THE DISTRIBUTION OF ISOTOPICALLY HEAVY WATER IN AN EVOLVING SOLAR NEBULA

Le Yang[1], Fred J. Ciesla[1], James R. Lyons[2]. [1] Department of the Geophysical Sciences, The University of Chicago, 5734 South Ellis Avenue, Chicago IL 60637, USA (leyang@uchicago.edu); [2] Institute of Geophysics and Planetary Physics, UCLA, Los Angeles CA 90095, USA.

Introduction: Earth, Mars and the asteroids are enriched in heavy oxygen isotopes, ^{18}O and ^{17}O, compared to the average oxygen isotopic composition of the solar nebula [1], however the mechanism responsible for the ^{18}O (^{17}O) enrichment is still uncertain. Most primitive meteoritic materials, like refractory inclusions (CAIs and AOA) and chondrules in chondritic meteorites, plot near a slope-1 line in the oxygen three-isotope ($\delta^{17}O_{SMOW}$ − $\delta^{18}O_{SMOW}$) plot [2,3], leading to the suggestion that these materials record the mixing of ^{16}O-riched silicates with an isotopically heavier oxygen reservoir, probably isotopically heavy water [4,5].

Previous studies have suggested that water with a range of oxygen isotopic abundances could be produced through self-shielding photodissociation of CO in the parent molecular cloud [6] or in the outer solar nebula [7]. Once present in the solar nebula, this isotopically heavy water would be subject to viscous transport, which could bring it to the locations where meteoritic materials and terrestrial planets formed. Once there, that water could exchange heavy oxygen isotopes with primitive ^{16}O-rich materials [8].

Previously, we simulated the transport and mixing of water within a forming and evolving protoplanetary disk by adopting the H_2O and CO abundances and isotopic compositions in the infalling molecular cloud materials calculated by [6]. We found that the oxygen isotopic compositions of CO and water in the solar nebula varied significantly as materials were added to the disk, but the variations began to smooth out due to the dynamics associated with disk evolution after infall ended [9]. However, the CO and H_2O isotopic compositions were assumed to be preserved throughout the period of infall and mixing, which may not be valid given that isotopic exchange could occur through a variety of chemical reactions.

Here we continue to investigate how the concentrations and isotopic ratios in CO and H_2O that are inherited from the parent cloud vary with space and time in the disk, but also consider how the oxygen isotopic variations in the solar nebula would be affected by exchange between water and other gaseous oxygen-bearing species as they are transported during disk formation and evolution.

Model Description: We generally follow our previous study [9] which considered a disk forming within its parent molecular cloud core in a background of external ultraviolet radiation field. As the molecular cloud undergoes inside-out collapse, the abundances of CO and H_2O isotopologues vary with time due to self-shielding photodissociation of CO in the molecular cloud, and the details depend sensitively on the intensity of incident UV photons [6]. Water and CO isotopologues, along with other infalling materials, are added to the disk at locations which depend on the specific angular momentum that each parcel of material had in the parent cloud. Once incorporated into the disk, they would be redistributed in the solar nebula through viscous evolution [10].

Further, the concentrations and isotopic ratios in CO and H_2O would evolve in the solar nebula due to ^{18}O (^{17}O) exchange with ^{16}O between gaseous oxygen-bearing species, like $C^{16}O+^{18}OH \leftrightarrow C^{18}O+^{16}OH$, and $H_2{}^{18}O+^{16}OH \leftrightarrow H_2{}^{16}O+^{18}OH$. Here we consider only neutral-neutral reactions since our dynamical model focuses on the very early stages of disk evolution when the effects of photochemistry and cosmic ray induced chemistry would be diluted due to the high surface densities and optical depths of the disk. In the chemistry network, over 50 reactions involving 12 gaseous species are considered: H_2, H, OH, H_2O, O, O_2, CO, CO_2, C where the oxygen-bearing species are composed of both ^{16}O and ^{18}O isotopologues. All rate coefficients of those reactions are taken from [5,11]. As gaseous species see different temperatures and pressures throughout the course of disk evolution, the oxygen isotopic exchange would proceed at rates that depend on their locations in the disk.

Preliminary results: Results for the complete dynamical and chemical evolution of the species considered here continue to be collected. Here we discuss the physical evolution of the disk and how the chemistry would occur in singular disk environments in order to illustrate how the various conditions expected in the solar nebula would affect the isotopic properties of various species.

Figure 1 shows how the disk midplane temperature varies with distance from the Sun throughout the time considered. During the infall stage, disk temperatures rise as the disk accretes mass from its parent cloud. The high temperatures in the inner disk develop due to the large amounts of viscous dissipation expected there, whereas the lower temperatures in the outer disk are largely set by irradiation from the central star. After infall stopped which is at 0.45 Myr in this case, viscous dissipation decreases in importance with time, leading to lower, irradiation dominated temperatures in the inner disk.

We applied the chemical network involving ^{18}O (^{17}O) − ^{16}O exchange to a variety of conditions expected from our disk evolution calculations. Taking $\delta^{18}O_{SMOW}(H_2O)$ = 100‰ and $\delta^{18}O_{SMOW}(CO)$ = -180‰ initially, we then calculated how the $\delta^{18}O_{SMOW}$ (H_2O) would evolve over time. Figure 2 shows how this evolution would proceed in a region where the gas pressure was 10^{-5} bar, a typical value for the pressure expected in the solar nebula at a variety of temperatures. At temperatures > 1000K, ^{18}O-^{16}O exchange could reach equilibrium within ~100 years, while the timescale for equilibrium gets much longer at lower temperatures 500K < T < 1000K (10^2-10^5 yrs). When T is below 500 K, the oxygen isotope exchange is minimal within the evolutionary timescale of a protoplanetary disk, and the initial $\delta^{18}O_{SMOW}$ (H_2O) could be preserved. The timescales for oxygen isotopic exchange are generally consistent with previous calculations done by [12]. We also considered other cases with different gas pressure and varying initial compositions, the trends shown here are robust. This means that ^{18}O-^{16}O exchange between those gaseous species would proceed to a certain extent in the hot inner region of disk, and be minimal at greater distances from the young Sun.

