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CO FORMATION IN SUPERNOVAE

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RESUMEN

Estudiamos los efectos de varias distribuciones de masa de la envolvente, de redes de reacciones y de constantes de las tasas de formación de CO en el primer mes de un colapso del núcleo de supernovas. Hemos encontrado que las abundancias de CO calculadas a partir de una distribución de la masa de la envolvente no uniforme se acerca a los valores observados. Como prueba de la "grumosidad" hemos hecho pruebas con fluctuaciones de densidad en la envolente que varían aproximadamente en forma sinusoidal con el radio. Estas fluctuaciones han triplicado la producción de CO en las regiones más profundas de la envolvente; sin embargo, la tasa global es un orden de magnitud menor que la observada. Las estructuras de densidad que se han añadido tienen efectos complejos en las tasas de reacciones químicas. Hemos usado un código 1–D, por lo que predecimos que si empleamos la formulación de transporte radiativo plenamente en 3–D con distribución de densidad se logrará una tasa de formación de CO acorde con los valores observados.

ABSTRACT

We are studying the effects of various envelope mass distributions, reaction networks, and rate constants on CO formation in the first month in core–collapse supernovae. We have found that a nonuniform envelope mass distribution does indeed bring the calculated CO abundances closer to the observed values. As a test case of "clumping", we have tested envelope density fluctuations that vary approximately sinusoidally with the radius. These fluctuations have tripled the CO production in the deeper areas of the envelope; however, the overall rate is still too low by an order of magnitude. The added density structures have complex effects on the chemical reaction rates, and we are using a 1–D code, so we predict that moving to a fully 3–D radiation transfer scheme and density distribution will bring the CO formation rate up to observed values.

Key Words: **MOLECULAR PROCESSES — SUPERNOVAE: GENERAL**

1. INTRODUCTION

Molecular formation in supernovae was first detected in SN 1987A, particularly the presence of CO and SiO (Lepp, Dalgarno & McCray 1990; Sharp & Höflich 1989). In fact CO features are present in the earliest spectra of most observed core–collapse supernovae. The chemistry of these molecules can yield valuable information about the progenitor and the evolution of the envelope and are important in such processes as the formation of dust grains from the ejecta (Gerardy et al. 2000; Höflich & Zorec 1989; Gearhart, Wheeler & Swartz 1999).

The models of CO formation in SN 1987A, for one, have been consistently producing only about 1% of the observed abundances. Even the most cursory analysis will show that the understanding of this very important mechanism is severely lacking. Explanations for the shortfall include an incomplete chemical reaction network, incorrect reaction rate constants, and, most importantly, inhomogeneities in envelope mass distributions. The solution to this problem is likely a lack of sophisticated models of simple physics, not any unknown processes. In this vein, we are systematically studying the effects of these three possibilities on the CO formation timescales (Rawlings & Williams 1990; Gearhart, Wheeler & Swartz 1999; Liu, Dalgarno & Lepp 1992).

2. MODEL

The model is run as a set of modular Fortran 77 programs modified to run in parallel on a Beowulf cluster. Various levels of detail can be attained by adding or subtracting the modules. This will facilitate future development of our envelope structure and chemical reaction network. However, the underlying model always includes time– and depth–dependent radiation transport and rate equations for CO, a depth–dependent density structure and composition derived from hydrodynamical calculations, and detailed equations of state for all relevant species (Petuchowski et al. 1989; Avrett et al. 1996; Höflich 1995).

3. CHEMISTRY OF CO FORMATION

Typical chemical reaction networks involved in the formation of CO have been readily modeled. However, these previous models fell short of observed CO abundances. In this aspect of the problem, we are studying the effects of varying the rate constants of the less–understood reactions and using different combinations of the reactions given by Gearhart, Wheeler & Swartz (1999).

Most of the dominant processes are well known and have been thoroughly studied (Dalgarno, Du & You 1990; Liu, Dalgarno & Lepp 1992; Petuchowski et al. 1989; Rawlings & Williams 1990; Gearhart, Wheeler & Swartz 1999). The effects of additional, minor reactions that also form and destroy C or O are usually ignored because they are likely to be negligible. However, in the interest of completeness, we are including them to determine what effect the uncertainties in the rates of these reactions has on the overall CO formation timescales.

4. CLUMPS

CO formation has been thoroughly studied in SN 1987A, but several other supernovae have also exhibited early CO features. Thus a particular chemistry can be ruled out. A more general, and perhaps plausible, explanation for the observed CO is clumping of the ejecta caused by Rayleigh–Taylor instabilities or asymmetric explosions (Gerardy et al. 2000). In addition, most previous models were one–zone models, so clumping was not possible in connection with a complete reaction network.

The chemical reactions involved are mostly two–body reactions which are very sensitive to the local number density of the reactants. The reaction rates in areas of overdensity would increase enough to more than compensate for the slower rates in the areas of underdensity. The quadratic nature of this process could bring about a substantial increase in CO production.

As a test case of "clumping", we have added density fluctuations that vary approximately sinusoidally with the radius (see Fig. (1)). This is a bit idealistic, but our test model is one–dimensional, and this simple case is useful in confirming the effects of density fluctuations without the added complexity of fully three–dimensional radiation transfer and hydrodynamical calculations. The structure of the fluctuations follows

$$\rho' = \rho \left[1 + A \sin \left(\frac{2\pi n}{f} \right) + R \right], \tag{1}$$

where ρ is the density, f is the spatial frequency of the sine wave over the radius, n is the depth point, R is a random number, and A is an amplitude chosen to satisfy $A \leq R + 1$ through the entire range of R (ρ must be nonnegative). We chose R between zero and one, so the largest useful amplitude factor was one. This is the top curve in Figure (2)).

