

THE CHEMICAL EVOLUTION IN A MODEL OF CONTRACTING CLOUD

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Abstract. The evolution of the different chemical species are followed in a model of contracting interstellar cloud. The central density increases from $n = 10 \text{ cm}^{-3}$ diffuse initial cloud model to a dense cloud with central density number of $n \geq 10^5 \text{ cm}^{-3}$ after a time of 1.2×10^7 yr. A network of 622 reactions has been involved. The chemistry of the cloud is integrated simultaneously with the hydrodynamic equations of contraction.

The results predict that the different molecular species increase in abundance as the contraction proceeds. The species which enhance significantly are CO, HCO, CS and NO. The fractional abundances of many of the other molecular species increase distinctly with contraction, e.g. CH, C₂H, CN, SO₂, CO₂, H₂O, C₂, NH₃, HCN, SO, OCS and SN. The transformation of the initial diffuse cloud model with small abundances of molecular species to a dense molecular cloud with enhancement of the different molecular species is confirmed. The results predict good agreements of our results with both the observations and other theoretical studies.

Key words: Interstellar chemistry.

1. Introduction

An important aim of astrochemistry is to understand the chemical evolution in interstellar clouds and using the various interstellar molecules as tracers of specific physical or chemical activity in the diffuse or dense interstellar clouds. What is driving the chemical selectivity, and how does it depend on stellar type or evolutionary state? Understanding the chemical and physical processes that lead to the observed abundances of the detected molecules is a challenging task.

The reverse question of how the initial chemical state of a cloud effects the starformation process is equally important. On theoretical grounds, the rates of collapse, and ultimately the efficiency of starformation in interstellar clouds are expected to depend on the chemical evolution of the gas. This would be realized through some known processes. The cooling and heating processes, which in turn, are governed by the chemical composition of the cloud, influence the rate of collapse. The ionization state which is controlled by the cosmic ray ionization rate and subsequent chemical processes may also play an important role in the chemical evolution of interstellar clouds. Magnetic field supports the interstellar clouds and clumps against gravity. The magnetic fields are coupled to the neutral gas through the charged particles. Ambipolar diffusion, as a result of the drift velocity between charged and neutral particles, may diminish or at least weaken the magnetic support

in the dense cores, hence the collapse rate increases. Thus the ionization state, which influences ambipolar diffusion, would indirectly influence the collapse rate. The grain evolution and the gas-grain chemical reaction may also play an important role in the chemical evolution of interstellar clouds.

The interstellar clouds can be distinguished on the basis of their physical characteristics. The most tenuous are the diffuse interstellar clouds. Ultraviolet photons from the interstellar radiation field can penetrate diffuse clouds and rapidly destroy most molecules, so that the atomic fraction is high and only the simplest diatomic species are found. Translucent clouds with visual extinction $A_v = 1-5$ mag. form the bridge between the diffuse and the dark molecular clouds. Their densities are somewhat higher and the temperatures are lower than those in diffuse clouds. The cold, dark molecular clouds are visible as dark patches on the sky, and show a complex morphology. The dense molecular clouds appear as small individual cores or clumps in the clouds, with densities of $n > 10^4 \text{ cm}^{-3}$ temperatures as low as 10 K. It is in these cores that low mass star formation (2 solar masses) has been observed to occur.

Some of the theoretical time dependent models were built on the steady state approximation, e.g. Herbst and Klemperer (1973) and Mitchell et al. (1978), and many scientists have included time dependence in their theoretical models, e.g. Langer et al. (1984), Millar and Nejad (1985), Langer and Gredel (1989), Herbst and Leung (1989), Nejad et al. (1990) and Williams and Hartquist (1991).

Models in which the physical parameters are no longer fixed, are called evolutionary models. The density increases with contraction from diffuse to a dense state. In other words, diffuse and dense clouds may be related in a dynamical and evolutionary sense. Such evolutionary models are developed by Gerola and Glassgold (1978), Suzuki (1983), Tarafdar et al. (1985), Prasad et al. (1987), Nejad et al. (1990), Prasad et al. (1991), and Amin et al. (1995a,b,c).

Amin et al. have studied the time dependent chemical evolution of contracting interstellar clouds. They have followed the chemical reactions in a magnetized cloud in two dimension. Cylindrical polar coordinates were used in the numerical treatment of the hydromagnetic equations which controlling the contraction process. In order to study the chemical evolution of the cloud model, a network of 557 reactions has been developed. The chemical kinetic equations were integrated as a function of time by using gear program. They have followed the chemical reaction system at low, intermediate and high cloud densities. Their procedure falls short of simultaneous integration of the chemical rate equations and the Magnetohydrodynamic (MHD) equations. This is because the calculations of contraction of magnetized cloud in two dimension requires a huge computer time, adding the chemistry to that would complicate the situation. The aim of the present work is to overcome this point, by integrating the chemical rate equations and the MHD equations simultaneously, where we have used a one dimensional program to simplify the treatment of contraction. In addition some developments have been carried out

in the chemical network. We have included some important reactions and a detailed chemical network of 111 reactions for negative ions.

In Section 2, the hydrodynamical equations of the problem are discussed. The chemical model and related assumptions are introduced in Section 3. The results are given in Section 4.

