A multiphase Monte Carlo model of gas-grain chemistry

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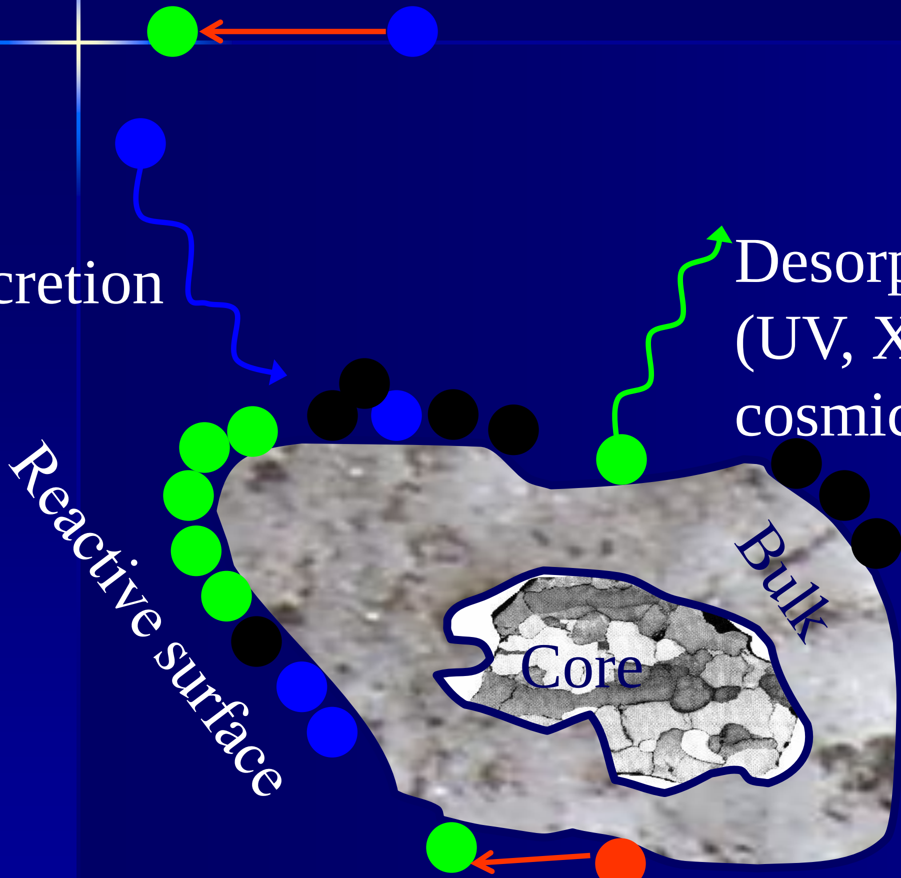
Formation and Destruction of Molecules

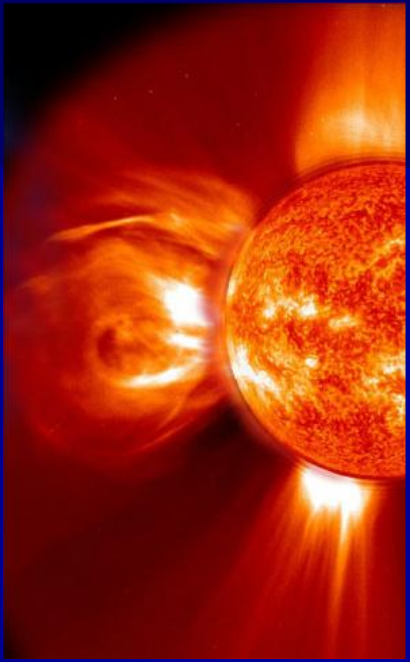
Collisions in gas phase

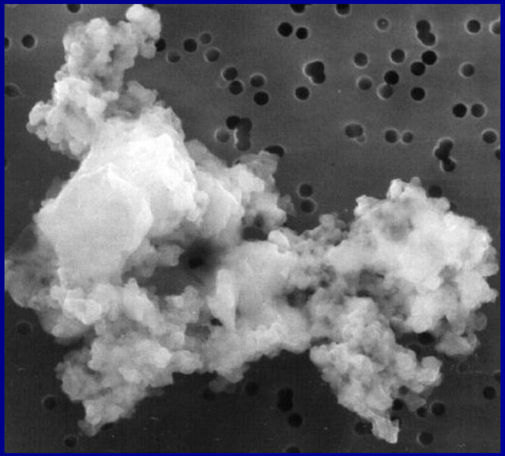
Accretion

Desorption (UV, X-ray, cosmic rays)



Surface reaction (thermal hopping, tunneling)





Based on a slide of D.Semenov

Observational and laboratory studies of ices:

Gibb et al. 2000

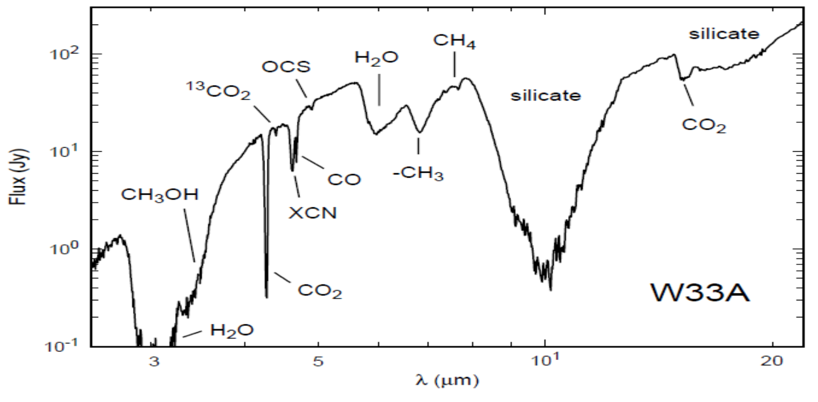
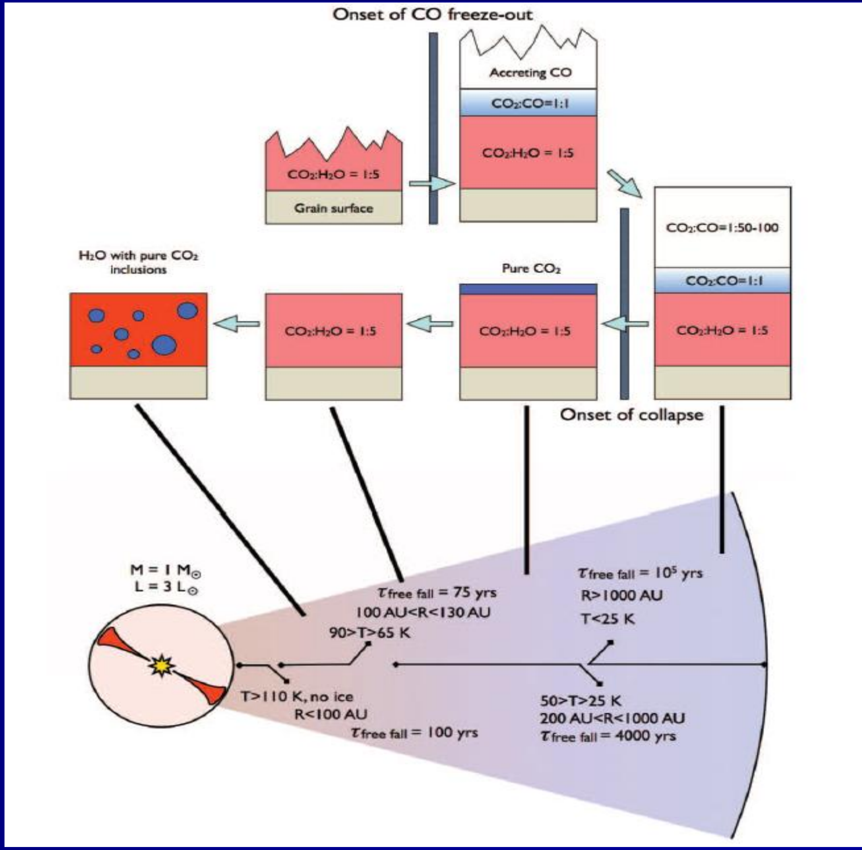


Figure 1 The ISO-SWS spectrum toward the protostar W33A (taken from Gibb et al 2000, Langer et al 2000). This cold and dense line of sight is characterized by large column densities of interstellar ices. Dominant absorption bands are visible at 3.0 μm (H_2O ice), 4.27 μm (CO_2 ice), 4.67 μm (CO ice), and 10 μm (silicates). The spectrum between 2 and 25 μm shows several additional species, many of them organic in nature.

Pontoppidan et al. 2008



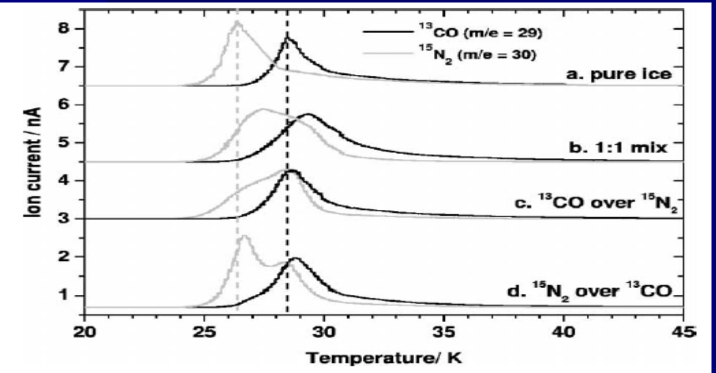


FIG. 1.—TPD spectra of (*a*) pure CO (40 L) and N_2 (40 L), (*b*) an intimately mixed equimolar CO-N_2 ice (80 L total exposure), (*c*) an N_2 layer (40 L) over a CO layer (40 L), and (*d*) a CO layer (40 L) over an N_2 layer (40 L). The ^{13}CO (m/e = 29) traces are in black; $^{15}N_2$ (m/e = 30) traces are in gray. The heating rate is 0.1 K $minute^{-1}$. The two dashed lines are superposed on the plot to show the positions of the desorption peaks of the 40 L pure samples of N_2 (*gray*) and CO (*black*).

