

## Physics 295 Final Report

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Essentially all Galactic star formation occurs within dense molecular clouds, so understanding how these clouds evolve is essential to the understanding of star formation. The production of two species,  $\text{H}_2$  and  $\text{CO}$ , is crucial to the development of the molecular cloud as they shield the cloud from UV radiation (Glover 2010). This allows cloud to cool, which then allows it collapse and form stars. We hope to track the evolution of  $\text{H}_2$ ,  $\text{CO}$ , and related species coupled with the dynamic development of the cloud in higher resolution than has been done before. This will further our understand of the time dependent evolution of these molecular clouds. The largest challenge is the computational power needed to integrate with high resolution the reaction rate equations of dozens of species in a more than million cell chemical network. One nice feature of these integrals is that they only depend on their neighbors. This allows the integrals to be solved in parallel on a GPU, and will hopefully reduce the overall computation time. One major challenge with this approach is that the self-shielding that  $\text{H}_2$  provides is not local and therefore is not trivial to parallelize.

Because these molecular clouds are primarily  $\text{H}_2$ , we started by recreating the hydrogen chemical network laid out in Glover & Mac Low 2007. First we developed a single-cell chemical network separate from the dynamic and temperature development of the cloud. This involved directly tracking the densities of  $\text{H}_2$  and  $\text{H}^+$ , using conservation laws for the densities of  $\text{H}$  and  $\text{e}^-$ , and assuming instantaneous equilibrium for helium, carbon, oxygen, and silicon. The conservation laws are written in terms of the abundances of the species, with 1 being one hundred percent of the atoms in the cloud being found in that species. The total abundance of dissociated hydrogen is defined as  $x_{\text{H},\text{tot}} = 1.0 - x_{\text{C}} - x_{\text{O}} - x_{\text{Si}} - x_{\text{He}}$  where

$x_C = 1.4 \times 10^{-4}$ ,  $x_O = 3.2 \times 10^{-4}$ ,  $x_{Si} = 1.5 \times 10^{-5}$ ,  $x_{He} = 0.1$ . This results in conservation laws for

hydrogen and electrons:

$$x_H = x_{H,tot} - x_{H_2} - x_{H^+}$$

$$x_e = x_{H^+} + x_C + x_{Si}$$

The values of  $x_{H_2}$  and  $x_{H^+}$  are determined by integrating the ODEs based on the eight reactions

this network involves. Those reactions are:

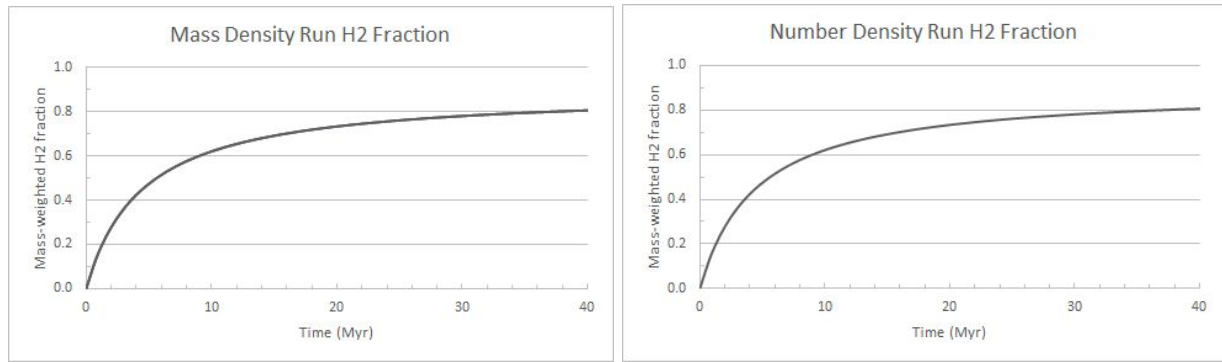
1.  $H + H + \text{grain} \rightarrow H_2 + \text{grain}$  ..... Hollenbach & McKee (1979)
2.  $H_2 + H \rightarrow 3H$  ..... Mac Low & Shull (1986) (low density); Lepp & Shull (1983) ( high density)
3.  $H_2 + H_2 \rightarrow 2H + H_2$  ..... Martin et al. (1998) (low density); Shapiro & Kang (1987) ( high density)
4.  $H_2 + \gamma \rightarrow 2H$  ..... Glover & Mac Low (2007)
5.  $H + \text{c.r.} \rightarrow H^+ + e^-$  ..... Glover & Mac Low (2007)
6.  $H + e^- \rightarrow H^+ + 2e^-$  ..... Abel et al. (1997)
7.  $H^+ + e^- \rightarrow H + \gamma$  ..... Ferland et al. (1992)
8.  $H^+ + e^- + \text{grain} \rightarrow H + \text{grain}$  ..... Weingartner & Draine (2001)

