MIXED OR LAYERED ICES IN THE OUTER SOLAR NEBULA? F. J. Ciesla[1] and S. Krijt[1], [1]Department of the Geophysical Sciences; University of Chicago; 5734 South Ellis Avenue; Chicago IL 60637; USA (fciesla@uchicago.edu).

Introduction: A major uncertainty in our understanding of the astrochemical evolution of volatiles in the outer solar nebula is the structure of ices on the grains. Often times, ices are treated as being layered, with the most volatile species freezing out last, and thus on top of the less volatile ices. In other studies, the mantles are thought to be mixed, with all species being available to interact with the gas phase; the availability at the surface would just correspond to the abundance of the species in the icy mantle.

Whichever of these pictures is correct is important to discern in developing our understanding of volatile evolution during the early stages of planet formation. It is only the outer-most layers of ice that are able to interact with the surrounding gas or are subject to processes such as photodesorption [e.g. 1]. Further, the ability of certain volatiles to freeze-out onto solids is controlled by the composition of the available substrate. For example, CO is retained by solids much less efficiently when it is frozen out on top of other CO molecules than when it freezes out on top of H_2O [2,3]. Thus the chemical evolution of the outer solar nebula was likely set by the physical properties of the disk.

Here we investigate the formation of an ice mantle as two different species, H_2O and the much more volatile CO, freeze out and are desorbed from a grain as it migrates through the disk in order to determine the likely physical structure of ices in the disk and how this would impact the distribution of volatiles during the early stages of planet formation.

Methodology: As a starting point, we focus on the vertical transport of a grain at a given location of the disk; we will generalize this to two dimensions in the future. We follow the vertical transport] using particle-tracking methods [4,5] to follow how a grain moves through various heights in the disk. The disk is assumed to be in a steady-state with the gas-phase abundance of each species determined by the balance of freeze-out and desorption processes. We have considered a variety of disk structures and properties. For our discussion below, we focus on a region 50 AU from the proto-Sun, at a midplane temperature of 15 K, and with an ambient radiation field of equal to 300x that of the ISM. The vertical temperature profile of the disk is assumed to follow [6], in that below 2 scale heights, the temperature is equal to the midplane temperature and above 3 scale heights the temperature is 3x the midplane temperature. In between, the temperature is found by linear interpolation.

As the grain migrates through these various regions, the loss/gain of CO and H_2O are determined and updated accordingly. In order to track the behavior of each species, the ice covering on the refractory grain core is divided into a mantle and a surface, following [7]. Species on the surface can be exchanged with the gas through adsorption, thermal desorption, and photodesorption. Mantle species represent surface species which were buried under a newly adsorbed particle. Mantle species can migrate to the surface when a surface species is desorbed.

Results: Figure 1 shows the abundance of the respective species in the gas phase for the case described above. We have assumed that the ices in the disk are originally layered, with a water ice layer surrounding the refractory core and a CO ice layer surrounding it. As a result, water cannot begin to enter the gas phase until all of the CO is lost from the gain, which occurs around 7.5 AU (nearly 2 scale heights) above the disk midplane. If the ices were mixed, water would be more abundant around the disk midplane than assumed here. Thus this is the most conservative assumption.

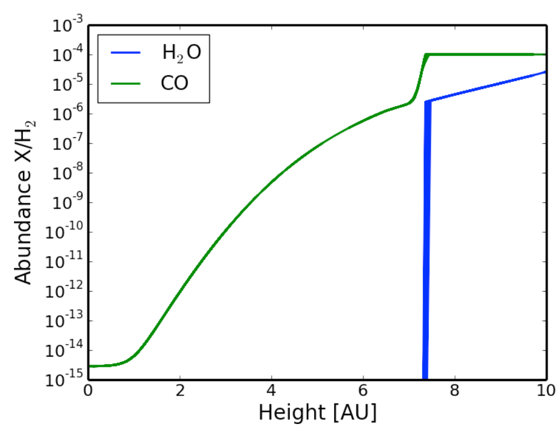

Figure 1: Plot of expected vapor abundances as a function of height above the disk midplane for the model described in the text.

Figure 2 shows the trajectory of a 1 μm grain in the disk, which starts slightly above 3 scale heights (~10.5 AU) at the beginning of the simulation. The grain undergoes a random walk in the disk due to the turbulence present (characterized by $\alpha=10^{-3}$), but largely migrates towards the disk midplane due to settling and the higher concentration of mass there [4].

