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On the Formation of Molecular Clouds in Three-Dimensional Expanding Supershells

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Abstract – The evolution of three-dimensional supershells produced by supernova explosions in OB associations has been studied for different assumptions of their location relative to the center and plane of the Galaxy. It has been shown that the formation of hydrogen molecules is possible in the advanced stages of the evolution of supershells located at galactocentric distances not exceeding 15 kpc. The total mass of molecular hydrogen clouds may be up to $\simeq 10^6 M_\odot$, and their distance from the galactic plane does not exceed 100 pc.

1. INTRODUCTION

Several high-resolution radio surveys of our Galaxy [1, 2] and nearby galaxies [3 - 7], conducted over the last few decades, resulted in the discovery of the large-scale cellular structure of the interstellar medium. The characteristic size of the structure constituents is 10^2 - 10^3 pc. The estimated kinetic energies of expanding supershells are up to 10^{53} erg, which is much higher than the energy released in the usual explosions of supernova. Our solar system is located at the edge of one of these cavities, which has a diameter of $\simeq 200$ pc and is centered at the Scorpio–Centaurus association [8]. The discovery of the large-scale cellular structure of the interstellar medium resulted in a drastic change of our ideas concerning the structure of the latter. Instead of the two-phase equilibrium models (cold dense clouds plus hot rarefied gas), models of a dynamic system regulated by a combination of strong local energy sources were suggested. The large-scale structure and energy balance of the interstellar medium are to a large extent determined by the aggregate action of massive stars that are members of OB associations. The latter may also result in the redistribution of heavy elements in the galactic disks [9], the formation and support of a hot galactic halo [10], and the ejection of gas enriched in heavy elements from dwarf galaxies [11 - 14]. Progress with the dynamic model of the interstellar medium requires us to study the complete chain of the circulation of matter in galaxies: gas–clouds–stars–gas. Special attention must be paid to the recent data on the possibility of the more active formation of a new generation of stars due to the drastic violation of the dynamic and thermal balance by extreme local energy evolution [15]. Evidence that this hypothesis may be true for small local structures is provided by the recent discovery of the enhanced density of pointlike IR sources in some supernova remnants [16] and the discovery of IR sources with an anomalous ratio of IR luminosity to the mass inside the extended H II regions [17]. On a large scale, the correctness of this hypothesis is confirmed by the existence of a gradient of stellar ages in complexes like Cep OB3 [15] and in the expanding supershell LMC-4 [18]. Observations also show that compact star formation regions are placed, as a rule, on the periphery of the largest supershells [19 - 21]. Therefore, it becomes particularly interesting to establish what conditions and which galactocentric distances are favorable for the formation of molecular clouds that serve as the birthplaces for a new generation of stars. We shall show below that the geometry of the supershells has a fundamental importance here.

For a proper description of the evolution of supershells, it is necessary to consider the inhomogeneity of gas distribution in the direction perpendicular to the galactic plane, as well as galactic differential rotation. As shown by Palous [19, 22] and Silich [23, 24], the Z component of the galactic gravitational field begins to play an important dynamic role in the advanced stages of dynamic evolution (at $t > 20$ Myr). Thus, a complete solution to the problem of the evolution of expanding supershells requires three-dimensional calculations.

The effects of the Z distribution of gas and the differential rotation of the galactic disk have been discussed many times [25 - 33]. Tenorio-Tagle and Palous [29] were the first to set forth the problem of molecular cloud formation in expanding shells. The possibility of the formation of gas molecules in expanding supershells was also noticed by McCray and Kafatos [35]. The possibility of the fragmentation of supershells due to gravitational instability was estimated in papers [29, 33, 35]. Tenorio-Tagle and Palous [29] and Palous *et al.* [30] performed two-dimensional calculations; therefore, they only investigated the effect of galactic differential rotation. The effect of inhomogeneous gas distribution in the direction perpendicular to the galactic plane and the role of the Z component of the gravitational field of the Galaxy were not considered. In the calculations by Tenorio-Tagle and Palous, the growth of the surface density of the supershell up to the value

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necessary for the screening of external UV flux and the formation of molecular hydrogen was attributed only to the sweeping of interstellar gas and to the distortion of the shell shape by galactic differential rotation. As we shall show below in our three-dimensional calculations, the column density of gas increases not only due to the sweeping of surrounding gas and the differential rotation of the galactic disk, but also because the shape of the shell is distorted when it moves through the inhomogeneous gas layer under the effect of the Z component of the galactic gravitational field. To understand these processes, we need to carry out three-dimensional calculations.

