

# HOW SUPERDIFFUSION ALTERS THE FRACTIONAL ABUNDANCES IN MOLECULAR CLOUDS

G. Marschalkó

Eötvös University, Department of Astronomy, H-1518 Budapest, Pf. 32, Hungary

E-mail: G.Marshalko@astro.elte.hu

## Abstract

The chemistry of molecular clouds is a complex system influenced by wide scale of different factors; amongst them one of the most important is the turbulent diffusion. Whilst the previous improved models laid emphasis on the chemistry, we wish to examine the turbulence with special regard to the superdiffusion.

**Keywords:** *turbulence, diffusion, ISM: clouds, ISM: abundances, ISM: molecules*

## 1 Introduction

The determination of fractial abundances of the constituents of molecular clouds has a long history. After the initial steady state gas-phase chemistry model of Herbst & Klemperer (1973) several (pseudo-)time-dependent models with fixed profiles of physical parameters were developed, considering more and more chemical reactions, however in the absence of photodissociation (Leung et al., 1984; Herbst & Leung, 1989; Millar & Herbst, 1990). Moreover, these models produced the observed fractional abundances (particularly in the case of C and complex organic molecules) too early and reaching the steady state these decreased notably below the expected values. However, the consideration of turbulence in later works solved these problems, significantly altering steady state abundances and radial profiles of the more important species (Xie et al., 1995).

Since then, these models have been refined: Willacy et al. (2002) demonstrated that HI is a tracer of turbulent diffusion and refined the ion-neutral reaction scheme, as well as took into account the gas-grains interaction and H<sub>2</sub> and CO self-shielding; Yate & Millar (2003) integrated in the model of Xie et al. (1995) the grain accretion effects and adsorption onto grains.

We examined the role of anomalous diffusion, namely how superdiffusion alters the evolved fractional abundances. After presenting a model with initial simplifying assumptions we conclude that the problem deserves the further studies.

## 2 Turbulence and anomalous diffusion

We would like to study the diffusive transport of certain species in a turbulent cloud using mixing length theory. Let  $n_{H_2}$  the number density of hydrogen,  $n_i$  the number density and  $f_i$  the fractional abundance of tracer  $i$ . Thus its diffusion equation is:

$$\frac{\partial n_i}{\partial t} = D \frac{\partial}{\partial r} \left[ \frac{\partial}{\partial r} n_i - f_i \frac{\partial}{\partial r} n_{H_2} \right] + S_i, \quad (1)$$

where  $S_i$  is the source and sink term, which comes from the chemistry reaction-scheme, and  $D$  is the diffusion coefficient, whose determination is fundamental.

It is known from the observations that there is an approximately power-law relation between the internal velocity dispersion and the size (or mass) of the cloud (Larson, 1980; Leung et al., 1982). Whilst the turbulent velocity is usually estimated to be approximately 1 km s<sup>-1</sup> in the case of a typical molecular cloud, the values of the correlation length vary on a larger scale in the different papers. Xie et al. (1995) define about 10% of the cloud as the correlation length, which is approximately 0.1-0.5 pc. Yate & Millar (2003) prefer smaller values than 0.5 pc, what they reckon as an upper limit, while in highly fragmented clouds they figure that the mixing length is between 0.003 and 0.03 pc. Hence these authors get different values of diffusivity, 3x10<sup>22</sup> - 2x10<sup>23</sup> and 10<sup>21</sup> - 10<sup>23</sup> cm<sup>2</sup>s<sup>-1</sup>, respectively.

The diffusion velocity of each species, thus the diffusion timescale, too, depend on its density scale heights being altered continuously by the chemical reactions, moreover it depends on the cloud radius and is influenced by the external radiation field (Xie et al., 1995). Hence, in the case of diffusion timescales only an upper limit can be given by  $R^2/D$ . To estimate the timescales we need to define the turbulent flux of a tracer after Xie et al. (1995):

$$\phi_i = Dn_i \frac{1}{H}, \quad (2)$$

where  $H = (\frac{1}{H_i} - \frac{1}{H_{H_2}})^{-1}$  is the relative density scale height, which one can calculate by the density scale height of hydrogen  $H_{H_2}$  and the different tracers  $H_i$  ( $H_j = -n_j(\frac{dn_j}{dr})^{-1}$ , where  $j = \{i, H_2\}$ ). Thus the diffusion velocity and the diffusion timescale are given on scale  $H$   $v_d \sim \frac{D}{H}$  and  $\tau_c \sim \frac{H^2}{D}$ , respectively. This timescale is comparable with the chemical timescale, both are around  $10^6$  years, but at higher densities the transport timescale exceeds the chemical timescale, so there is less effect of the turbulence (Scalo & Elmegreen, 2004).

