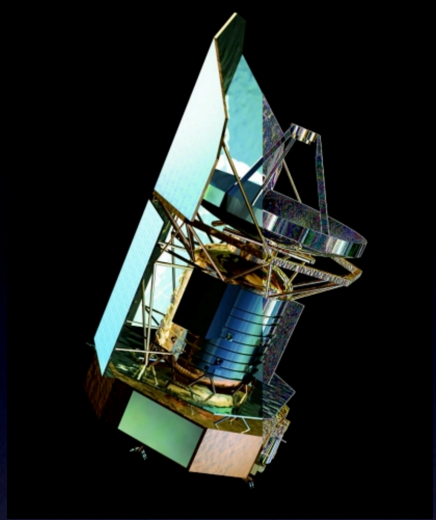
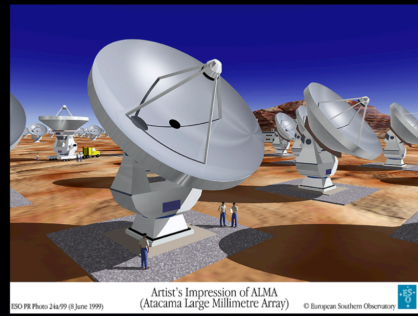


Welcome



A new generation of databases for interstellar chemical modeling in preparation for HSO and ALMA

Goal of the team: Address the difficult question of uncertainties in reaction rate coefficient in order to improve chemical databases for astrochemistry modeling.

Meeting 1: General consideration about uncertainties
Meeting 2: Work on specific reactions

Publication of a review paper on this topic

Program

Monday afternoon: Session 1

Introduction to astrochemistry and gaz-phase databases

Tuesday morning: Session 2

Estimated uncertainties in rate coefficients and how they are used

Tuesday afternoon: Session 3

Theory and temperature extrapolation

Wednesday morning: Session 4

Gas-phase experiments and uncertainties in rate coefficients

Wednesday afternoon: Session 5

Surface chemistry and uncertainties

Thursday morning: General discussion

Abundance Uncertainties and Sensitivity Analyses in cold and hot sources

Valentine Wakelam
Laboratoire d'Astrophysique de Bordeaux
University Bordeaux 1 / CNRS
France

Uncertainties in rate coefficients in osu

✓ osu network: created and used by the Ohio State University Astrochemistry team (leaded by Prof. Eric Herbst)

✓ Mainly for low temperature objects

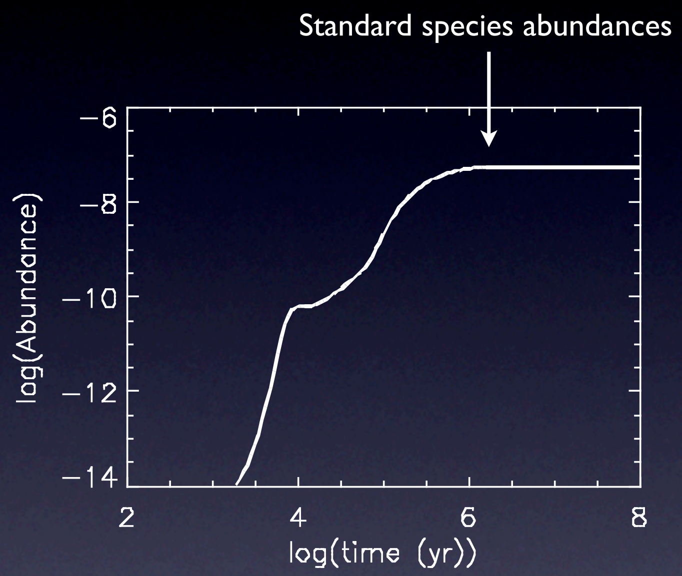
✓ Uncertainties recently added similarly to UMIST

Model used: 0D pure gas-phase model, single fixed gas temperature and density, time dependent chemistry

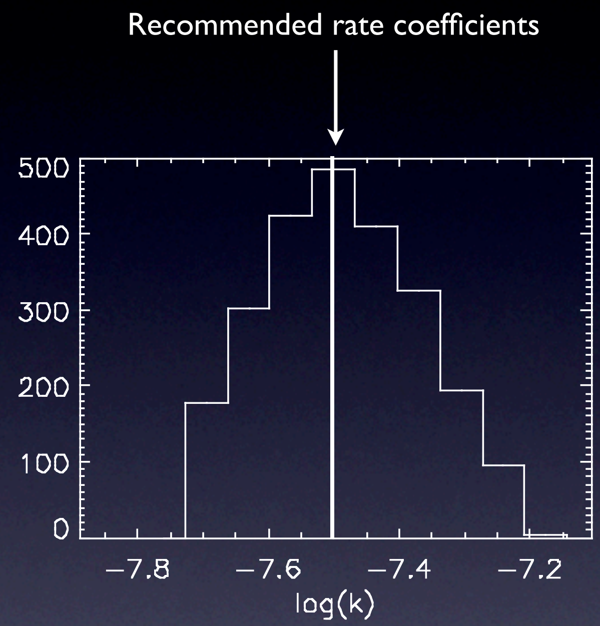
OSU and Srates database

Two types of sources:
- dark clouds ($T=10K$, $n(H_2)=10^4 cm^{-3}$, $Av=10$)
- “hot corinos” ($T=100K$, $n(H_2)\sim10^7 cm^{-3}$, $Av=10$)