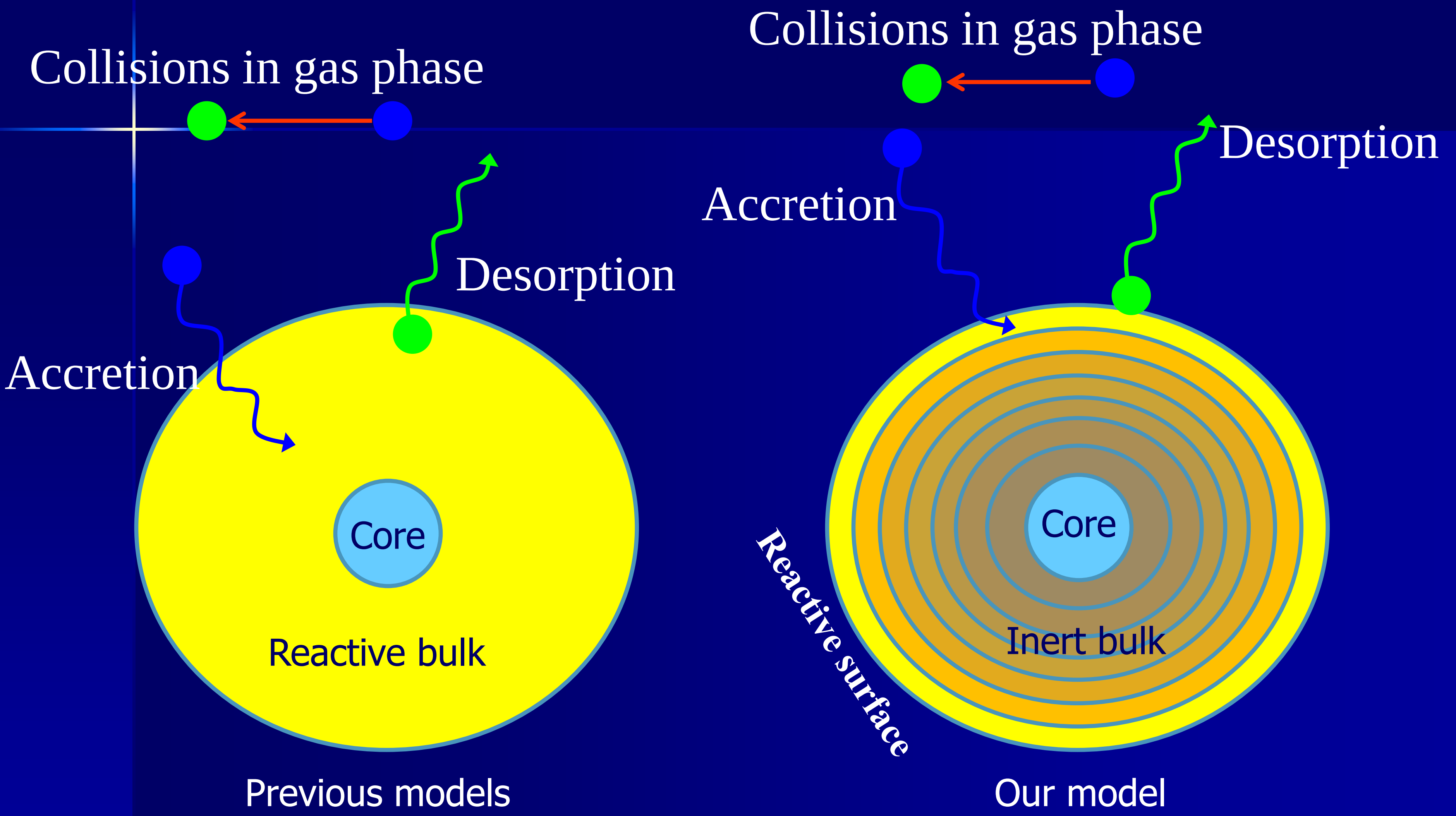
Öberg et al. 2005-2010

Motivation:

Complex structure of ice mantles (H_2O:CO:CO_2) and its variation with physical conditions revealed with observations (e.g., van Dishoeck 2004, Bergin et al. 2005, Pontoppidan et al. 2008)

Laboratory studies of ices (Öberg et al. 2005-2010, Fayolle et al. 2011): zero-order desorption, ice segregation, entrapment of volatiles in H_2O ice – processes not included in rate-equations models

Our model vs. previous models:



Previous work:

- Tielens & Hagen (1982)
- Hasegawa & Herbst (1993)
- Charnley (1997, 2001), - also a poster here
- Viti et al. (2004)
- Collins et al. (2004)
- Cuppen et al. (2005 - 2010)
- Vasyunin et al. (2009)

The aim of the current study:

- To simulate the coupled gas-grain chemistry, taking into account the multi-layered structure of a grain mantle as well as recent lab results on ice properties

- To assess the impact of the new approach on the results of astrochemical modeling

The MONACO code:

(Vasyunin et al. 2008, Vasyunin et al. 2011 in prep.)

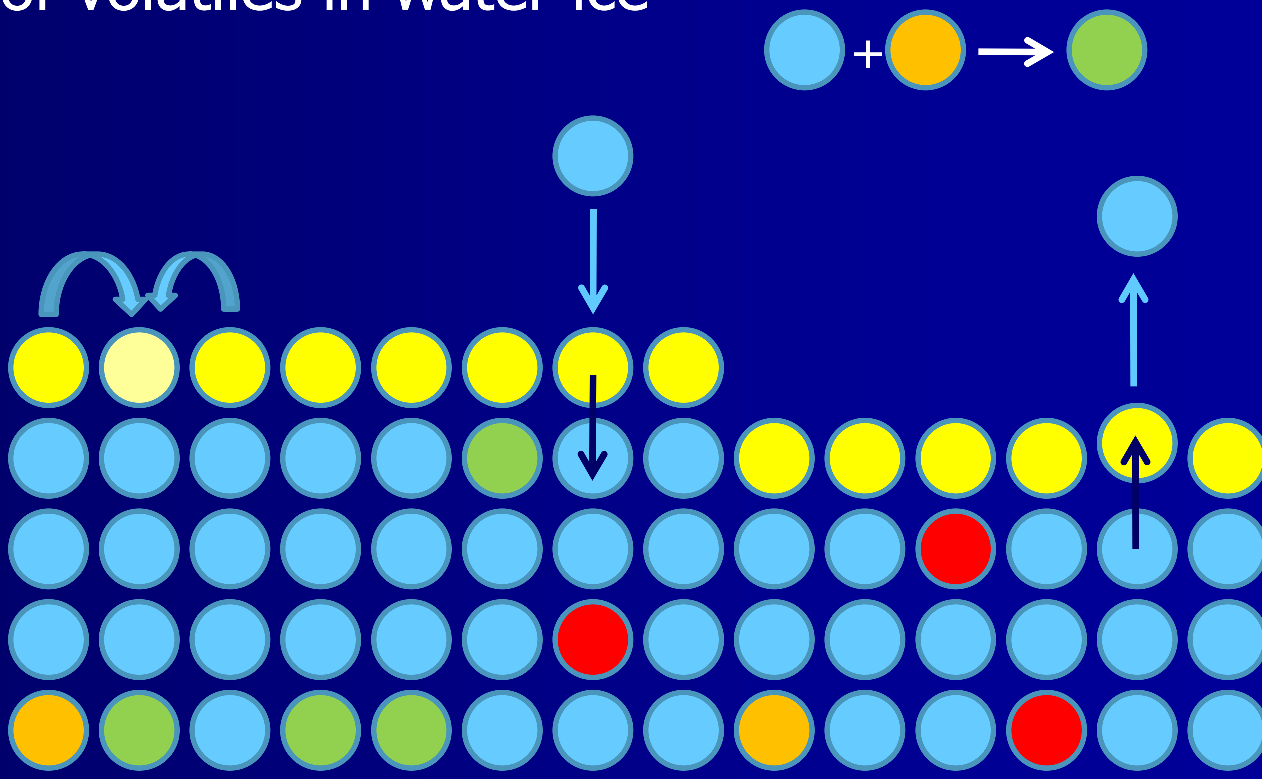
- Exact Monte Carlo treatment of both surface and gas-phase reactions, based on the KIDA database (Administrator: V. Wakelam, the latest published version: Semenov et al. 2010)
- Time-dependent layer-by-layer tracking of the structure of the ice mantle

