

OXYGEN ISOTOPE RESERVOIRS IN THE SOLAR NEBULA. P. Mane^{1,2}, S. J. Desch³, E. T. Dunham⁴, and C. D. Williams⁵ ¹Lunar and Planetary Institute, USRA, Houston TX, ²NASA Johnson Space Center, Houston TX (pmane@lpi.usra.edu) ³Arizona State University, Tempe AZ (steve.desch@asu.edu), ⁴University of California, Los Angeles, Los Angeles, CA, ⁵University of California, Davis, CA.

Introduction: The oxygen isotopic composition of the solar system materials is an important tool in understanding the birth of our solar system. Various solar system materials show a wide range in their oxygen isotopic composition varying from $\Delta^{17}\text{O}$ values of -40‰ to $+250\text{‰}$ [1,2]. We present a hypothesis for how the different oxygen isotope reservoirs in the solar nebula were established. We discuss the meteoritic evidence in support of this hypothesis and suggest further tests.

Oxygen in Calcium-rich, Aluminum-rich Inclusions (CAIs): CAIs are the oldest solids formed in the solar system and are made of minerals that condensed from solar nebula gas. They record the earliest stages of chemical and isotopic evolution of the nebular gas. Most pristine CAIs from different chondrites record a ^{16}O -rich isotopic composition $\Delta^{17}\text{O} \sim -24 \pm 2\text{‰}$ [3,4] or $-23.4 \pm 1.1\text{‰}$ [5]. The $\log f_{\text{O}_2}$ values determined for type A and B CAIs are -19.9 ± 0.6 (at 1500K) [6], suggesting that these CAIs formed under highly reducing conditions with $\text{C/O} \approx 0.93$ (0.91 - 0.98), more reducing than solar composition gas with $\text{C/O} \approx 0.55$ [7] $\log f_{\text{O}_2} = -17.9$ (at 1500K).

Our Model: We assume there were three main reservoirs of oxygen in the Sun's molecular cloud—silicate dust, water, and carbon monoxide gas—and that all three were initially isotopically homogeneous, with $\delta^{17}\text{O} \approx +2\text{‰}$, $\delta^{18}\text{O} \approx +4\text{‰}$, and $\Delta^{17}\text{O} = \delta^{17}\text{O} - 0.517 \times \delta^{18}\text{O} \approx 0\text{‰}$. Such homogenization may be expected after long residence in the interstellar medium. Assuming the Sun formed in a high-mass star-forming region, UV irradiation of the molecular cloud could have photodissociated CO in an isotopically selective way, leading to excess dissociation of C^{16}O (and therefore ^{16}O -rich H_2O and ^{16}O -poor CO) near the cloud surface, from where these species escape; and excess dissociation of C^{17}O and C^{18}O in the cloud interior, leading to ^{16}O -rich CO and ^{16}O -poor H_2O [8]. We hypothesize that the H_2O reservoir was at $\Delta^{17}\text{O} \approx +85\text{‰}$, to match the cosmic symplectite [9], and the CO reservoir was at $\Delta^{17}\text{O} \approx -167\text{‰}$, consistent with mass balance and molar ratio $\text{CO}/\text{H}_2\text{O} = 0.50$. Silicates would not participate in this chemistry, and would remain at $\Delta^{17}\text{O} \approx 0\text{‰}$. We assume that in the molecular cloud, the fraction of O in H_2O was $f_{\text{H}_2\text{O}} \approx 50\%$, the fraction in CO was $f_{\text{CO}} \approx 33\%$, and the fraction in silicates was $f_{\text{sil}} \approx 17\%$, yielding $\Delta^{17}\text{O} \approx 0\text{‰}$ in the bulk molecular cloud.

We next hypothesize that during accretion, magnetic fields held back $\approx 43\%$ of the small, charged dust grains

from the solar nebula, as described by [10]. Such a process can lead to a reduction in silicate-to-gas ratios of $\geq 40\%$. Similarly, the abundance of H_2O condensed as ice mantles on dust grains would be reduced in a high-mass star-forming region where temperatures reach ~ 100 K, whereas, CO would remain in the gas phase and be fully accreted onto the Sun. This process would have changed the proportions of oxygen in each reservoir, to $f_{\text{H}_2\text{O}} \approx 45.4\%$, $f_{\text{CO}} \approx 40.6\%$, and $f_{\text{sil}} \approx 14.0\%$, yielding $\text{CO}/\text{H}_2\text{O} = 0.89$. These proportions are consistent with a water-to-silicate mass ratio ≈ 1.5 , consistent with the estimates ≈ 0.9 to ≈ 1.9 [11]. The CO/O ratio would be 0.40, but presumably after including C not in CO, the ratio would match the protosolar $\text{C/O} = 0.55$ [7]. The Sun and bulk solar system would have $\Delta^{17}\text{O} \approx -29.1\text{‰}$. This is consistent with values inferred for the Sun from the *Genesis* mission, $-28.4 \pm 3.6\text{‰}$ [12], and with values measured in some CAIs, $-29.1 \pm 0.7\text{‰}$ [5].