For the calculations in this paper, we apply a 2.5D numerical scheme [24, 34] based on the well-known thin layer approximation. We follow the evolution of three-dimensional supershells located at different galactocentric distances for the different distances of energy sources (OB associations) from the galactic plane. In Section 2 we describe the initial conditions, numerical method, and fundamental parameters of the problem. In Section 3 we discuss the peculiarities of the evolution of supershells located at different galactocentric distances and the possibility of the generation of conditions favorable to the formation of molecular clouds. In Section 4 we summarize the main results.

2. NUMERICAL METHOD, INITIAL CONDITIONS, AND BASIC PARAMETERS

For our calculations, we applied the 2.5D numerical scheme suggested by Bisnovatyi-Kogan and Silich [34] and Silich [24]. This scheme is based on the thin-layer approximation. We performed our calculations for the case of continuous energy injection into a cavity by sequential supernova explosions in a parent OB association [35]. Inhomogeneous gas distribution in the Z direction, differential rotation of the galactic disk, energy losses from a shock front, and the galactic gravitational field were taken into account. It was assumed that the supershell was initially spherical and that it was at a distance R_0 from the center of the Galaxy and at a distance Z_0 from the galactic plane. Thus, at $t = t_0$ the coordinates of the supershell center were $x = R_0$, $y = 0$, $z = Z_0$. The initial radius of the supershell was assumed to be $R_e = 50$ pc, which is much less than the characteristic scale of gas inhomogeneities. Initially, the supershell was split into $N = 1522$ Lagrangian elements by planes parallel and perpendicular to the galactic plane.

The motion of each Lagrangian element is described by seven equations: equations of mass and momentum conservation and equations of the variation of coordinates [24, 34]. Therefore, if one also considers the equation of energy conservation, the problem is then reduced to the solution of approximately 11 000 ordinary differential equations. This system was solved by the 12th-order Adams numerical method in the galactocentric Cartesian coordinate system. The coordinates were chosen such that initially,

$$x = R_0 + R_e \sin\theta \cos\varphi, \tag{1.1}$$

$$y = R_e \sin\theta \sin\varphi, \tag{1.2}$$

$$z = Z_0 + R_e \cos\theta. \tag{1.3}$$

McCray and Kafatos [35] and MacLow and McCray [26] have shown that supershells reach the radiative phase in a very short period of time (before the inhomogeneity of undisturbed gas significantly influences their dynamics). The energy injection into the cavity due to sequental supernova explosions in the OB association can be considered quasi-continuous. Therefore, the initial expansion velocity, thermal energy, and time at which $R = R_e$ were assumed to follow the analytical solution of Weaver *et al.* [36]:

$$U_0 = 0.6\,(125L_0/154\pi\rho_0)^{1/5} t_0^{2/5}, \tag{2.1}$$

$$E_{t0} = (5/11)L_0 t_0, \tag{2.2}$$

$$t_0 = (154\pi\rho_0 R_e/125L_0)^{1/3}, \tag{2.3}$$

where L_0 is the energy injection rate, ρ_0 is the density of the undisturbed gas near the supershell center, U_0 is the initial expansion velocity, and E_{t0} is the initial thermal energy of the supershell. Then, in the galactocentric reference frame, the initial velocity components are:

$$U_x = U_0 \sin\theta \cos\varphi - V_R \frac{y}{R}, \tag{3.1}$$

$$U_y = U_0 \sin\theta \sin\varphi + V_R \frac{x}{R}, \tag{3.2}$$

$$U_z = U_0 \cos\theta, \tag{3.3}$$

where $V_R(R)$ is the rotational velocity of the galactic disk. We assumed that undisturbed gas revolves in circular orbits about the galactic center under the influence of the gravitational field