The MONACO code: details of the model

Reactive surface vs. inert bulk

Zeroth-order desorption of species

Entrapment of volatiles in water ice

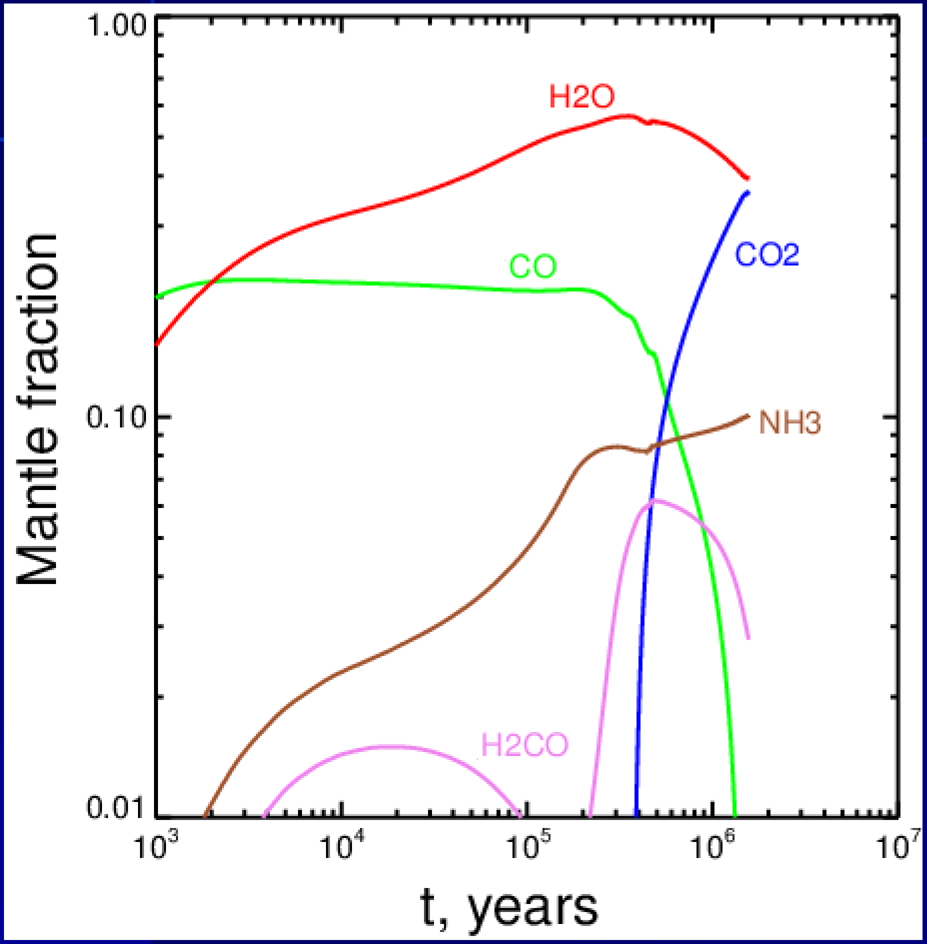


Warm-up chemistry with multiphase model

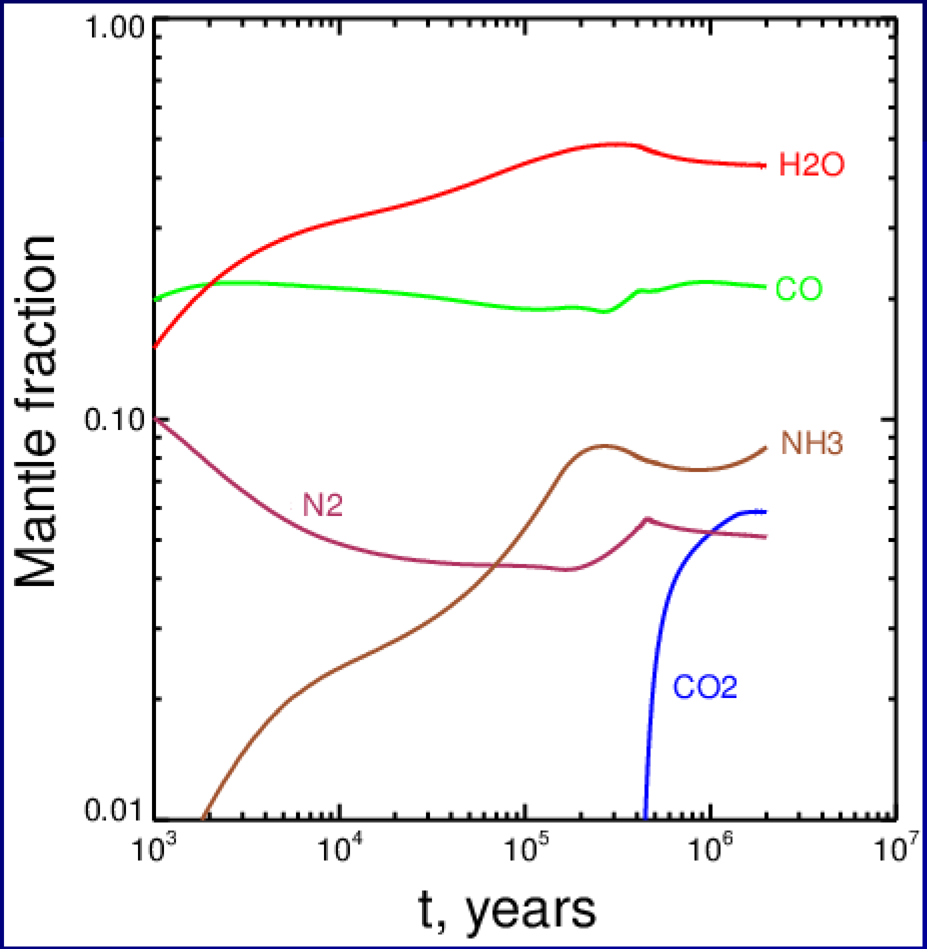
- Early warm-up from 10K to 20K ($3 \cdot 10^5$ years), then plateau for 10^6 years, $n_H = 10^4$ cm^{-3}.

- Late warm-up: constant temperature 10K over 10^6 years, then quick ($2 \cdot 10^5$ years) heat-up to 200K, $n_H = 10^4$ cm^{-3}.

Early warm-up: two-phase vs. multiphase model:



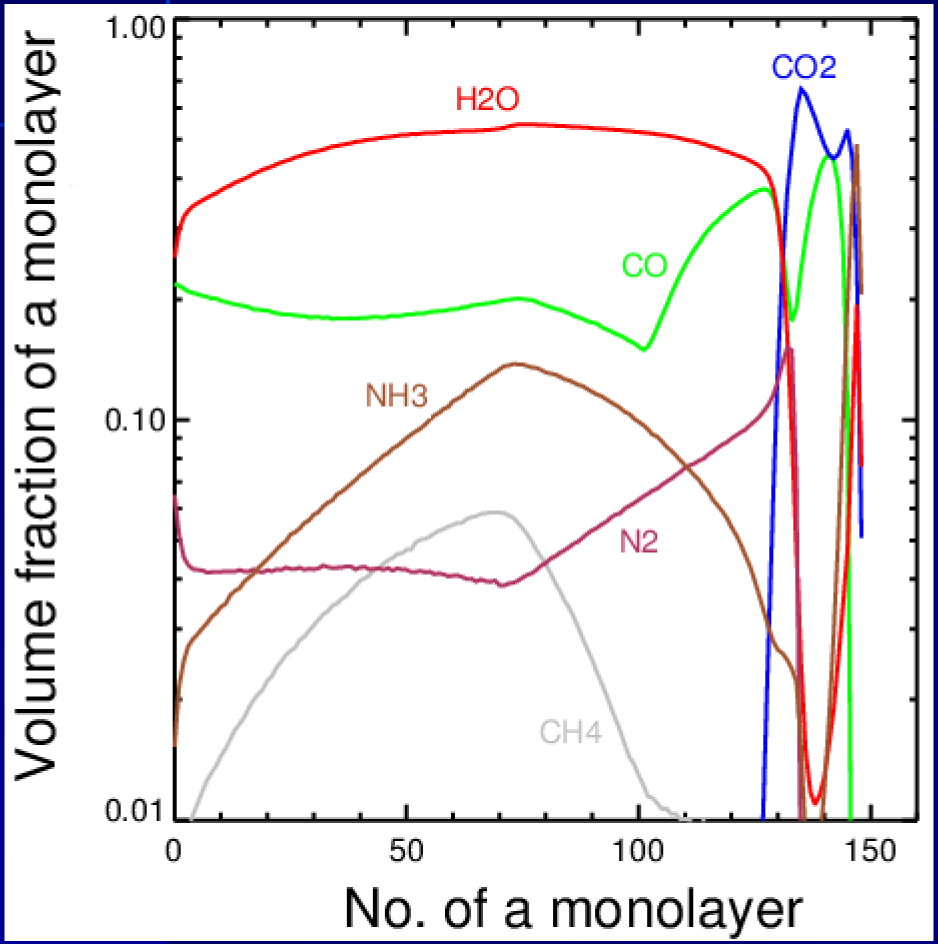
Standard two-phase model

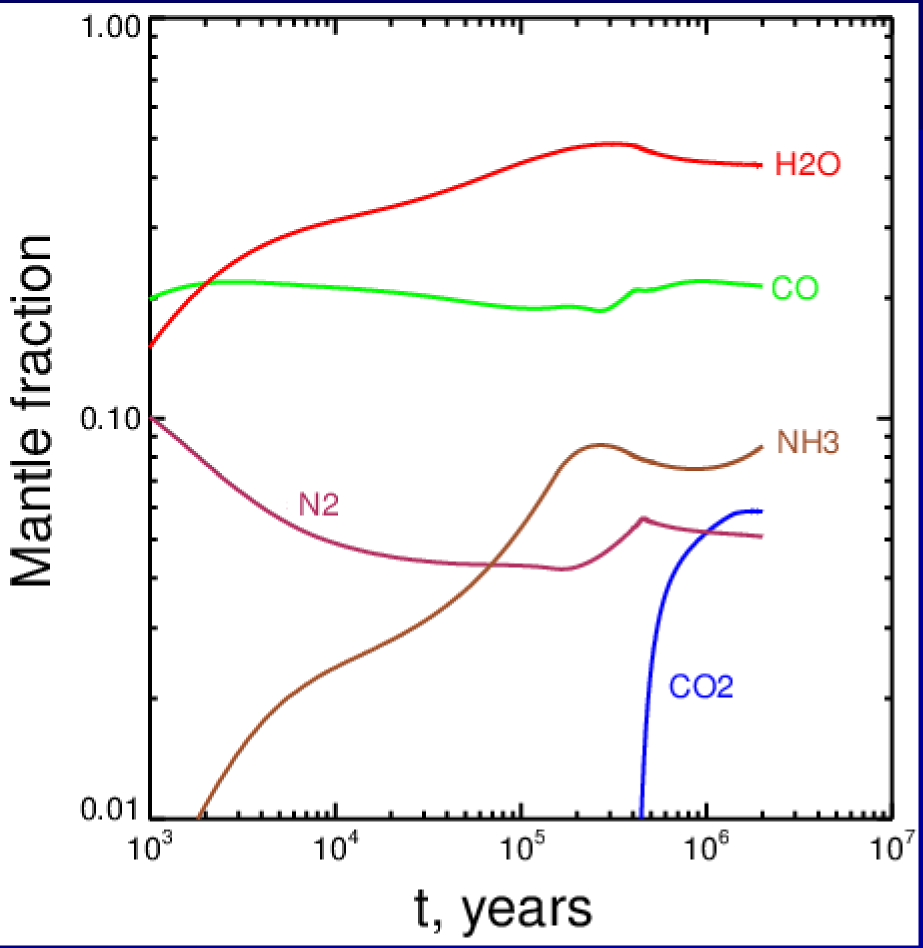


Multiphase model

Good agreement with obs. data in e.g. Zasowski et al. 2009

Early warm-up: multiphase model

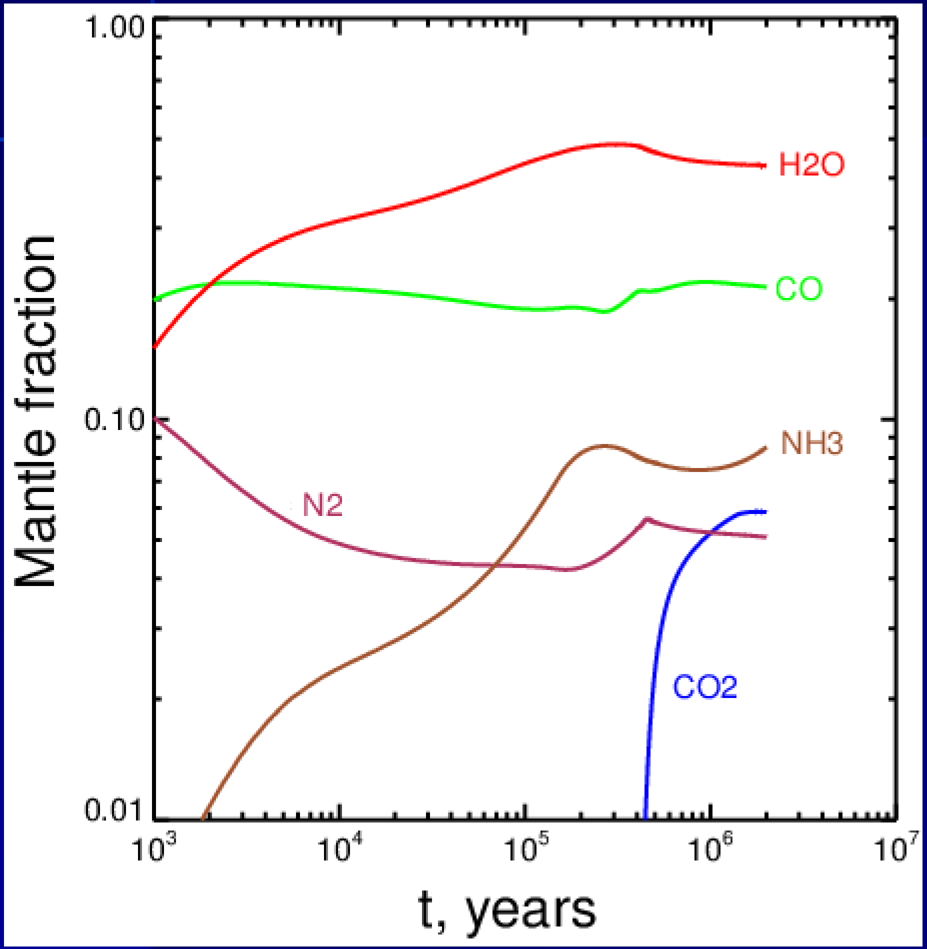


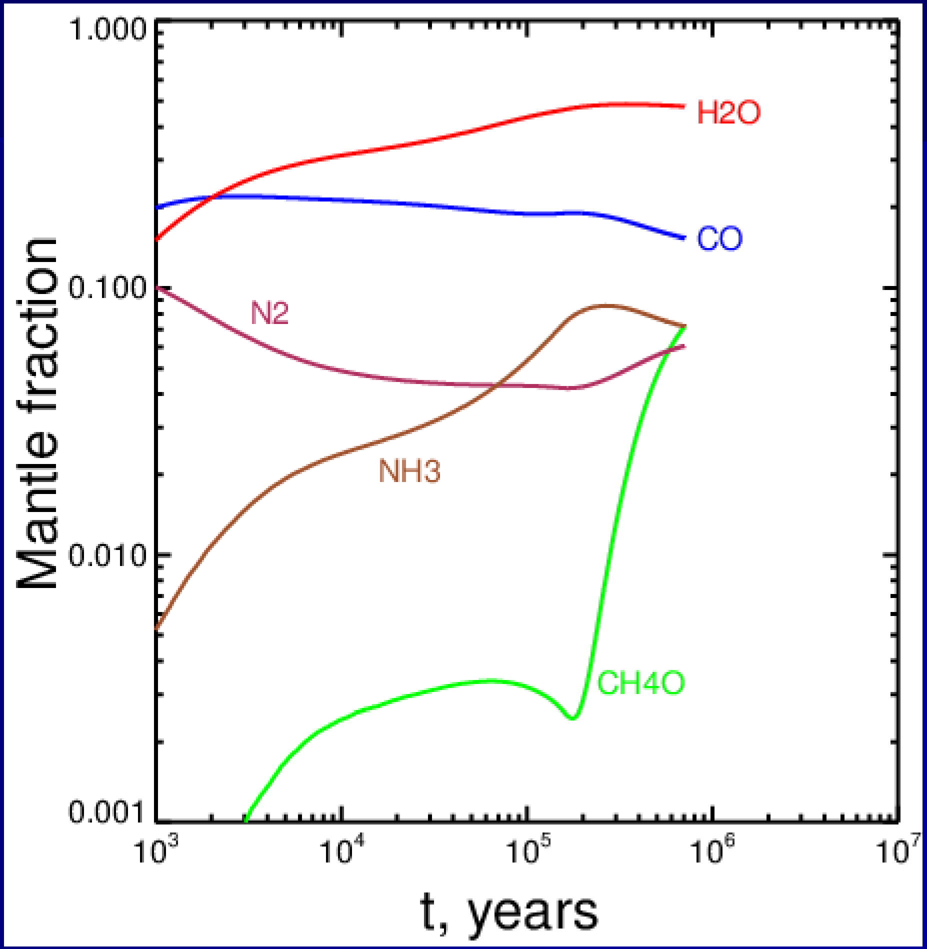


Individual monolayers

The bulk

Ice composition: importance of heating history





