

Space chemical reactor of protoplanetary disk

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According to our main hypothesis, Life originated in the solar system before the Earth formation at the stage of protoplanetary disk existence. For some time the protoplanetary disk operated as a space chemical reactor synthesizing the organic compounds from the simple molecules. The primary chemical species of the disk included H₂, He, and CO. The dust particles appear to have been composed mainly of metal compounds such as iron, that are the classic catalysts of synthesis of complex organic molecules from the space "syn-gas" of the molecular clouds and disks. Taking into account the loss of H₂ and He, we have determined that more than 10²⁸ g of organic substance with respect to CO could have been produced by global organic synthesis. The appearance of 10¹⁸ g of dry biotic substance on the Earth surface represents only a "fluctuation" at the space - Earth interface as compared to the above giant flows of organic compounds. Due to the predominance of H₂, the reactions giving CH₃OH, CH₂O, NH₃, HCN, hydrocarbons, and other prebiotic molecules should prevail.

The mathematical model was developed for computer simulation of the physico-chemical processes in the protoplanetary accretion disk. The physico-chemical processes are described by a system of non-stationary multidimensional equations of mathematical physics among them Vlasov's equation, equations of hydrodynamic type and Poisson equation for gravitational field.

The goal of computer simulation of space chemical reactor is to determine the zone of synthesis and retention of organic compounds. Did this zone extend to the orbit of Mars? How close did this zone approach the Solar? The immediate task of mathematical modelling is to refine parameters of medium in the disk and verify the physico-chemical notions of the formation and operation of the global catalytic reactor. As a result of computer simulation we have found the space and time distribution of density, velocity, temperature and other macroscopic parameters of two-phase medium in the protoplanetary accretion disk. The conditions of planetesimals formation by instability in the protoplanetary disk with catalytic reactions were found.

References

- Snytnikov V.N., Vshivkov V.A. and Parmon V.N., (1996), *Abs. 11th Intern. Conf. on the Origin of Life*, P. 65.
Snytnikov V.N., Vshivkov V.A., Nikitin S.A. and Parmon V.N., (2002), *Russian J. Computational Technologies*, 7, No. 3, in press.

Kinetics of melts crystallization.

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In the process of cooling melts ordered [1]. Clusters form centers crystallization of [2, 3]. Centers of crystallization are stable only by supercooling. The center of crystallization can grow only when total free energy of the system center of crystallization – adjacent part of melt decreases.

At the equilibrium crystallization's temperature (T_k) liquid and solid phase are in equilibrium and have equal energies, capable of make the equal work: $G_L = G_S$ (1), where G_L – Gibbs' free energy in liquid and G_S – free energy of crystalline phase. The free energy (G) is: $G = E - TS + PV$ (2). The center of crystallization can grow by supercooling melt on the front of crystallization of nuclei crystallization. The more is the radius of nuclei the less is supercooling. The changing of degree of ordering (by transition liquid phase to solid one) can be represents as changing of entropy: $\Delta S = L/T_k$ (3), where L – latent heat of crystallization, T_k – thermodynamic temperature of crystallization. The final probability (P) of liquid phase transition to solid depends on possibility to transit other the energetic barrier ΔG_{max} : $P = C e^{-\Delta G_{max}/k}$ (4), where C – constant which significance depends on conditions of a process realization, k – Boltzman's constant. The rate of stable centers of crystallization formation is proportional to \dot{N} . For formation an equilibrium center of crystallization it is necessary to overcome energetic barrier (ΔG_{max}), which is equal one third of surface energy of nuclei:

$\Delta G_{max} = 1/3 \Sigma S_i \gamma_i$ (5), where S_i – square, γ_i – specific surface energy of i field of the surface of equilibrium nuclei. In the case of homogeneous nuclei formation all facet of which have the same surface tension in relation to liquid: $\Delta G_{max} = 1/3 S \gamma$ (6). Equation for the radius (r) of equilibrium nuclei is: $r = 2\gamma T_k / L \Delta T$ (7). From (7) is clear that nuclei is stable and can grow in the case if its radius $> r$. For the nuclei of cubic form (cube's edge $= 2r$) when it crystallizes from supercooled melt: $\Delta G_{max} = 1/3 \gamma S = 1/3 \gamma 6(2r)^2 = 32 \gamma^3 T_k^3 / L^2 (\Delta T)^2$ (8) and correspondingly $\lg P = \lg C - [32 \gamma^3 T_k \lg e / L^2 (\Delta T)^2 k]$ (9).

By formation nuclei of silicate minerals the supercooling varies from 15% up to 20% relatively to their melting temperature (°C). For acid aluminosilicate melts the supercooling of formation nuclei varies in the limits 100 – 400 °C.

References

1. Frenkel Ya. I. Kinetic theory of liquids. Academia of Sciences of USSR. 1975. 513 p. (in Russian).
2. Mayson B. (1995), *European J. of Mineralogy*. 7, 4, 745–766
3. Feltz A. Amorphe und glasartige anorganische festkörper. Akademie – Verlag. Berlin. 1983. 553 p.