$$g_x = -\frac{V_R^2}{R^2} x, \tag{4.1}$$

$$g_y = -\frac{V_R^2}{R^2} y. \tag{4.2}$$

The galactic rotation curve was taken after Wouterloot *et al.* [37]:

$$V_R(R) = V_c (R/R_c)^{0.0382} \text{ km s}^{-1}, \tag{5}$$

where $V_c = 220$ km s^{-1} and $R_c = 8.5$ kpc. The Z component of the galactic gravitational field was computed according to the analytical expression given by Kuljken and Gilmore [38]:

$$g_z = -2\pi G \sigma_D \frac{z}{\sqrt{z^2 + Z_D^2}} - 4\pi G \rho_h z, \tag{6}$$

where σ_D and Z_D are the surface density and characteristic inhomogeneity scale height of the density distribution in the stellar disk, respectively; and ρ_h is the effective density of the matter in the galactic halo. An additional relation between σ_D and ρ_h, which follows from the consistency of the calculated and observed galactic rotation curves [38], was also taken into account:

$$\rho_h = 0.015 - 0.0047\left(\frac{\sigma_D}{50 M_\odot \,\mathrm{pc}^{-2}}\right), M_\odot \,\mathrm{pc}^{-2}. \quad (7)$$

In accordance with Kuljken and Gilmore [38] and Caldwell and Ostriker [39], it was assumed that the surface density of the stellar disk along the galactic radius is distributed as

$$\sigma_D(R) = \sigma_D(R_\odot)\exp\left(\frac{R_\odot - R}{L}\right) \quad (8)$$

with a characteristic scale of $L = 4.5$ kpc and a surface density in the vicinity of the Sun equal to $\sigma_D(R_\odot) = 46 M_\odot \,\mathrm{pc}^{-2}$.

It was assumed that gas distribution in the Z direction may be described by the three-component model [40] combining cold and warm Gaussian and extended exponential atmospheres:

$$n(z) = n_1 \exp\left[-(z/Z_1)^2\right] + n_2 \exp\left[-(z/Z_2)^2\right] + n_3 \exp\left(-|z|/Z_3\right). \quad (9)$$

In the solar vicinity: $n_i = 0.395$ cm^{-3}, $Z_1 = 127$ pc, $n_2 = 0.107$ cm^{-3}, $Z_2 = 318$ pc, $n_3 = 0.064$ cm^{-3}, and $Z_3 = 403$ pc. It was assumed that the characteristic scale heights Z_i ($i = 1, 2, 3$) for each component vary with their galactocentric distance according to the law that gives the overall half-height of the H I layer:

$$Z_i(R) = \alpha Z_i(R_\odot), \qquad \alpha = Z_{1/2}(R)/Z_{1/2}(R_\odot). \quad (10)$$

All components of the atmosphere were assumed to obey the same relation along the galactic radius:

$$n_i(R) = \beta n_i(R_\odot). \quad (11)$$

The numerical value of β depends upon the ratio of the total surface density of H I at galactocentric distance R to that in the solar vicinity and upon the parameter α:

$$\beta = \frac{\sigma_{\mathrm{H\,I}}(R)}{\sigma_{\mathrm{H\,I}}(R_\odot)}\alpha^{-1}. \quad (12)$$

The values of $Z_{1/2}(R)$ and $\sigma_{\mathrm{H\,I}}(R)$ were taken following Wouterloot *et al.* [37]: in the vicinity of the Sun, $Z_{1/2}(R_\odot) = 150$ pc and $\sigma_{\mathrm{H\,I}}(R_\odot) = 8.57\, M_\odot \,\mathrm{pc}^{-2}$. The gas temperature in the galactic plane was assumed to be $T_0 = 6000$ K; it depends upon the height over the galactic plane as

$$T(z) = T_0 n_0 / n(z), \quad (13)$$

where $n_0 = n_1 + n_2 + n_3$ is the number density of the gas particles at $z = 0$. The gas pressure was assumed to be constant and equal to $P_{\mathrm{ext}} = k n_0 T_0$.