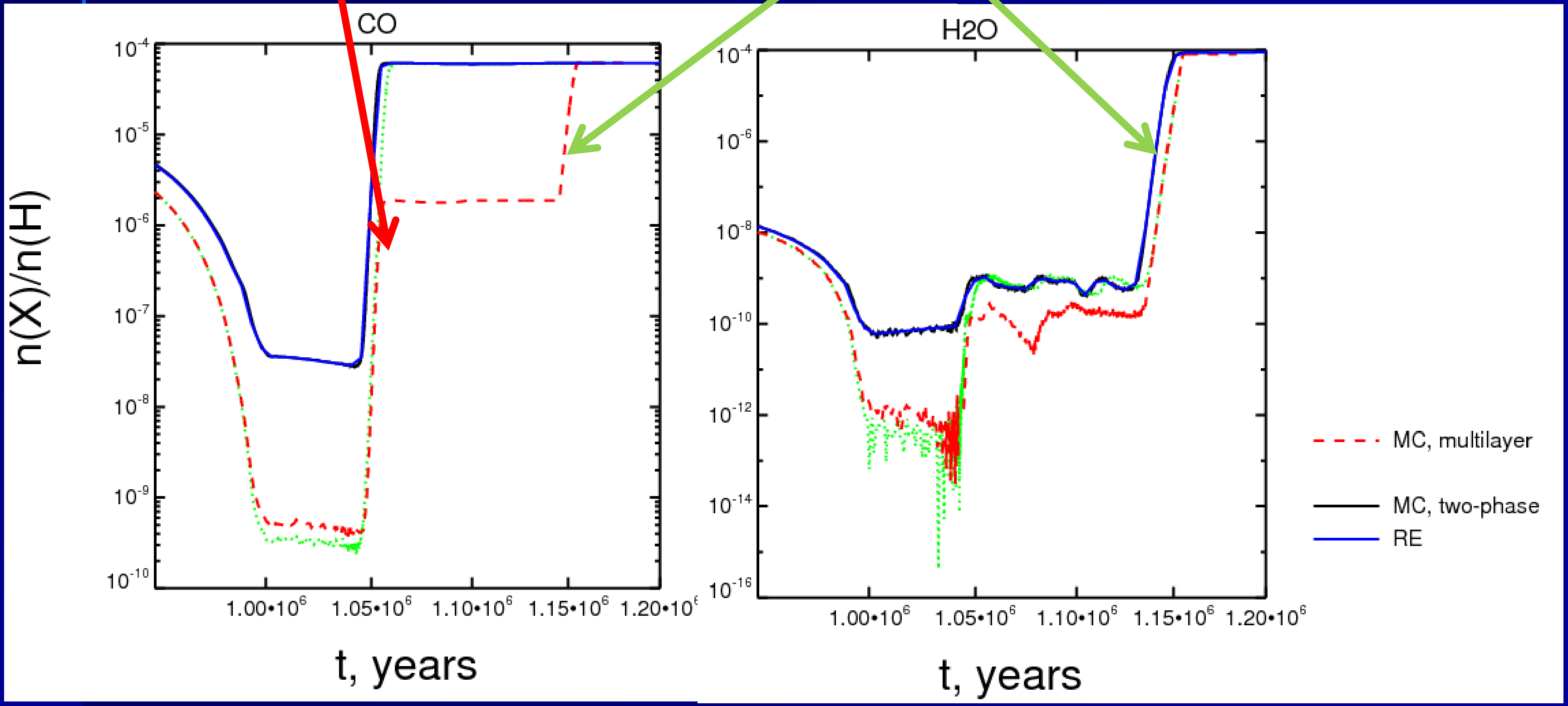
Early warm-up

Late warm-up

Gas-phase abundances: CO and H_2O

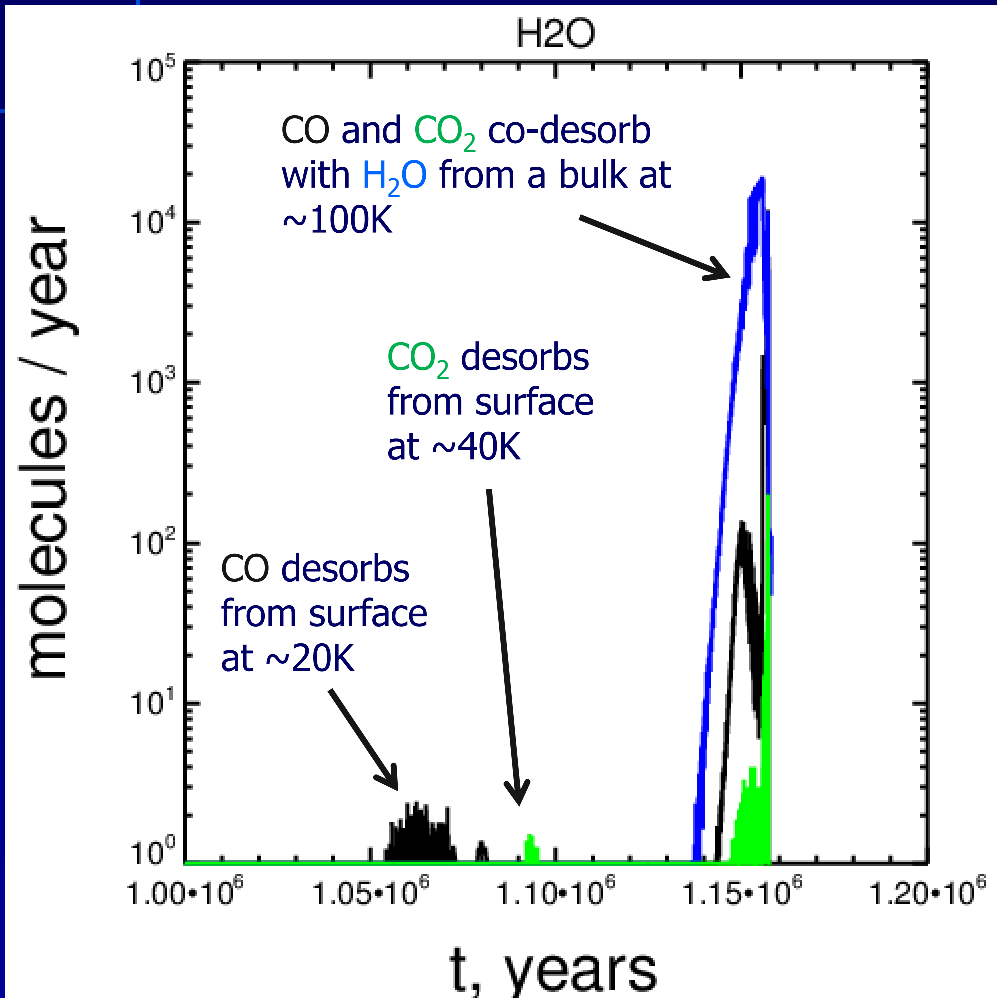
CO desorbs from the surface of mantle

CO and H_2O co-desorb from the bulk



Late warm-up

Desorption of volatiles at late warm-up:



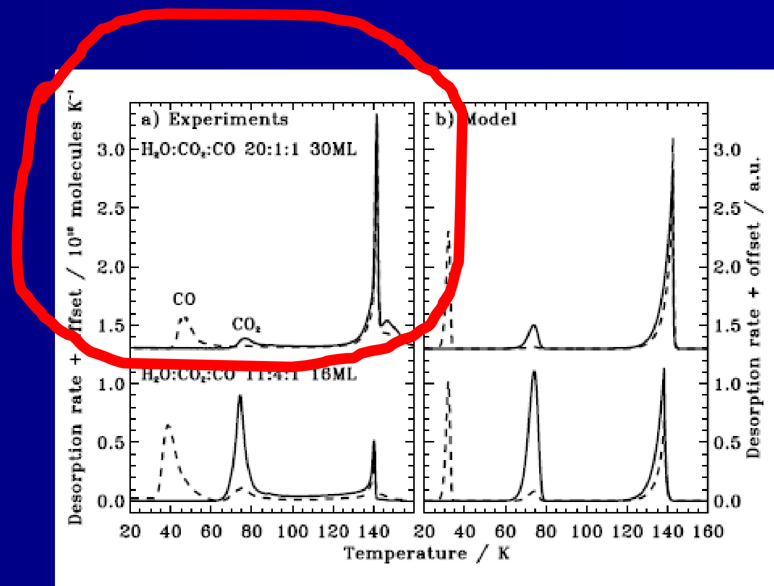


Fig. 4. a) Desorption rate of CO_2 (solid line) and CO (dashed line) from two tertiary water dominated ice mixtures (Exps. 18 and 19) with a 1 $K.min^{-1}$ heating rate. – b) Implemented three-phase model desorption rate for the same eperiments.

Fayolle et al. 2011

Conclusions:

- A multiphase Monte Carlo code MONACO is developed, which allows to simulate full-scale chemistry in the ISM with account for "multilayer" structure of a grain mantle and several recent experimental findings
- Layer-by-layer modeling of an ice mantle growth allows to reproduce observed abundances of its major constituents
- Warm-up history is of crucial importance for the final composition of ice
- Entrapment of volatiles in water ice may affect abundances of gas-phase species in warm environments

Thank you for your attention!