

THE EVOLUTION OF CHARGED PARTICLES IN A MODEL OF CONTRACTING CLOUD

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Abstract. The evolution of the charged particles are followed during contraction of a model of an interstellar cloud, with initial density number of $n = 10 \text{ cm}^{-3}$. The contraction is followed up to density increase by five orders of magnitude. Special care is given to the details of the negative ions. In addition, we have tested the ambipolar diffusion according to the results of the ion density.

The results predict the importance of atomic ions in the diffuse regions. H^+ and C^+ are distinctly enhanced in the beginning of contraction but decrease as contraction proceeds. Molecular ions enhance as contraction proceeds and becomes important in dense regions. The most enhanced molecular ions are HCO^+ , O_2^+ , C_2H_3^+ , H_3O^+ and SO^+ . H_3^+ is less abundant. The atomic ions (except metallic ions) decrease noticeably as density increases. In general the negative ions are of negligible fractional abundances. It has also been found that the time of ambipolar diffusion is shorter than the dynamical time, hence the magnetic field should be weakened in the central core as the central density increases to $n = 10^4 \text{ cm}^{-3}$.

Key words: Interstellar chemistry.

1. Introduction

Magnetic field supports interstellar clouds against gravity, and may slow down the speed of contraction in the direction perpendicular to the lines of magnetic field. Ambipolar diffusion is important in transforming a super-critical cloud into a sub-critical one leading to its collapse. The ion density is an important factor in studying ambipolar diffusion. In addition, the charge state plays an important role in the chemical evolution of interstellar clouds through the ion-molecule reactions. The density of charged particles is influenced by many processes which are well summarized by El-Nawawy (1990).

Many observational efforts have been made to define the density of the charged particles in interstellar clouds, e.g. Van Dishoeck et al. (1992), Petrie et al. (1991), Balm and Jura (1992) and Heck et al. (1993). The following molecules have been identified in interstellar clouds: CH^+ , SO^+ , HOCO^+ , HCNH^+ , H_3O^+ , H_2D^+ , HCO^+ , HOC^+ , N_2H^+ and HCS^+ . There are many molecular ions which are difficult to be detected. It is expected that new discoveries will increase in the future owing to the continuing improvements in detector sensitivities and the availability of new large observational facilities at millimeter and submillimeter wavelengths.

On the other hand, theoretical studies of the physical parameters affecting the charge state, in diffuse and dense interstellar clouds have been followed by

many authors, e.g. Oppenheimer and Dalgarno (1974a,b), Elmegreen (1979), Umebayashi and Nakano (1980), Umebayashi (1983), Langer (1985) and El-Nawawy et al. (1992). Studies of grain charging can be found in many articles, e.g. Brown and Charnely (1990), El-Nawawy et al. (1992) and Hasagawa and Herbst (1993). Amin and El-Nawawy (will appear in the present volume, henceforth referred to as paper I), studied the time dependent chemical evolution of a contracting interstellar model, the contraction is followed using a 1-D computer code to study the contraction of spherically symmetric cloud in one dimension. They have integrated both the chemical rate equations and the hydrodynamic equations simultaneously. The details of the physical and chemical scheme, the numerical method of solution of both the hydrodynamic equations of contraction and the equations of the chemical model, the rate coefficients and the abundances of the neutral species were presented in paper I.

The objective of the present study is to study the evolution of charged particles during contraction. Special care is given to the details of the negative ions. In addition we test the ambipolar diffusion according to the results of the contracting model.

In Section 2 we discuss the importance of the negative ions in cloud chemistry. The evolution of ionic species in a contracting interstellar cloud is interpreted in Section 3. Ambipolar diffusion are studied in Section 4.

