THE D/H RATIO OF WATER IN A FORMING AND EVOLVING PROTOPLANETARY DISK.

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Introduction: Previous models studying the deuterium over hydrogen ratio (D/H) distribution in the solar system [1,2] showed that D/H increases with increasing distance from the Sun. However, those models conflict with the most recent published results from the Herschel Space Observatory [3]. According to this measurement, the (D/H) of Jupiter-family comet Hartley2 is $(1.61\pm0.24)\times10^{-4}$, which is indistinguishable from that of Earth's ocean water within measurable uncertainties, but is a factor of two lower than that of other comets whose D/H ratios have been measured [4-7]. Being a Jupiter-family comet, Hartley 2 is thought to originate beyond the region where the giant planets formed, whereas all previously measured comets were Oort cloud comets, and thus believed to have formed within the region the giant planets formed. Thus, the D/H does not increase monotonically with distance from the Sun as previous models predicted.

Those previous models of the D/H distribution in the solar system investigated the isotopic exchange that would occur between gaseous water and molecular hydrogen in a turbulent solar nebula. The initial D/H ratio of water was set to be 25 times that of protosolar hydrogen gas, which was the highest D enrichment observed in LL3 meteorites, and interpreted to be the value of protosolar water. This ratio decreased dramatically in the inner, hot region of the nebula due to isotopic exchange with H_2 [8]. Diffusion and advection within the evolving nebula mixed the isotopically light water with the unprocessed interstellar water, leading to a D/H ratio which would increase with increasing distance from the young Sun.

However, these previous studies neglected the effects of disk building on the evolution of the nebula. We have recently shown that molecular cloud material may be exposed to high temperatures and pushed to the outer edge of the solar system throughout the time that the cloud material falls onto the growing solar nebula, allowing processed material to migrate outward beyond the otherwise pristine materials [9]. We couple our model with a kinetic study of isotope exchange to explore how the D/H ratio of water would evolve in a growing solar nebula.

Model Description: Our model begins with a collapsing molecular cloud core. In simulating the evolution of the solar nebula, we use our previous model of material transport in a protoplanetary disk that accretes materials from its parent molecular cloud [9]. Once in the disk, materials are exposed to the mass and angular momentum transport associated with disk evolution, which we describe using standard α-model.

The D/H of water ice in the cloud has been suggested to be higher than what those previous models assumed, possibly in the range 0.001-0.01 due to ion-molecular reactions in the molecular cloud [10], values supported by astrophysical observations [11]. However, the D/H of water would evolve in the solar nebula due to D exchange with H between hydrogen gas (H_2) and water (H_2O):

$$HD + H_2O \xleftrightarrow{k^+,k^-} H_2 + HDO$$

The reaction rate k^- has been measured by [12]. Since k^+ has not been determined by any experiments, k^+ is set as $k^- \cdot A(T)$, where $A(T)$ is the fractionation at equilibrium given by [13]. k^- and $A(T)$ sensitively depend on temperature. These same reaction rates were used in previous models for the evolution of the D/H ratio of water in the solar nebula [1,2], and thus facilitate comparisons between our results and theirs.

In our model, we track the surface density of HD, H_2O, H_2, HDO, respectively, as described by

$$\frac{\partial \Sigma_i}{\partial t} + \frac{1}{R}\frac{\partial R\Sigma_i \upsilon_r}{\partial R} = \frac{1}{R}\frac{\partial}{\partial R}\left[RD\Sigma\frac{\partial}{\partial R}\left(\frac{\Sigma_i}{\Sigma}\right)\right] + S_i(R,t)$$

where Σ_i is the surface density of each species, D is the diffusion coefficient, and $S_i(R,t)$ is the source term of materials. The source term is determined by the material added from infall as described in [9] and isotopic exchange. We calculated the source terms of isotopic exchange following the previous D/H studies by calculating reaction rates for the entire column assuming the conditions (number densities and temperature) at the disk midplane.

As the number density and temperature in a viscous disk will vary with height, we are also investigating how isotopic exchange occurs when the vertical structure of the disk is taken into account. We compared the rates at which the surface density of a given species varied using the method of previous studies and one where the vertical structure and vertical mixing was allowed for—that is, calculating the isotopic exchange rate in a column of the disk, accounting for density and temperature variations with height and vertical diffusion. We found that the vertically integrated reaction rates for the cases where vertical structure is accounted for are ~0.25 times those that assume midplane conditions, with only a small dependence on parameter choices. Thus, to provide a more realistic representation of the isotopic exchange rates we calculate the corresponding source term as described in previous paragraph and then multiply it by a constant factor of 0.25.

