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ABSTRACT

1. INTRODUCTION

2. METHODOLOGY - DRAFT

2.1. *The Protoplanetary Disk Model*

The results of this report were simulated using a theoretical model of a protoplanetary disk. This section explores how exactly the model was constructed. Here, we consider the assumptions and calculations she employed to determine the gaseous and grain abundances of elements within the modeled disk.

2.1.1. *Assumptions*

For constructing the disk model, we first acknowledge the assumptions that were built into the framework of the disk. We assume initially that the material in the disk is dispersed evenly in the angular ϕ direction. In other words, slices of the disk in a fixed R-z plane along a sliding ϕ axis are assumed to be identical.

In addition, we assume that stellar radiation is the only source of heating within the disk. With this assumption, we exclude the heating effects of accretion. This exclusion significantly alters the positions of snow lines relatively close to the central star; however, as this report focuses upon the more distant snow lines, such as that of N_2, the neglection of accretion heating has a negligible effect.

Related to temperature, we also assume that the change in temperature with respect to height is negligible. Throughout this report, we use the midplane temperature to apply for the entirety of the disk at a given radial distance.

For calculations of the elemental abundances, we assume that each molecule has an equivalent adsorption and desorption rate (see **??** for the equations themselves). Furthermore, we assume no chemical reactions (?better term?) occur within the model, such that the concentration of each molecule (with respect to Hydrogen) remains constant throughout the disk. Furthermore, we assume that each molecule can be in only either gaseous or grain form.

2.1.2. *Model*

With these assumptions in mind, the authors first formed the base pf the model, which simulated the base of an actual protoplanetary disk, containing a central star surrounded by a disk of pure Hydrogen nuclei. To model the star and the abundant Hydrogen nuclei, the authors used temperature and number density profiles that mapped out the structure of the disk over its radius and height.

$$T = T_{atm} + (T_{mid} - T_{atm}) cos \left\{ \frac{\pi z}{8H} \right\}^{2\delta}$$

Temperature Profile. Equation 1 offers the temperature profile used for the protoplanetary disk model, where z is the height above the midplane. The midplane and atmosphere temperatures T_{mid} and T_{atm} are given in Equation **??**, respectively. The scale height H is given in Equation 9 **?**. (1)

$$\rho = \frac{\Sigma}{\sqrt{2\pi}H} exp \left\{ -\frac{1}{2} \left\{ \frac{z}{H} \right\}^2 \right\}$$

Density Profile. Equation 2 details the density profile used for the protoplanetary disk model. Here, Σ refers to the column density, given in Equation 10, while H refers to the characteristic scale height, given in Equation 9. z represents the vertical distance. **?** (2)

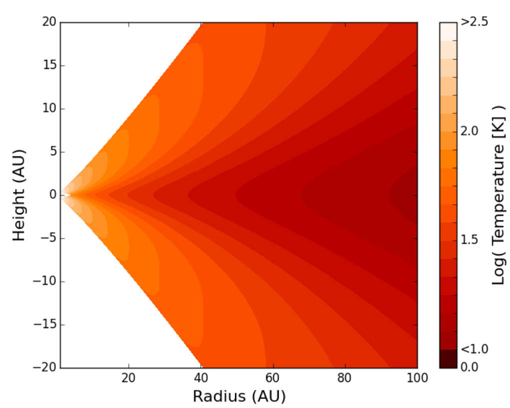

Figure 1. Temperature Gradient. Figure 2.1.2 displays the temperature distribution of a cross-sectional slice of the disk model. The x-axis and y-axis provide the radius and height of the disk, respectively, while the color indicates the log scaling of the temperature itself. Equation 1 offers the mathematical formation of the gradient.