2. Hydrodynamic Equations of the Problem

The equations governing the contraction of an interstellar cloud (non-magnetized) of density ρ , velocity v , gas pressure p , gravitational potential ψ , and temperature T , are: The continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{V}) = 0 \quad (1)$$

The momentum equation:

$$\frac{\partial(\rho \bar{V})}{\partial t} + \nabla \cdot (\rho \bar{V} \bar{V}) = -\rho \nabla \psi - \nabla P \quad (2)$$

The gravitational potential ψ is given by solving Poisson's equation

$$\nabla^2 = 4\pi G \rho \quad (3)$$

where G is the gravitational constant.

Equations (1)–(3) were solved using the finite difference method originally given by Black and Bodenheimer (1975). This method has been refined by Norman et al. (1980) to study the contraction of a rotating cloud and later modified by El-Nawawy et al. (1988), to study the contraction of a magnetic non-rotating cloud. The numerical computer code of El-Nawawy et al. is simplified by El-Nawawy et al. (1992) to follow the contraction process in the non-isothermal regime in spherically symmetric cloud in one dimension (1-D). This final form of 1-D computer code is used in the present work. The pressure at the cloud boundary was considered uniform and constant. The original grid was divided into shells with equal spacing. The coordinates were constructed to move approximately with the matter, but with the inner shell under a constraint of a constant mass. All operators of the form,

$$\frac{\partial D}{\partial t} = -\bar{\nabla} \cdot D \bar{V} \quad (4)$$

where D stands for each of the variables ρ and ρv , were treated in the same manner as follows

$$\frac{\partial}{\partial t} \int d^3 \times D = - \int_Q D \bar{V} \cdot da \quad (5)$$

Equation (5) describes the changes in D due to flow in and out of a shell bounded by surface S . Most of the details of the numerical method can be found in El-Nawawy et al. (1988). We have restricted ourself to follow the contraction from the low density number $n = 10 \text{ cm}^{-3}$ up to $n = 10^5 \text{ cm}^{-3}$, just to study the chemical evolution from diffuse to dense molecular clouds. The cloud model is assumed to be isothermal, which is almost the case in interstellar clouds of density numbers lower than 10^9 cm^{-3} .

3. The Chemical Model

The various molecular, atomic and ionic species included in our chemical scheme are altogether 104 species from the families of H, C, O, S, Si, Cl, metals and grains. The number of possible mutual interactions between the different species is extremely large. We have considered only reactions involving two body interactions. Photo-dissociation and cosmic ray ionization were considered for all species. For every species, there were at least two reactions leading to its formation and two leading to its destruction. This resulted in a large network involving 622 reactions with 111 reactions for negative ions. The numerical treatment is given in Amin et al. (1995a). For modelling interstellar cloud chemistry, it is necessary to know the reaction rate coefficients for the different reactions at temperatures below 100 K. The rate coefficients of our system are taken from Millar et al. (1991), and updated with some modifications given by Anicich (1993), Pineau des Fortes et al. (1993), Gerlich (1993), Clary et al. (1993), Herbst and Yamashita (1993) and Slancil et al. (1993). The rate coefficient for the dissociative recombination of H_3^+ .



is taken by the value $k = 1.0 \times 10^{-7} (\text{T}/300)^{-5} \text{ cm}^3 \text{ s}^{-1}$, as given by Stemberg and Dalgarno (1994).

The chemical kinetic equations were integrated as a function of time. The abundance of each species at time step $t = t_0 + \Delta t$ was taken from that at the previous time step. The corresponding density at the same time was taken from the contraction equations. Our procedure do simultaneous integration of the chemical rate equations and the hydrodynamic equations as shown in the schematic diagram in Figure 1. The fractional abundance of a species is denoted by $x = n(i)/n(\text{H}) + 2n(\text{H}_2)$, where $n(i)$, $n(\text{H})$ and $n(\text{H}_2)$ are respectively, the density numbers of a species, hydrogen atoms and hydrogen molecules. The chemical networks for the Oxygen, Carbon, Nitrogen and Sulphur families are as given by Amin et al. (1995a,b) with some modifications regarding the reactions with SO_2 , which is readily form from SO and is widely observed, as follows:

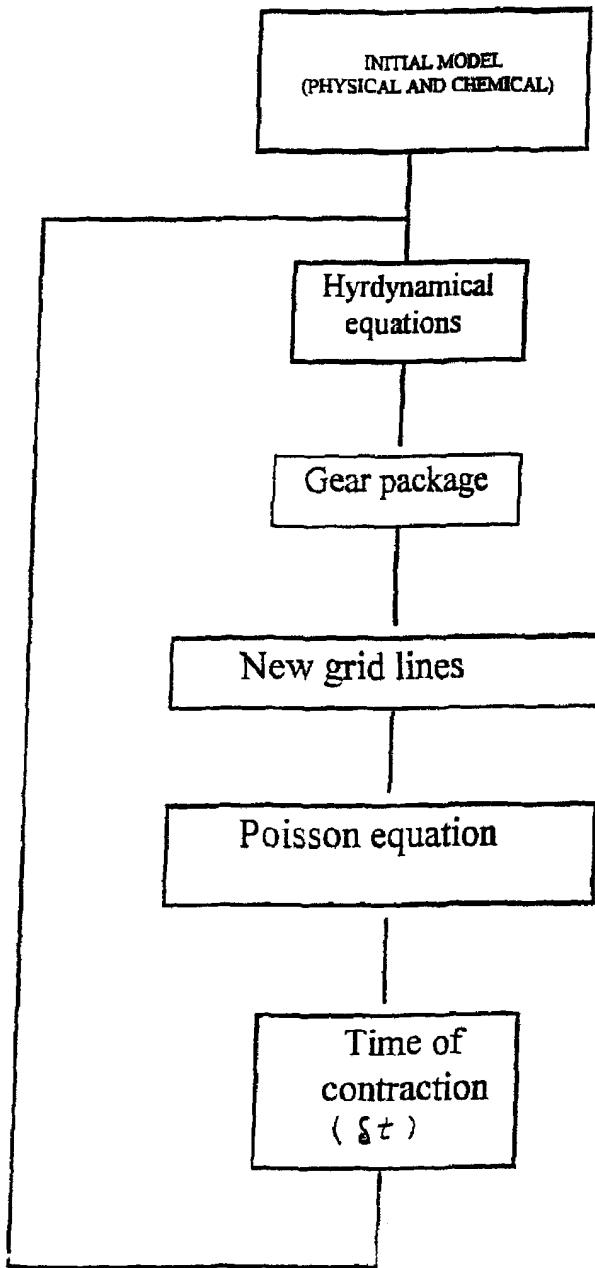


Figure 1. The scheme of contraction.

Table I
Initial abundances

Element	Abundance	Element	Abundance
H	1	Mg	1.0 (-6)
C	7.0 (-5)	Mg ⁺	1.0 (-6)
O	2.0 (-4)	Fe	3.0 (-7)
N	4.28 (-5)	Fe ⁺	3.0 (-7)
S	1.0 (-5)	He	1/12
Si	1.0 (-6)	S ⁺	1.0 (-5)
Gram	1.0 (-12)		

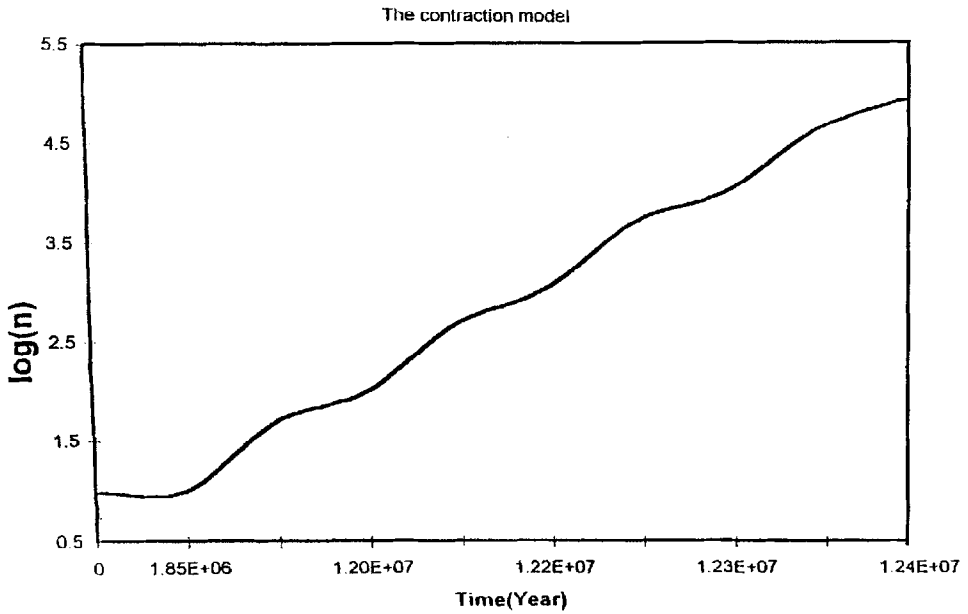


Figure 2. The central density number (in cm^{-3}) versus time.

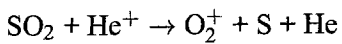
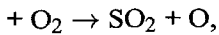
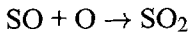
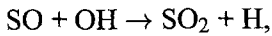