2. Negative Ions

Negative ion-atomic collisions have been the subject of detailed and accurate experimental measurements. In an $A^- - B$ collision, electron detachment is the most important process (Gauyacq, 1980):



According to Wayne (1985), attachments of an electron to a neutral molecule to form a negative ion requires the removal of excess energy, in the same way that neutralization does. Detachment processes convert negative ions back to neutrals. Dalgarno and McCray (1973) have considered gas-phase reactions in which they involved the negative ions. The association detachment process of,



based upon a complex potential formulation are discussed by Bieniek and Dalgarno (1979). The infrared emission of H_2 in planetary nebulae resulting from reaction (r2) was calculated by Black et al. (1977). The radiative attachment reaction,



Table I
The physical parameters of the models
2–4

Model	n (cm ⁻³)	T (K)	A_v
2	500	110	0.63
3	2500	22	1.01
4	10 ⁴	10	10

Table II
The initial fractional abundances with respect to
total hydrogen which has been used in the models
2, 3 and 4. In model 4 the hydrogen is assumed
to be initially in molecular form only

Species	x (initial)	Species	x (initial)
H	1	He	0.14
O	1.74 (-4)	C	7.30 (-5)
N	2.14 (-5)	S	8.00 (-6)
Si	8.00 (-7)	Fe	3.00 (-7)
Na	2.00 (-7)	Mg	7.00 (-7)

has a complex temperature behaviour, as discussed by Rawling and Williams (1988).

We have included in our chemical network 111 reactions for negative ions. The sources of the rate coefficients are explained in paper I. Three cloud models were studied to follow the abundances of negative ions: models 1 and 2 simulate the outer and inner components of the cloud toward ζ Oph. In model 3, we assumed a high value of density. This is to represent the situation in TMC-1 cloud. Table I summarizes the initial parameters of the three models. These three models (termed as models 2, 3 and 4) are studied using the same numerical code (Gear package) of Amin et al. (1995a), in steady state models (i.e. the density and temperature are considered fixed). This has been carried out in order to study in detail the chemical reactions of negative ions. We have assumed that, the initial abundances of the molecular species, negative ions and the other ionic species are equal zero. The initial values of the fractional abundances of the elements are assumed to be those of H, C, O, S, Si and metals as given in Table II. The time-dependent evolution of the three models is followed until reaching chemical equilibrium for the majority of the species. This occurs at a time of $t = 10^7$ year in diffuse clouds and at $t = 10^8$ year in dense regions. Models 2–4 are devoted to study the reactions of negative ions under different densities of neutral hydrogen, as in diffuse, intermediate and dense regions.

Table III
The calculated fractional abundances of some selected negative species compared with electrons (e)

Species	Model 1	Model 2	Model 3
H ⁻	4.0 (-10)	3.5 (-11)	5.5 (-13)
C ⁻	6.4 (-15)	1.4 (-14)	2.6 (-16)
O ⁻	7.4 (-13)	1.8 (-13)	7.0 (-17)
S ⁻	6.7 (-17)	1.3 (-16)	1.7 (-16)
OH ⁻	1.1 (-16)	1.1 (-15)	1.9 (-13)
CN ⁻	6.8 (-22)	2.7 (-21)	1.0 (-16)
CH ⁻	9.2 (-20)	6.4 (-19)	5.5 (-18)
e	3.6 (-4)	9.4 (-5)	1.2 (-6)

In Table III we present the maximum fractional abundances of the various negative species calculated by models 2, 3 and 4. The results predict that the negative ions H⁻ and O⁻ should not be neglected at least in diffuse clouds. The molecular ions are of negligible fractional abundances. The formation of negative hydrogen H⁻ opens reaction paths for the formation of heavier molecules. For example, the following sequence of reactions;



can occur (Dalgarno and McCray, 1973). Also, Ammonia can be produced by the sequence:



As shown in Table III, the fractional abundance of H⁻ increases in diffuse clouds with high temperature and decreases with increase of density.

O⁻ is important in producing OH through the reactions,



or



The S^- can undergo a variety of reactions analogous to those for O^- ,



and CH_2 can itself be produced from CH^- through the associative detachment reactions,



The negative ions H^- , C^- and S^- can be removed by the reactions with ionic metals Me^+ ,



In other words one should expect that metallic ions decrease due to the above mentioned reactions.

