

FORMATION OF LAYERED VS. MIXED ICES IN PROTO-PLANETARY ENVIRONMENTS. M. N. Barnett¹ and F. J. Ciesla¹, ¹The University of Chicago, Department of Geophysical Sciences (meganbarnett@uchicago.edu)

Introduction: Protoplanetary disks are an initial incubator for complex organic molecules, which can then be incorporated into forming planets and be available for biological processes over time. As more organic molecules are being detected in proto-planetary disks [1-3] it is more important than ever to understand the formation of these organic molecules during the various environments that would exist during planet formation.

Organic molecules can form either in gas phase or grain-surface reactions [4]. In a recent study, CH₃CN formation is suggested to be primarily grain-surface reaction based [5] and this may be true for many other organic molecules formed in disks, provided the reactants are able to find one another. As such, understanding the structures and compositions of the ice mantles around dust grains is necessary to understanding organic molecule synthesis during planet formation.

Here, we seek to characterize the extent to which mixed ices and layered ices would form in various molecular cloud and protoplanetary disk environments. We focus on studying how simple molecules with a range of volatilities freeze-out and are distributed under a variety of physical environments. We then use this to evaluate which of these environments could support grain-surface reactions or grain-gas reactions which could form organic molecules.

Methods: We use the Astrochem chemical modeling code [6] to simulate the chemical reactions that would occur at different number densities of hydrogen and temperatures. To start, we use a simplified chemical network selected from the UMIST12 version 2 database [7], focusing on thermal desorption off the grain, freeze out, and UV driven photo-desorption. This is so we can isolate only the processes and resulting formulation/destruction of ice mantles and their compositions without separate grain surface and gas-grain reactions occurring during model evolution, which we will explore in future studies.

For each set of initial conditions we compare two sets of molecules, N₂-CO as examples of species with similar volatilities [8] and H₂O-CO as examples of those with very different volatilities. Each species begins entirely in the vapor phase at the start of evolution, and the behavior of each molecule in both vapor and ice phase is tracked for 1 million years. We start by exploring the evolution under static conditions holding the gas/grain temperature, optical depth, UV irradiation field (Go), and total abundances of all species and dust grains constant throughout evolution.

For each model, during evolution, the ratio of the abundances of each species in the deposited ice is

determined at each time step. We focus on the ratio during the timestep where the greatest increase in the ice layer occurs to determine whether the ice is mixed or layered. The initial ratio of abundances of the species is defined as $\chi_0 = \frac{n_{\text{species } 1}}{n_{\text{species } 2}}$, and the resulting contour maps of the models display the concentration enrichment factor in terms of χ_0 . Ice is considered mixed when the ratio of ice creation of the two species approaches the initial ratio of abundances of the species in the vapor phase. Conversely, ice is considered layered when the ratio of the two species at maximum ice creation is very large compared to the initial vapor abundance ratio, indicating that the ice is dominated by one species.

Initial Results and Discussion: For our ice evolution models, we consider a different range of temperatures for the N₂-CO system vs. the H₂O-CO system. For the N₂-CO models, we consider a range of temperatures from 14 to 20K, while we consider a temperature range between 8 and 35K for the H₂O-CO models. For both sets of models we consider a range of n_H values between 10⁵ and 10¹³ [cm⁻³], and we consider a range of UV irradiation values from 0 Go to 100 Go. This range of conditions is meant to simulate all possible conditions seen in molecular clouds and protoplanetary disks.

Figures 1 and 2 show the results of our models for the N₂-CO and H₂O-CO systems respectively. Not surprisingly, the temperature where ices transition from mixed (red) to layered (blue) is a strong function of gas density, and correlates to the freeze-out temperature of the less volatile molecule. In some cases, it is possible that trapping of the less volatile species allows ices to be effectively mixed at conditions where layered ices would form. This would likely be the case at the higher gas densities, where very high deposition rates were possible [9], something we are working to quantify.

These findings show that the formation location or history of ice mantles will play a critical role in determining the structure of the ices and the types of chemistry that could occur. If mixed ices are needed to allow particular chemical reactions to occur, then these ices must form in conditions where deposition occurs at temperatures below the freeze-out temperature of the most volatile species of interest. That is, if interactions between molecules of different volatilities on grain surfaces are important (such as those that might lead to organic production through UV irradiation [e.g. 10]), then these ices must have formed at very low temperatures. If instead, the ices formed through slow, gradual cooling of a system, the less volatile species would freeze-out first, followed by the freeze-out of the more volatile

species, yielding a layered structure. This would limit the interactions that could occur between them, and thus the types of chemistry that would be permitted.