CAIs would sample bulk solar system and have $\Delta^{17}\text{O} \approx -29.1\text{‰}$ if they condensed from a gas with the three main reservoirs of oxygen present in the same proportions as in the Sun. Some CAIs are characterized by more ^{16}O -rich compositions than the Sun [13], including two grossite-bearing CAIs from Isheyevo (CH chondrite) with $\Delta^{17}\text{O} \approx -33 \pm 1\text{‰}$ and $\Delta^{17}\text{O} \approx -34.5 \pm 1\text{‰}$ [14]. We interpret those, and most CAIs (with $\Delta^{17}\text{O} \approx -23.4\text{‰}$), to be sampling the three oxygen reservoirs in different proportions from the Sun.

The main cause of variations in oxygen isotopes would be concentrations or depletions of H_2O relative to the other reservoirs, e.g., through radial distribution and trapping at snow lines; and concentrations of solids relative to the gas. Within a warm region of the solar nebula, H_2O vapor and CO gas would combine. In any region with $T > 200$ K, H_2O and CO would equilibrate and both have $\Delta^{17}\text{O} \approx -34\text{‰}$. If silicates and solids then were to evaporate in a region with a solar silicates-to-gas ratio, the resulting vapor would be solar in composition, with $\Delta^{17}\text{O} \approx -29.1\text{‰}$ and $\text{C/O} = 0.55$. If CAIs were to condense in a region with increased solids-to-gas ratio, or reduced H_2O vapor abundance, they would have increased $\Delta^{17}\text{O}$. Increased solids-to-gas ratio could occur due to settling of solids to the midplane, or silicate condensation fronts. Decreased water-to-gas ratio could occur due to loss of water vapor from the inner disk to beyond the snow line, where it is cold trapped. In particular, if the silicate-to-gas ratio were increased by a factor of $F_{\text{sil}} = 1.5$, and the water-

to-gas ratio decreased by a factor $F_{\text{H}_2\text{O}} = 0.15$, the system would have $\Delta^{17}\text{O} \approx -23.4\%$. If the solids-to-gas ratio were decreased to ≈ 0 , the resulting vapor would have $\Delta^{17}\text{O} \approx -34\%$.

Discussion: Our model explaining the oxygen isotope variations in the CAI-forming region robustly predicts that the oxygen isotopic ratio $\Delta^{17}\text{O}$ correlates with oxygen fugacity, as parameterized by the C/O ratio in the gas. To convert C/O into oxygen fugacity $f_{\text{O}_2} \approx p_{\text{O}_2}$, we use the relation $\log_{10} p_{\text{O}_2} = 2 \log_{10} (p_{\text{H}_2\text{O}} / p_{\text{H}_2}) - 10.37$ [15], assuming that all C is bound in CO, and any O not bound in CO is in H₂O. In the absence of chemical fractionations, we assume O/H = 6.59×10^{-4} and C/H = 3.62×10^{-4} [7], but we assume that the silicates-to-gas ratio is reduced or increased by a factor F_{sil} , and the water-to-gas ratio reduced by a factor $F_{\text{H}_2\text{O}}$. We assume that at $p_{\text{H}_2} = 10^{-4}$ bar and 1600 K, $\log_{10} p_{\text{O}_2} = -10.44$ at the iron-wüstite (IW) buffer. From these assumptions we find the oxygen fugacity relative to the IW buffer is $\Delta\text{IW} = -5.69 + 2 \log_{10}[0.454 F_{\text{H}_2\text{O}}]$. A solar gas with variable C/O would yield the same ΔIW with C/O=1-0.454 $F_{\text{H}_2\text{O}}$. The corresponding oxygen isotopic composition is:

$$\Delta^{17}\text{O} = (-34.0\%) [1 - 0.140 F_{\text{sil}}] / [0.454 F_{\text{H}_2\text{O}} + 0.406 + 0.140 F_{\text{sil}}].$$

A solar composition gas with $F_{\text{sil}}=1$ and $F_{\text{H}_2\text{O}}=1$ has $\Delta\text{IW} = -6.38$ (C/O=0.55) and $\Delta^{17}\text{O} = -29.1\%$.