3. Evolution of Ionic Species in a Contracting Interstellar Cloud

In paper I, we have discussed the results of evolution of the different neutral species during contraction of a spherical interstellar cloud. In this section, we describe the results of evolution of the ionic species during contraction. The results shown in Figures 1 represents the fractional abundances of some selected ionic species and its evolution with time during contraction. The atomic ions, particularly the metal ions are the dominant ions in diffuse regions. H^+ and C^+ are distinctly enhanced in the beginning of contraction but decrease as contraction proceeds. The most enhanced molecular ions are HCO^+ , O_2^+ , $C_2H_3^+$, H_3O^+ , and SO^+ . H_3^+ decreases quickly with density increase. But there is a general increase in the abundances of the other different molecular ions as the cloud model contracts. The fractional abundances of the ionic species are drawn versus density and the results are shown in Figure 2. It can shown that the different molecular ions enhance as density increases. The most dominant of them are explained above. The atomic ions (except metallic ions) decrease noticeably as density increases. The metallic ions are assumed initially with small abundances than in diffuse regions. The results of evolution predict a fixed value approximately of Fe^+ and Mg^+ . In Figure 3, the results on the abundances of negative ions are drawn versus density. OH^- appears to be the most dominant

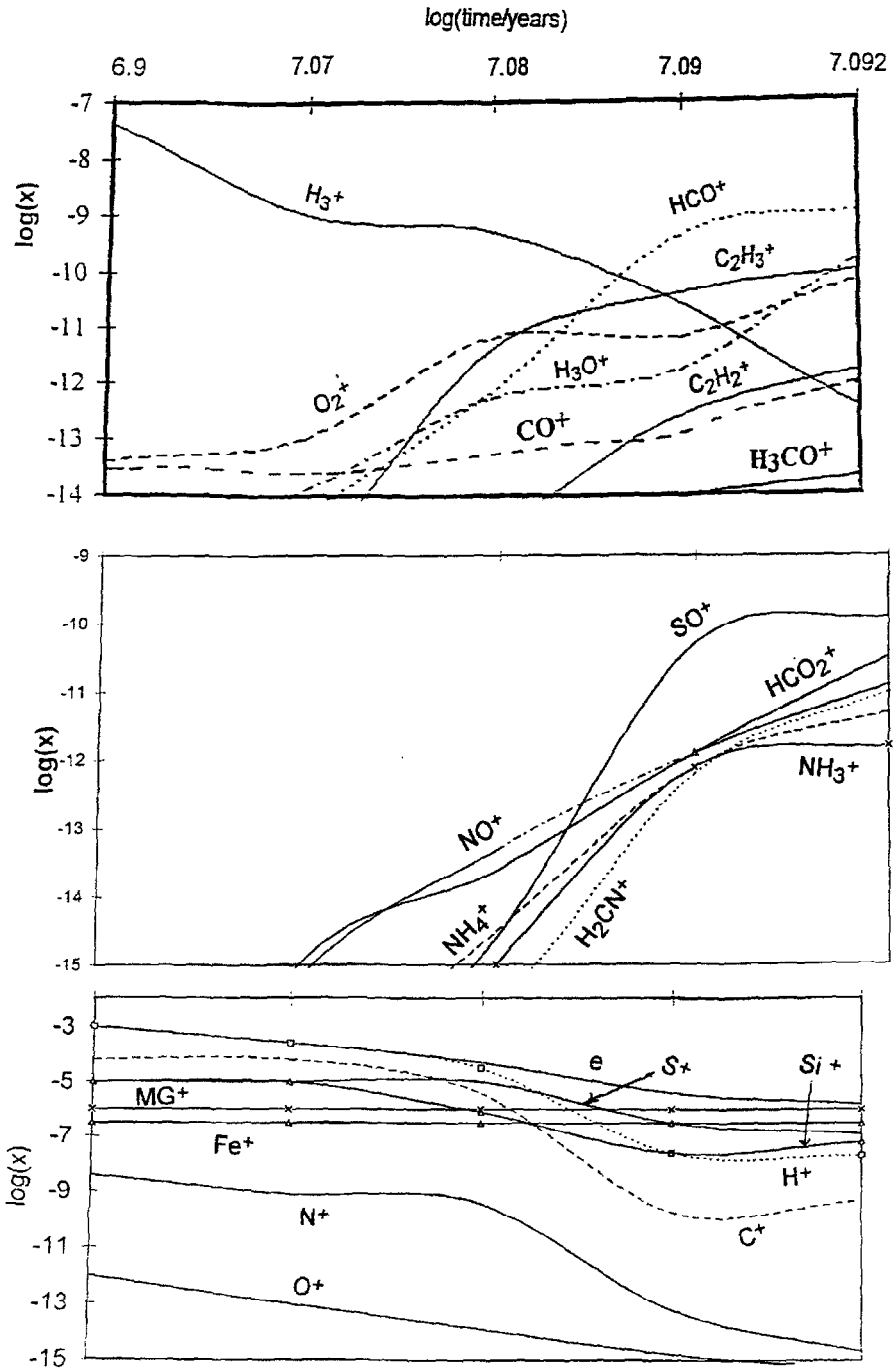


Figure 1.

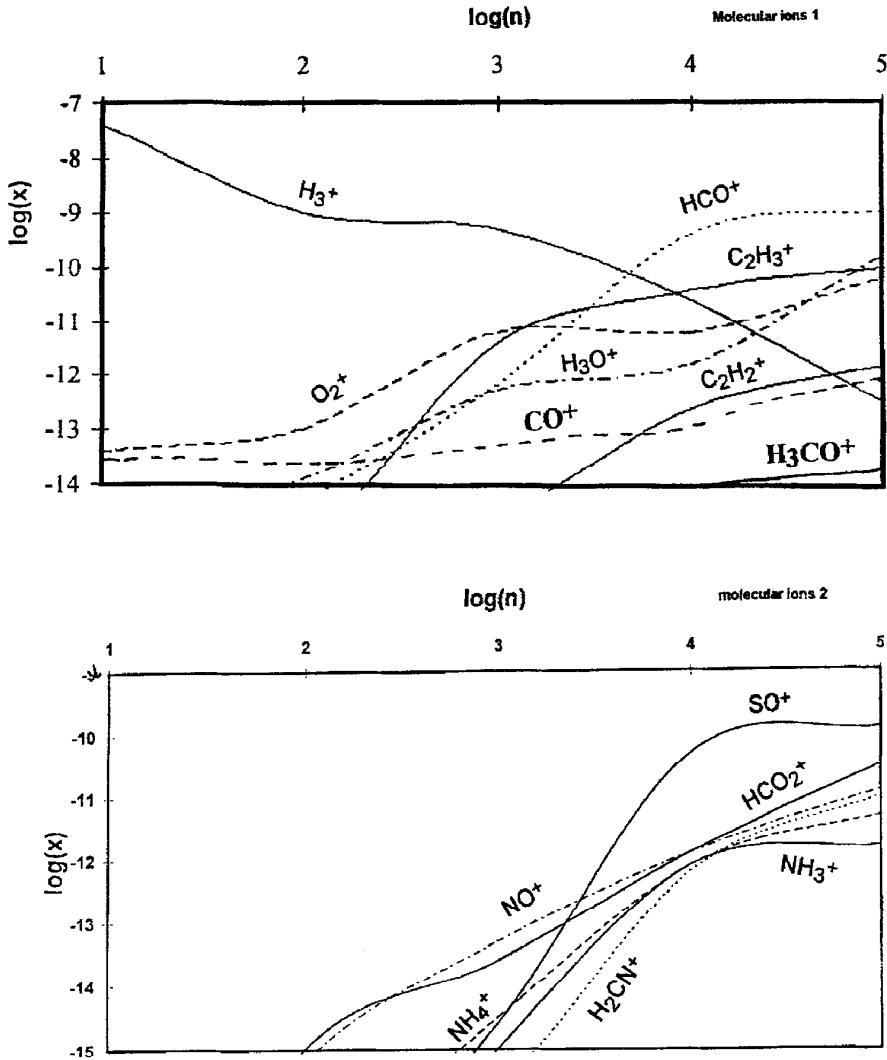


Figure 2.

negative ion. S^- increases with density, but the other negative ions mostly decrease with contraction.