Numerical calculations were performed for three values of galactocentric distance $R = 5$, 8.5, and 15 kpc, and for three values of the height of the energy source of the initial OB association over the galactic plane $Z_0 = 0$, 50, and 100 pc.

The rate of energy injection into the cavity by sequential supernova bursts in OB associations was assumed to be constant over 30 Myr and varied from $L = (0.3 - 3) \times 10^{38}$ erg s^{-1}. After 30 Myr the energy injection was switched off, because all massive stars in an OB association finish their evolution by exploding as supernova.

We assumed that mass accumulation by a given Lagrangian element stops when the expansion velocity of the relevant part of the envelope becomes equal to the sound velocity in the surrounding gas. The motion of the element then continues under both the influence of gravity and the difference between the internal and external pressure.

Altogether we calculated 12 models of supershell evolution. The initial parameter values are listed in

Table 1. Initial model parameters for different computations

R, kpc	5	8.5	15
Z_0, pc	0; 50	0; 50; 100	0
L_{38}, 10^{38}erg s^{-1}	0.315; 1.05; 3.15	0.315; 1.05; 3.15	0.315; 1.05; 3.15
σ_D, $M_\odot$ pc^{-2}	100.1	46	10.8
Z_D, pc	300	300	300
$\sigma_{\mathrm{H\,I}}$, $M_\odot$ pc^{-2}	8.57	8.57	5.3
Z_1, pc	127	127	257
Z_2, pc	318	318	644
Z_3, pc	403	403	817
α	1	1	2.03
β	1	1	0.3
n_1, cm^{-3}	0.395	0.395	0.12
n_2, cm^{-3}	0.107	0.107	0.032
n_3, cm^{-3}	0.064	0.064	0.019
ρ_h, $M_\odot$ pc^{-2}	5.59×10^{-3}	1.067×10^{-2}	1.4×10^{-2}

Table 2. Results of computations

R, kpc	L_{38}, 10^{38}erg s^{-1}	Z_0, pc	t_m, Myr	h, pc	$D_{\max}$, pc	$D_{\min}$, pc	ζ	M_{cl}, $10^5 M_\odot$
5	0.315	0	28.5	1460	1090	550	1.98	6.4
	1.05	0	27.3	2430	1280	670	1.91	15.2
	1.05	50	27.8	2190	–	–	–	10.3
	3.15	0	25.4	3580	1440	790	1.82	22.6
8.5	0.315	0	37.3	1800	1170	690	1.70	3.2
	1.05	0	35.7	3150	1350	800	1.69	8.2
	1.05	50	36.8	2800	–	–	–	4.3
	1.05	100	38.1	2560	–	–	–	–
	3.15	0	33.7	4760	1510	920	1.64	12.7
15	0.315	0	63.3	1930	2290	1480	1.55	–
	1.05	0	60.5	3240	2570	1630	1.58	–
	3.15	0	57.4	5350	2840	1790	1.59	–