Uncertainty Method

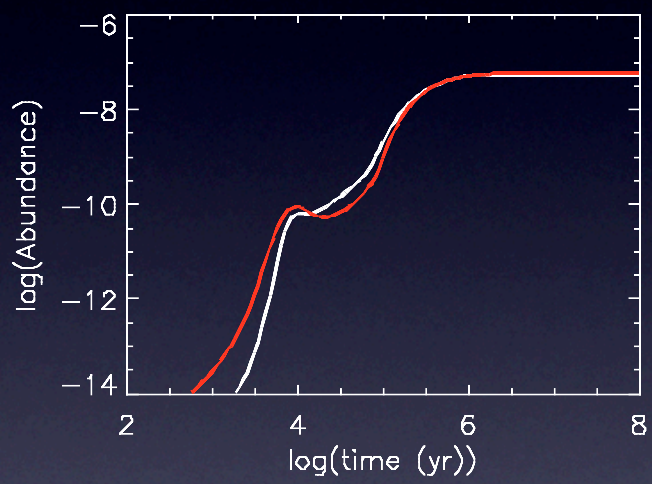


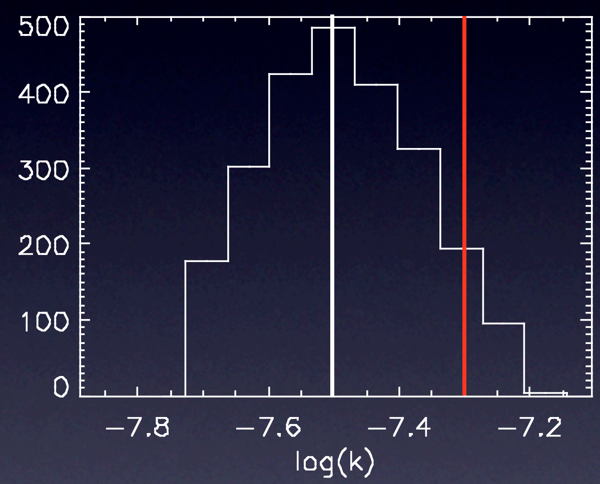
SO abundance



Distribution of k assuming the uncertainty in the rate coefficients is lognormal

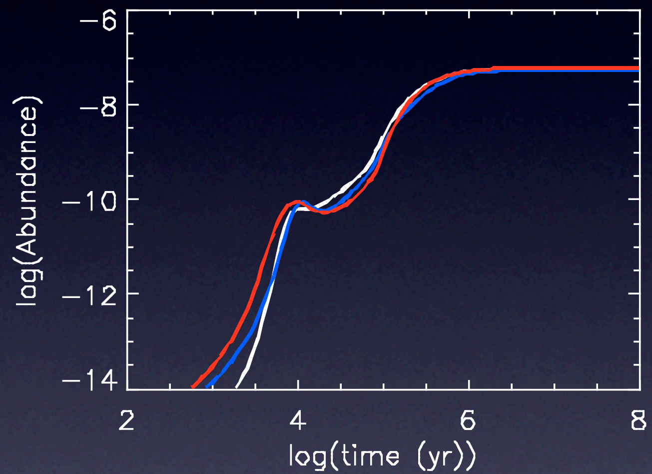
Uncertainty Method

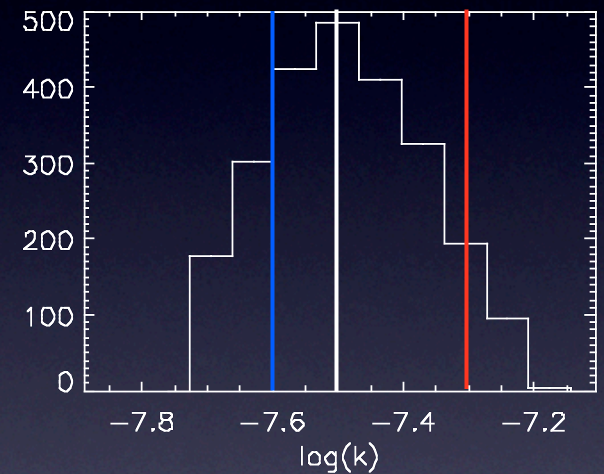




Random variation of k within the uncertainty range

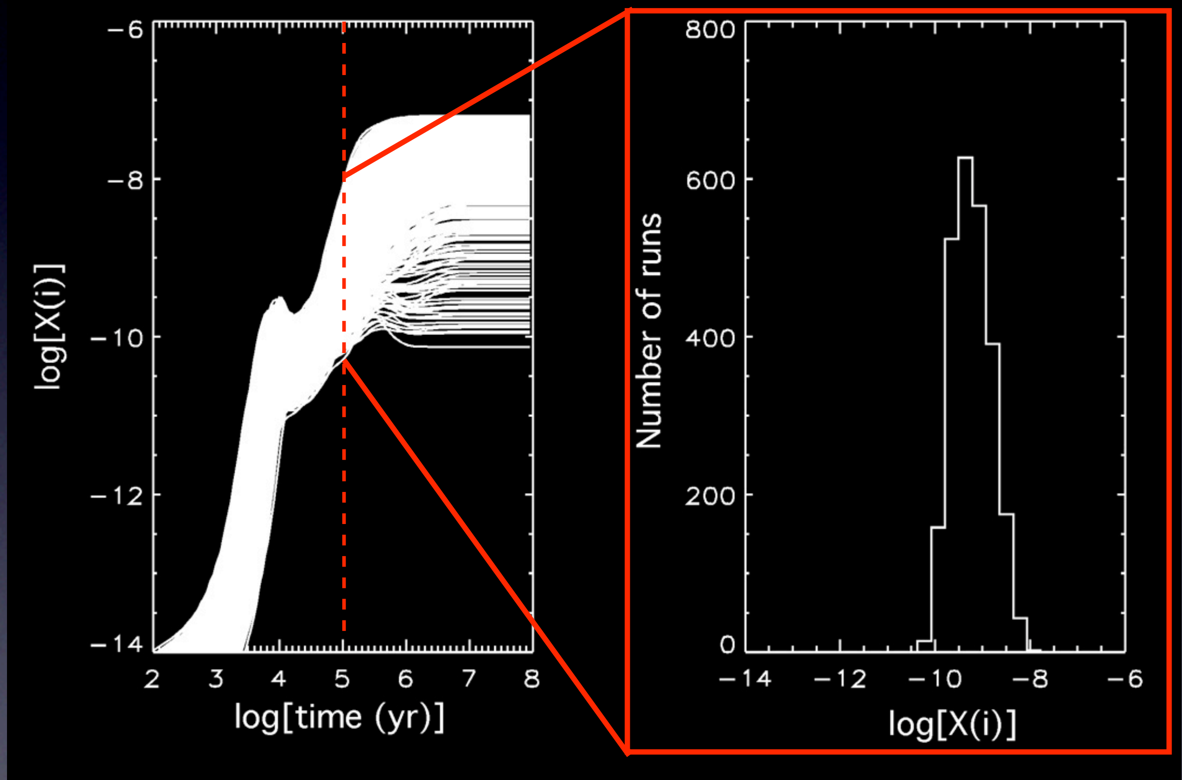
Uncertainty Method





Random variation of k within the uncertainty range

