CHEMICAL AND PHYSICAL PROCESSING OF ICES IN A DYNAMIC SOLAR NEBULA. F. J. Ciesla[1], [1]Department of the Geophysical Sciences, University of Chicago, 5734 South Ellis Avenue, Chicago IL 60637 (fciesla@uchicago.edu).

Introduction: Ciesla and Sandford [1] suggested that organic molecules could have formed via irradiation and warming of ices in the outer solar nebula. In their model, turbulence carried icy grains through a variety of nebular environments which exhibted a wide range of temperatures and radiation fluxes. In the very upper regions of the nebula, the radiation flux seen by the icy particles were often orders of magnitude greater than what would have been seen at the disk midplane. While the residence time in these regions of the solar nebula at any given time may have been brief, the integrated effects of migrating in and out of such environments may still have been sufficient to break molecular bonds and allow more complex species to form from the resulting ions and radicals [1].

While Ciesla and Sandford demonstrated that icy grains could receive the needed UV dosage to produce organic molecules, the detailed chemical evolution of the ices over the course of the particles' lifetimes were not considered. Here we couple the particle-tracking methods for calculating the dynamical evolution of grains in the solar nebula [1-4] with chemical models for the evolution of ices in the outer solar nebula [5,6] to explore in detail how icy grains would be affected by their transport prior in various regions of the solar nebula, and where the needed C, H, O, and N would be retained in the ices of the grains to allow organic species to form in this manner.

Motivation: Experiments have shown that the total UV fluences seen by the grains in the model of [1] would have been sufficient to break apart the molecular bonds of the ices on the surface, allowing the resulting ions and radicals to reform into more complex organic species. Ultraviolet irradiation of ices could also have a number of other effects on the chemical and physical properties of the ices on these grains. In addition to breaking molecular bonds, UV photons could lead to the photodesorption of frozen-out species or induce structural changes in the solids with which they interact. Further, the higher temperatures that would be present at disk surfaces could also lead to changes in the icy grains. Temperatures at the disk surface in the outer disk may be tens of K greater than the temperatures in the disk midplane due to this region being directly irradiated by the central star [7]. Thus volatile species which were frozen out on a dust grain at the disk midplane may become thermally desorbed, and lost from the grain, while at higher altitudes.

Model: To explore the detailed chemical evolution of ices on a dynamically evolving micron-sized grain within a protoplanetary disk, we use the disk model of [8], where a 2D azimuthally symmetric disk is assumed, with the UV radiation intensity determined everywhere. We then apply the particle-tracking methods of [1-4], to follow the paths of particles released at various points in the protoplanetary disk. The particles evolve for a period of 10^5-10^6 years, and we track the pressure, temperature, and radiation flux that each particle sees throughout this period.

We then apply a chemical model which determines how water and carbon monoxide are exchanged between the ice mantle and surrounding nebular gas. As a starting point, each species is allowed to behave as a pure substance—no trapping of CO in the water ice of any form is assumed. The binding energy of each molecule for thermal desorption calculations is taken from the latest UMIST database [6], while the photodesorption yields are taken to be Y=0.001 [9,10]. Abundances of CO and H_2O were calculated from the molecular abundance ratios of Lodders [11].

Results: Figure 1 shows the environmental conditions seen by one particle in the simulation over the first 10^4 years of the calculation (more time was calculated but file size limitations prevent showing the full evolution here). This particle was released at the disk midplane 50 AU from the central star. The temperatures and UV field that the particle was exposed to during this time are shown. Figure 2 shows the fraction of the original H2O and CO remaining on the grain throughout this evolution.

Due to the higher binding energy of water compared to CO (E/k=5300 and 1150 K, respectively [6]) water survives on the grain more readily than CO, which is lost from the grain when it gets lofted to sufficient heights above the disk midplane, where UV fluxes and temperatures are higher—a correlation with CO fraction on the grain and environmental conditions is readily seen. The grain shown here is lofted to regions with higher temperatures and UV fluxes than seen in the first 10^4 years shown here. These later excursions lead to greater loss of CO, but also to reaccumulation of the CO as it freezes out again on the surface of the particles.

