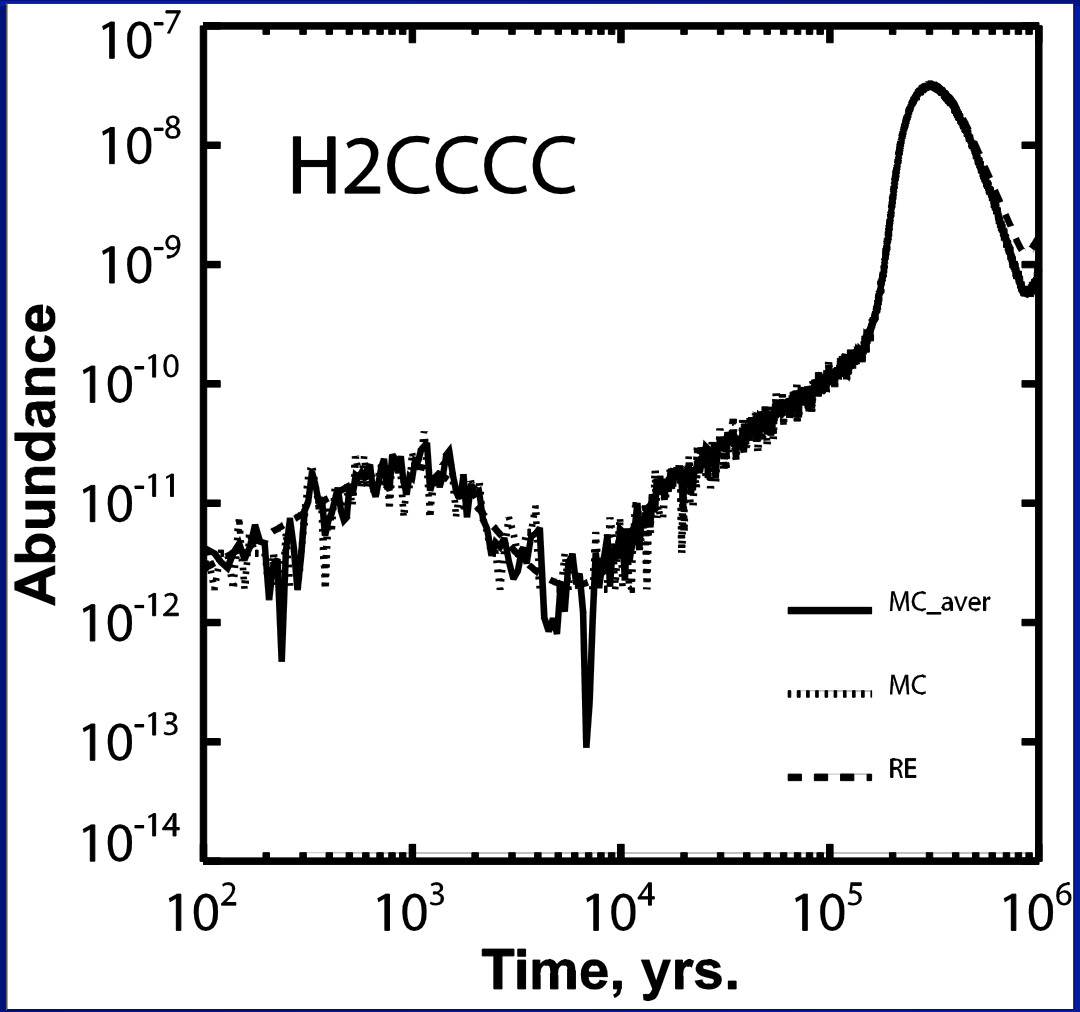
Our Monte Carlo model

- Monte Carlo (Gillespie's SSA): gas-phase coupled with surface chemistry
- 600 species, >6000 reactions
- RATE06 gas-phase ratefile (Woodall++ 07)
- Surface network (Garrod & Herbst 06)
- 0.1μm uniform olivine grains
- "Low metals" initial abundances (Lee++ 97)
- ISM conditions: $n_H \leq 10^5$ cm^{-3}; T=10-50K;
- 1 Myr

Comparison of (modified) rate equations with Monte Carlo approach

- Two models of surface chemistry:
  - T: “fast”, tunneling for H & H_2, E_b/E_D=0.3 (Hasegawa et al. 1992)
  - H: “slow”, thermal hopping only, E_b/E_D=0.77 (Katz et al. 1999)
- Methods:
  - Rate Equations
  - Modified RE (Caselli et al. 1998, Garrod 2008)