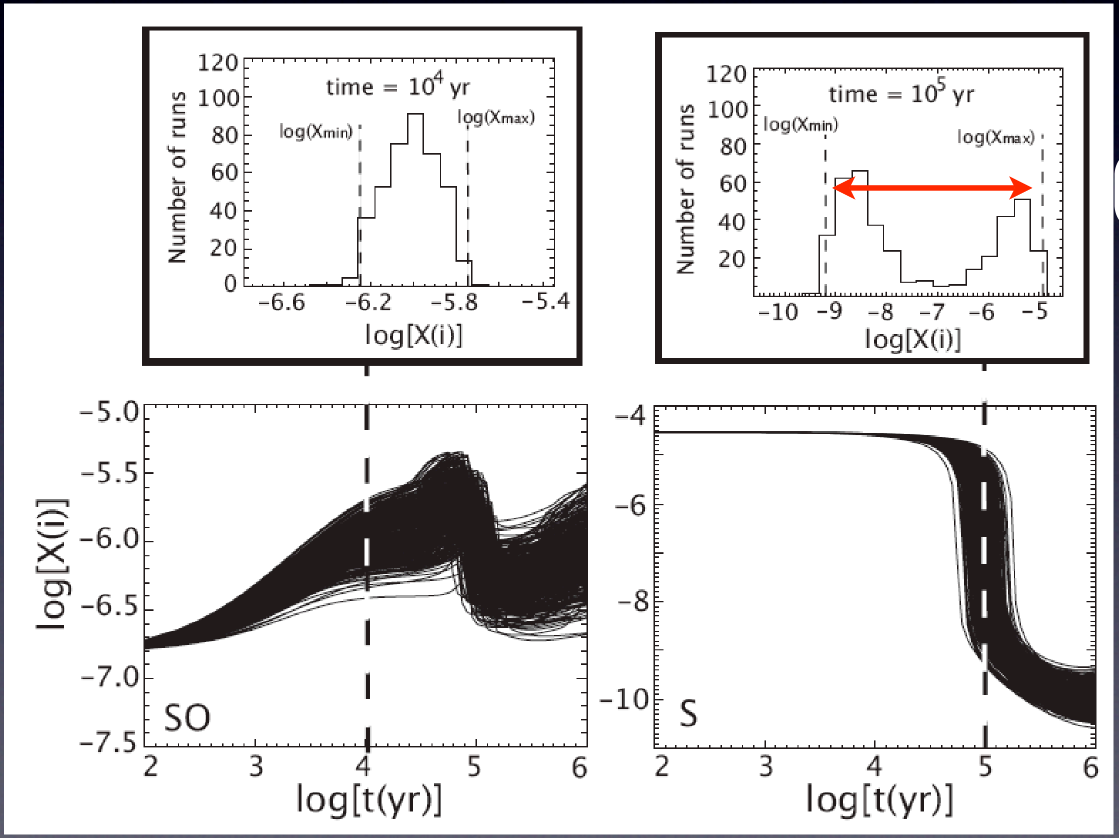
Uncertainty Method



SO abundance: each line is the result of one run

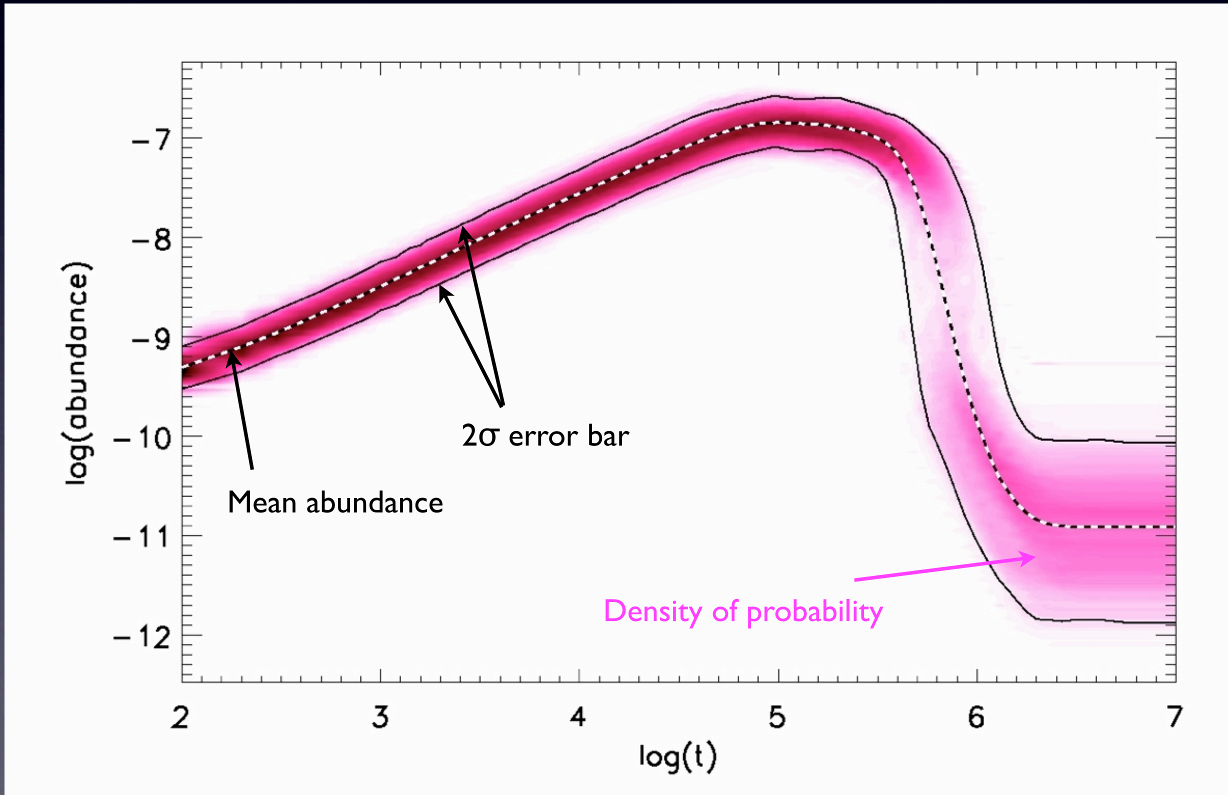
Distribution of SO abundance at 10^5 yr

Defining uncertainties in abundance species

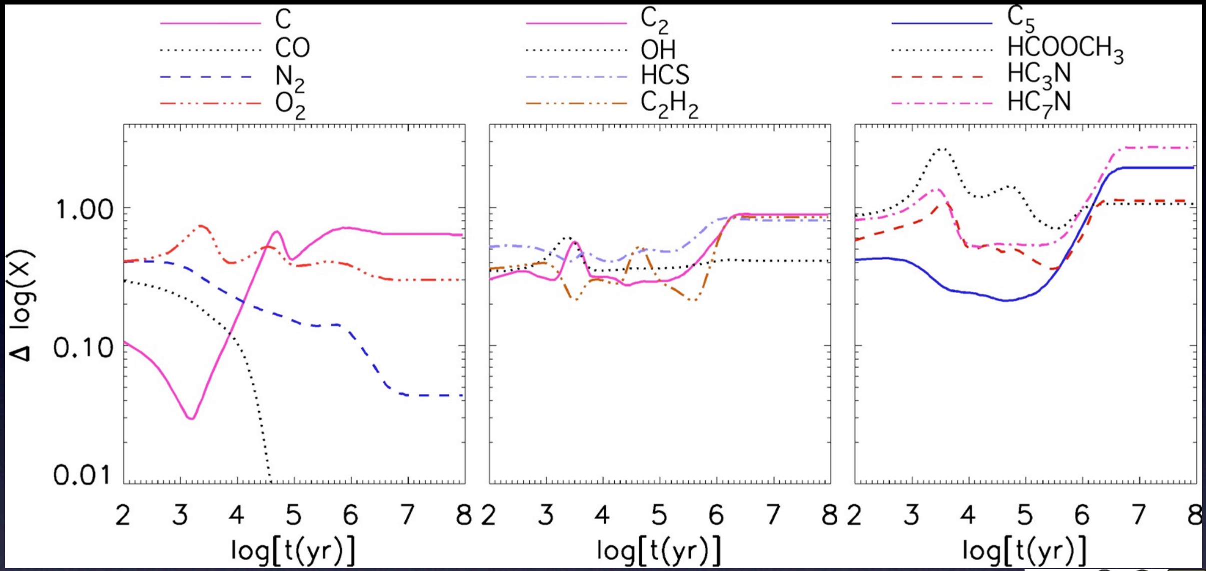


Δlog(X)
contains 94.5% of the curves

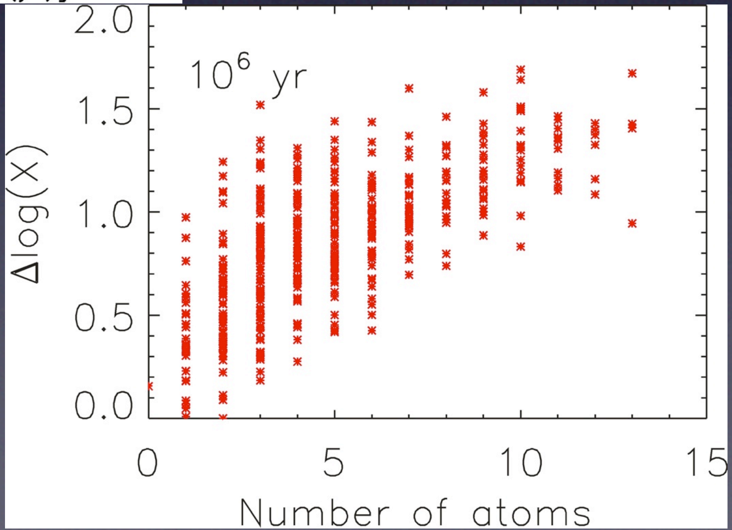
Typical results: H_2CS in hot cores



Some quantitative results
Uncertainties in molecular clouds