Table II
The resulting maximum fractional abundances for some selected molecules

Species	Our calculated values	Observed values	Other calculations
N ₂	4.0 (-8)	5.0 (-8) ^A	3.1 (-8) ^T
CN	1.5 (-8)	6.0 (-8) ^O 2.0 (-8) ^A	7.2 (-8) ^T 1.2 (-7) ^W
NO	1.3 (-7)		1.9 (-7) ^N
NH	1.0 (-8)		5.4 (-8) ^N
NH ₂	1.1 (-8)		1.0 (-8) ^H
NH ₃	7.9 (-8)	2.0 (-8) ^A	2.6 (-8) ^H
HCN	1.0 (-8)	2.0 (-8) ^{A,F}	2.5 (-8) ^N
C ₂	1.0 (-11)	5.0 (-8) ^A	2.4 (-11) ^N
HCO	1.2 (-8)		2.0 (-9) ^L
H ₂ CO	1.0 (-8)	2.0 (-8) ^A	3.9 (-8) ^T
CH	1.0 (-8)	2.1 (-8) ^A	2.0 (-8) ^L
CH ₂	1.0 (-11)		1.4 (-10) ^T
C ₂ H	1.0 (-8)	3.0 (-8) ^F 8.0 (-8) ^A	7.2 (-8) ^H 2.0 (-9) ^L
CO	6.3 (-5)	8.0(-5) ^{A,F,O}	6.2 (-5) ^T
CO ₂	1.2 (-7)		2.6 (-7) ^T
OH	1.0 (-7)	3.0 (-7) ^A	1.2 (-7) ^T
H ₂ O	4.0 (-7)	2.0 (-7) ^B	3.5 (-7) ^T
CS	3.1 (-8)	2.0 (-8) ^A 5.0 (-8) ^O	5.0 (-9) ^L 4.0 (-7) ^N
SO	1.0 (-9)	5.0 (-9) ^F	3.1 (-9) ^C
SN	4.4 (-10)		1.3 (-10) ^T
OCS	1.0 (-9)	2.0 (-9) ^A 9.0 (-9) ^{A,F}	2.0 (-9) ^N 1.7 (-9) ^W
HS	1.1 (-11)		2.3 (-11) ^T
H ₂ S	1.4 (-11)	1.0 (-7) ^O 3.0 (-9) ^F	2.1 (-10) ^H 3.2 (-10) ^N
SO ₂	1.3 (-9)	1.0 (-9) ^A	9.2 (-9) ^H
HCO ⁺	1.0 (-9)	8.0 (-9) ^A	9.5 (-9) ^H

Where $a(-b)$ signifies $a \times 10^{-b}$.

A: For TMC-1 cloud observed by Irvine et al. (1987).

O: For Orion Plateau cloud, by Hydbeck and Hjalmarson (1985).

F: For Orion ridge cloud, by Hydbeck and Hjalmarson (1985).

L: Langer and Graedel (1989).

H: Herbst and Leung (1989).

N: Nejad et al. (1990).

W: Williams and Hartquist (1991).

T: Tatsuhiro and Herbst (1993).

C: Caselli et al. (1993).

B: Black et al. (1986).

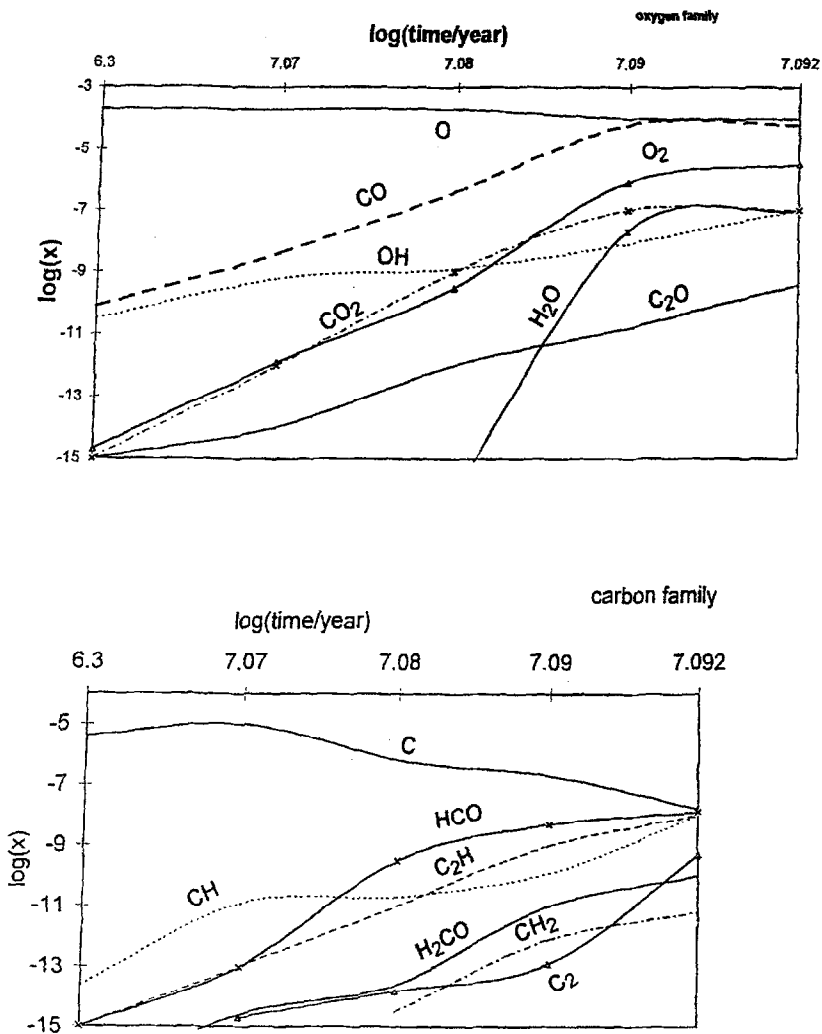
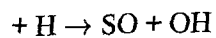
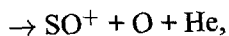
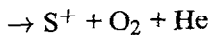


Figure 3.



