

MODELING NITROGEN ISOTOPE CHEMISTRY IN THE SOLAR NEBULA. J. Garani¹ and J. R. Lyons¹,
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Introduction: In the early 2000s the Genesis mission was sent to the L1 to collect solar wind particles. From this mission, we know that there is a 400‰ difference in the $^{15}\text{N}/^{14}\text{N}$ ratio between bulk Earth and the Sun [1]. N_2 photodissociation and the process of self-shielding in the solar nebula may account for this drastic difference. Self-shielding of CO has been used to account for discrepancies seen in oxygen isotopes throughout the solar system, which is why we believe it could be applied to N_2 [2]. Here we start the analysis of N_2 isotopes based on N_2 self-shielding and explore different parameters of a disk model.

N_2 Photodissociation and Self-Shielding: In H-rich environments, N_2 is photodissociated from 91-100 nm. We consider two isotopologues of nitrogen, $^{28}\text{N}_2$ and $^{29}\text{N}_2$. With the substitution of the heavier isotope, the absorption spectrum of the isotopologue changes. This means that in order to photodissociate, $^{28}\text{N}_2$ and $^{29}\text{N}_2$ absorb photons of slightly different wavelengths. As the photons penetrate into columns of gas in the solar nebula, the $^{28}\text{N}_2$ becomes optically thick and dissociates very slowly. Beyond this point, no photons of wavelengths that dissociate this isotopologue make it through. However, since $^{29}\text{N}_2$ dissociates at different wavelengths, those photons still make it past this point. This results in an accumulation of ^{15}N because only $^{29}\text{N}_2$ is dissociating.

Methods: Using a 2-D solar nebula disk model, 394 chemical reactions are modeled through simulated turbulent mixing in a vertical column with diffusion from the mid-plane to the upper UV surface of the disk. We observe the effects of self-shielding in a column of the disk with UV photons assumed to be hitting the top of the disk from a nearby O or B star. The UV radiation is assumed to be perpendicular to the disk, allowing for 1-D radiative transfer modeling.

Two main parameters have been investigated. α is the parameter that characterizes the amount of turbulent viscosity in the disk. The lower the value of α , the less turbulent mixing is present. The other parameter is ϵ , which scales the UV flux incident on the disk. The N_2 photodissociation rate constant is proportional to the product of ϵ and the photodissociation rate coefficient due to the local ISM field, J_{ISM} , where $J_{\text{ISM}}=2.0 \times 10^{-10} \text{ s}^{-1}$. The higher the value of ϵ , the more UV flux is hitting the top of the disk. In this model, $\epsilon = 1$ corresponds to $50 * J_{\text{ISM}}$ for N_2 [3]. We also changed the molecular cloud value (MCV) of HCN.

Results: From looking at the mixing ratios and $\delta^{15}\text{N}$ values for N_2 and HCN_{gr} at times from 10 to 10^7

years (Figure 1), we see that $\alpha = 0.01$ or 0.001 may be the most likely to explain the 400‰ difference. We used both of these values to test different ϵ values from 1 to 10^5 . For $\alpha=0.01$, an ϵ value of 10 most closely accounts for the 400‰ difference. This is shown in Figures 2 and 3. As N_2 is photodissociated, N atoms react to form HCN and condense onto grains.

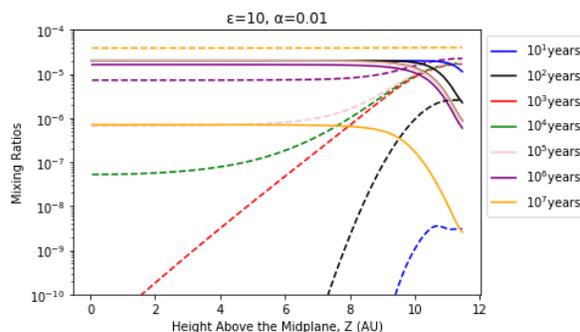


Figure 1. Mixing ratios of HCN_{gr} and N_2 vs. Z at various times. Dashed lines represent HCN_{gr} and solid lines represent N_2 . This shows that HCN_{gr} increases and N_2 decreases over time.

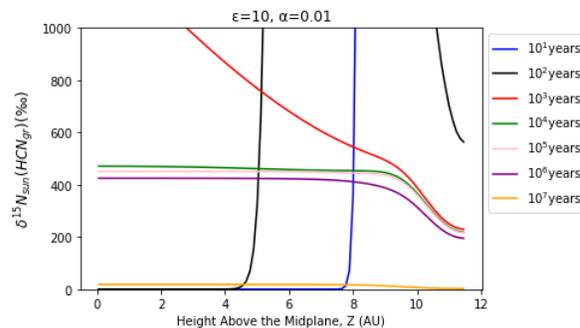


Figure 2. $\delta^{15}\text{N}(\text{HCN}_{\text{gr}})$, which shows that at 10^6 years (purple line), the δ -value is about 400‰ relative to the Sun.

From Figure 2, there is a 400‰ difference from the beginning of disk evolution to the 10^7 years, providing a possible set of conditions in the model that can explain the observed difference in isotope ratios. We also looked at the midplane results for N_2 and HCN_{gr} which are shown in Figure 4. Approximately half of the N_2 at the midplane for $\epsilon=10$ is dissociated by three million years.