In addition to being isotopically heavy in oxygen, water in molecular clouds would be highly deuterated through ion-molecular and grain surface reactions at low temperature [13]. As water is redistributed in the disk, it would also exchange deuterium with other hydrogen-bearing species [14]. We evaluated the ^{18}O−^{16}O exchange together with D−H exchange between isotopically heavy water and other species under a variety of disk conditions. Figure 3 shows that the D-H exchange proceeds much faster than ^{18}O-^{16}O exchange, which means when water undergoes isotopic exchange with other gaseous species in the disk, its initial high (D/H) signature would be erased more efficiently compared to its initial high $\delta^{18}O$ value.

Discussion: We continue to explore how isotopic exchange occurs in various disk environments and how transport affects the spatial variations in isotopes over time. We will report our latest results at the meeting.

References: [1] McKeegan K. D. et al. (2011) *Science*, Vol. 332, 1528. [2] Clayton R. N. (1993) *Annu. Rev. Earth Planet. Sci.* **21**, 115 [3] Liu M. C. et al. (2009) *GCA*, **73**, 5051 [4] Clayton R.N. and Mayeda T.K. (1984) *EPSL* 67, 151. [5] Young E. D. (2007) *EPSL* 262, 468**.** [6] Lee J. E. et al. (2008) *MaPS*, vol. 43, 1351. [7] Lyons J.R. and Young E.D. (2005) *Nature*, 435, 317. [8] Yu Y. et al. (1995) *GCA* 59, 2095. [9] Yang L. et al. (2011). 42nd LPSC, abstract # 1608 [10] Yang, L. and Ciesla, F. (2012), *MaPS* 47 , Nr 1, 99–119. [11] Woodall J. et al. (2007) *A&A*, 466, 1197. [12] Lyons J.R. et al. (2009) *GCA*, 73, 4998. [13] Roberts H., and Millar T. J. (2000) *A&A* 361, 388. [14] Yang L. et al. (2013). In Preparation.

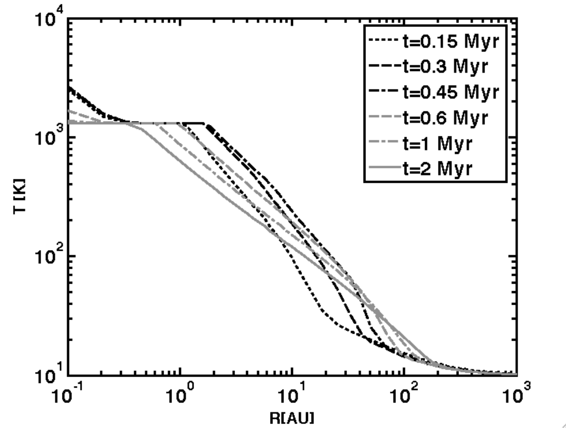

Fig. 1 The spatial variations in the disk midplane temperature at different times. Infall stopped at 0.45 Myr.

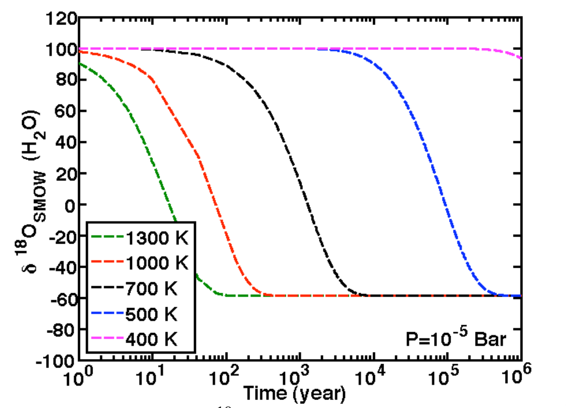

Fig. 2: Evolution of $\delta^{18}O_{SMOW}$ (H_2O) in our chemical model at a pressure of 10^{-5} bar at a variety of temperatures. Isotopic exchange is rapid at high temperatures (>1000 K), but minimal at temperatures less than 500 K.

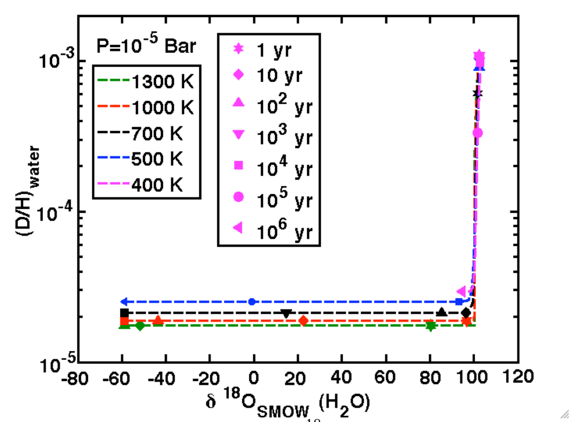

Fig. 3: Comparison of how $\delta^{18}O_{SMOW}(H_2O)$ and $(D/H)_{water}$ vary with time as isotopically heavy water exchanges D and ^{18}O with other gaseous species at different temperatures in the solar nebula.