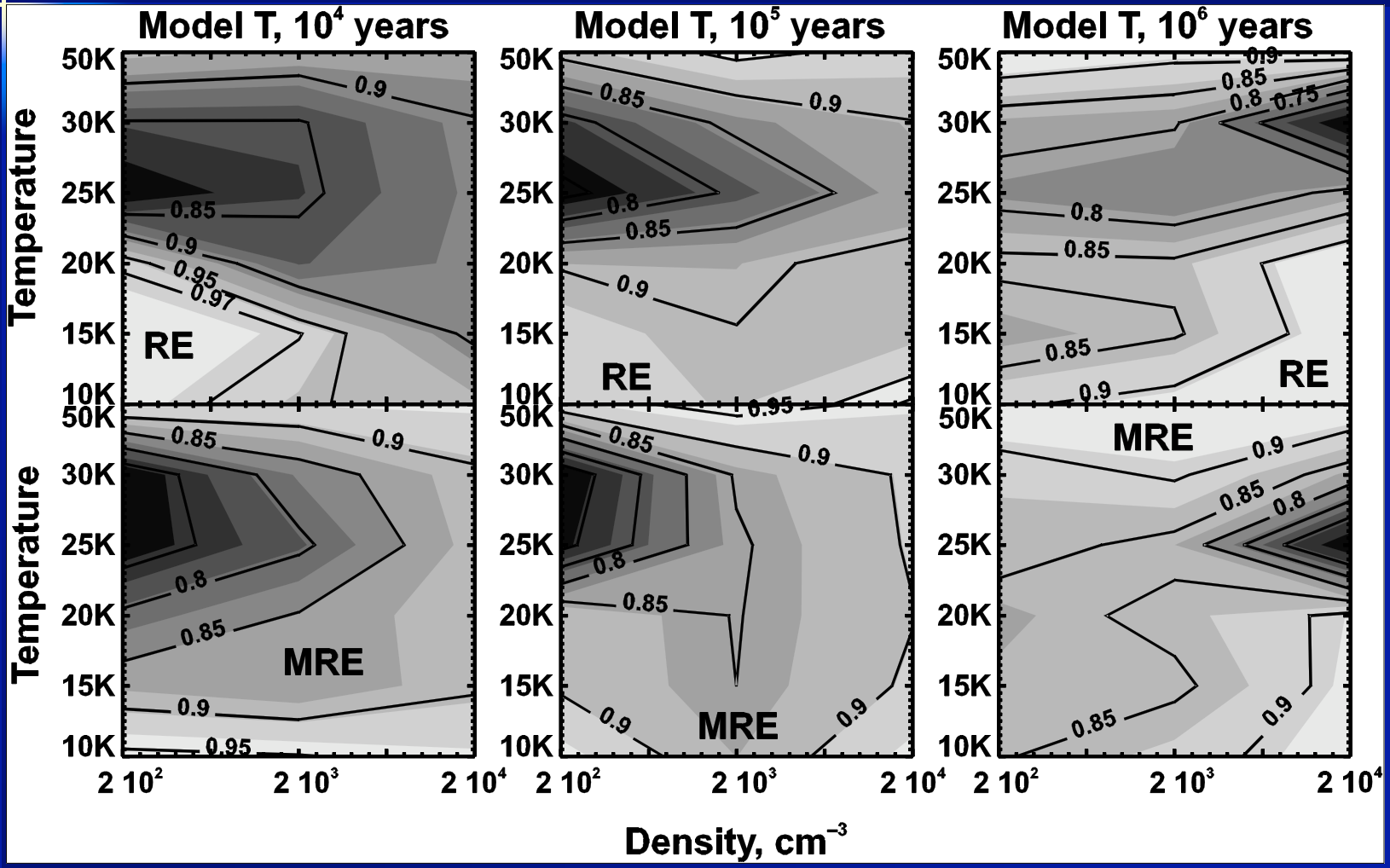
Test case:


H2CCCC
Abundance
Time, yrs.
MC_aver
MC
RE
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}