Each of these reactions has a temperature dependent rate coefficient that can be found in the corresponding reference. The rate coefficient of a reaction is the product of the cross section of the reactants and the reactants' relative velocity; it is temperature dependent because temperature affects the species' velocities, which in turn affects their cross section. To get the reaction rate equation for a certain reaction, the rate coefficient is multiplied by the densities of the reacting species. This is because the higher the concentration of the reactants, the more likely they are to collide and react. This gives, for example, the reaction rate contribution for  $H_2$  from equation 1 to be

$$n_H \times n_H \times k_1(T),$$

where  $k_1(T)$  is the temperature dependent reaction rate coefficient for equation 1. One decision we had to make was whether we would use number density (units  $cm^{-3}$ ) or mass density (units

$g \times cm^{-3}$ ) of the species. We tested both in the Glover & Mac Low network and found that it does not seem to make a difference (as can be seen in Figure 1 below). We decided to use number density because it did not require a factor of  $1.67 \times 10^{-24} g$  from the mass of a proton. We were concerned that this small of a number might have caused numerical stability issues later on. The number density of a given species that was not directly tracked with the integrator is simply calculated by multiplying its abundance by the total number density. A good approximation of the mass density of a species can be recovered by multiplying its number density by the mass of a proton and the number of nucleons in the species.



**Figure 1.** A comparison of running the network with mass density versus running the network with number density. Both runs produced nearly identical results. (Both runs had a total number density of  $300 cm^{-3}$  and temperature of 50 K).

The total reaction rate equation for  $H_2$  depends on the reaction that creates  $H_2$  (reaction 1) minus the reactions that destroy  $H_2$  (2, 3 and 4). The reaction rate equation for  $H^+$  is calculated similarly with reactions 5, 6, 7, and 8. This setup models a single cell, so we can assume a constant shielding from UV radiation. To calculate the photoionization rate after this shielding we use equation 31 from Glover & Mac Low with  $f_{shield}(N_{H_2}) = 1$  and an assumed column density of

$8 \times 10^{21} \text{ cm}^{-2}$ . In addition to photons, there are gamma-rays that are so high energy they are not shielded against. It is assumed that they lead to a constant ionization rate of  $10^{-17} \text{ s}^{-1}$  (Glover & Mac Low 2007).

Once we set up the conservation laws and the two ODEs for  $\text{H}_2$  and  $\text{H}^+$ , we needed to decide on an integrator. The two ODEs are coupled, and the different terms in the ODEs may cause them to have different characteristic timescales, so we decided to use a stiff integrator. We decided on the fourth-order Rosenbrock stiff integrator from “Numerical Recipes in C - Second Edition.” To use this integrator we needed to calculate the jacobian of the ODEs. This can be done by hand for the Glover & Mac Low paper, but we wanted to verify our calculations. To do this we also ran the integrator using a two-point central difference differentiator that calculates the jacobian numerically at runtime. Both methods produced essentially identical results.

Once our model of the Glover & Mac Low 2007 paper was completed, we moved on to trying to reproduce the more complex network laid out in Glover et al. 2010. Our general setup is identical to before, but this larger network tracks hydrogen, carbon, and oxygen in the form of 32 species with 218 reactions. In the paper they directly track fourteen species, assume thirteen species are instantaneously in equilibrium, and use conservation laws for the remaining five. In our model we also use conservation laws for those five species, but we directly track all the remaining 27 species. We can do this because at first we are only modeling one cell of the network, so the number of computations required is reasonable. This will allow us to see if we agree with Glover et al. about which species can be assumed to be instantaneously in equilibrium. We will do this by examining all the species’ time dependent evolutions and determining which evolve on a timescale much shorter than the rest.

Because there are so many ODEs in this model, we can not calculate its jacobian by hand. Instead, we calculate it at run time with the numerical differentiator used to test the previous

network. We also wanted to ensure that there was no human error when typing up all the reaction rate constants and combining them to create the 27 ODEs. To do this we created a script that checks conservation laws for the equations that are inputted to the program. This then combines the reactions in the correct fashion of creation and destruction terms for the ODEs. Unfortunately, there are still stability issues while trying to get this more complex network to run. We hope to relieve this by adjusting the initial conditions for the stiff integrator and verifying there are no terms in the ODEs that are radically unstable.

## References

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