Values of the uncertainties in the abundance species as a function of time and complexity of the molecule

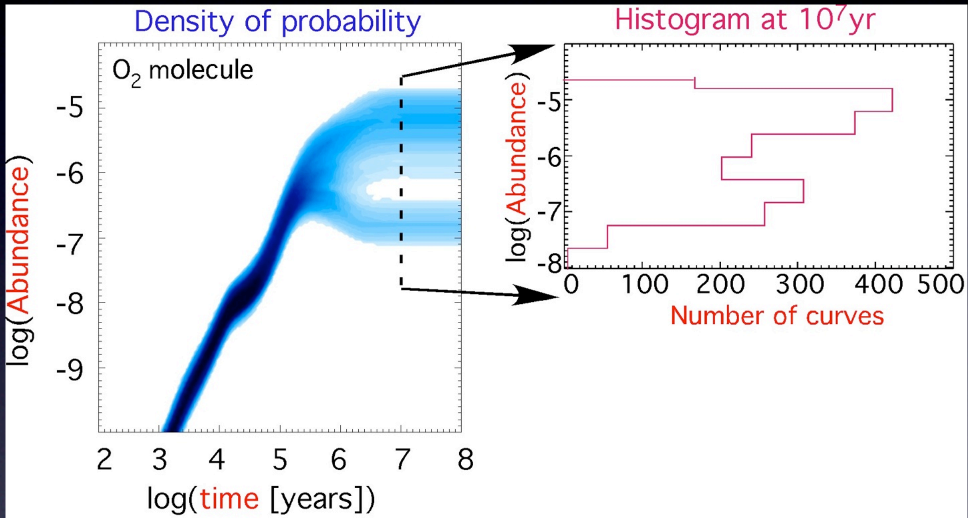


$\Delta\log(X)=0.1$ means $X/1.25 \leq X \leq X*1.25$

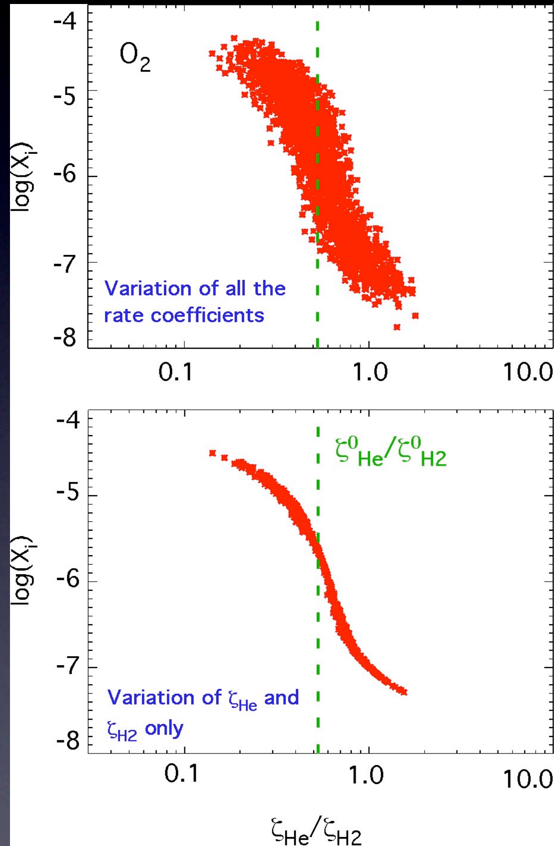
$\Delta\log(X)=1$ means $X/10 \leq X \leq X*10$

Finding hypersensitivity and bistability

High metal elemental abundances - varying all rate coefficients at the same time



O_2 abundance as a function of ζ_{He}/ζ_{H2}

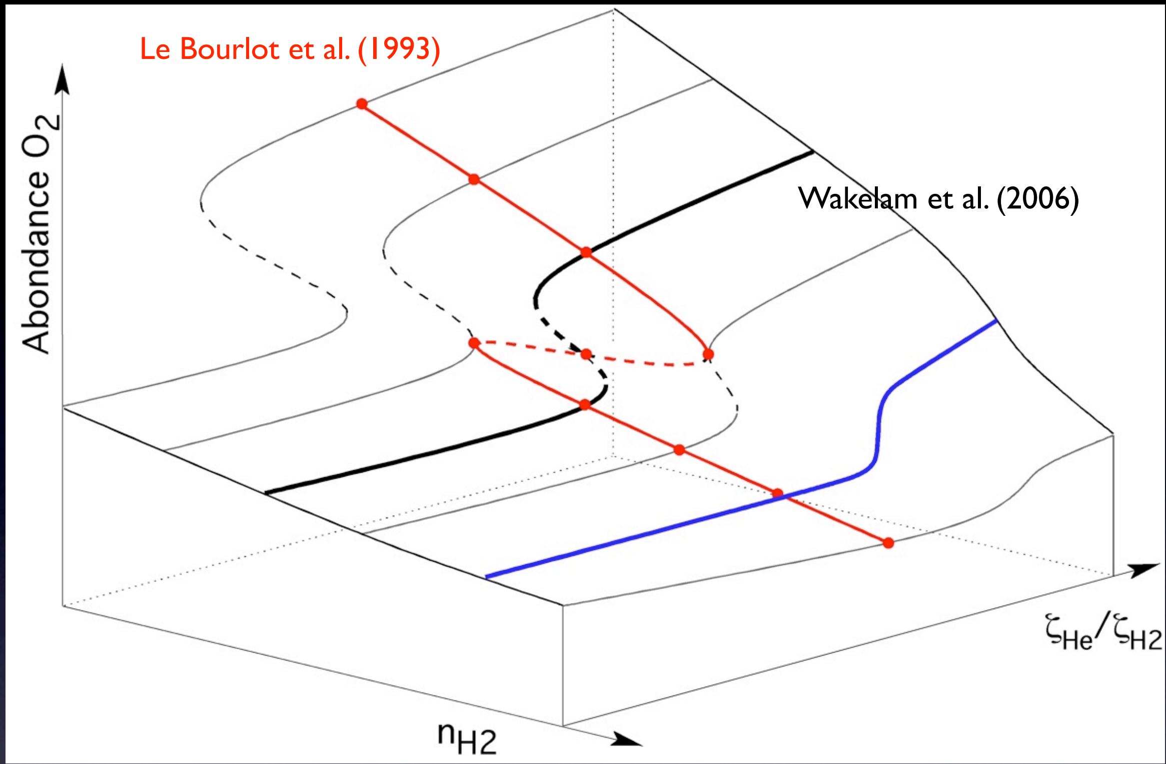


Cosmic ray ionization:

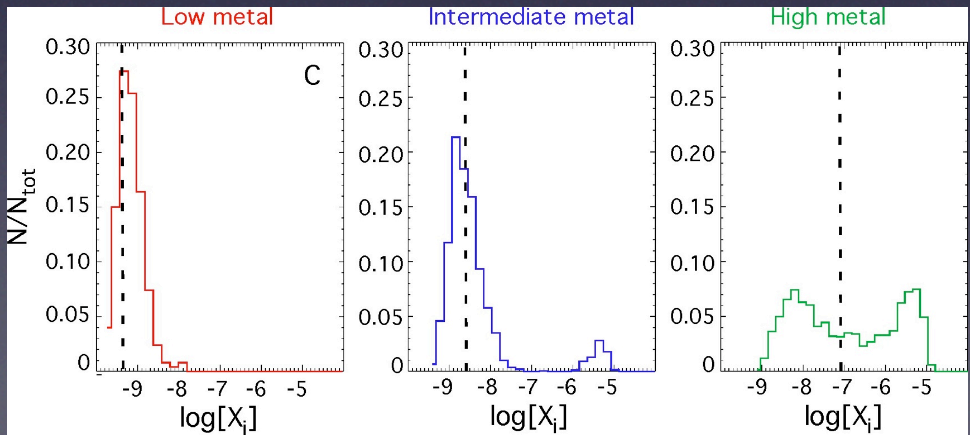
He + cosmic ray → $He^+ + e^-$ ζ_{He}

H_2 + cosmic ray → $H_2^+ + e^-$ ζ_{H2}

Wakelam et al. (2006)



Le Bourlot et al. (1993)
Wakelam et al. (2006)
Abondance O2
nH2
ζHe/ζH2

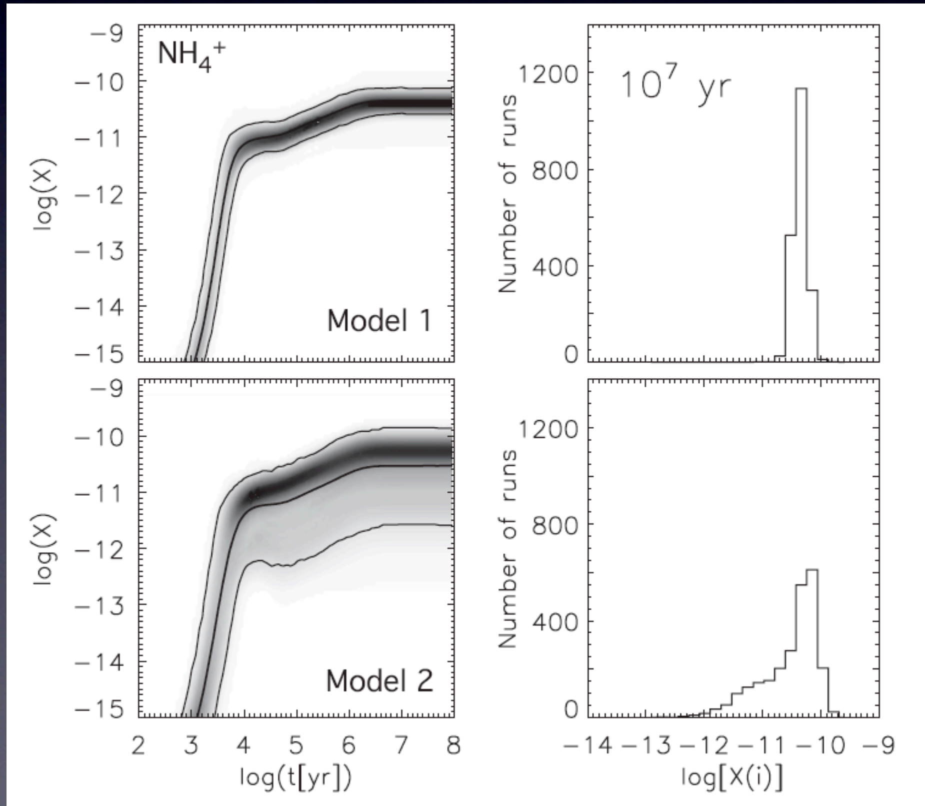


Low metal
Intermediate metal
High metal
C
N/Ntot
0.30
0.25
0.20
0.15
0.10
0.05
0
-9 -8 -7 -6 -5
log[Xi]

Uncertainties in physical conditions in molecular clouds

Variation of 50% of T and $n(H_2)$ around typical values (10K and $10^4 cm^{-3}$)
Increase the uncertainty for some species especially N-bearing species

Nitrogen chemistry starts with
$N^+ + H_2 \rightarrow NH^+ + H$ $k=10^9 exp(-85/T)$
Not efficient à low T



What can we do with the uncertainties in abundance species?

Compare the theoretical and observed abundances taking into account the both error bars in order to:

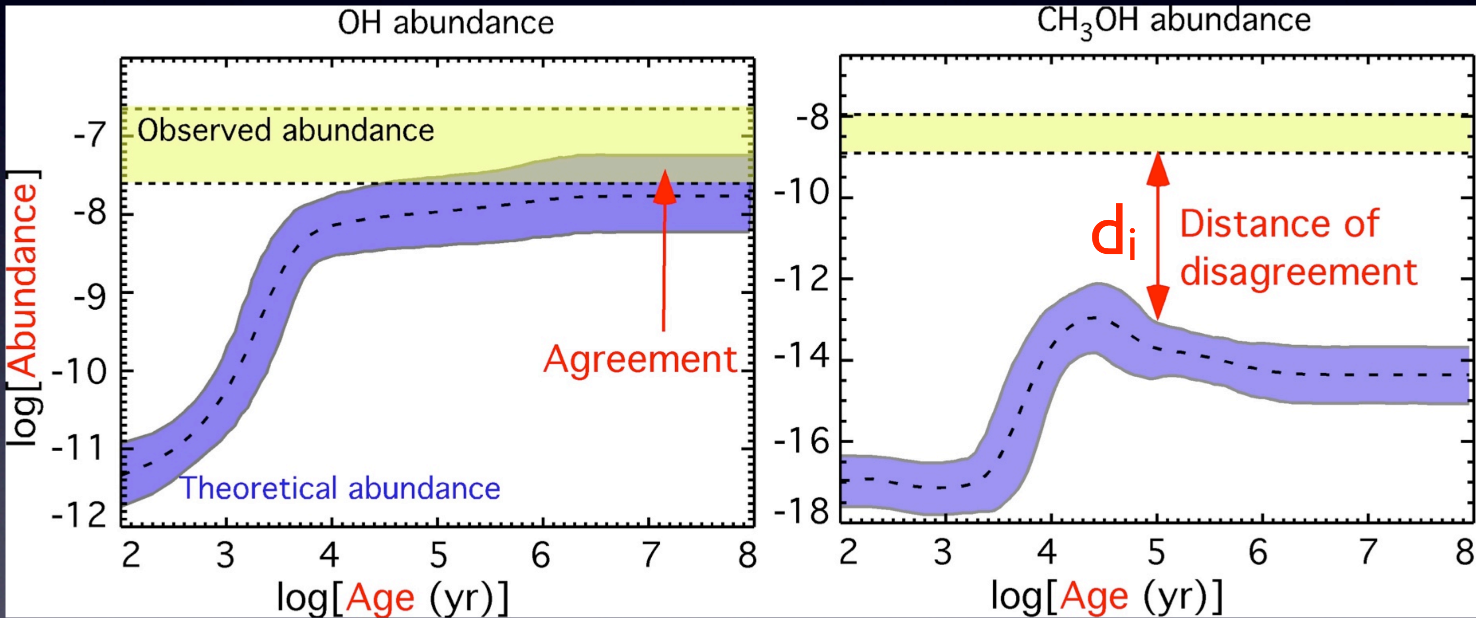
✓ define the most problematic species (really not reproduced by models)

