Icarus 226 (2013) 256–267

Contents lists available at SciVerse ScienceDirect

Icarus

journal homepage: www.elsevier.com/locate/icarus

The D/H ratio of water in the solar nebula during its formation and evolution

Le Yang [a,*], Fred J. Ciesla [a], Conel M.O'D. Alexander [b]

[a] Department of the Geophysical Sciences, The University of Chicago, 5734 South Ellis Avenue, Chicago, IL 60637, USA
[b] DTM, Carnegie Institution of Washington, Washington, DC 20015, USA

ARTICLE INFO

Article history:
Received 25 January 2013
Revised 6 May 2013
Accepted 15 May 2013
Available online 7 June 2013

Keywords:
Cosmochemistry
Comets, Composition
Origin, Solar System
Solar nebula

ABSTRACT

We couple a dynamic model of material transport and mixing within a forming and evolving protoplanetary disk with a kinetic study of D–H isotopic exchange amongst gas-phase molecules to explore the isotopic evolution of water in a young protoplanetary system. We begin with water that was highly deuterated in the parent molecular cloud core, then track its isotopic evolution within the protoplanetary disk. Our model shows the $(D/H)_{water}$ is low in the hot inner disk due to rapid isotopic exchange with molecular hydrogen, and then increases toward the cold, outer disk where exchange reactions are more sluggish. These results are consistent with previous studies. However, counter to previous studies, we find that the $(D/H)_{water}$ decreases again in the outer regions of the disk because water that exchanged at high temperatures near the young star would have been transported outward during the early evolution of the disk. As a result, water ice in the outermost region of the disk may have, on average, a lower $(D/H)_{water}$ ratio than found closer to the star. This non-monotonic gradient in D/H could explain the recent observations showing that the $(D/H)_{water}$ of a Jupiter Family Comet, 103P/Hartley 2, is lower than that of previously measured Oort cloud comets.

1. Introduction

In the last decade, theoretical studies of interstellar chemistry have revealed that water becomes enriched in deuterium relative to molecular hydrogen through ion–molecule and grain surface reactions at $T < 50$ K in astrophysical environments (Brown and Millar, 1989; Millar et al., 1989; Roberts and Millar, 2000; Roberts et al., 2004). These models predict that water in molecular cloud cores, where temperatures may be 10–20 K, develops D/H ratios ranging from 0.001 to 0.01, which are about 2–3 orders of magnitude higher than the cosmic (D/H) value ($\sim 1.6 \times 10^{-5}$; Linsky, 2003) and also greater than the bulk solar (D/H) value ($\sim 2 \times 10^{-5}$; Geiss and Gloeckler, 1998). This prediction is supported by astronomical observations showing that the $(D/H)_{water}$ in hot cores ($T \sim 100$–200 K) where water ice is being evaporated are $\sim 3 \times 10^{-4}$–3×10^{-2} (Jacq et al., 1990; Gensheimer et al., 1996; Rodgers and Millar, 1996; Lerate et al., 2006; Persson et al., 2007; Bergin et al., 2010; Liu et al., 2011; Coutens et al., 2012).

However, such high D/H values are not necessarily preserved in water throughout the process of planet formation. When water is incorporated into the hot, inner region of a protoplanetary disk, it would undergo isotopic exchange reactions with other hydrogen-bearing species, erasing some, or all, of the memory of the molecular cloud. This process was examined in a number of studies that modeled how deuterated water was processed and redistributed in viscously evolving disks (e.g., Drouart et al., 1999; Mousis et al., 2000; Hersant et al., 2001; Horner et al., 2007; Kavelaars et al., 2011; Petit et al., 2011). These studies allowed for isotopic exchange via the reaction $H_2O + HD \leftrightarrow HDO + H_2$ (Geiss and Reeves, 1981; Lécluse and Robert, 1994) in the various environments found in the solar nebula in order to determine how the isotopic composition of water would vary across the Solar System. Because isotopic exchange occurred rapidly at high temperatures, these models found that water would equilibrate with the hydrogen and acquire a $(D/H)_{water} \sim 2 \times 10^{-5}$ in the inner regions of the nebula. While in the outer disk, where low temperatures led to sluggish isotopic exchange, water would preserve its high $(D/H)_{water}$ ratio. While the details of these models varied depending on the assumed initial conditions, their overall results generally agreed with available data of the D/H ratio of water-bearing Solar System bodies. In particular, it was found that water in Oort cloud comets, which may have formed amongst the giant planets, had greater deuterium enrichments than found in Earth's water or the aqueously altered meteorites, all of which were thought to form closer to the Sun (Balsiger et al., 1995; Bockelée-Morvan et al., 1998; De Laeter et al., 2003; Robert, 2006).

---

* Corresponding author.
E-mail address: leyang@uchicago.edu (L. Yang).

0019-1035/$ - see front matter © 2013 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.icarus.2013.05.027

These models have recently been challenged by the Herschel/HIFI observations of a Jupiter Family Comet (JFC), 103P/Hartley 2 (Hartogh et al., 2011). Being a JFC, Hartley 2 may have originated beyond the region where Neptune formed (Dones et al., 2004; Morbidelli, 2005; Duncan, 2008). While it is uncertain exactly where Oort cloud comets formed (e.g., Dones et al., 2004; Levison et al., 2010; Brasser et al., 2012) the similar D/H ratio of these comets and water from Saturn's moon Enceladus (Waite et al., 2009) supports the theory that they formed in the Jupiter and Saturn forming regions. As the JFCs may have formed beyond this region, the models described above would predict that the $(D/H)_{water}$ in the JFCs would be equal to or greater than what is seen in the Oort cloud comets. However, the D/H value of water in Hartley 2 was found to be $1.61 \pm 0.24 \times 10^{-4}$, approximately a factor of two lower than those values measured in Oort cloud comets ($\sim 3 \times 10^{-4}$; Balsiger et al., 1995; Bockelée-Morvan et al., 1998, 2012; Meier et al., 1998; Villanueva et al., 2009; Brown et al., 2012) and comparable to what is found in the Earth's oceans today.