Additional particles have been considered, with particles originating at various locations in the disk. All particles migrate in and out of the hot, high UV flux regions of the disk, leading to loss of volatiles from their surface and the reaccumulation of those volatiles on their surface closer to the midplane.

Discussion: The photoprocessing of ices that results from grains migrating through a range of environments within a protoplanetary disk will lead to the desorption and freezing-out again of volatile species. Complex organic formation will occur provided that these ices retain some C, H, O, N during irradiation. Retention of the most volatile species (CO, HCN, N_2) is easiest at very low temperatures, far from the central star, where temperatures and UV fluxes are low. However, turbulence in the outer disk would lead to grains being brought to regions where such species would likely be lost.

This loss would difficult to prevent if such species were present in their pure form. However, trapping of volatiles in water ice will likely lead to greater retention of these volatiles [12], something that will be considered in the next stages of the model. Further, as the molecules are liberated from the grain, they will undergo further reactions driven by UV photons in the gas phase. This could allow for the formation of other molecular species which would then freeze out onto the dust grains again. This, too, will be the focus of the next stages of development of this model.

Summary: Some of the most volatile molecules to condense onto grains in the solar nebula, such as CO, are likely to be lost as those grains migrate to the upper regions of a protoplanetary disk where temperatures and UV fluxes are much greater than would be found in the dark, cold midplane. Loss of such molecules could limit the yield or complexity of molecules formed in the manner outlined by Ciesla and Sandford [1]. However, water ice is effective at trapping these species, and would increase the retention of these molecules over what is seen when they are treated as pure substances. The next focus will be to determine where in the solar nebula such volatiles were retained and thus the spatial variations in volatile and organic content in primitive Solar System bodies.

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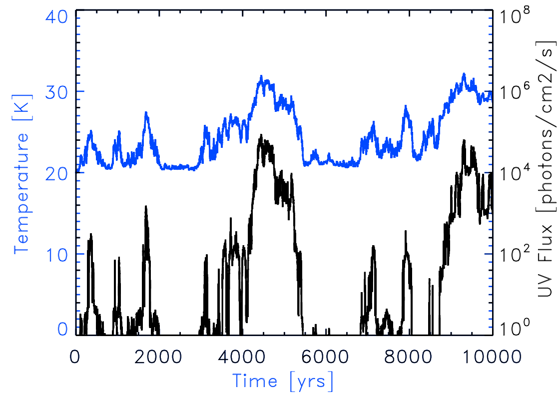

Figure 1: Temperature (blue, left axis) and UV flux (black, right axis) seen by a particle in the model for the first 10^4 years of its evolution (a subset of the calculated lifetime). The increases in temperature and UV flux correspond to times the particle is lofted above the disk midplane where irradiation from the central star is stronger (leading to higher fluxes of photons and greater warming of the disk).

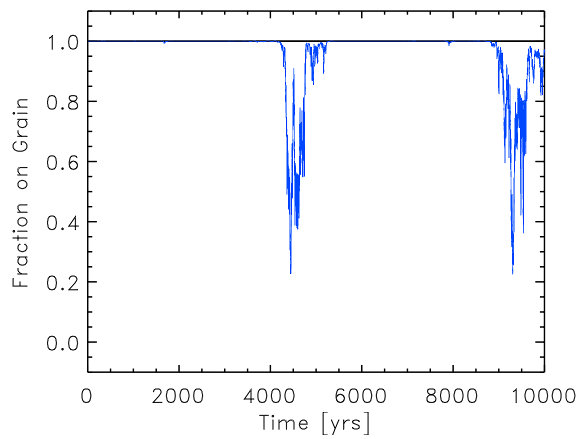

Figure 2: Fraction of H_2O (black) and CO (blue) molecules which remain on the grain migrating through the different environments shown in Figure 1. Note that the CO fraction on the grain drops sharply where temperatures and radiation intensities increase. Such behavior is expected for pure CO. CO which was trapped in the water would be retained more readily, and thus may be necessary for the formation of organics.