✓ define the need for including other processes (gas-grain interactions for instance)

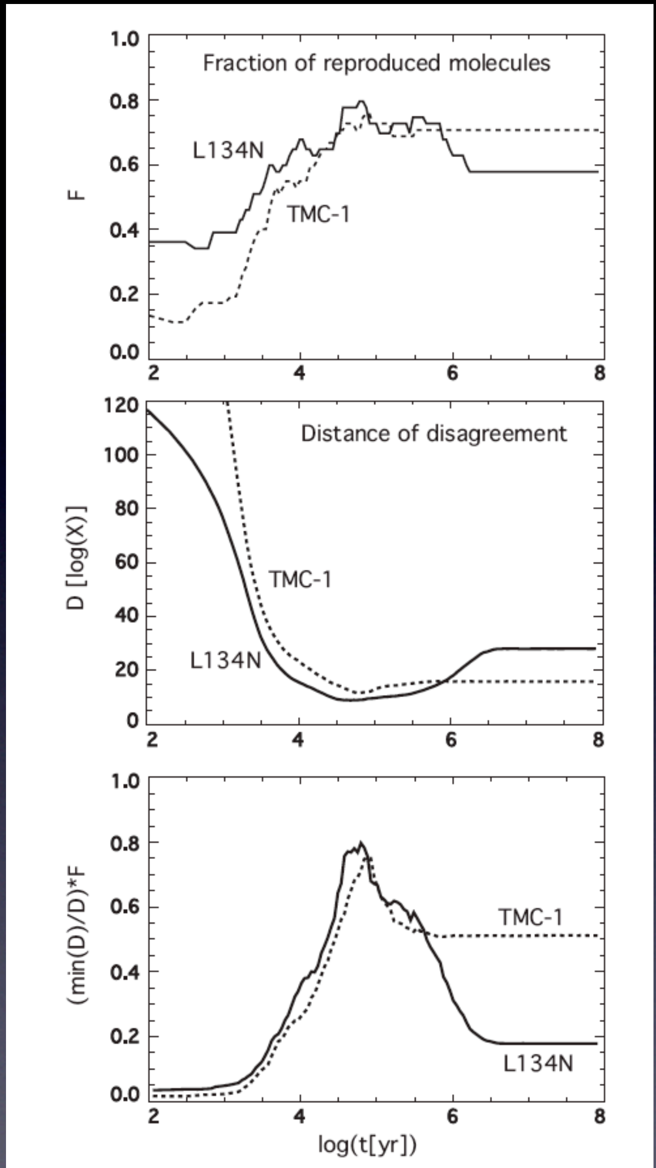
✓ laboratory needs

Problem: how do we compare?

Proposed method to compare observed and modeled abundances



Wakelam et al. (2006)



F(t) = fraction of reproduced species as a function of time

⇒ Constrain non reproduced species

D(t) = $\Sigma\, d_i$ for non-reproduced species as a function of time

[min(D)/D(t)]*F(t)
Takes into account both agreement and disagreement

⇒ Constrain the chemical age

Reproduce around 80% of observed molecules in L134N and TMC-1 assuming a factor of 3 uncertainty in observed abundances.

BUT:

✓ Values in the observed uncertainties (different approximations and telescopes)

✓ Values in the rate coefficient uncertainties

✓ Observed abundances in TMC-1 reproduced only if C/O > 1

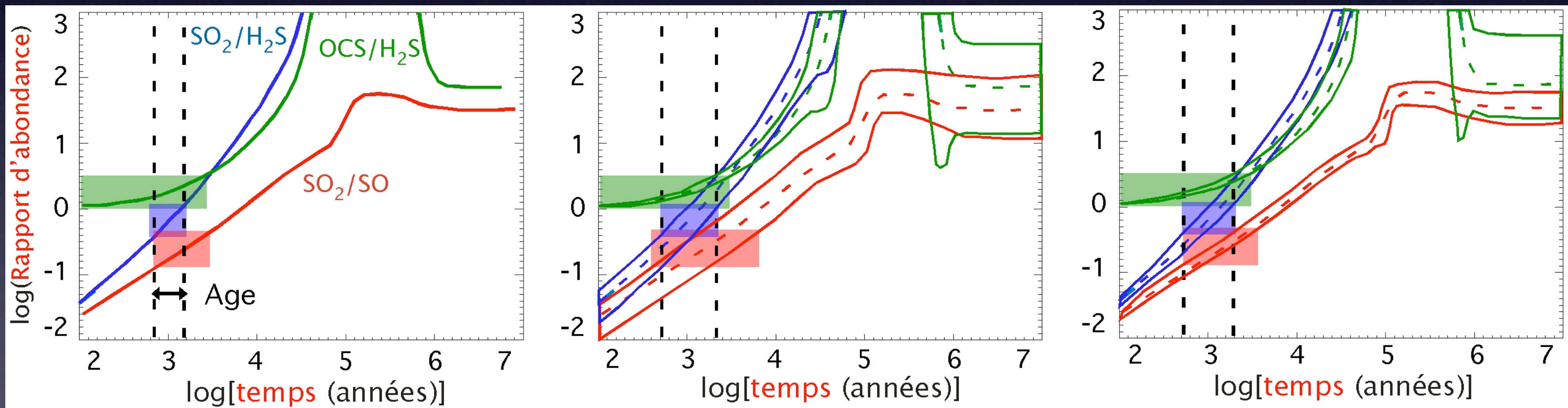
Dating low mass protostars

0D gas-phase chemical model for low mass protostar.
Comparison with observations in IRAS16293-2422

Without uncertainties

With uncertainties

Reducing uncertainties on a list of 5 selected reactions



Wakelam et al. (2005)

Sensitivity Methods

Identification of important reactions that may be wrong or can be improved
Linear correlations:
- varying rate coefficients one after an other (method 1)
- linear correlation coefficients (method 2)

Non-linear correlations (to be done in ISM chemistry)

Method 1

Varying rate coefficients one after an other

Recommended rate coefficients → Abundances of reference

$k_{rec}^{1}, k_{rec}^{2}, \ldots, k_{rec}^{n} \longrightarrow X^{ref}_{1}, X^{ref}_{2}, \ldots, X^{ref}_{m}$

Modifying one rate coefficient (by a certain factor) → Modified abundances

$k_{mod}^{1}, k_{rec}^{2}, \ldots, k_{rec}^{n} \longrightarrow X^{mod}_{1}, X^{mod}_{2}, \ldots, X^{mod}_{3}$

Compute at each time step, how much each reaction influences the abundance of each species:

$$R^{i}_{j}(t) = \frac{(X^{i}_{j}(t) - X^{ref}_{j}(t))}{X^{ref}_{j}(t)}$$

If $R^{i}_{j}(t) = 0.1$, it means that the modification of reaction i rate coefficient by a certain factor induces an increase of 10% in the species j abundance at a time t.