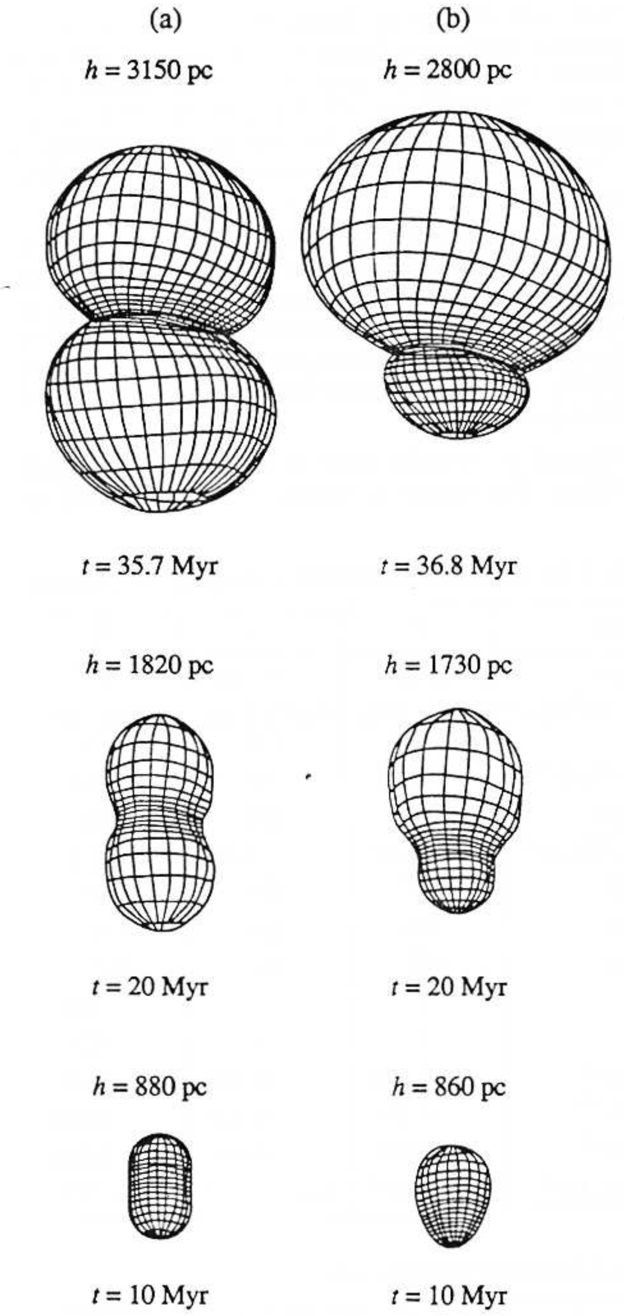

Fig. 1. Evolution of supershells for different locations of the parent OB association: (a) $Z_0 = 0$ pc and (b) $Z_0 = 50$ pc. h is the size of supershells in the Z direction.

Table 1. In this table, R is the galactocentric distance of the parent OB association, Z_0 is the height of the association over the galactic plane, and L is the rate of energy injection. The results of our calculations are summarized in Table 2. In this table, t_m is the time at the end of the calculations; $h = Z_{\max} - Z_{\min}$ is the size of the supershell in the direction perpendicular to the galactic disk; $D_{\max}$ and $D_{\min}$ are the maximal and minimal diameters of cross-sections of the shell by the plane $z = 0$, respectively; $\zeta = D_{\max}/D_{\min}$ is the ratio of these diameters; and $M_{\rm cl}$ is the mass of the gas for which conditions for the formation of molecular hydrogen are satisfied. For models with the energy source located over the galactic plane, we did not calculate the diameters of the cross sections of the supershells by the equatorial plane of the Galaxy.

3. DISCUSSION

Figure 1 shows the shapes of the supershells and their temporal evolution for different locations of parent OB associations over the galactic plane. Clearly, the location of the source has a considerable effect upon the shape of a supershell. If the source of energy is in the galactic plane, the shape of the supershell is slightly distorted by differential rotation, and it resembles a three-dimensional figure eight. When the energy source is displaced from the galactic plane, a strongly asymmetric figure forms, which resembles a balloon; it is distorted by galactic differential rotation. In both cases, in the advanced stages of evolution, a typical "neck" forms near the $z = 0$ plane, which separates the upper and lower parts of the supershell.

As shown in our earlier paper [24], supershell dynamics are strongly affected by the Z component of the galactic gravitational field. Initially, attraction by the galactic disk decreases the Z component of the expansion velocity. Later, it causes the entire supershell to fall down to the galactic plane, thus limiting the lifetime of supershells in the inner regions of the Galaxy. Therefore, supershells do not have enough time to become considerably stretched under the action of galactic differential rotation. The ratio of the large axis of the cross section of the shell by the $z = 0$ plane to the small ζ one never exceeds two (see Table 2).