In Figure 4 we compare the fractional abundance of electrons results from our calculations to that given by El-Nawawy et al. (1992). There is a good agreement between both. The calculated values of $x(CO^+)$ and $x(H_3CO^+)$ are shown in Figures 2 and 3. The maximum fractional abundances of CO^+ and H_3CO^+ are in agreement with the observations given by Black et al. (1987) for the Orion molecular cloud in the external ridge. The molecular ion HC_3NH^+ is one of the observed species, but not included in our scheme of chemical species.

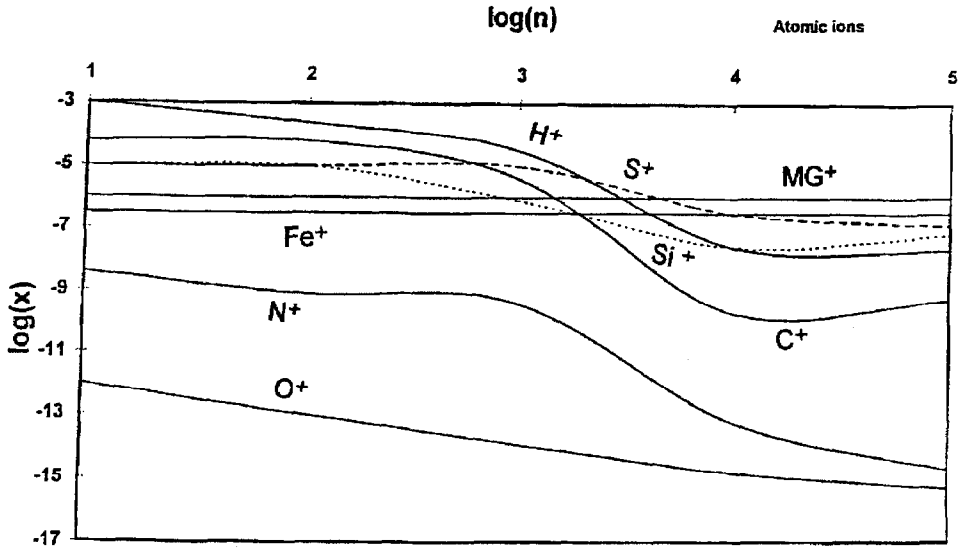


Figure 2. Continued.

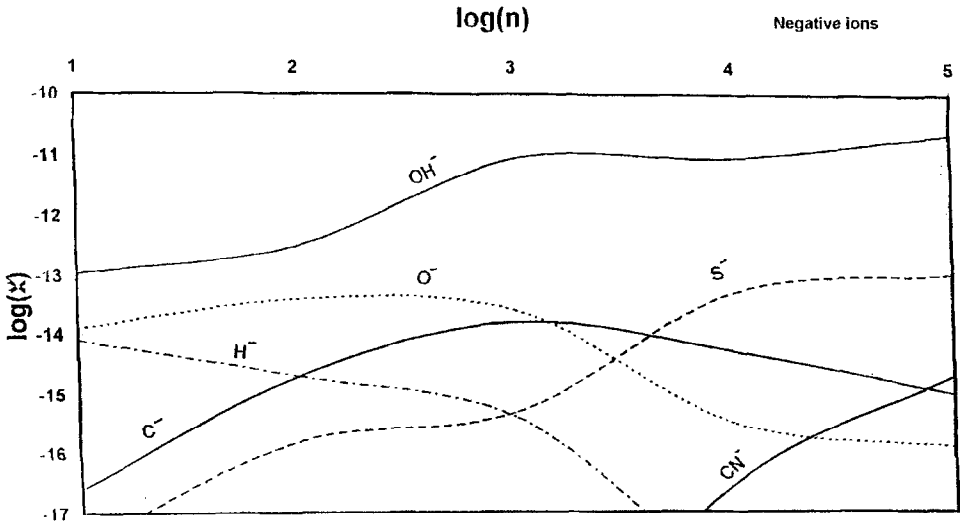


Figure 3. The fractional abundances of selected negative ions are drawn as functions of density numbers (cm^{-3}).