Method 2

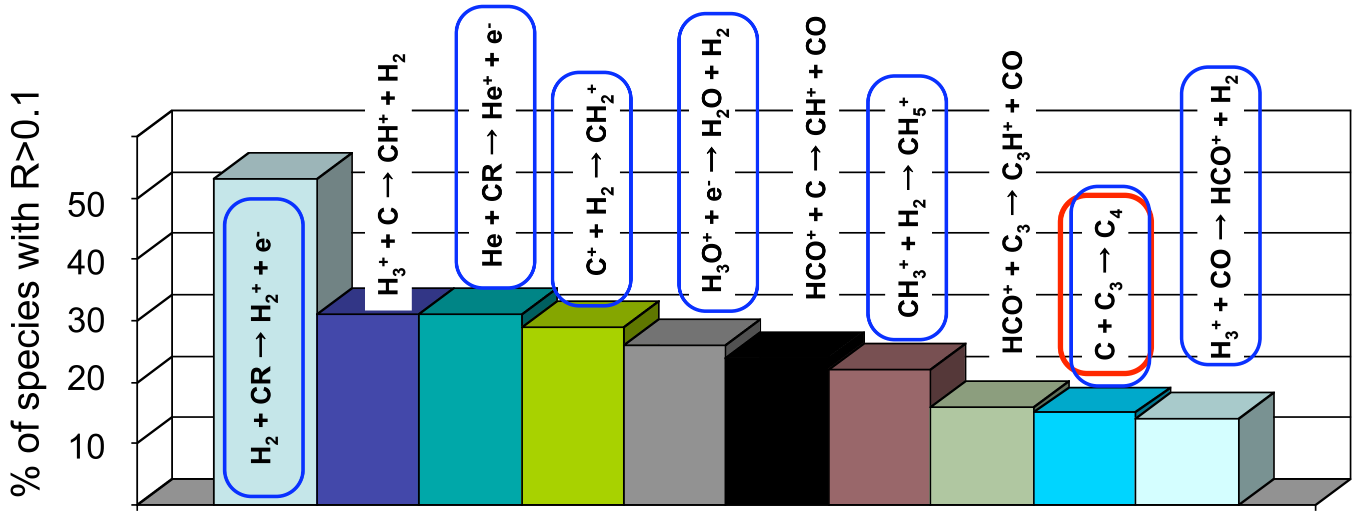
Pearson correlation coefficients

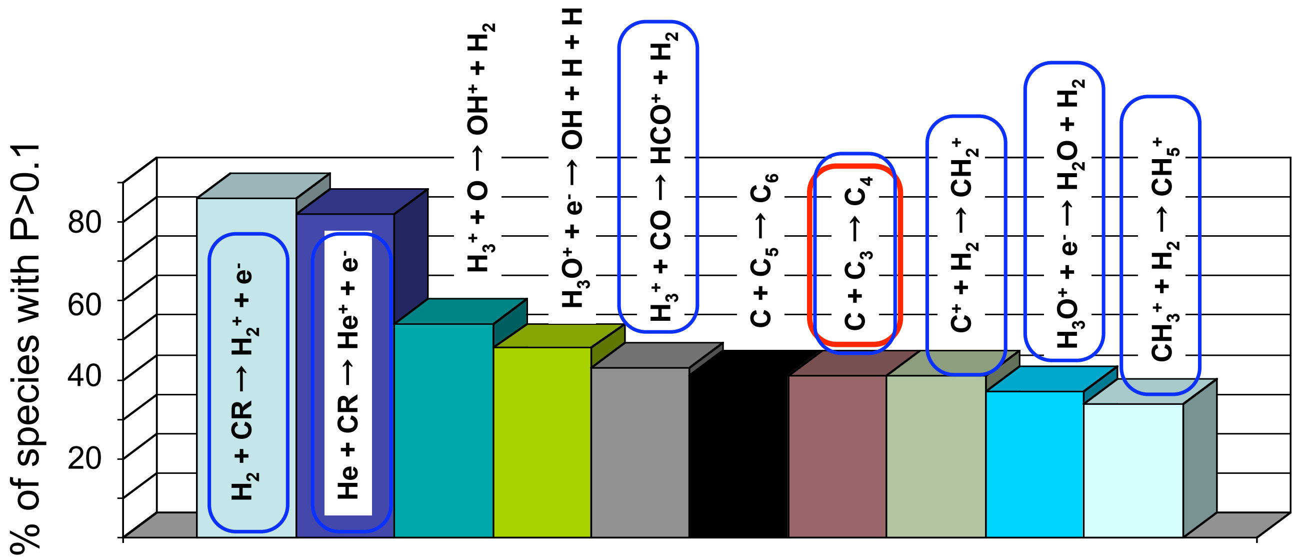
Random modification of all rate coefficients at the same time in their uncertainty range → results of the uncertainty calculations

$$P_j^i(t) = \frac{\sum^l (X_j^l - \bar{X}_j)(k_i^l - \bar{k_i})}{\sqrt{(\sum^l (X_j^l - \bar{X}_j)^2 \sum^l (k_i^l - \bar{k_i})^2}}$$

X abundance species, $\overline{X}$ mean abundance
k rate coefficient, $\overline{k}$ mean rate coefficient

