Chemistry in dark clouds at low metallicity

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A time-dependent model of a dark cloud was constructed, in an attempt to model these clouds in low metallicity environments such as other galaxies. The models were calculated with varying initial elemental abundances of carbon, oxygen, nitrogen and sulphur. These abundances were taken from observations of HII regions in the Large and Small Magellanic Clouds [1]. The model results were compared with those of Millar and Herbst (1990) [2], who previously modelled dark clouds in the LMC and SMC. It was found that the results were in reasonable agreement with Millar and Herbst (1990). The model results were used to identify potential metallicity tracer species in dark clouds. It was found that CO was a good tracer of the underlying carbon abundance at both early time and steady state. H_2CS was found to be a potential tracer of the underlying sulphur abundance. NH_3 was found to be a poor metallicity tracer.

Background:

Dark clouds are regions of star formation, and have been observed and modelled within the Galaxy to a good degree of accuracy. These regions are important, as they provide insight into the star formation process, as well as yielding information regarding metallicity and chemical enrichment on both solar and galactic scales. With the advent of new facilities, such as ALMA [3], detailed observations of dark clouds will be achievable in external galaxies. We have thus attempted to model a dark cloud in the low metallicity extragalactic environments of the Large and Small Magellanic Clouds (henceforth LMC and SMC), using observations of chemical abundances taken from HII regions [1]. The wider motivation behind this work is a desire to increase understanding of how individual star forming regions have evolved over cosmological timescales.

The Model:

A time-dependent gas-phase chemical model (e.g. Herbst and Leung, 1985 [4]) was adopted to model homogeneous dark clouds in low metallicity environments. The physical conditions shown in Table 1 were all held to be constant for the duration of the simulations. The models included a Galactic model (G), an LMC model and an SMC model. The initial elemental abundances of carbon, oxygen, nitrogen and sulphur were varied as shown in Table 2. The LMC and SMC abundances were taken from Garnett (1999) [1]. The sulphur abundances in Garnett (1999) were higher than the Galactic dark cloud sulphur abundances taken from the UMIST database 06 paper [5]. This was because the Garnett (1999) abundances were taken from an HII region rather than a dark cloud. The model input sulphur abundances were depleted from the Garnett (1999) values, by a ratio found from Galactic HII region/dark cloud sulphur abundances. The reactions used in the model were taken from the UMIST database [5], although only those reactions involving H, He, C, O, N, S, Fe, Na and Mg were used, as trace species were not included in the simplified model. The results were used to try and identify suitable species which could be used as metallicity tracers in dark clouds, particularly in other galaxies.

Temperature	10K
H_2 density	1×10^4 cm^{-3}
A_V	10 magnitudes
CR ionisation rate	1.3×10^{17} s^{-1}

Table 1: Parameters used in the models.

Model	O	C	N	S
G	3.52(-4)	1.46(-4)	2.48(-5)	4.00(-8)
LMC	1.26(-4)	3.97(-5)	3.97(-6)	1.15(-8)
SMC	5.00(-5)	1.26(-5)	1.58(-6)	4.58(-9)

Table 2: The initial elemental abundances used in the models. Note: a(-b) refers to $a \times 10^{-b}$.

	G/LMC	G/SMC	LMC/SMC
O	2.8	7.0	2.5
C	3.7	11.6	3.2
N	10.8	27.0	2.5
S	3.5	8.7	2.5

Table 3: Relative metallicities in the models (using initial elemental abundances).