4. Ambipolar Diffusion

In a magnetic interstellar cloud, magnetic field influences the motion of charged particles. Consequently, the motion of neutral particles will be effected by the magnetic field via the frictional force between ions and neutrals. If the differ-

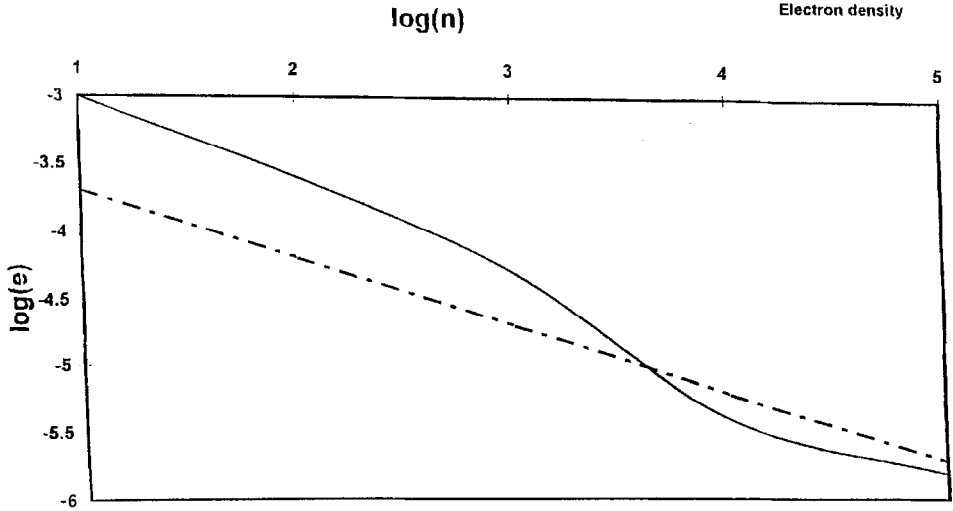


Figure 4. The electron density (e) as a function of density (solid curve) as given in our calculations are compared with that of El-Nawawy et al. (1992).

ence between the velocities of ions and neutrals, called the drift velocity v_D , is considerably large, then the magnetic field will diminish via ambipolar diffusion.

The drift velocity v_D of ions relative to neutrals can be expressed as follows (El-Nawawy, 1990):

$$v_D = \left\{ \frac{m_i + m_n}{4\pi \langle \sigma v \rangle_{in}} \right\} \frac{B^2}{\rho \rho_i R}. \quad (1)$$

where m_i and m_n are the ion and neutral masses respectively. ρ , ρ_i , R and B are the neutral and ion densities, the radius of the cloud core and the magnetic field strength, respectively. $\langle \sigma v \rangle_{in}$ is the momentum-transfer rate coefficient for an ion colliding with neutral averaged over the Maxwellian velocity distribution. The time of ambipolar diffusion is given by,

$$t_D = \frac{R}{v_D} = \left(\frac{4\pi \langle \sigma v \rangle_{in}}{m_i + m_n} \right) \left(\frac{\rho R}{B} \right)^2 x_i. \quad (2)$$

where we have inserted the drift velocity from Equation (1), $x_i = \rho_i/\rho$. Equation (2) predicts that the time scale of ambipolar diffusion increases with $(\rho/B)^2$. The abundances of the ions (x_i) affecting clearly the time scale of ambipolar diffusion in addition to the geometry of the cloud. The above physical and chemical variables would complicate the situation for the determination of the critical density for ambipolar diffusion. The grain charge has not been considered for simplicity. This assumption is not bad in clouds of low density. The charged grains must be considered only at densities of $n \geq 10^8 \text{ cm}^{-3}$ (El-Nawawy, 1990).