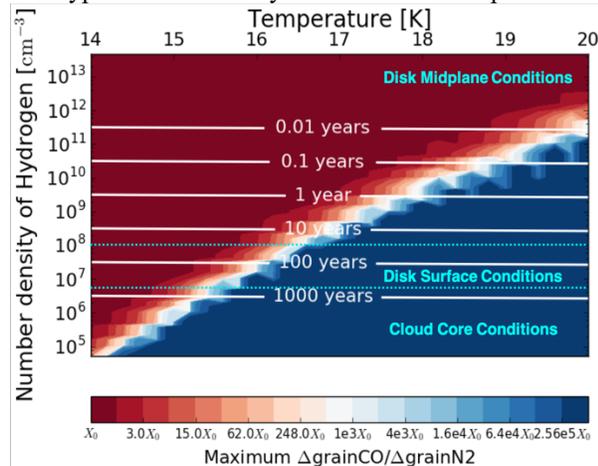


Figure 1: CO to N_2 ratios in the ice at times of maximum deposition for a range of temperatures and gas densities. All models contain no UV radiation. The white contour lines mark various freeze out timescales for the models. The cyan dotted lines indicate boundaries for different environments in the disk, labeled in cyan [11].

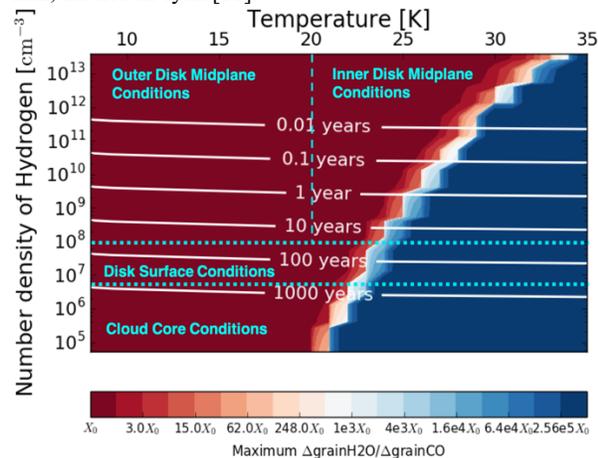


Figure 2: Same as Figure 1, but for CO and H_2O . The dashed cyan line marks the boundary between the outer disk midplane conditions and the inner disk midplane conditions, which we define as the CO snow line ($\sim 20K$) [11].

UV photons can greatly affect the structures that develop, particularly at low hydrogen gas densities. In these cases, photo-desorption effectively removes molecules that have frozen out on grain surfaces, independent of volatility. This is shown in Figure 3, where UV introduces an additional removal mechanism for frozen out molecules, preventing mixed ice mantles from forming in low density environments, leaving either pure ices of lower volatility or mixed films on grain surfaces.

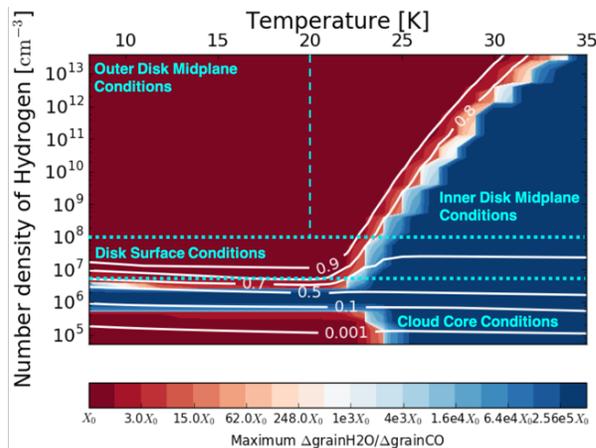


Figure 3: H_2O to CO ice compositions as in Fig 2 with incident UV irradiation of 100 Go. Solid white contour lines show total fraction of H_2O and CO deposited after 1 Myr.

Future Work: Our above results include only ices that develop in static environments. However, in protoplanetary disks, grains will be migrating from one environment to the next, which may impact the forming ice structures. To follow up on our initial results, we will combine our chemical model to investigate the evolution that occurs as grains are turbulently mixed within a protoplanetary disk, tracking the conditions that they are exposed to [12,13]. As shown in Figures 1 and 2, areas of the disk have different freeze-out timescales which means that the timescale of dust particle movement can vary the ice mantle composition dramatically.

In using a dynamical model, we can predict both the composition of the ice mantle on the moving dust grains, but also the real-time chemistry that would occur on the grain surface and in the gas. We will expand the chemical network to include grain-surface reactions between species in the ice. Through this method, we will investigate how much dust grain movement affects the molecules ultimately created through the dust grain evolution, and how dust grain movement can potentially transport these molecules to other sections of the disk.

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