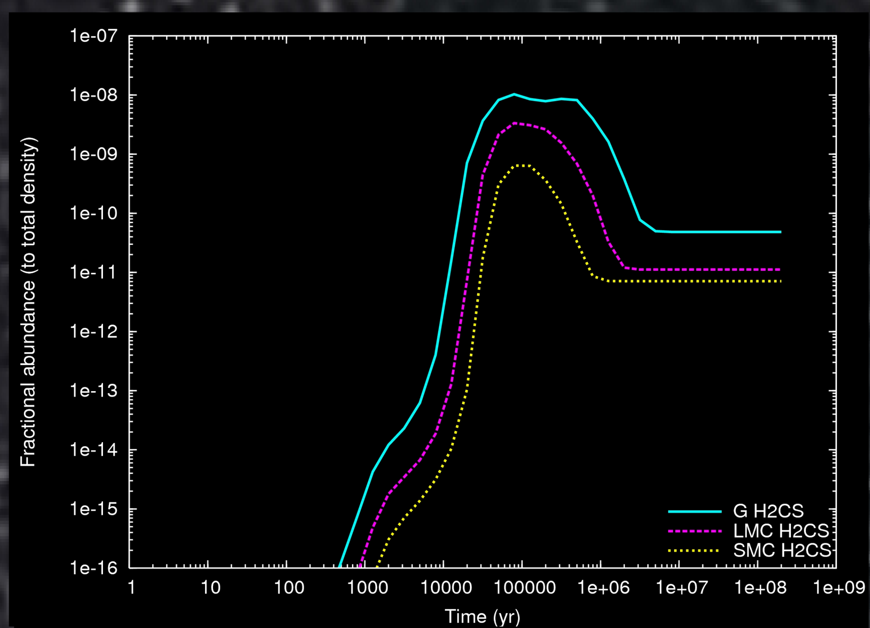

Figure 3: The H_2CS abundance in each model traces the underlying S abundance.

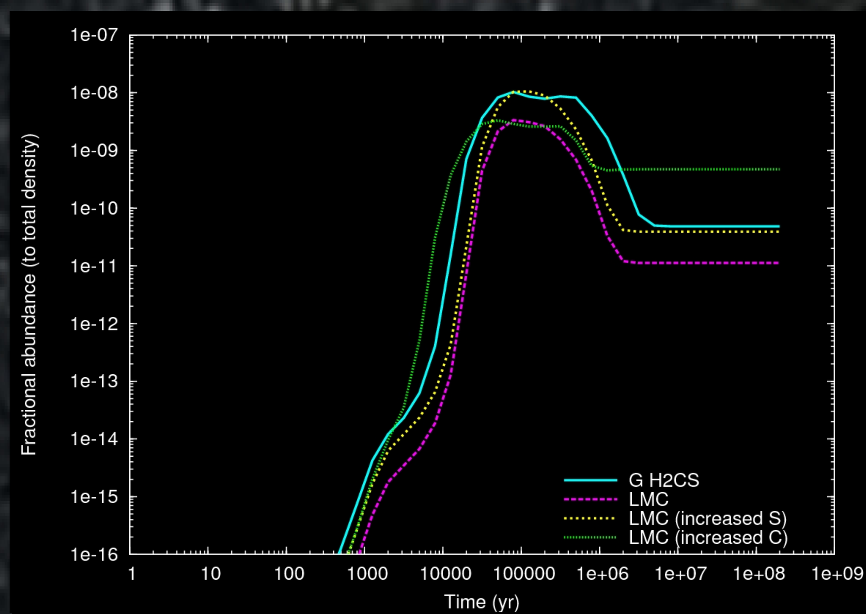

Figure 4: Increasing the initial abundance of C or S in the LMC model to that used in the G model, shows that the H2CS abundance is tracing the underlying S abundance rather than C abundance.