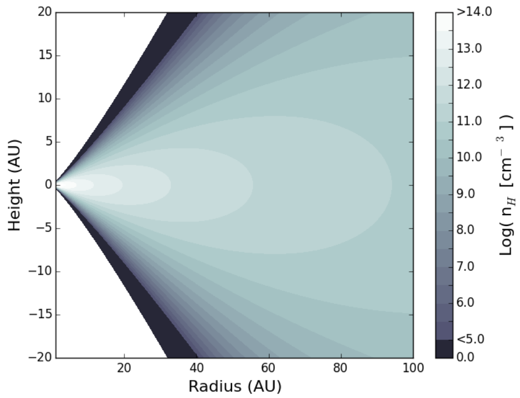

Figure 2. n_H **Gradient.** Figure 2.1.2 illustrates the distribution of the base number density of Hydrogen nuclei within a cross-sectional slice of the disk model. The x-axis and y-axis show the radius and height of the disk, respectively. The color illustrates the log scaling of the density. Equation **??** shows the mathematical formation corresponding to the gradient.

Equations **??** and 2 give the temperature and density profiles of the disk. In turn, Figures 2.1.2 and 2.1.2 illustrate the resulting gradients of the temperature and density profiles, respectively, as a function of radius and height. These gradients, which capture a view of the cross-section of the disk, demonstrate the model's basic structure.

Once the 'base' of the protoplanetary disk was constructed, the authors then added in molecules, to join the Hydrogen nuclei. For each of these molecules, the authors equated the adsorption and desorption rates. Here, adsorption rate refers to the rate at which molecules would attach and 'stick' to grains within the disk. In contrast, desorption rate gives the rate at which molecules would break away from the surface of grains inside of the disk.

$$\frac{-\delta n_{A[gas]}}{\delta t} = (n_{gr})(n_{A[gas]})\sigma s v$$

Adsorption Equation. Equation 3 illustrates the adsorption equation of the molecule-grain collisions in the disk for a given molecule A. Here, $n_{A[gas]}$ is the number density of molecule A in gaseous form. n_{gr} is the number density of the grains, set as 1e-10% of the Hydrogen density for this report. Furthermore, σ is the cross-sectional area of the grains, with a radius assumed to be (0.1e-4)cm, while s is the coefficient of sticking between the molecules and grains, assumed as 1. Finally, v is the velocity of the molecules, as given in Equation 5 **?**. (3)

$$\frac{\delta n_{A[gas]}}{\delta t} = (n_{A[gr]})\nu_0 e^{-E_{des}/T}$$

Desorption Equation. Equation 4 illustrates the desorption equation for sublimation (?) of gas from grains. For this equation, $n_{A[gas]}$ and $n_{A[gr]}$ represent the number densities of the molecule A in gaseous and grain form, respectively. E_{des} is the desorption energy (K), while T is the disk temperature at the given location. ν_0 is the oscillation frequency, as detailed in Equation 6 **?**. (4)

Table 1

Model Molecules. This table displays the molecules added to the protoplanetary disk model. Column 1 gives the chemical formula for each molecule. The remaining columns show a few of the characteristics of each molecule that were necessary for the adsorption and desorption rate calculations.

Molecule	Abundance (x 10^{-5} of n_H)	E_{Des} (K)
CO	14.0000	1389
CO_2	3.0000	2440
H_2O	9.0000	5773
N_2	10.7236	1053
NH_3	0.4950	2965
Grains (C)	Check!	-
Silicates (O)	Check!	-

Equations 3 and 4 showcase the adsorption and desorption rates, respectively. Equating these two rates allowed the authors to subsequently determine the gaseous and grain abundances for the molecules, using the base number density of Hydrogen nuclei and the assumptions given in Section 2.1.1.

Table 2.1.2 lists the molecules that were poured into the modeled disk. Additionally, Table 2.1.2 offers some of the relevant parameters for those molecules that were needed to calculate the gaseous and grain abundances from the equated rates.

The authors used the calculated *molecular* abundances to then derive the gaseous and grain abundances of each *element* contained within the disk.