Agreement map, high surface rates

RE

MRE

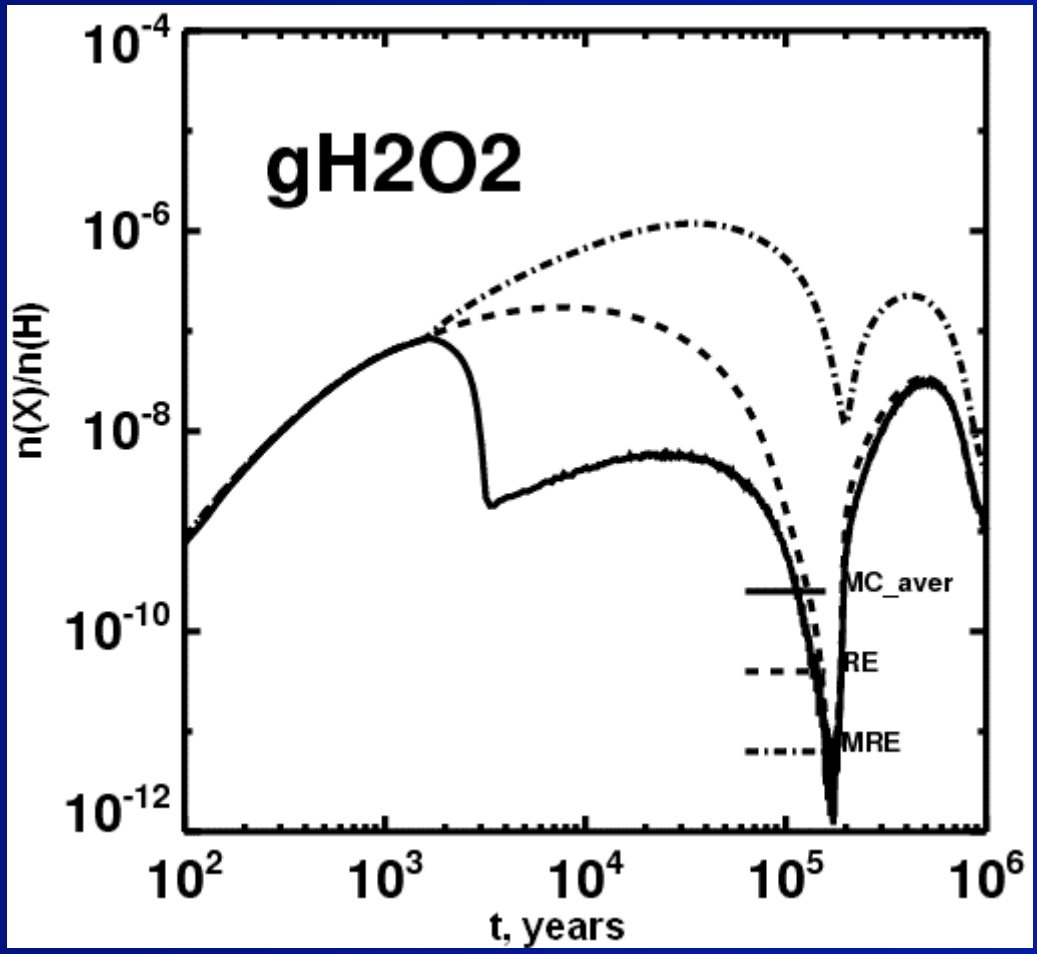


Some processes are missed in (M)RE calculations?

nH=2*10^4 cm^{-3}

T=10K

Fast surface rates



Warm medium (25-30K): gas-phase abundances are affected!