It can be seen that the diffusion and the chemistry form a very complex system, so one needs to make some simplification, for example to use constant diffusivity over the whole cloud. We can take into account eddies with different sizes using superdiffusion, namely the eddies exceeding the separation  $r$  do not contribute to the further separation of fluid parcels at separation  $r$ .

The equation that describes the rms separation of two tracers

$$r = 2Kt^\zeta, \quad (3)$$

can be rewritten to get a unique relation between  $r$  and  $t$  ( $r = 2K'(r)t^{1/2}$ ), so we can formally introduce a 'scale-dependent diffusion coefficient' (Petrovay, 2001):

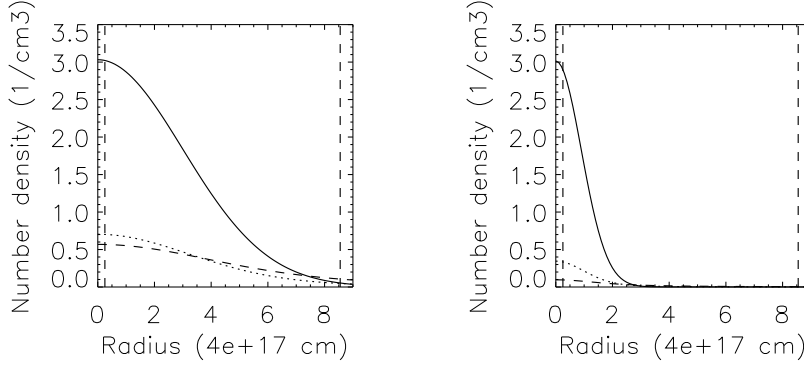
$$D(r) = K'^2 = K^{1/\zeta} r^{2-1/\zeta}. \quad (4)$$

One can speak about a simple diffusion process if  $\zeta = \frac{1}{2}$ , while the case  $\zeta \neq \frac{1}{2}$  corresponds to anomalous diffusion: superdiffusion if  $\zeta > \frac{1}{2}$  and subdiffusion if  $\zeta < \frac{1}{2}$ .

### 3 Our results

At first we studied a simplified problem, neglecting the chemical processes and estimating the source term by means of the diffusionless solution based on relaxation timescales in referenced papers. Our cloud is spherically symmetrical, the density of  $H_2$  is constant and we look for a stationary solution. Thus the equation of diffusion:

$$\frac{\partial n}{\partial t} = D\nabla^2 n + S, \quad \text{where } S = \frac{n_0 - n}{\tau_c}, \quad (5)$$



**Figure 1:** Number density of a tracer as a function of the radius. The solid line represents the initial (or diffusionless) state, the dashed line the diffusive case and the dotted line the superdiffusive case. The upright dashed lines represent the inner and outer computational domain of the cloud. Left: Gaussian,  $D = 10^{23} \text{cm}^2 \text{s}^{-1}$ ,  $\tau_c = 10^6 \text{year}$  Right: Gaussian with lower standard deviation,  $D = 1.2 \times 10^{23} \text{cm}^2 \text{s}^{-1}$ ,  $\tau_c = 10^6 \text{year}$

$n_0$  is the diffusionless equilibrium solution of number density of the tracer and  $\tau_c$  is the characteristic time. Transforming the initial partial differential equation into the Fourier space we get

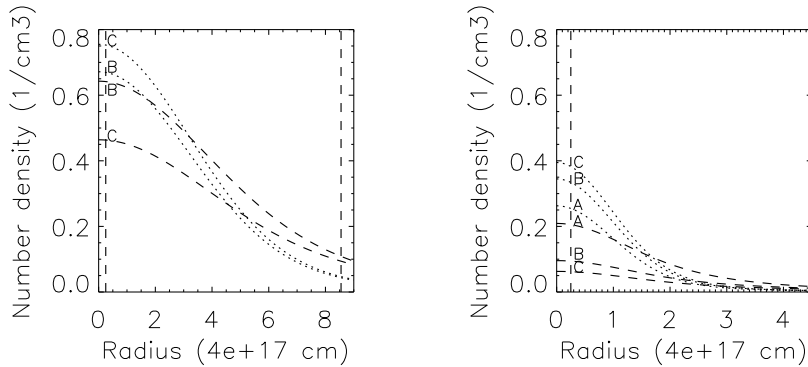
$$\frac{\partial \hat{n}}{\partial t} = -Dk^2 \hat{n} + \hat{S}, \quad \text{where } \hat{S} = \frac{\hat{n}_0 - \hat{n}}{\tau_c}, \quad (6)$$

finally we find the stationary solution of this equation:

$$\hat{n} = \frac{\hat{n}_0}{1 + \tau_c D k^2}. \quad (7)$$

To make the Fourier transform we apply the theorem that an  $n$  dimensional Fourier transform can be replaced a one dimensional Hankel transform, if the transformable function depends only on  $r = \sqrt{\sum x_i^2}$  (Sneddon (1951)). So in the case of  $n = 3$  the transformation formulae are:

$$\hat{n}(k) = \int_0^\infty r^{\frac{3}{2}} n(r) J_{\frac{1}{2}}(kr) dr \quad \text{and} \quad n(r) = \int_0^\infty k^{\frac{3}{2}} \hat{n}(k) J_{\frac{1}{2}}(kr) dk. \quad (8)$$