3. RESULTS

3.1. *Comparison*

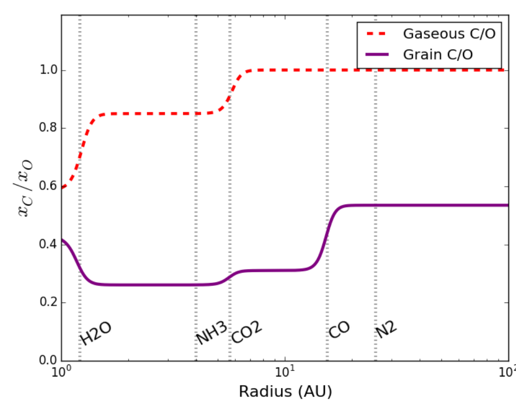

Figure 3. **Midplane C/O.** Figure 3.1 displays the elemental abundances for the Carbon to Oxygen ratio specifically along the modeled disk's midplane. The x-axis displays the radius (in AU), while the y-axis gives the elemental abundance ratios. The dashed red line shows the gaseous abundance, while the solid purple line shows the grain abundance. Snow lines are picked out in dotted gray lines.

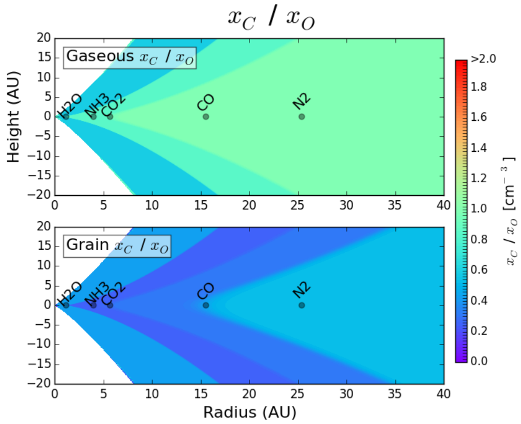

Figure 4. Disk $\frac{C}{O}$. Figure 3.1 maps out the gaseous and grain elemental abundances for the ratio of Carbon to Oxygen. The x-axis and y-axis give the radius and height (both in AU) of the disk, respectively. The elemental abundance ratios are indicated with color. Snow line locations along the midplane are dotted and labeled in black.

3.2. *Variation in Ice Structure*

In this section, we consider the effect of ice structure on the C\O gaseous and grain abundances. In particular, we vary the structure of CO and N_2 icy grains between two extremes: pure ices and mixed (layered) ices. The authors altered the ice structures by changing the desorption energies, using values provided by (!cite the papers!) **??**.

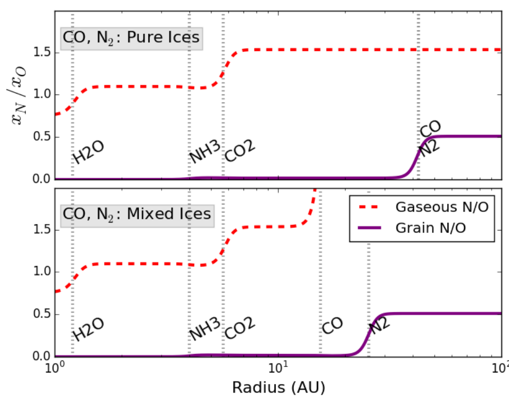

Figure 5. Midplane C\O: Varied Ice Structures. Figure 3.2 illustrates the effect of altered ice structures of CO and N_2 upon the C\O ratio in the modeled disk. The plots are structured similarly to Figure **??** (see Figure **??** for a description of how the plots work). The top plot's disk model contains CO and N_2 in pure ices, while the bottom plot's disk model features CO and N_2 in mixed (layered) ices. Ice structures were varied using differing desorption energies E_{Des} **?**.

The extreme of pure ices, as shown in Figure 3.2, shifts the snow lines of CO and N_2 such that they overlap. In other words, the molecules of CO and N_2 will be in gaseous form over the same region of the disk. Furthermore, both molecules will freeze out of the disk atmosphere into icy grain form past the same radius. At the other end of the spectrum, the extreme of mixed ices separates the snow lines of CO and N_2 by a considerable distance of nearly 10 AU. In this case, the CO snow line proceeds the N_2 snow line, such that the region between the two snow lines contains CO frozen into icy grain form and N_2 still in gaseous form.