Comparison methods 1 and 2
The 10 most important reactions





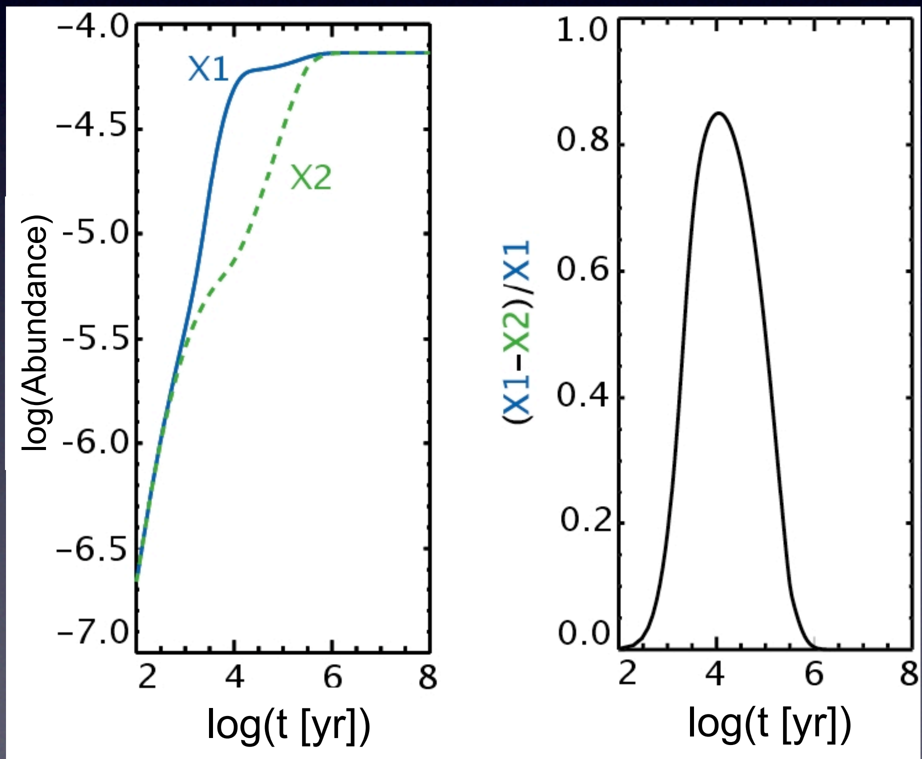
Example: Reaction $C + C_3 \rightarrow C_4$

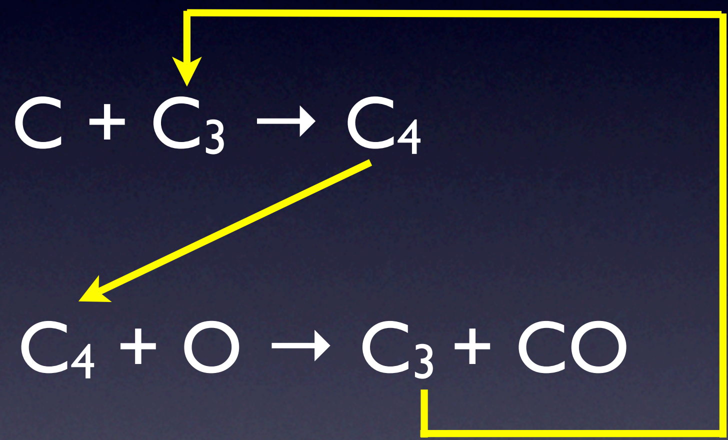
Previous value of k: 10^{-10} $s^{-1}cm^{-3}$ Smith et al. (2004)

Proposed new value: ~10^{-12} $s^{-1}cm^{-3}$

k1
k2

CO abundance as a function of time





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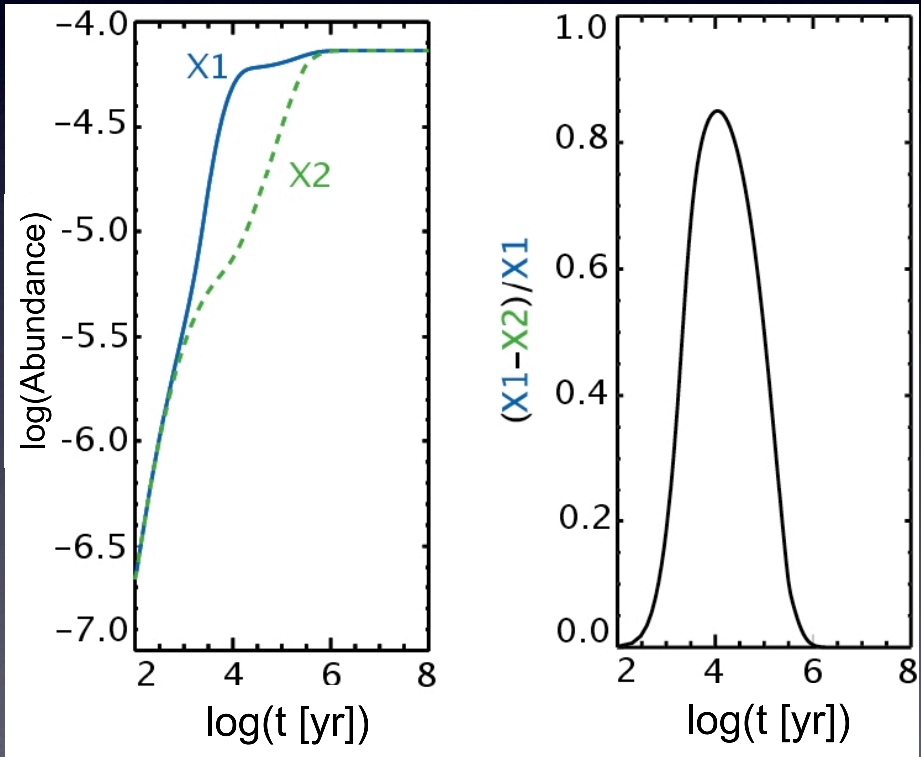

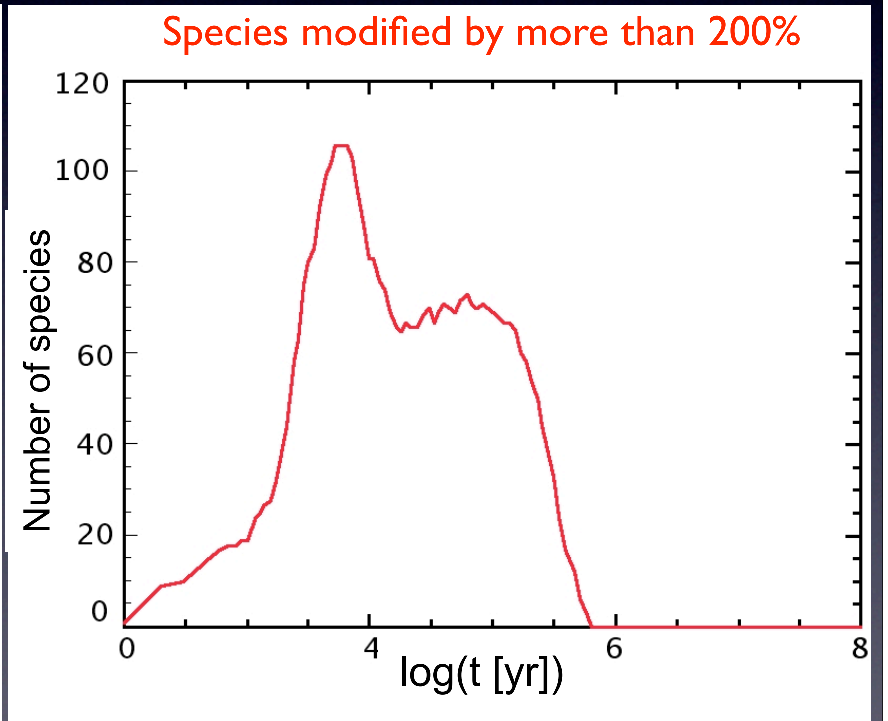

The main problem: the definition of the rate coefficient uncertainties