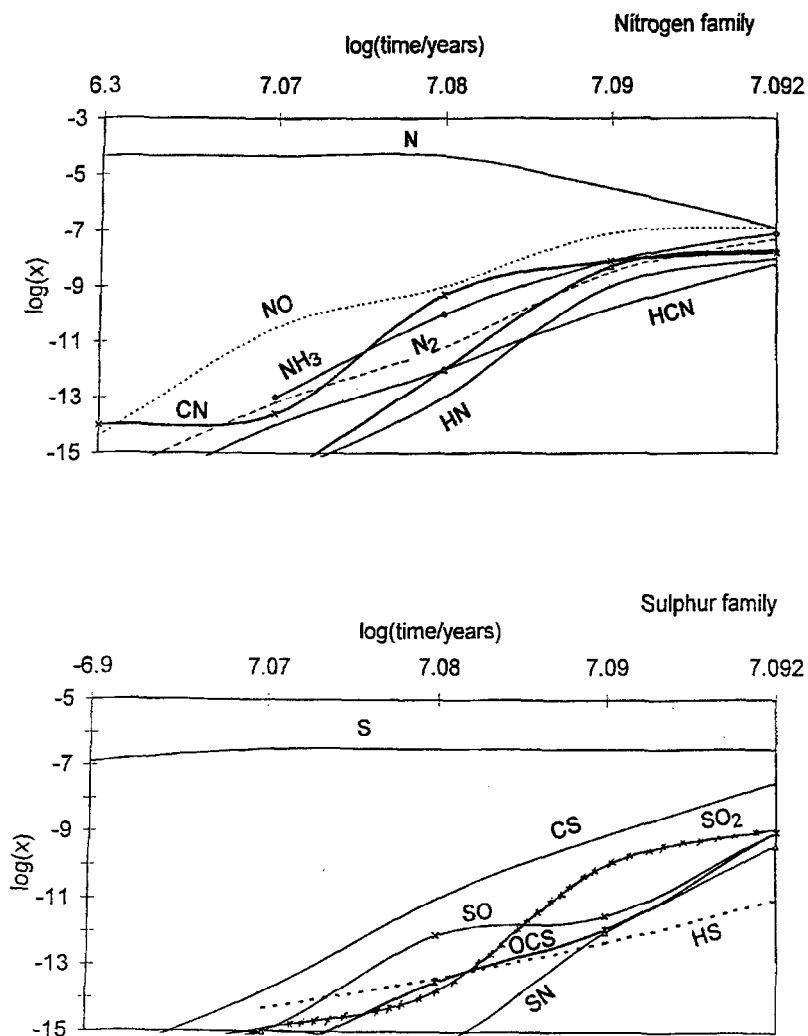
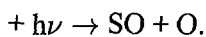
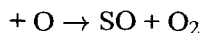


Figure 3. Continued.



In addition, a network of 111 reactions for negative ions is involved.

The following physical assumptions were used to get the solution for the chemical equations:

1. The hydrodynamical parameters (e.g. density, velocity) remain unchanged during a run of the Gear program.

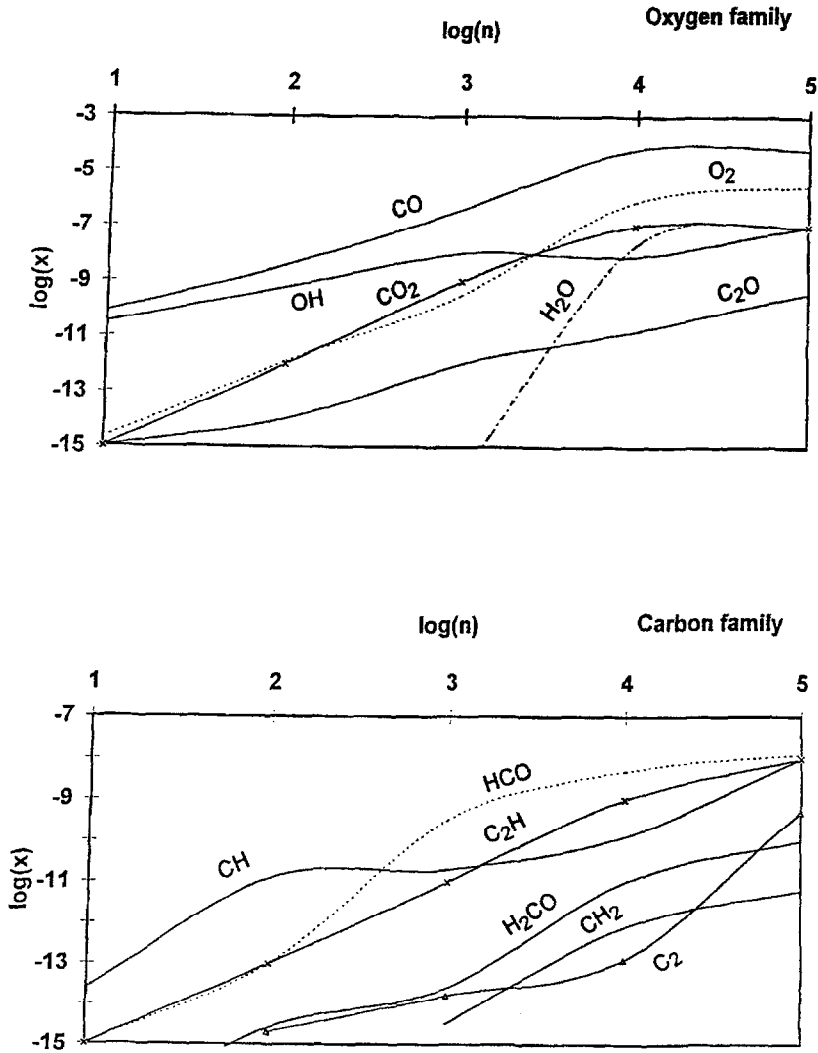


Figure 4.