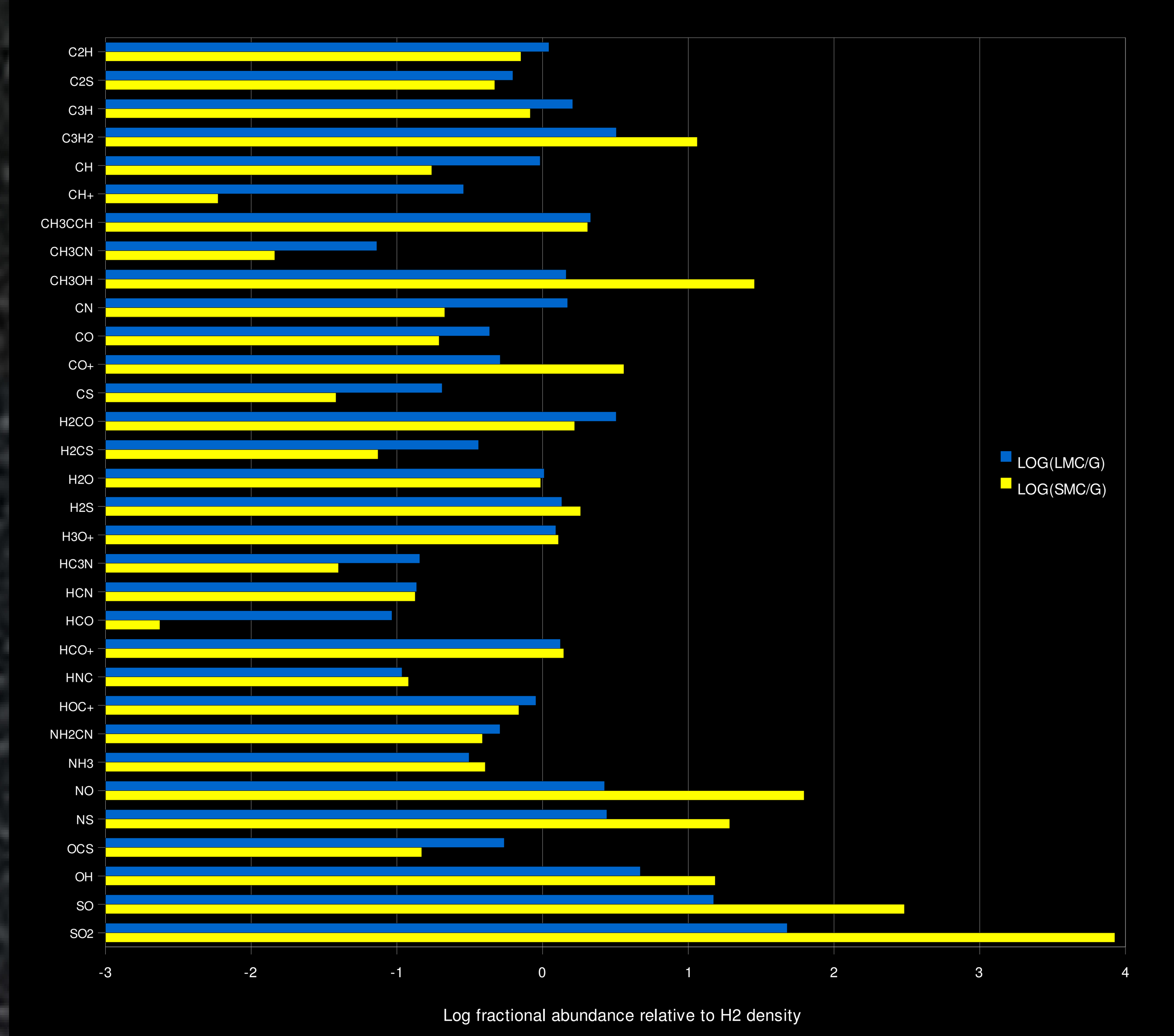

Figure 1: The early time log fractional abundances (to H_2) produced by models LMC and SMC, as a ratio of the abundances produced by the galactic model G. These species have all been detected in extragalactic sources.

Potential metallicity tracers:

•Figures 1 and 2 show the abundances of different species as a ratio between the abundances obtained from the Galactic model, and those obtained from the LMC and SMC models. A good metallicity tracer will reflect the ratio of the underlying elements, as seen in Table 3. A bad metallicity tracer will be produced in similar amounts in the different models. This will result in a log fractional abundance ratio of zero.

• CO is a good tracer of the underlying C abundance at both early time (~ 10^5 years) and steady state (~ 10^7 years) . At steady state the CO abundance scales directly with the underlying C abundance. The models are all oxygen rich, which means that the majority of the carbon gets locked-up in the stable CO molecule at steady state. At early time, the CO abundance does not scale directly with the underlying C abundance. However, as seen in Figure 5, the ratio between the models remains fairly constant, and this ratio can be used to estimate the underlying C abundance in a cloud.

• H_2CS is a potential tracer of the underlying S abundance at early time. It can be seen in Figure 3 that the H_2CS abundance in each model is distinct, and reasonably constant, between around 10^5 years and 10^6 years. Figure 4 shows that the H_2CS abundance appears to trace the S abundance rather than the C abundance. The models G and LMC in this graph are the same as those in Figure 3. The "increased" models show the effect of increasing either the C or the S in the LMC model to the same level used in the G model. When the S is increased to the level used in the G model, the H_2CS abundance at early time is similar to that seen in the G model. When the C is increased to the level used in the G model, the H_2CS abundance at early time barely changes (although at steady state it is much increased). Figure 4 therefore demonstrates that the H_2CS abundance in these models appears to trace the S abundance, rather than the C abundance.

H_2CS is also a good tracer of S abundance at steady state, as is C_2S.

• HC_3N could possibly be used as a tracer of the underlying nitrogen abundance in a cloud. Similar abundances are produced in the LMC and SMC models at early time. However, the abundance produced in the G model is much higher at this time. The HC_3N abundance could therefore be used to derive an upper limit on the underlying N abundance in a cloud, rather than a specific N abundance. At steady state, HC_3N traces the C abundance reasonably well.

