EVOLUTION OF OXYGEN ISOTOPES IN THE SOLAR NEBULA. J. R. Lyons[1] and E. D. Young[1,2], [1]Institute of Geophysics and Planetary Physics, Center for Astrobiology, UCLA, Los Angeles, CA 90095-1567, jrl@ess.ucla.edu , [2]Department of Earth and Space Sciences, UCLA, Los Angeles, CA 90095-1567, eyoung@ess.ucla.edu.

Introduction:

Clayton recently proposed [1] that self shielding of CO at the X-point of the solar nebula was responsible for the formation of an ^{16}O-poor gas capable of shifting the oxygen isotopes of the rocky component of the inner solar system ~ + 50 ‰ in both ^{17}O and ^{18}O. In this proposed model the most refractory mineral phases (e.g., CAI's) retained their original (interstellar) isotope ratios, and self shielding of CO produced H_2O strongly depleted in ^{16}O. Although we believe that self shielding at the X-point would be difficult [2], we also believe that self shielding is an excellent mechanism for the formation of distinct oxygen isotope reservoirs, especially in the surface region of the nebula [3]. We recently showed that large fractionations will result from CO photodissociation at the surface of a static nebula [4]. Here we calculate the time-evolution of fractionation during CO photodissociation in a disk that undergoes vertical mixing.

We evaluated the self-shielding at the nebula surface by employing a one-dimensional photochemical model to compute the time-dependent CO isotopomer mole fraction profiles. The model is still quite rudimentary but allows us to explore isotopic evolution and the $\delta^{17}O/\delta^{18}O$ ratio in the nebular gas. Radiative transfer is treated in one-dimension only, namely along the normal axis of the disk, rather than along the path from the central protostar. This simplification greatly reduces computational requirements without sacrificing any of the fundamental physical processes, and is likely a fair representation of photodissociation via enhanced far ultraviolet (FUV) radiation in a star-forming region.

Photochemistry in a one-dimensional disk:

We utilized the analytical flared-disk model of Aikawa and Herbst [5] which describes the two-dimensional distribution of H nuclei. Here we present results evaluated at a distance of R = 5 AU from the protosun, where the temperature is 125 K and the H_2 number density is 4 x 10^{12} cm^{-3} in the midplane. We assumed a solar composition nebula for which CO/H_2 = 2 x 10^{-4} by mole.

We have restricted the photochemistry to the non-mass dependent fractionation step, namely the photolysis reactions of CO isotopomers:

$$C^{16}O + h\nu \rightarrow C + {}^{16}O$$

$$C^{17}O + h\nu \rightarrow C + {}^{17}O$$

$$C^{18}O + h\nu \rightarrow C + {}^{18}O$$

where photodissociation occurs in the wavelength range 91.2 to 110 nm in the presence of abundant hydrogen [6], and where both ^{12}C and ^{13}C isotopes have been included (i.e., all six CO isotopomers are in the model).

To follow the time evolution and vertical distribution of CO and its isotopomers in the disk, we solved the coupled one-dimensional continuity and flux equations for each isotopomer:

$$\frac{\partial f_i}{\partial t} = \frac{1}{n}\frac{\partial}{\partial z}\left(\nu_t n \frac{\partial f_i}{\partial z}\right) + \frac{P_i}{n} - L_i f_i$$

where f_i is the mole fraction of the CO isotopomer 'i', n is the number density of the background gas (mostly H_2), z is the height above the disk midplane, and t is time measured from the initiation of FUV radiation on the disk. Vertical motion is characterized by the turbulent viscosity, $\nu_t = \alpha cH$, where c is the speed of sound and H is the vertical scale height in the nebular gas, and $\alpha \leq 1$ is a free parameter commonly used in disk models to describe the strength of turbulent mixing. The vertical scale height is H ~ 0.1R. P_i and L_i are the production rate (molecules cm^{-3} s^{-1}) and loss rate (molecules s^{-1}), respectively, for CO isotopomers.

To quantify the effects of self and mutual shielding (i.e., shielding of one isotopomer by another), we employed the results of van Dishoeck and Black [6] developed for molecular clouds in the interstellar medium (ISM). Using fits to their derived shielding functions, expressions for the photodissociation rate constant (L_i) for each isotopomer may be determined (not shown here). The effects of dust opacity and absorption by H_2 are also included.

Results:

For a radial distance of 5 AU, the model was run from time zero to 10^7 years for a range of values of α and FUV multiplying factor. Figure 1 shows the time evolution of $\delta^{17}O$ and $\delta^{18}O$ of residual CO and product O at the disk midplane for $\alpha = 10^{-3}$ and 1 x FUV. In

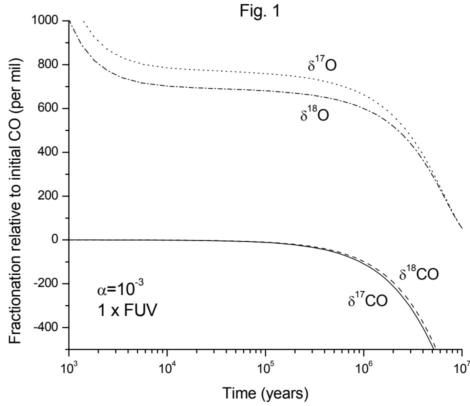

Fig. 1

our model 1 x FUV corresponds to the FUV flux from the modern sun during solar maximum; at 5 AU this is ~ 100 x the modern ISM FUV flux. Figure 1 demonstrates the formation of ^{16}O-poor O and ^{16}O-rich CO due to self shielding during CO photodissociation.