HCN is produced photochemically in the solar nebula, but it is also likely to have been produced in the parent molecular cloud. We define total HCN on the grains, $\text{HCN}_{\text{gr,t}}$, as the sum of initial HCN from the

cloud, $\text{HCN}_{\text{gr},i}$, and the HCN_{gr} produced photochemically in the solar nebula. Figure 5 shows the δ -values of total $\text{HCN}_{\text{gr},t}$ relative to atmospheric N_2 for four different molecular cloud values of $\text{HCN}_{\text{gr},i}$. Assuming molecular cloud HCN with a solar $^{15}\text{N}/^{14}\text{N}$ ratio (i.e. no self-shielding in the parent cloud), the molecular cloud value that brings the δ -values closest to zero at 10^6 years is 10^{-7} or less. This is a quite low fraction of cloud HCN.

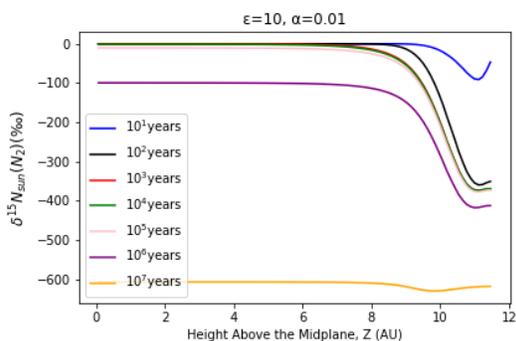


Figure 3. $\delta^{15}\text{N}$ values for N_2 , which shows that at 10^6 years, the value is about -400‰. Unfortunately, this is not observable for gas phase N_2 due to the lack of a N_2 dipole moment.

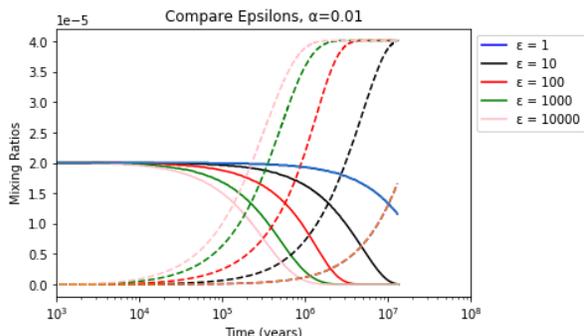


Figure 4. This figure shows the mixing ratios for N_2 and HCN_{gr} at the midplane over time. Dashed lines represent HCN_{gr} and solid lines represent N_2 . With time, the amount of HCN_{gr} increases as the amount of N_2 decreases due to N_2 photodissociation.

Figure 5 shows that for an α value of 0.01, an ϵ value of 10, and a low initial MCV of HCN, the model comes within about 80‰ of explaining inner solar system nitrogen isotopes. More testing of the parameters needs to be done, together with additional N chemical species and reactions. Species not presently in the code include NH_3 , NH_4^+ , CN , and NO . This model also does not include the vibrationally excited states of hydrogen, H_2 (v), which has been found to be an important factor in other models [4]. Adding this chemistry is our next step in the modeling process.

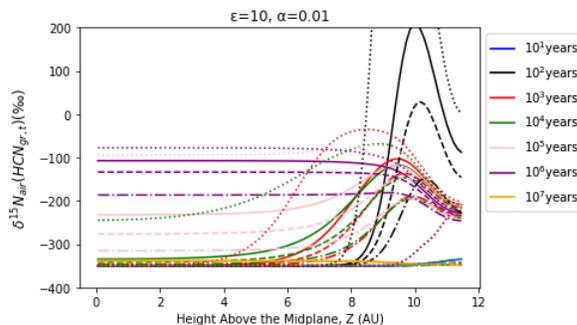


Figure 5. This graph shows the $\delta^{15}\text{N}$ values for total HCN_{gr} compared to atmospheric N_2 . The model was run with the molecular cloud value (MCV) of initial $\text{HCN}_{\text{gr},i}$ at 10^{-6} (solid lines), 2×10^{-6} (dashed lines), 5×10^{-6} (dotted and dash-dotted lines) and 10^{-7} (dotted lines). Because the δ -values are now referenced to air and not the Sun, the numbers for total HCN_{gr} should be compared to zero.

Conclusion: In these trials of different parameters, we have found a combination that nearly explains the 400‰ difference in nitrogen isotope ratios from the inferred solar value and the Earth atmospheric value. However, the model is incomplete and there is considerable reaction chemistry to be added followed by parameter testing. The fact that this additional chemistry is not in the model, yet the model nearly reproduces observations may suggest this additional chemistry is not of great significance.

Given that using a low initial MCV of $\text{HCN}_{\text{gr},i}$ comes within about 80‰ of explaining the nitrogen isotope distribution we see in the solar system, about 20 % or more of the N_2 self-shielding signature may derive from the parent cloud that formed the solar nebula, as has been suggested for O isotopes [5],[6]. If so, it's also possible that most of the self-shielding occurred in the parent cloud, and that the contribution from the disk may have been minor, at least within the inner solar system. Exploring this possibility will be the next step in this research.

References: [1] Marty B. et al. (2011) *Science*, 332, 1533. [2] Lyons, J. R. (2019) *LPSC LI*, Abstract #3107. [3] Lyons J.R. and Young E.D. (2005) *Nature* 435, 317. [4] Visser, R. et al. (2018) *A&A*, 615, A75. [5] Yurimoto H., Kuramoto K. (2004) *Science* **305**, 1763-1766. [6] Lee J.-E., Bergin E. A. and Lyons J. R. (2008) *Meteorit. Planet. Sci.* **43**, 1351-1362.