Poor metallicity tracers:

• At early time, oxygen bearing species including H_2O, H_3O^+ and HCO^+ appear to be poor tracers of metallicity. The abundances of these species in the LMC and SMC are very similar to those produced in the Galactic model. As all the models are oxygen rich, this could mean that the abundances of these species are tracing the H_2 density rather than the metallicity, with the H_2 density as the limiting factor in their production. These oxygen bearing species are also seen to be overabundant in the LMC and SMC models (compared to G) at steady state, making them poor metallicity tracers at all times.

• NH_3 appears to be a poor metallicity tracer – Figure 6 shows that shortly after 1×10^5 years, the NH_3 abundance in the highest and lowest metallicity models (G and SMC) is the same. NH_3 is also a poor metallicity tracer at steady state – the three models produce similar abundances of this species. Any observations of NH_3 could not be used to differentiate between these models and thus determine the underlying metallicity. This can be seen on Figure 6 at times greater than around 10^6 years.

C_2H and C_3H are also poor tracers of metallicity – similar abundances of these species are produced in all models at early time.

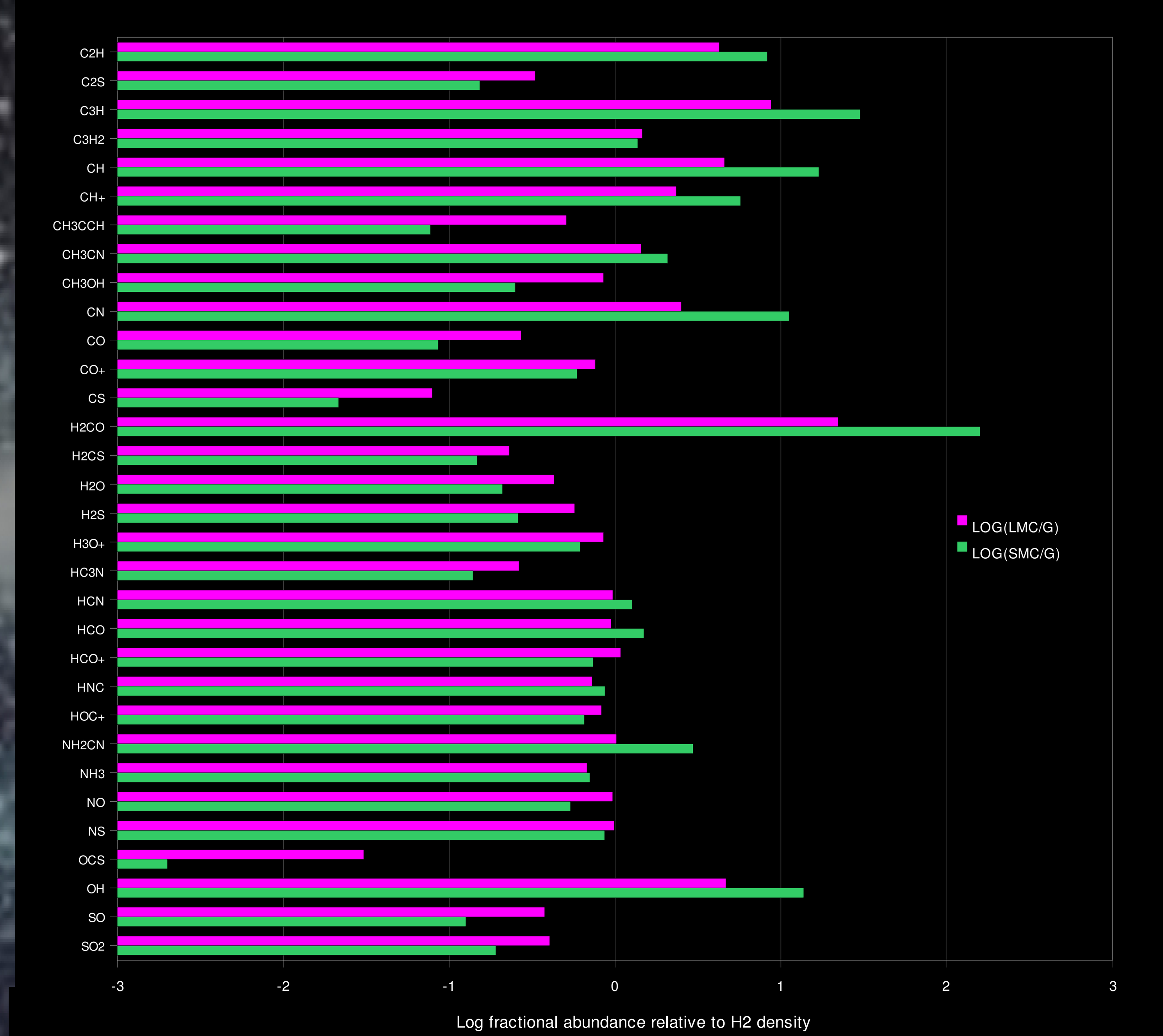

Figure 2: The steady state log fractional abundances (to H_2) produced by models LMC and SMC, as a ratio of the abundances produced by the galactic model G. These species have all been detected in extragalactic sources.

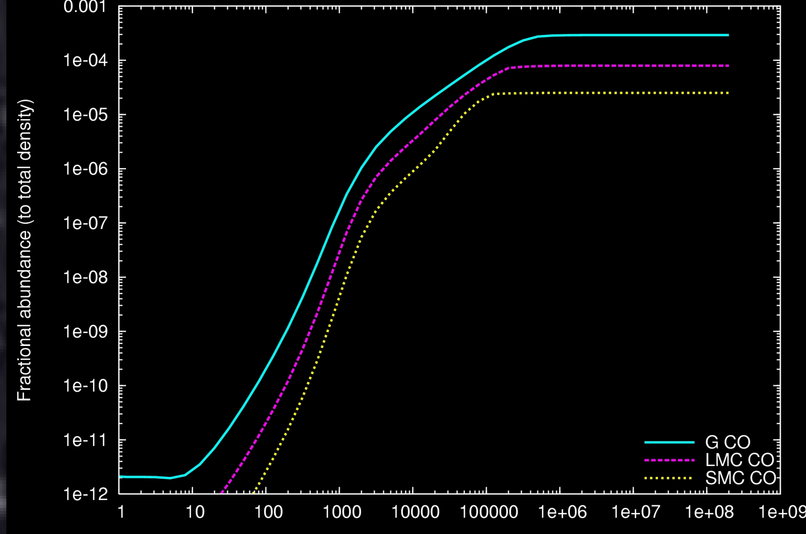

Figure 5: The CO abundance is a good metallicity tracer. In the three different metallicity models, CO abundance traces the underlying C abundance fairly well, at all times.

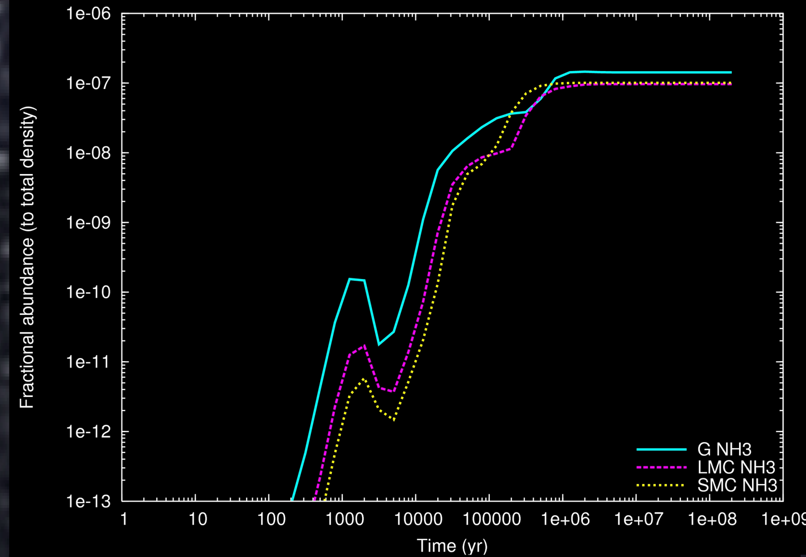

Figure 6: The NH_3 abundance is a poor metallicity tracer. In the three different metallicity models, NH_3 abundance is similar or the same at all times after ~ 10^5 years.

CONCLUSIONS:

• The majority of the model results are in reasonable agreement with those of Millar and Herbst (1990) [2]. Any differences are thought to be caused by improvements in reaction rate information since 1990.

• Initial model results indicate that the species most able to trace metallicity in dark clouds are CO, which traces the underlying carbon abundance, and H2CS, which traces the underlying sulphur abundance.

• NH3 and HCO+ are poor metallicity tracers at early time and steady state.

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