With the passage of time, the surface density at the poles drops, while near the neck it grows (Fig. 2). The growth of the surface density in this region is caused not only by the sweeping of the surrounding gas, but also by the purely geometrical effect of diminishing the surface area of the Lagrangian elements. The latter effect becomes dominant when the supershell velocity becomes subsonic, and it results in a dramatic growth of surface density (Fig. 2) before the shell fragments that are moving in opposite directions along the Z axis merge. The column density of hydrogen atoms in the neck region may exceed the critical density required for the screening of external UV radiation and the generation of molecular hydrogen [41, 42]

$$N_c = 10^{21}\left(\frac{\chi_{\odot}}{\chi}\right)\text{cm}^{-2}. \tag{14}$$

In equation (14), χ is the abundance of heavy elements in the gas. In the vicinity of the Sun, $\chi_{\odot} \simeq 1.5 \times 10^{-2}$; at the galactocentric distance $R = 5$ kpc, $\chi \simeq 2\chi_{\odot}$, and at $R = 15$ kpc, $\chi \simeq 2/3\chi_{\odot}$ [43].

In Fig. 3a we show the relative distribution of the surface density (N/N_c) in the vicinity of the neck for three galactocentric distances R. As one can see, in the supershells at $R = 5$ and 8.5 kpc from the galactic center,

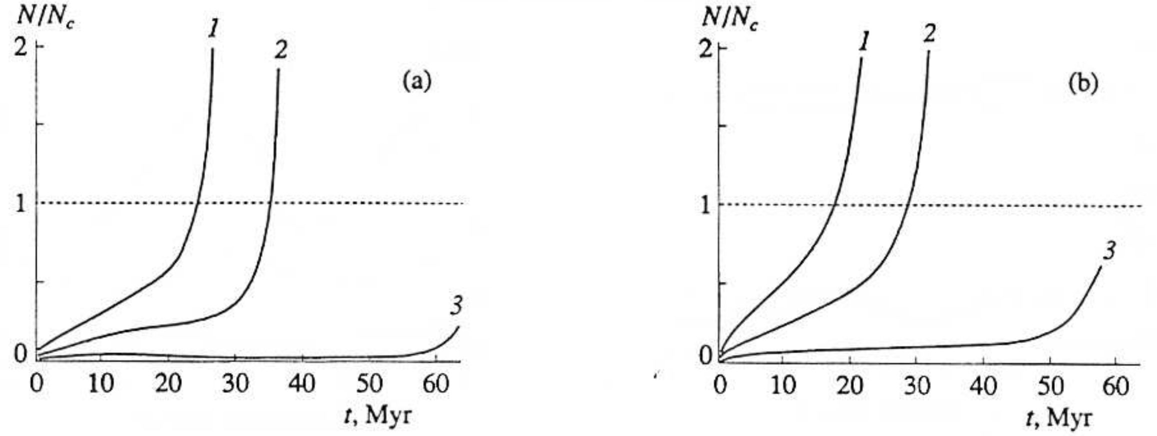

Fig. 2. Variation of the relative column density of hydrogen (N/N_c) at the supershell equator with time. Curves *1*, *2*, and *3* correspond to the galactocentric distances 5, 8.5, and 15 kpc, respectively. Panel (a) is for $L_{38} = 0.315$, and panel (b) is for $L_{38} = 3.15$.

the conditions for the formation of molecular hydrogen may be satisfied. At $R = 15$ kpc, however, the column densities do not reach the critical value and molecular clouds in the expanding supershells cannot form. The possibility of the formation of molecular hydrogen in expanding supershells also depends strongly upon the distance of the parent OB association from the galactic plane. In Fig. 3b we show the distribution of column densities of atoms near the neck of supershells located in the vicinity of the Sun ($R = 8.5$ kpc) at different distances from the galactic plane Z_0. It can be seen that if the distance of the energy source from the symmetry plane $z = 0$ exceeds 50 kpc, the critical column density is never achieved, and molecular hydrogen does not form.