Time scales

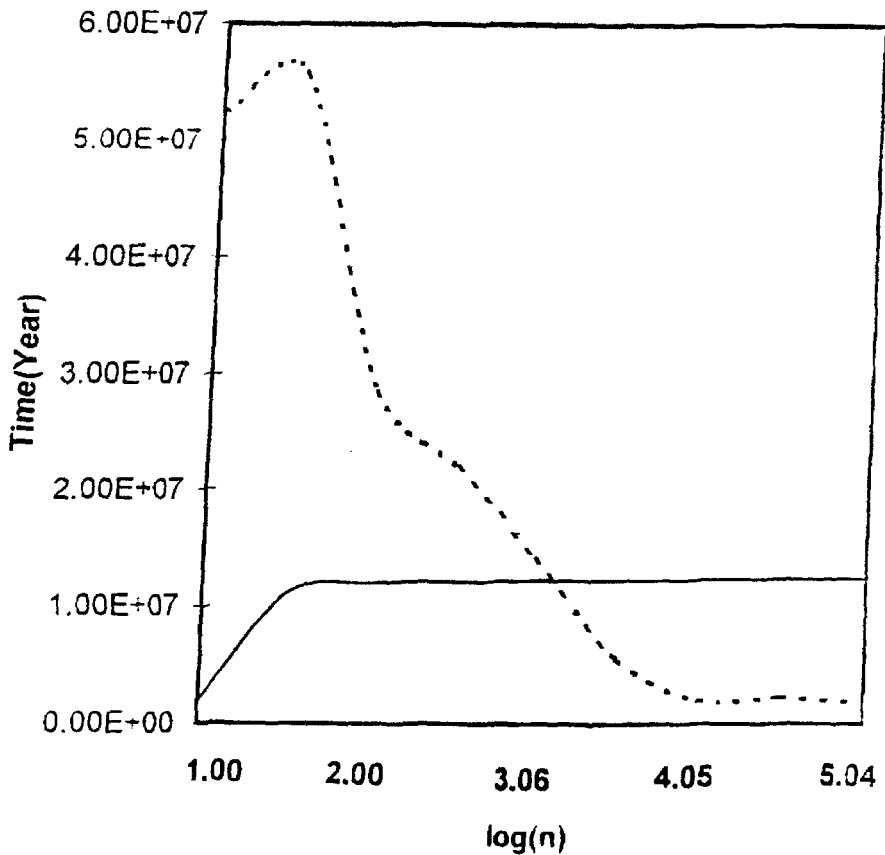


Figure 5. The time scale for both, ambipolar diffusion (dashed curve) and the dynamical contraction (solid line) as functions of density number (in cm^{-3}).

The magnetic field strength in a flattened cloud is given by the following relation (El-Naway, 1990),

$$B_f \sim 8C_s \rho^{1/2}. \quad (3)$$

Substituting Equation (3) into Equation (2) we get,

$$t_D = \left(\frac{\pi \langle \sigma v \rangle_{\text{in}}}{(4c_s)^2 (m_i + m_n)} \right) \rho R^2 x_i. \quad (4)$$

Equation (3) predict an increase of the magnetic field strength with contraction. This would be the situation as long as the magnetic field is frozen in the interstellar cloud. As ambipolar diffusion is working, the magnetic field may decrease. Hence,

Equation (3) gives an upper limit of the magnetic field in this case. Consequently, Equation (4) gives a lower value of the time of ambipolar diffusion. The value of the density ρ is taken from the model of contraction and x_i is substituted from the resulting electron abundance of the model of chemical evolution. The resulting time t_D of ambipolar diffusion in the central core (central shell) is compared with the time of contraction. The momentum-transfer rate coefficient for an ion colliding with neutral $\langle\sigma v\rangle_{\text{in}} \approx 1.5 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$, El-Nawawy et al. (1992). In order to know how ineffective is the ambipolar diffusion in dissipating the magnetic flux, it is more convenient to compare the time of ambipolar diffusion t_D with the dynamical time of contraction t_d . If $t_D < t_d$, then the magnetic field dissipates effectively, otherwise the magnetic field is frozen in the matter. The time of ambipolar diffusion is compared with that of dynamical contraction and the results are shown in Figure 5. The time of ambipolar diffusion is larger than that of contraction in the diffuse region up to densities of $n \leq 10^3 \text{ cm}^{-3}$. At higher densities, t_D becomes shorter than the time of dynamical contraction. This means that ambipolar diffusion will reduce the magnetic flux in the central core as the density increases to values higher than $3 \times 10^3 \text{ cm}^{-3}$. As we have mentioned before, the values of t_D is calculated in its lower limit. The real values of the time of ambipolar diffusion should be somehow higher.

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