2. The value adopted for the ionization rate by cosmic ray equals $4 \times 10^{-17} \text{ s}^{-1}$ recommended by Hollenbach and Mckee (1989).
3. The initial values of the different species are assumed to be zero except those contained in Table I.
4. The temperature is taken equals to 10 K all the time of contraction.
5. We have developed two networks: one for diffuse clouds up to density number of $n \approx 10^3 \text{ cm}^{-3}$, and the other network is used to follow the chemistry in the dense core with $n > 10^3 \text{ cm}^{-3}$.
6. The time of chemical evolution is assumed to be that of contraction.

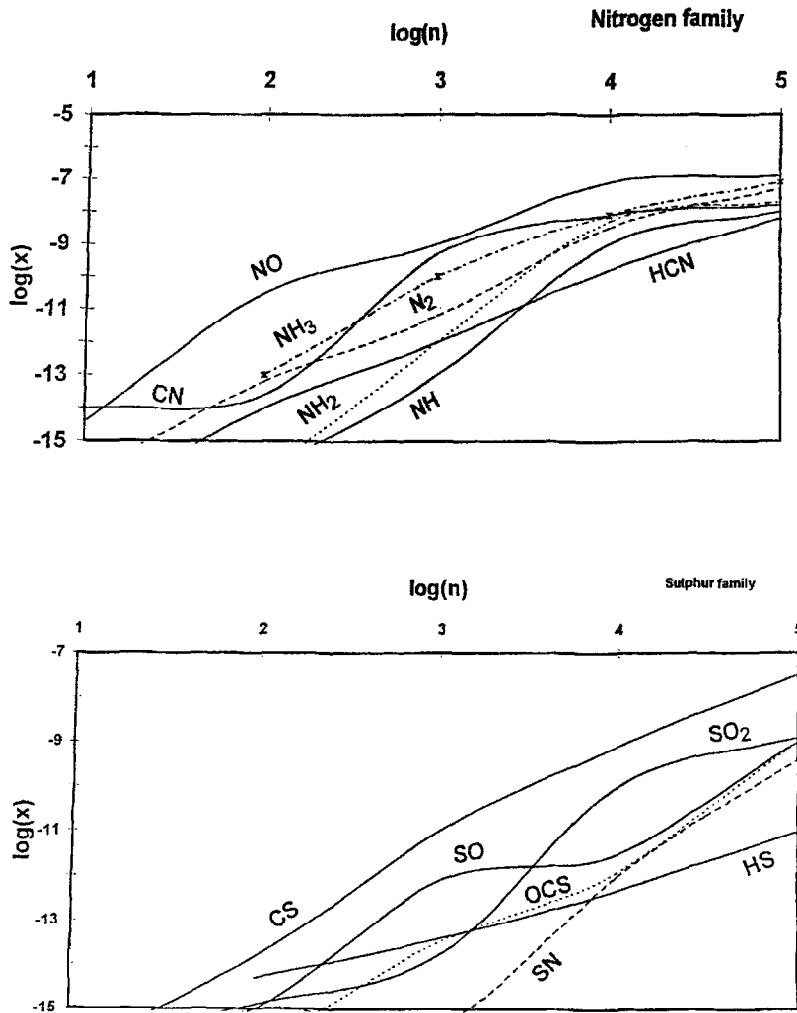
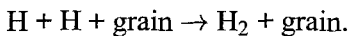


Figure 4. Continued.

7. The gas-grain interactions are neglected, as a matter of simplification, except the reaction:



8. The Interstellar cloud model is divided to 100 shells, with equal spacing only in the initial model. The coordinates were constructed to move approximately with the matter. Therefore the central core contracts in size and increases in mass. The 1-D hydrodynamics is calculated at the different shells starting from the center of the cloud and ending at the cloud boundary. The variations in the different physical parameters like, density, temperature, extinction and velocity has been followed in the different shells of the cloud. The chemical