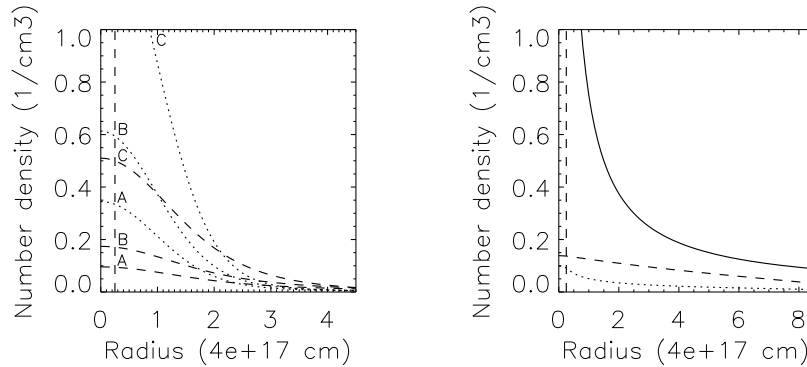


**Figure 2:** Abundances of a tracer as a function of the radius. Line coding as in Fig. 1.  $\tau_c = 10^6$  year, the diffusivities are  $4 \times 10^{22}$  (A),  $10^{23}$  (B) and  $1.6 \times 10^{23}$  (C)  $\text{cm}^2 \text{s}^{-1}$ . Left: Gaussian Right: Gaussian with lower standard deviation

In the superdiffusive case we assumed Kolmogorov spectra ( $\zeta = \frac{3}{2}$ ) and scaled the turbulent diffusivity according to the formula  $D = D_0 (\frac{k}{k_0})^{-\frac{4}{3}}$ . We only needed defining  $k_0$  to know what size of eddies can assign to  $D_0$ , in the simple diffusive case used diffusion coefficient.

To simplify the calculations we made the equations dimensionless and approximated the initial density distribution of the tracer with Gaussian distributions. One of them has the same value at the outer border of the cloud like the real reciprocal distribution, but the total mass of it greater, the other has the same total mass, but its outer border is at the half of the real value. We performed our calculations with different diffusivities and characteristic times in both cases, concentrating particularly on the difference between the diffusive and superdiffusive case.

The results from the Gaussian distribution approximation show that further studies are warranted because the difference between these two cases approaches a factor of two in certain parts of the cloud. This can be seen better on the Gaussian distribution with lower standard deviation (see Fig. 1). It is also visible that with increasing diffusivity the difference between the diffusive and superdiffusive cases also increases (see Fig. 2). However this difference is the largest in the innermost part of the cloud; there, as we have mentioned above, the turbulence has little effect, so our approximation is less suitable within the



**Figure 3:** Abundances of a tracer as a function of the radius. Line coding as in Fig. 1. Left: Gaussian with lower standard deviation,  $D = 10^{23} \text{ cm}^2 \text{ s}^{-1}$ , the characteristic times are  $10^6$  (A),  $7.6 \times 10^5$  (B) and  $1.2 \times 10^5$  (C) year. Right: real,  $\tau_c = 10^6$  year,  $D = 10^{23} \text{ cm}^2 \text{ s}^{-1}$

radius  $10^{17}$  cm. The difference between the two cases also increases with larger characteristic time (see Fig. 3 on the left side). Finally we made our calculations using a real reciprocal number density profile of a tracer, after Xie et al. (1995), within the above mentioned radius with constant density. The obtained results show that in this case also there are similar remarkable differences (see Fig. 3 on the right side).

## 4 Conclusion

We studied the effect of the superdiffusion on fractional abundances in molecular clouds using a simplified model. Approximating the initial tracer distribution with a Gaussian, and using constant density of  $\text{H}_2$ , the received results show that there are significant differences between the diffusive and superdiffusive case. In the future we plan to study this question dropping the assumption of a constant distribution of  $\text{H}_2$  - since a gradient in the density of the main component affects the fractional abundance of a tracer (see Equation (1), where  $f_i = n_i/n_{\text{H}_2}$ ) - looking for a non-stationary solution of the diffusion equation.

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