The best results were obtained by using the maximum amplitude (A=1) and a high spatial frequency (f=50). These are shown in Figure (2). The fractional CO concentration with this particular density structure was most affected in the deeper layers, where it was $\sim$3.2 times higher than that of the normal structure. If one assumes that clumping in each dimension will produce a rise in CO production of this order, then a density structure with 3–dimensional clumps should result in CO concentrations that are $\sim$30 times higher. This alone would then bring the popular models into the range of the observed abundances.

The sinusoidal structure is of course arbitrary, and more sophisticated patterns might increase CO production further. Nevertheless, this simple model introduces enough uncertainty in the envelope density distribution

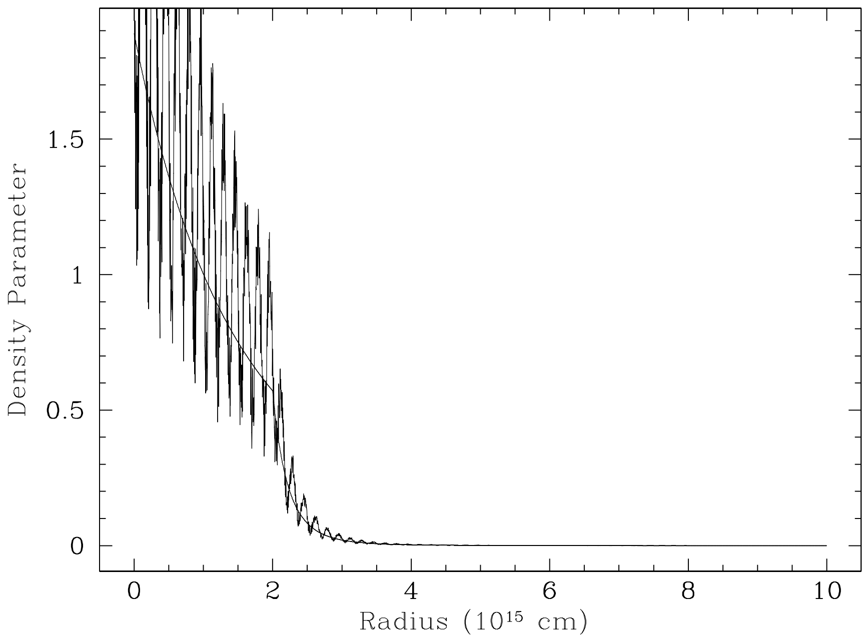

Fig. 1. The added density fluctuations are sinusoidal with a small random component. This particular distribution was chosen with a spatial frequency of 50 over the entire radius and maximum amplitude of one. Superimposed is the uniform, unfluctuated, power–law density distribution.

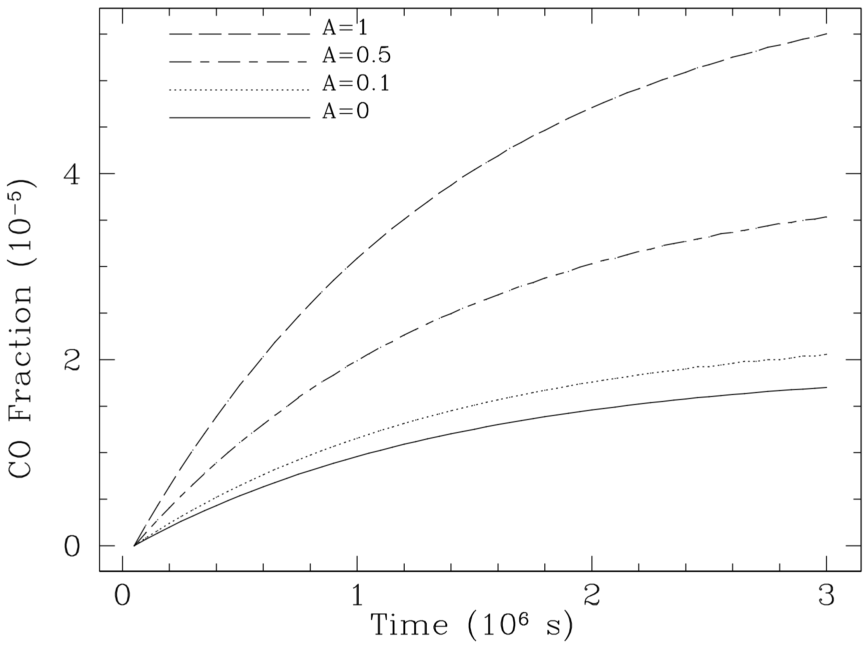

Fig. 2. The fraction of CO formed from the available C and O increases substantially with increasing fluctuation amplitude. Here we show the evolution of the CO concentration for the unfluctuated envelope and the fluctuated envelope with three amplitudes ($A = 0.1, A = 0.5, A = 1$) and a spatial frequency of 50.

at early times to easily account for the seemingly large discrepancy between the observed and calculated abundances of CO.

5. SUMMARY AND FUTURE WORK

Density fluctuations significantly affect the CO formation rate, with a simple sinusoidal fluctuation producing a threefold increase. The effects of varying the chemical reaction rates and the reaction network is very complicated, but they are unlikely to prove significant and do not generalize to arbitrary supernovae.

Future work will include verifying the validity of our models by comparison with previous models, such as those of Gearhart, Wheeler & Swartz (1999). Then a complete reaction network will be included with the clumping, and 3–D radiation transfer and non–spherically symmetric envelope density structures will be added to produce more realistic clumping.

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