It should be mentioned that conditions for the formation of molecular hydrogen are satisfied only in very narrow (in the Z coordinate) layers (Fig. 4). Most of the molecular gas accumulates at two nearly opposite edges of a ring-shaped layer (Fig. 5). The position of this ring with respect to the galactic plane ($z = 0$) depends upon the location of the energy source with respect to this plane. If the OB association is in the plane, then the neck and the molecular ring also form in the plane. If the association is above the galactic plane, then the neck and the ring form below the plane (Fig. 4). Anyhow, molecular layers form at distances that do not exceed 100 pc from the galactic plane. This is in excellent agreement with observational data on the distribution of molecular hydrogen in the Galaxy [44]. Despite the negligible thickness of the molecular ring, as compared to the total size of the supershell, the mass of gas that can be transformed into molecules is rather high and may exceed $10^6 M_{\odot}$ (Fig. 6). But this is exactly the mass typical of giant molecular clouds. What is the fate of this gas? Can it form separate molecular clouds, and what would be their parameters? To answer these questions, one must do a detailed analysis of the stability of the emerging molecular layer. Estimates of the gravitational stability of supershells based on an analysis of the homogeneous plane or spherical layers

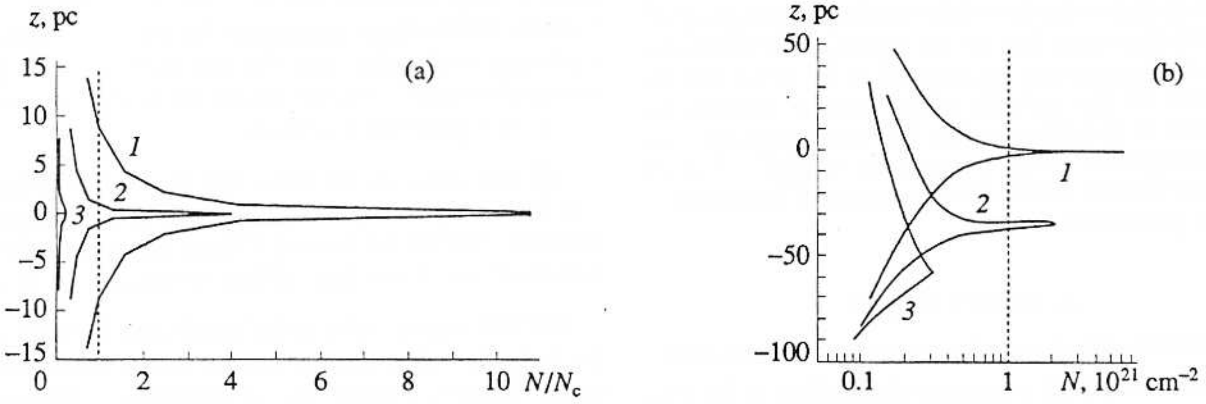

Fig. 3. Distribution of the relative column density of hydrogen (N/N_c) along the surface of a supershell. Panel (a) shows the distribution for different galactocentric distances. Curves *1*, *2*, and *3* correspond to distances of 5, 8.5, and 15 kpc, respectively. Panel (b) shows the distribution for different positions of the parent OB association with respect to the galactic plane. Curves *1*, *2*, and *3* correspond to $Z_0 = 0$, 50, and 100 pc, respectively. Galactocentric distance $R = 8.5$ kpc, and energy injection rate $L_{38} = 1.05$.

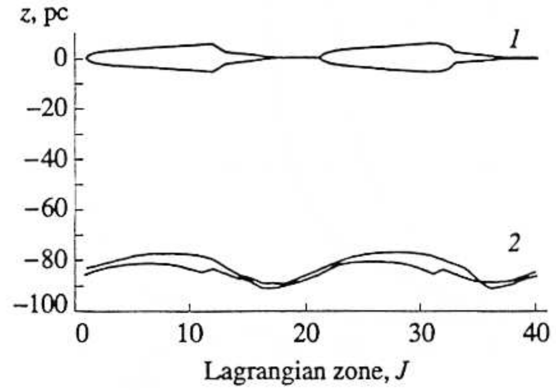

Fig. 4. Profile of the H_2 layer for different locations of the parent OB association with respect to the galactic plane: (*1*) Z_0 = 0 pc, (*2*) Z_0 = 50 pc. Galactocentric distance R = 8.5 kpc, and energy injection rate L_{38} = 1.05.