Preliminary Results: Figure 1 shows the result of a typical model simulation. For this run we considered a $1M_{\odot}$ molecular cloud core at a temperature of 15 K. The D/H of water ice in the cloud core is set as 0.001, and the D/H of hydrogen gas is 2×10^{-5}, which is the protosolar value [14]. Water abundance relative to hydrogen gas in the molecular cloud is set as 2×10^{-4} [15]. We assumed a value of $\alpha = 10^{-3}$ throughout the disk to describe its evolution, but augment it in regions that become gravitationally unstable as in [9].

Figure 1 shows how the D/H of water varies with location in the disk at various times. We treat water as being either a vapor or small dust particles, meaning their dynamical behaviors are identical. Since water condenses at ~160K, isotopic exchange does not occur, meaning microscopic ice records the D/H of the water vapor from which it condenses.

As shown in Figure 1, the D/H of water inside of 2 AU is found to equal that of the hydrogen gas as temperatures are high enough for rapid isotopic exchange. Those materials from that region get redistributed throughout the rest of the disk, especially in the early stage, which allows the D/H of water at greater distances from the Sun to be as low as the equilibrated value. At later times, the high D/H ratio of pre-solar water ice mixes with this equilibrated water as it is added to the cooler regions of the disk, increasing the average D/H ratio in the outer disk. The peaks shown in the 0.2 Myr and 0.3 Myr snapshots are due to the added pristine ice, as molecular cloud materials are incorporated into the disk at these times out to ~3 and ~10 AU respectively. This material is never added to the disk outside of 10 AU in this model, and instead only migrates to larger distances by mixing with processed water already present there. As such, the D/H of water is not monotonically increasing away from the central star, and this non-monotonic distribution persists even after millions of years of evolution.

Discussion: Here we have shown the results of only one model run. Different parameter choices lead to different isotopic gradients in the disk. However, the result that evolution during infall leads to non-monotonic gradients in the disk is robust.

We are currently focusing on understanding how coagulation and migration of dust aggregates affect the D/H of water in solar nebula. We will use a new model describing the dynamics of multiple species of solids developed by [16] to investigate how these effects impact the D/H of water in the protoplanetary disk. We are also exploring how other hydrogen-bearing species affect the D/H of water, as discussed in [17].

We continue to explore these model runs and compare our results to measured D/H values in primitive bodies. We will consider how the time of formation for various bodies impacts the D/H ratio recorded in chondritic meteorite parent bodies and comets. We will report on these results.

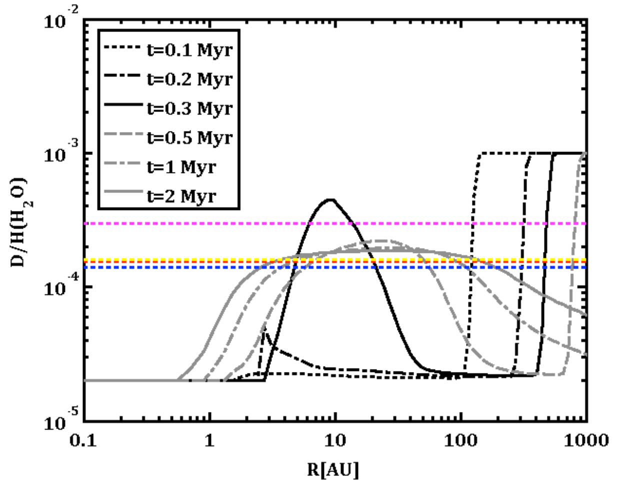

Fig. 1 the D/H of water distributions in the disk at different time. Black lines represent times when infall continues, while grey are those times after infall ceases (at ~0.3 Myr). Those horizontal dotted lines represent the measured D/H values for solar nebular objects. The purple line shows the mean D/H ratio of six comets from the Oort cloud, which is $(2.96 \pm 0.25) \times 10^{-4}$ [18]. The yellow line shows the D/H ratio of $(1.61 \pm 0.24) \times 10^{-4}$ [3] in the Jupiter-family comet 103P/Hartley 2. The red line and the blue line show the D/H values for Earth's ocean [19] and CI carbonaceous chondrites [20], respectively.

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