If Hartley 2 is representative of other JFCs, we must ask whether it is possible for the D/H variations in water ice in the outer nebula to be less than those found in the giant planet formation region. Here we attempt to address this by extending previous models to consider the time period prior to when other models began. That is, previous modeling efforts began their simulations with a fully formed solar nebula that was no longer accreting mass from its parent molecular cloud. However, solar nebula formation is expected to occur over a finite period of time, resulting in materials being processed and redistributed prior to the time the disk reached its final mass. As a result, materials processed at high temperatures can be pushed outwards by disk early evolution, before being diluted by freshly added cloud materials (Dullemond et al., 2006; Yang and Ciesla, 2012). Here, we revisit the dynamical and isotopic evolution of water in the early solar nebula and explicitly consider the effects of disk building in order to evaluate how this would impact the isotopic distribution of water in the solar nebula.

In the next section, we present the model used here, describing both the physical and chemical models that we used in our study. We then apply the model to explore how $(D/H)_{water}$ varies within an early evolving disk. Following that, we discuss how variations in key parameters would affect the results. We end with a discussion of how our results could be applied to interpret previous measurements, and how our model could be tested by future studies of meteoritic and cometary materials.

2. Model description

We consider a disk forming within its parent molecular cloud core as it undergoes inside-out collapse (Shu, 1977), and its evolution as mass and angular momentum are redistributed by internal processes. Assuming that materials within the molecular cloud are well mixed prior to infall, water, whose D/H ratio would be enhanced over the bulk value for the cloud (Roberts and Millar, 2000; Roberts et al., 2004), would be accreted into the star + disk system as a constant fraction of the infalling materials. Where infalling materials are added to the disk depends on the specific angular momentum that each parcel of material had in the parent cloud (Hueso and Guillot, 2005). Once incorporated into the disk, the water would be redistributed in the solar nebula through viscous evolution, along with other hydrogen-bearing species and their deuterium isotopologues, most notably H_2, HD, OH, and OD. Since those gaseous materials see different environments (temperature and pressure) throughout the course of disk evolution, water would undergo isotopic exchange with these other species at rates that depend on their locations in the disk.

2.1. Disk model

Our dynamic model calculates how the surface density profile, $\Sigma(R, t)$, changes with time as the disk evolves as a result of angular momentum transport during and after the period when the disk accreted material from its parent molecular cloud. Here we qualitatively describe the physical effects that determine how the disk evolves. Detailed equations and treatments can be found in Yang and Ciesla (2012), which adopted many of the same methodologies used in previous models (e.g., Hueso and Guillot, 2005; Dullemond et al., 2006; Zhu et al., 2010).

During the period of disk building, infalling materials from the molecular cloud are added to and well mixed-vertically within the disk at locations inside the centrifugal radius, which is defined as the distance from the central protostar where the orbital angular momentum of the material in the disk equals the maximum angular momentum in the shell of molecular cloud core being accreted at that time (Dullemond et al., 2006; Hueso and Guillot, 2005; Zhu et al., 2010). Some of the mass inside of the centrifugal radius is pushed outwards due to the viscous spreading associated with angular momentum conservation. Viscous evolution continues even after infall ceases.

Here, we adopt the classical α-viscosity formalism (Shakura and Sunyaev, 1973; Lynden-Bell and Pringle, 1974), as this provides a computationally simple method for representing the mass and angular momentum evolution of the disk over long timescales. Here we assume that the turbulent viscous parameter, α, has a uniform value of 0.001, but can be augmented in gravitationally unstable regions (Armitage et al., 2001). We will return to discuss how different values of α would affect our results later.

All gaseous species involved in the D–H exchange reaction network are transported by advection and diffusion within the disk:

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

where Σ_i is the surface density of gaseous species that are considered. D is the diffusion coefficient, which is assumed to be equal to the viscosity ν. $S_i(R, t)$ is the source term of a specific gaseous species that is added from infall, if applicable, and also that is altered through the chemical reaction network that is described in the following section.

The thermal evolution of the disk is determined by balancing the energy received from viscous dissipation, irradiation from the central star, and radiation from the cloud envelope with the energy lost from the disk surface. In our calculations, disk opacity is dominated by dust, and thus is assigned a low value in regions above the dust sublimation temperature (for details see Yang and Ciesla, 2012).

2.2. Chemical model

In the models of Drouart et al. (1999) and Mousis et al. (2000), isotope exchange between water and hydrogen was assumed to be determined by the reaction $H_2O + HD \leftrightarrow HDO + H_2$, with the forward and backward reaction rates provided by Lécluse and Robert (1994). More recent studies (e.g., Willacy, 2007; Willacy and Woods, 2009; Thi et al., 2010) have explored how this D–H exchange would have occurred by considering a suite of possible reactions involving the major chemical species that would have been present in the solar nebula gas. This was done because water molecules would not have been limited to react with just H_2 in the disk, and the water abundance would vary with temperature.

As shown by Thi et al. (2010), water deuteration would have strongly depended on the behavior of the hydroxyl radical, OH.