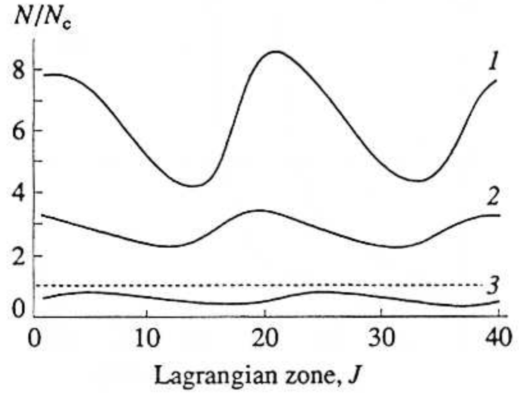

Fig. 5. Distribution of the relative column density of hydrogen along the equator of a supershell for different galactocentric distances. Curves *1*, *2*, and *3* are for R = 5, 8.5, and 15 kpc, respectively. Distance to the galactic plane Z_0 = 0 and energy injection rate L_{38} = 1.05.

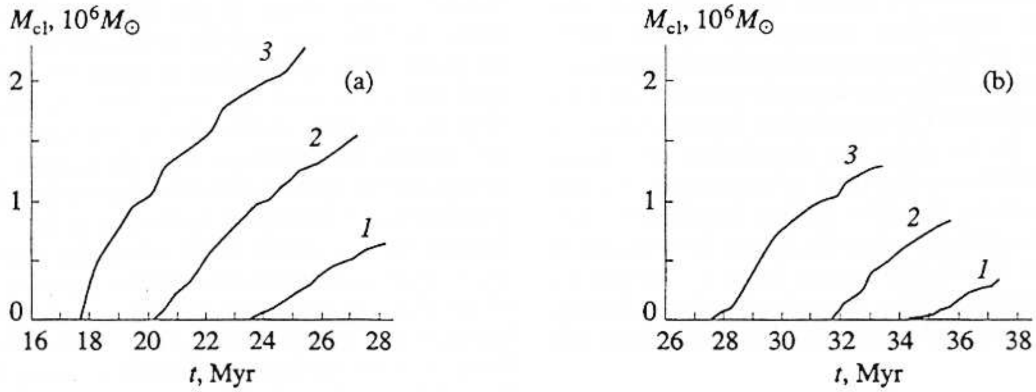

Fig. 6. Dependence of the molecular hydrogen layer mass on time for (a) R = 5 kpc and (b) R = 8.5 kpc. Curves *1*, *2*, and *3* correspond to the rate of the energy injection into the cavity L_{38} = 0.315, 1.05, and 3.15, respectively.

[29, 33, 35] do not say definitely whether if fragmentation is possible. One must also consider the possibility that a crucial role may be played by an inhomogeneity that arises due to the thermal instability of the gas [33]. Also, it is important that the formation of the molecular ring occurs against the background of the descent of the supershell to the galactic plane and its destruction. Therefore, it is quite possible that molecular gas may form complexes with parameters typical of giant molecular clouds, which are the centers of formation of the next generation of stars.

4. CONCLUSION

Let us now summarize the basic results of this study.

(1) We carried out a numerical modeling of the evolution of three-dimensional supershells that form around rich OB associations, for different assumptions regarding their location with respect to the galactic center and to the galactic equatorial plane.

(2) We have shown that at the advanced stages of the evolution of large supershells, the conditions for the formation of molecular hydrogen with a total mass of $\simeq 10^6 M_\odot$ may be satisfied. Giant supershells that form around large associations are, therefore, an effective medium for the transformation of atomic hydrogen into hydrogen molecules and for the formation of giant molecular complexes, which are the formation centers of the next generation of stars.

(3) Our calculations show that molecular hydrogen can form only in supershells located at galactocentric distances that do not exceed 15 kpc, and only if the OB association is closer than 100 pc to the galactic plane.

(4) The regions where the conditions necessary for the formation of molecular gas are satisfied have a very small extension along the Z coordinate. Molecular rings or ring segments and clouds, which are formed within them, cannot arise at distances from the galactic plane greater than 100 pc. Most of the molecular gas accumulates at the opposite edges of the molecular ring that corresponds approximately to the direction of galactic rotation.

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