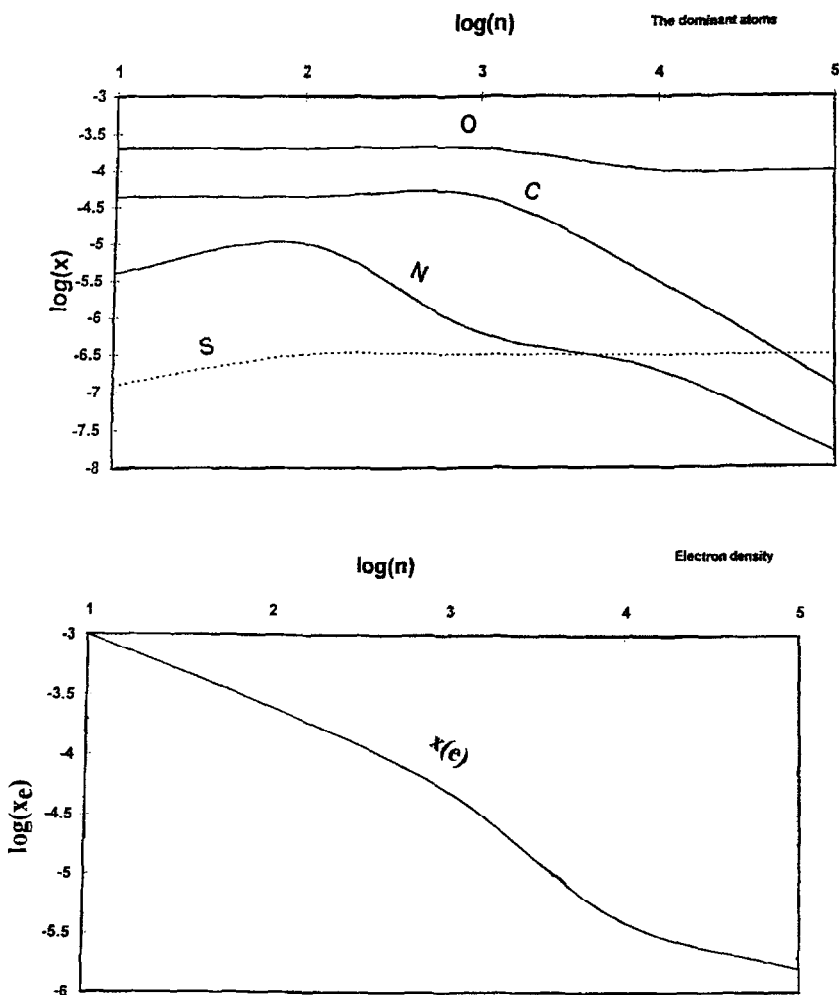


Figure 4. Continued.

evolution is followed only in the central zone. This has been done to simplify the calculations. Otherwise, to follow the chemistry in different shells of the cloud one needs a huge computational time and large memory. There is a plan to follow the chemical evolution in a simple model of chemistry and follow the molecular transform between the different shells. Such calculations would increase the efficiency of the computational evolutionary programs, but it really needs computers with high facilities.

The chemical evolution, at different values of central density, is followed until reaching steady state (about 10 million years). The time scale for molecule formation is larger than that of dynamical stability.

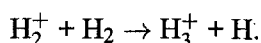
4. The Results

We have followed the contraction in one dimension from an initial density of $n = 10 \text{ cm}^{-3}$ up to density of $n \sim 10^5 \text{ cm}^{-3}$. The density increases with time as contraction proceeds as shown in Figure 2. The results from the full collapse model are presented in Table II and in Figures 3 and 4. The maximum calculated fractional abundances for some selected molecules are compared with both observations and other theoretical calculations as given in Table II. The comparison confirms the accuracy of our calculations where there are good agreements with either the observations or the considered theoretical studies.

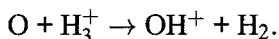
Figure 3 presents the results obtained for some dominant molecules in addition to the atoms O, C, N, and S. The fractional abundances are given by number relative to hydrogen and drawn against the time of contraction. The increase of the abundances of the different molecules with contraction are shown clearly in Figure 3. In the same time, the atomic species decrease as the cloud evolve to a molecular dense cloud. The species which enhance significantly are CO, HCO, CS and NO. Many of the other molecules increase distinctly with contraction e.g. HCO, CH, C₂H, CN, CS, SO₂, CO₂, H₂O, C₂, NH₃, N₂, HCN, SO, OCS and SN. Some of the molecular species increases in abundance rapidly with time of evolution and possibly reach their values at densities of $n > 10^3 - 10^4 \text{ cm}^{-3}$. This would not refer to a negligible values of these species in the diffuse regions. For example, we cannot predict that the diffuse clouds should be observed without gas-phase water. Gas-grain interactions confirm the presence of many molecular species, particular the previous mentioned example, the gas-phase water.

Figure 4 presents the results of evolution, obtained for the same species shown in Figure 3, with increase of density during contraction. The atomic species are the dominant abundant species at low density. When the cloud density increases to a value of $n \approx 10^5 \text{ cm}^{-3}$ some of the molecular species dominate, in particular CO, O₂, OH, H₂O, CO₂, NO and NH₃. Indeed many other molecules become important, as shown in the figures. These results confirm the evolution of a diffuse interstellar cloud with small abundances of molecular species to a dense molecular cloud with enhancement of the different molecular species. Molecules such as the hydrocarbons and related species increase in abundances distinctly. This is because, there is a significant abundance of C atoms which drive the hydrocarbon chemistry. On a longer time-scale, carbon is chemically processed into the extremely stable CO molecule which takes most of the available carbon. Therefore, other than H₂, CO is the most abundant molecule in interstellar clouds as shown in Figures 3 and 4.