Agreement map, low surface rates

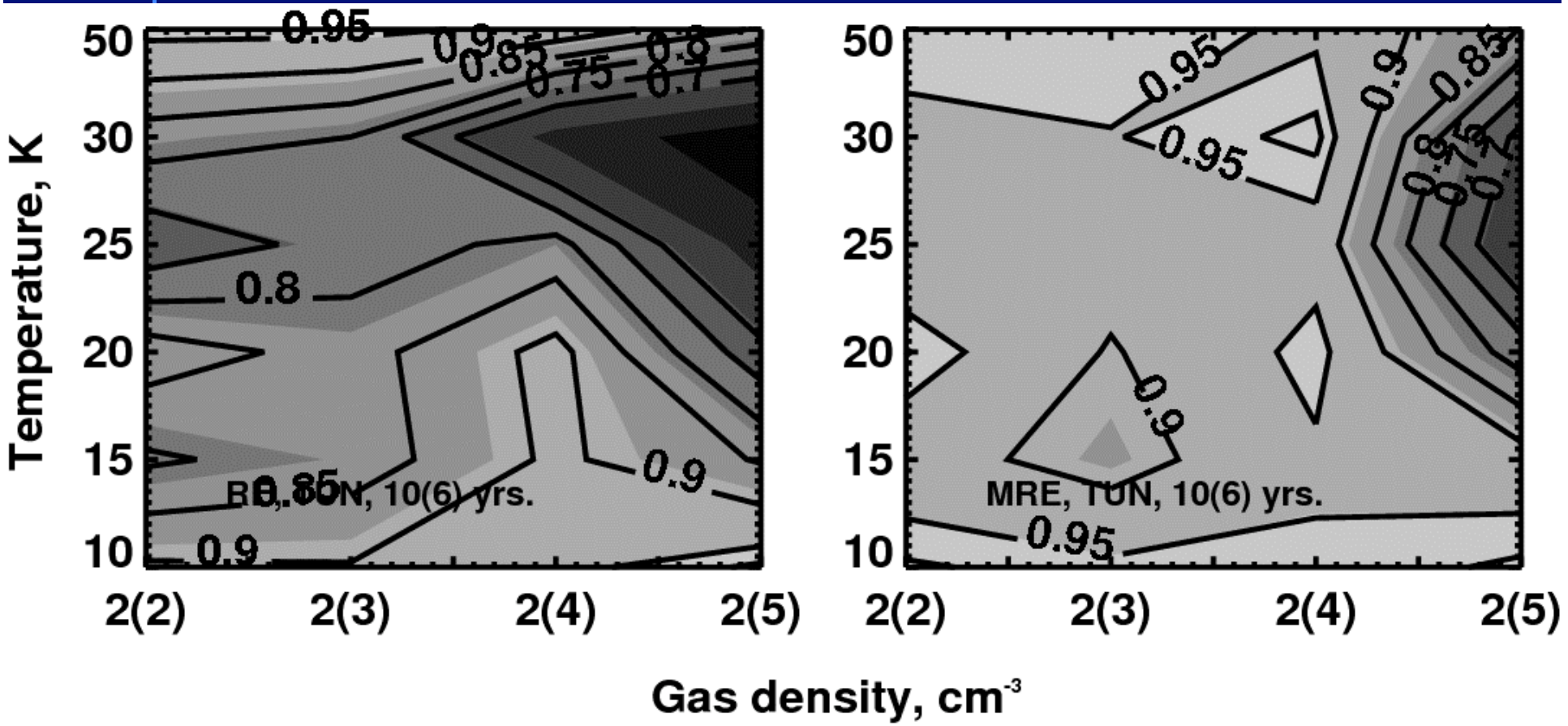
RE

MRE

Disk chemistry:

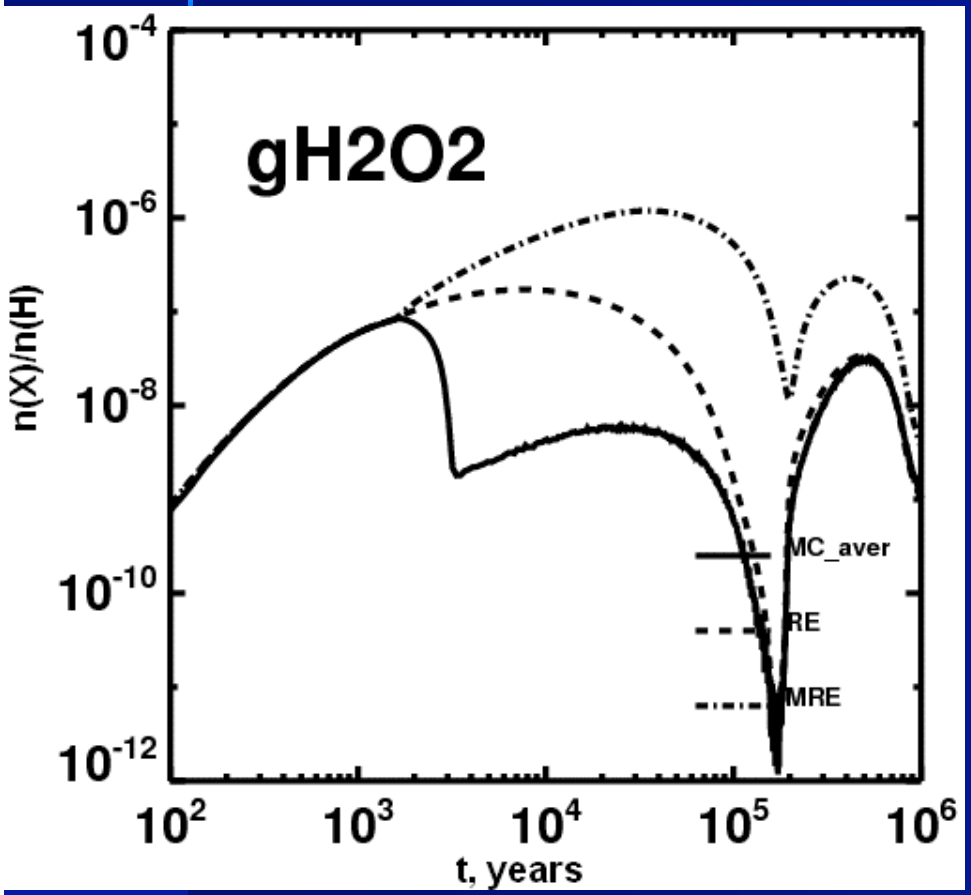
- Too dense for Monte Carlo to be applicable ($n_H > 10^5$ cm^{-3})
- Approximate methods should be employed to account for stochastic effects