We assume complete conversion of photoproduct O to H_2O, by reactions on grain surfaces and by ion-molecule reactions. If we then add the photodissociation-derived H_2O to the complement of H_2O expected in the collapsing molecular cloud (which has initial isotope values of –50 ‰, -50‰), we obtain the total nebular H_2O. (It should be noted that CO and H_2O will not reach chemical equilibrium by purely thermal processes in 10 Ma at temperatures ~ 100 K.) Figure 2 shows the resulting $\Delta^{17}O_{smow}$

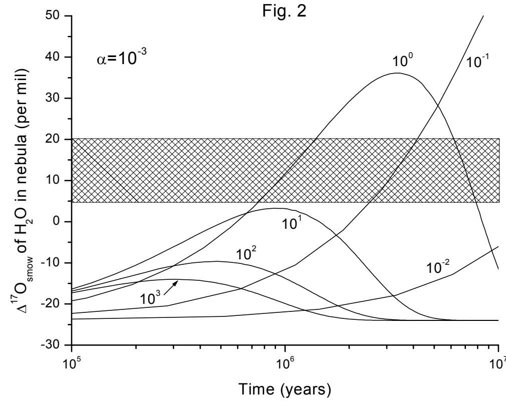

Fig. 2

for total nebular H_2O versus time for a range of FUV fluxes (each curve is labeled with the FUV multiplying factor). The shaded region of the figure shows the range of $\Delta^{17}O$ of initial water (or gas) inferred by Clayton and Mayeda [7] and by Young [8] from analyses of carbonaceous chondrites. For $\alpha = 10^{-3}$ an FUV flux ~ 1 x modern sun is optimal for ages < 2 Ma. Higher FUV fluxes dissociate too much $C^{16}O$, reducing the magnitude of the fractionation. For $\alpha \leq 10^{-4}$ all curves fall below the shaded region implying that vigorous mixing was required in the nebula.

Figure 3 shows the 1 x FUV and 10 x FUV nebula H_2O curves of Fig. 2 on a 3-isotope diagram. CCAM, slope 1 and slope .52 lines are shown for reference. Also shown are the inferred initial water values from [7] and [8]. Although both curves are close to the inferred water values, both curves are at slopes ~ 1.05 – 1.10. This results from the model assumption that self shielding by $C^{17}O$ and $C^{18}O$ differs only by the column abundance of these two isotopomers. In making this assumption we have neglected potential line-by-line differences in the absorbing character of the individual isotopomers.

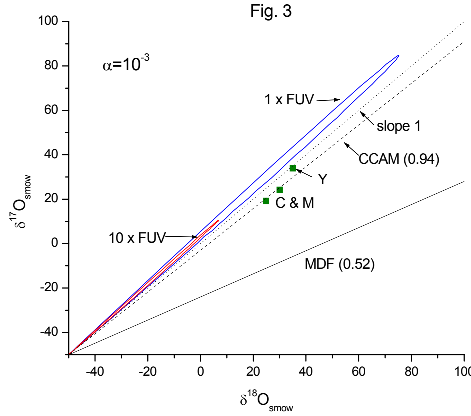

Fig. 3

Conclusions: We have used a one-dimensional photochemical model to demonstrate that CO self shielding could have produced mass-independent fractionation in nebula H_2O consistent with that required by analyses of carbonaceous chondrites. The model results are strongly dependent on the vigor of vertical mixing and on the FUV flux incident on the disk. Preservation of the fractionation in H_2O at higher temperatures requires an excess of H_2O over CO at the midplane. An analysis of this possibility, together with a new derivation of shielding functions, is in progress.

References: [1] Clayton R.N. (2002) *LPS XXXIII,* abstract #1326. [2] Lyons J.R. and Young E.D. (2003) *LPSC XXXIV,* abstract #1981. [3] Lyons J.R. (2003), abst., NASA Astrobio. Inst. Meet., Phoenix, Feb. 9-12. [4] Young E.D. and Lyons J.R. (2003) *LPSC XXXIV,* abstract #1923. [5] Aikawa Y. and Herbst E. (1999) *Astron. Astrophys., 351*, 233-246. [6] van Dishoeck E.F. and Black J.H. (1988) *Astrophys. J., 334,* 771–802. [7] Clayton R.N. and Mayeda T.K. (1984) *Earth Planet. Sci Lett., 67,* 151-161. [8] Young E.D. (2001) *Phil. Trans. R. Soc. Lond. A., 359*, 2095-2110.