The dominant pathway for any species is a reaction with molecular hydrogen unless the reaction is very slow or endothermic. Thus H₂⁺ rapidly forms H₃⁺ through the ion-molecule reaction,

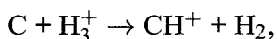


The proton transfer initiates the formation of other species. For example,



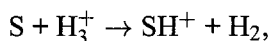
followed by reactions lead to the formation of H_3O^+ .

Like the Oxygen family, that of Carbon is initiated by a proton transfer reaction,



followed by sequences of reactions which lead to the formation of many molecules like CH, CH_2 or molecular ions such as, CH_3^+ , C_2H_3^+ .

The Sulphur does not follow the pattern shared by Oxygen and Carbon (Millar and Rerbst, 1990). The proton transfer reaction,



proceeds, but the hydrogen abstraction reactions in the sequence leading to the production of H_3S^+ are endothermic. However, at temperature of $T \geq 10^3$ K the formation of SH and H_2S are enhanced. Since our calculations are carried out at low temperature ($T = 10$ K), therefore our results of the abundance of H_2S is lower than the observations as shown in Table 2. Comparing our results with those of Amin et al. (1995a,b) one notices better improvements in the present results of the abundances of many species e.g. HCN, CH, C_2H , CS, SO. This may return to the developments in the numerical treatment and the updating of the rate coefficients with its most recent published values.

References

- Amin, M. Y., El-Nawawy, M. S., Ateya, B. G., and Aiad, A.: 1995a, *Earth Moon and Planets* **69**, 95.
 Amin, M. Y., El-Nawawy, M. S., Ateya, B. G., and Aiad, A.: 1995b, *Earth Moon and Planets* **69**, 113.
 Amin, M. Y., El-Nawawy, M. S., Ateya, B. G., and Alad, A.: 1995c, *Earth Moon and Planets* **69**, 127.
 Anicich, V. G.: 1993, *Ap. J. Suppl.* **84**, 215.
 Black, D. C. and Bodenheimer, P.: 1975, *Ap. J.* **199**, 619.
 Black, G. A., Anicich, V. G., and Huntress, W. T.: 1986, *Ap. J.* **300**, 415.
 Clary, D. C., Thierys, S., and Wickham, A. G.: 1993, *J. Chem. Soc. Faraday Trans.* **89**(13), 2199.
 El-Nawawy, M. S., Aiad, A., and El-Shalaby, M. A.: 1988, *MNRAS* **232**, 809.
 El-Nawawy, M. S., Shalabiea, O., Ali, A., and Aiad, A.: 1992, *Astrophysics and Space Science* **198**, 237.
 Gerlich, D.: 1993, *J. Chem. Soci, Faraday Trans.* **89**(13), 2199.
 Gerola, H. and Glassgold, A. E.: 1978, *Ap. J. Suppl.* **37**, 1.
 Herbst, E. and Klmpere, W.: 1973, *Ap. J.* **185**, 505.
 Herbst, E. and Leung, C. M.: 1989, *MNRAS* **222**, 689.
 Herbst, E. and Yamashita, K.: 1993, *J. Chem. Soci, Faraday Trans.* **89**(13), 2199.
 Hollenbach, D. and Mckee, C. F.: 1989, *Ap. J.* **306**.
 Langer, W. D., Graedel, T. E., Frerkljng, M. A., and Armentrout, P. B.: 1984, *Ap. J.* **277**, 581.
 Langer, W. D. and Grael, T. E.: 1989, *Ap. J. Suppl.* **69**, 241.

- Millar, T.J. and Nejad, L. A. M.: 1985, *MNRAS* **217**, 507.
- Millar, T. J., Rawlings, J. M. C., Bennett, A., Brown, P. D., and Charnely, S. B.: 1991, suppl., **87**, 585.
- Mitchell, G. F., Ginzburg, J. L. and Kunfz, P.J.: 1978, *Ap. J. suppl.* **38**, 39.
- Nejad, L. M., Williams, D. A., and Charnley, S. B.: 1990, *MNRAS* **246**, 193.
- Norman, M. L., Wilson, T. R., and Barton, R. T.: 1980, *Ap. J.* **239**, 968.
- Pineau des Fortes, G., Roueff, E., Schilke, P., and Flower, D. R.: 1993, *MNRAS* **262**, 915.
- Prasad, S. S., Tarafdar, S. P., Villere, K. R., and Huntress, W. J.: 1987, 'Chemical Evolution of Molecular Clouds', in D. Hollenbach and H. A. Thronson (eds.), *Interstellar Processes*, D. Reidel, Dordrecht, pp. 631–666.
- Prasad, S. S., Heere, K. R., and Tarafdar, S. P.: 1991, *Ap. J.* **373**, 123.
- Slancil, P. C., Babb, J. F., and Dalgarno, A.: 1993, *J. Chem. Soci, Faraday Trans.* **89**(13), 2199.
- Sternberg, A. and Dalgarno, A.: 1994, *Center for Astrophys.* preprint, ser. No. 3916.
- Suzuki, H.: 1983, *Ap. J.* **272**, 579.
- Tarafdar, S. P., Prasad, S. S., Wesley, T., Huntress, J. R., Villere, K. R., and Black, D. C.: 1985, *Ap. J.* **289**, 220.
- Williams, D. A. and Hartquist, T. W.: 1991, *MNRAS* **251**, 351.