Using our model, we find isotopic composition that match CAIs. A family of solutions with different F_{sil} and $F_{\text{H}_2\text{O}}$ could yield $\Delta^{17}\text{O} = -23.4\%$, but they each are characterized by different oxygen fugacities $\log_{10} f_{\text{O}_2}$. We predict that CAIs formed from regions with slightly elevated solids-to-gas ratio, $F_{\text{sil}}=1.50$, and considerably depleted water-to-gas ratio, $F_{\text{H}_2\text{O}}=0.15$, have $\Delta^{17}\text{O} = -23.4\%$ and $\log_{10} f_{\text{O}_2} = -19.2$ (at 1500 K), or $\Delta\text{IW} = -7.7$. Regions with solar water-to-gas ratio, $F_{\text{H}_2\text{O}}=1$, and elevated solids-to-gas ratio, $F_{\text{sil}}=2.75$, would produce CAIs also with $\Delta^{17}\text{O} = -23.4\%$, but with $\log_{10} f_{\text{O}_2} = -18.1$ (at 1500 K), or $\Delta\text{IW} = -6.6$. We favor the former case because it yields an oxygen fugacity consistent with the majority of CAIs. In fact, if $F_{\text{sil}}=1.50$, variations of $F_{\text{H}_2\text{O}}$ between 0.05 and 0.30 will lead to variations of $\Delta^{17}\text{O}$ between -22.7% and -24.4% , and variations of $\log_{10} f_{\text{O}_2}$ (at 1500 K) between -20.1 and -18.7 . These are consistent with the range observed in the majority of CAIs.

Variations in $F_{\text{H}_2\text{O}}$ could be attributed to radial redistribution of water beyond a snow line. At early times, $F_{\text{H}_2\text{O}}=1$ can be expected throughout the solar nebula. Exterior to the snow line, water exists as ice; interior to the snow line it exists as vapor, isotopically equilibrated with the CO, with $\Delta^{17}\text{O} = -34\%$. Over time, as water vapor diffuses outward past the snow line,

it can be “cold-trapped” as ice, depleting the inner disk in vapor, potentially by factors $F_{\text{H}_2\text{O}} \ll 1$ [16].

Variations in F_{sil} could be attributed to redistribution of silicates at a condensation front for refractory minerals in the solar nebula, or a “CAI snow line”. Formation of CAIs begins with evaporation of silicates and condensation of refractory minerals. As with other condensation fronts, the solids-to-gas ratio should increase in the region where the minerals form, just beyond the condensation front; variable enhancements by factors $F_{\text{sil}} \sim 2$ would be typical [16]. Other regions will be depleted in silicates. We find that for $F_{\text{sil}} \ll 1$ and $F_{\text{H}_2\text{O}} \sim 0.1$, $\Delta^{17}\text{O} = -34\%$ and $\Delta\text{IW} = -7.7$ (C/O=0.90), consistent with formation CAIs with have $\Delta^{17}\text{O} < -23.4\%$.

Conclusions: Our model explains the different isotopic compositions of oxygen reservoirs in the solar nebula using few assumptions. We assume the three main reservoirs of oxygen in the molecular cloud—silicates, water and CO—started with identical $\Delta^{17}\text{O} \approx 0\%$. Self-shielding and photodissociation of CO created isotopically light CO and heavy H₂O. Depletion of $\sim 40\%$ of H₂O ice-mantled silicates grains gave the solar system a net $\Delta^{17}\text{O} \approx -29\%$. Formation of CAI minerals at a “CAI snow line,” with reasonable enhancements ~ 1.5 in silicates-to-gas ratio, plus depletion of water vapor by a factor $\sim 0.05 - 0.3$, reproduces the range in $\Delta^{17}\text{O} \approx -23.4 \pm 1\%$, as well as the range in $\log_{10} f_{\text{O}_2} \approx -19.9 \pm 0.7$. Isotopic ratios $\Delta^{17}\text{O} \approx -34\%$, as found in some CAIs, also can be explained. Our model predicts a general correlation of $\Delta^{17}\text{O}$ with oxygen fugacity, which can be tested by coordinated analyses of f_{O_2} and oxygen isotopes in CAIs.

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