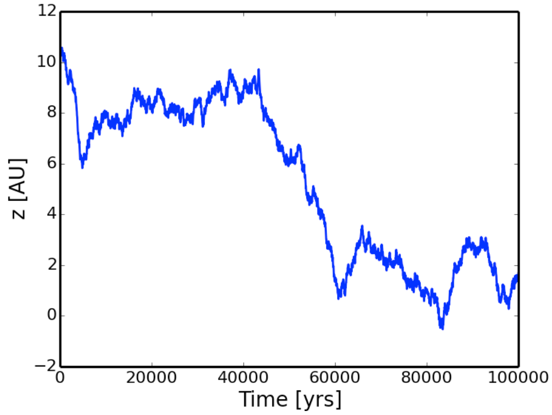

Figure 2: Time evolution of the particle's position above the disk midplane over time.

Comparing Figures 1 and 2, it is seen that the particle migrates above and below the region 7-8 AU above the disk midplane multiple times, providing multiple opportunities for the grain to experience times when freeze-out of solids (and loss from the grain as well). Figure 3 shows the trajectory with a log scale on the x-axis to focus on the early evolution of the particle and the addition of CO and H_2O over time. While water largely accumulates on the grain early, where temperatures are so high in the upper layers that CO does not freeze out, CO is rapidly added once the particle drops to the colder regions of the disk, a few thousand years into the simulation. At this point, it is largely CO that is freezing out, forming a layered structure, though trace amounts of water would be mixed into the CO. However, further upward migration brings the grain to the region where water freezes out on top of the CO layer, for a period lasting until roughly 400,000 years. The deposited water then further buries the CO, possibly trapping it as amorphous ice or leading to more mixing via diffusion within the ice mantle [7].

While all particles are expected to follow unique paths, the example here demonstrates that cycling of grains into the warm molecular-layer of the solar nebula can liberate volatile species and allow them to refreze again onto the grains. This would likely cause grains to evolve from a layered structure to a mixed ice structure over time. This effect would be particularly important for volatiles like CO and N_2, whose binding energies (freeze-out temperature) in layered ices (when they bond to themselves) is lower than when they are co-deposited with water in a mixed ice [3]. Thus this effect could effectively trap such volatiles to a greater extent than predicted in models. Further, the mixing of ices would be more significant for species with similar binding energies, rather than the strong differences for CO and H_2O assumed here. This could facilitate reactions between species trapped in ice mantles, and the production of organic molecules by bringing the species together in a water-rich environement [8]. We will continue to quantify this effect and investigate the ability of various ices to be mixed together in the solar nebula.

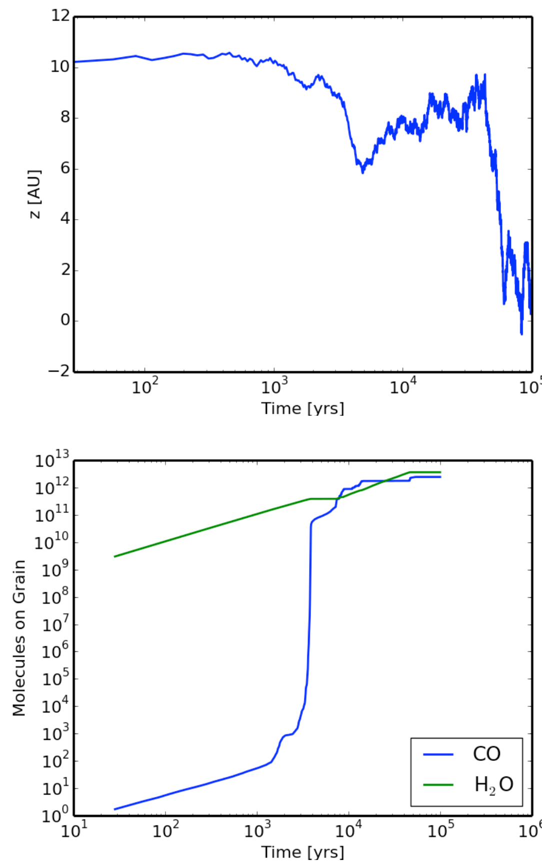

Figure 3: *Top*: Same as Figure 2, but a log scale on the x-axis to highlight the early dynamical behavior of the particle. *Bottom:* Total number of molecules frozen out in the icy mantle of the grain over time.The rapid freeze-out of CO corresponds to the rapid drop in the grains altitude a few thousand years into the simulation.

References: [1] Oberg K. et al. (2009) *A&A* 496, 281-293. [2] Cleeves L. et al. (2014) *Science* 345, 1590-1593. [3] Fayolle E. C. et al. (2016) *Astroph. J. Let.* 816, L28. [4] Ciesla F. J. (2010) *Astroph. J.* 723, 514-529. [5] Ciesla F. J. (2014) *Astroph. J. Let.* 784, L1. [6] Xu R. et al (2017) *Astroph. J.* 835, #162. [7] Fayolle E. C. et al. (2011) *A&A* 529, A74. [8] Fresneau A. et al. (2014) *MNRAS* 443, 2991-3000.