We can use these plotted models to constrain what we know of various cometary parameters. For example, in their (!year!) report, Mumma and Charnley (!spell check! and other authors?) discuss detailed measurements of cometary volatile abundances with respect to water, as determined from reported spectroscopic surveys. In their report, they provide evidence for measurements of (relatively) large abundances of CO, as well as a lack of evidence for measurements of any N_2. These observations suggest that the comets formed in a regime containing CO in icy grain form (allowing the molecules to be built into the forming comet) and containing N_2 in gaseous form (essentially excluding direct involvement of N_2 in the comet formation). Of the two extreme ice structures considered, mixed ice structure best fits these two criteria. As a result, we can infer that the CO molecules of the disk would be realistically contained in mixed icy grains, so as to allow this regime to exist. Constraints on the form of N_2 ices are less certain. Notably, N_2 in pure ice form would allow a wider regime of comet formation than for N_2 in mixed ice form.

3.3. *Variation in Molecular Abundances*

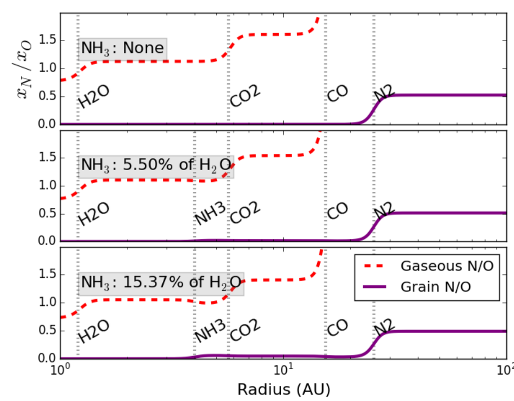

Figure 6. Midplane C\O: Varied Ammonia Abundances. Figure 6 demonstrates the effect of varying abundances of NH_3 (in respect to H_2O) on the modeled disk's C\O ratio. The plots have structures similar to those found in Figure **??** (see Figure **??** for a description of how the plots work). NH_3 abundance values were extracted from values measured in the (!reference c2d Spitzer paper!). The disk model for the top plot has no NH_3, the model for the bottom plot contains the maximum amount of NH_3 measured, while the model in the middle plot features the accepted amount of NH_3 measured overall **?**.

4. EQUATIONS

$$v = \sqrt{\frac{8k_BT}{\pi m}}$$

Thermal Velocity. **?** (5)

$$\nu_0 = \sqrt{\frac{2k_BE_{des}N_{sites}}{\pi^2 m}}$$

Oscillation Frequency. **?** (6)

$$T_{mid} = T_m \left\{ \frac{R}{1AU} \right\}^{-q_m} \tag{7}$$

$$T_{atm} = T_a \left\{ \frac{R}{1AU} \right\}^{-q_a}$$

Temperature Profile Components. Equations 7 and 8 give the midplane temperature T_{mid} and the atmosphere temperature T_{atm}, where R is the radial distance in the disk. For this report, the constants T_a and q_a were set to 343.269K and 0.54, respectively. Additionally, the constants T_m and q_m were set as 200K and 0.62 **? ?**. (8)

$$H = \left\{ \frac{k_BT}{\mu m_H} \frac{R^3}{GM_s} \right\}^{\frac{1}{2}}$$

Scale Height. Equation 9 offers the scale height H at a lateral distance R in the modeled disk with temperature T. Here, G and k_B are the Newtonian Gravitational Constant and the Stefan-Boltzmann Constant (???), respectively. m_H is the mass of the Hydrogen atom, while μ is the mean molecular weight. Finally, M_s is the mass of the central star. **?**. (9)

$$\Sigma = (2 - \gamma) \frac{M_D}{2\pi m_H (1AU)^2} \left\{ \frac{R}{1AU} \right\}^{-\gamma}$$

Column Density. Equation 10 shows the column density of the modeled disk. Notation-wise, m_H is the mass of the Hydrogen atom, and M_D is the mass of the total disk, assumed to be 4(10)