Rob Garrod's new MRE scheme (2008A&A...491...239G):

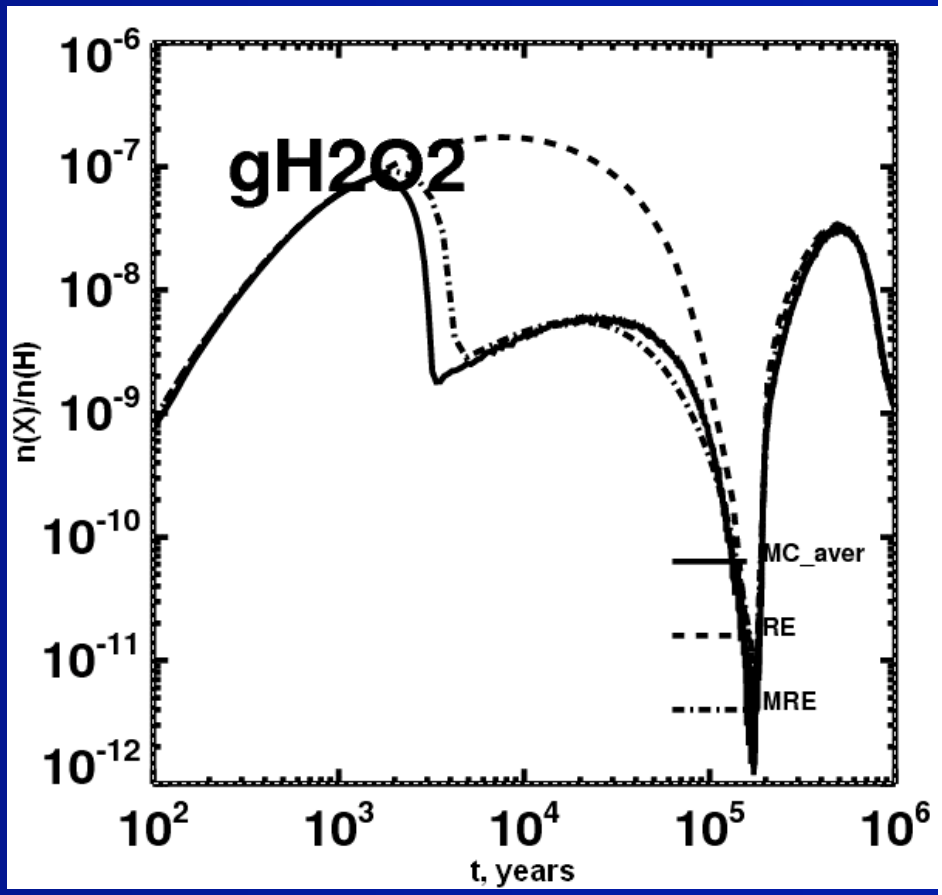


Rob Garrod's new MRE scheme (2008A&A...491...239G):

Old:



New:

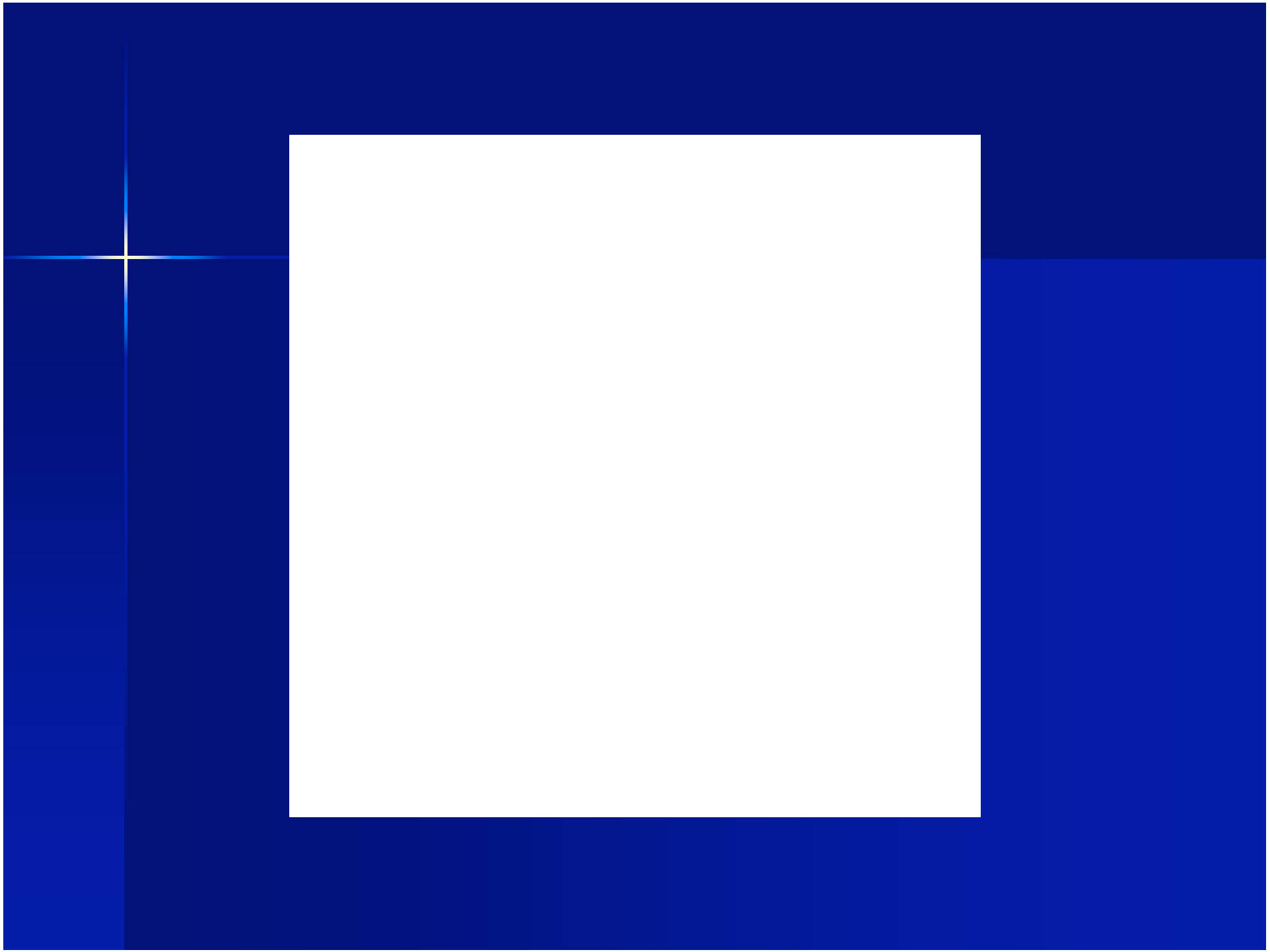


Conclusions

- A Monte Carlo code capable to simulate realistic astrochemical model is developed
- In many cases results of RE and MRE are far from results of MC. Differences are not only quantitative but sometimes qualitative
- Critical temperature range: 25K-30K. Even gas-phase abundances of key species are affected by stochastic effects
- “Hot corino” chemistry can be a “stress test” for this case

Conclusions

- New modified rate approach (Garrod 2008) seems to be the most accurate approximate method at the moment
- Unlike MC it is also suitable for disk chemical modeling!

Thank you for your attention!

$$\overline{X} = \frac{\sum_{i=1}^{N} X_i \Delta t_i}{\sum_{i=1}^{N} \Delta t_i}$$