

Information transmission possible mechanisms in natural capsule

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Introduction

Water sorption processes as information medium by cells (membranes, organelle, etc) components surface and in particular cells protoplasts biopolymers (information "absorption" by water) and , in particular, by biopolymers of the cells' protoplast(water information "absorption", and desorption (information "liberation" and its further transfer in cytoplasm) are, in our opinion, exceptionally important for understanding information transmission mechanism in natural capsules - cells of living organisms. At the heart of models' construction, the studies of natural results received while studying mixes of water-soluble polymers are accepted, allowing to model complex processes of water interaction with biopolymers, as well as Frenkel's representations about water nonmonotonic sorption by macromolecules.

Results and Discussion

It is quite obvious that macromolecular structures have hierarchy and consequently obtained data on waters sorption by polymeric mixes, possessing nonmonotonic character with the expressed extremum at certain correlation of components require theoretical approaches to explain the received regularities. One of such approaches has been undertaken by us as well.

During the process of solvent sorption by cell structure polymer one can observe the dynamic effect expressed in fluctuations of absorbed solvent by polymer concentration. S.Ya.Frenkel et al have made the phenomenological analysis of the given situation [1]. In authors' opinion, the reason of abnormal sorption is aggregation varying degree that due to decrease in density of cross-linkage can change solubility of polymer. However, such fluctuations can also be observed in slightly soluble polymers, when the change of nodes number can be neglected. Below the microscopic mechanism of dynamic effect using an example of rather simple polymer macromolecule, slightly dissolved in the solvent [2, 3] is given.

As is known, the process of polymer swelling is accompanied by entropy increase (ΔS_s – mixing entropy) (2) resulting in thermodynamic potential decrease. However, the number of solvent molecules (N_s) occupies part of a macromolecule volume thus making it inaccessible to polymer nodes. Thereof, at volume expansion, system's entropy decreases - D_{SP} , that, in its turn, increases thermodynamic potential. Finally, it results in that the system polymer-solvent achieves its equilibrium condition by fluctuations around equilibrium saturation level. Thus, in this situation it is pertinent to make analogy to ball fluctuations in a bowl (fig. 1) where the bowl surface is determined by changes of system's entropy and the ball's position models the solvent absorption value [4].

In this model the system makes small fluctuations close to steady equilibrium value $N_0 \sim n_0/5$ (from Flori formula [4]), where n is the number of nodes, N is the number of solvent molecules absorbed by the polymer (рис.2). Equilibrium deviation results in force occurrence :

$$\frac{dV}{dN} = F$$

preventing absorption, where

$$V = kT\Delta S = kT(\Delta S_s + \Delta S_p) = kT \left(n - \frac{n^2}{N} + \ln N - \frac{3}{2} \ln n - \frac{3}{2} \frac{N^{2/3}}{n} - \frac{3}{2} \right)$$

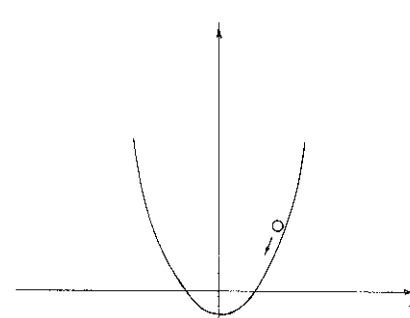


Fig 1. The ball fluctuation in the bowl

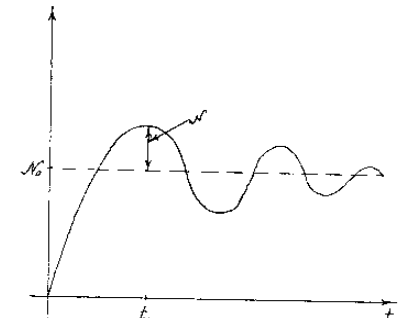


Fig 2. Fluctuations of solvent sorption by polymer

For small deviations the expression is true:

$$V(N) - V(N_0) = \frac{d^2V}{dN^2} \Big|_{N_0} (N - N_0)^2$$

Considering that the variable number of solvent molecules is a single degree of freedom, it is possible to write down system's langrajian:

$$L = \frac{mV_s^{2/3} \dot{N}^2}{2} - \frac{1}{2} \frac{d^2V}{dN^2} \Big|_{N_0} (N - N_0)^2$$

Where m and V_s is a molecular mass and solvent molecules volume accordingly. Hence it is easy to receive free fluctuations frequency of solvent molecules value:

$$\omega_0 = \sqrt{\frac{d^2V}{dN^2} \Big|_{N_0} / m \cdot V_s^{2/3}} = \sqrt{\frac{1}{3} \frac{kT}{n^{13/5} m V_s^{2/3}}}$$

However, one more force f_{fp} is involved in polymer-solvent system. It is friction force of a macromolecule against the solvent that is proportional to speed of solvent inflow into a macromolecule:

$$f_{fp} = -\xi \frac{dN}{dt}$$

Insofar as in the equilibrium **swelling condition** the solvent molecules value is $N_s \sim \alpha^3 n^{3/2} \gg n$ (where n - is the **nodes value**, α - is the coefficient of macromolecule volume expansion at swelling) then for estimation of friction coefficient (ξ) it is possible to be limited by approximation of polymer-solvent solution. Thus we consider that the solvent is at rest and the macromolecule moves. In the **beads'** model approximation of radius r_0 for a macromolecule [4], the friction coefficient is connected with solvent viscosity (η) by correlation of Stocks $\xi \approx 6\pi\eta r_0 n^{1/2}$, where l - is the link length. Thus it is possible to write down the equation for solvent molecules fluctuation value at polymer's swelling:

$$N + N\omega_0^2 + 2\lambda = 0$$

Whence the amplitude of fading fluctuations will be

$$N = N^0 e^{-\lambda t} \sin(\omega t),$$

Where N^0 is initial amplitude

$$\omega = \sqrt{\omega_0^2 - \lambda^2}$$

$$\lambda = \frac{\xi}{2mV_s^{2/3}}$$

$$N^0 = (N - N_0); t = t_1$$

Thus, we undertake an attempt of modeling of solvent sorption mechanism by polymer where the macroscopical physical and chemical model using an example of rather simple macromolecule is presented, describing oscillatory water's sorption character by polymeric systems through formation and destruction of clusters that is one of the processes occurring in dynamic structures. The model has been developed to explain water sorption nonmonotonic character by polymeric structures, cells membranes (natural capsules surface) and is based on clusters formation and destruction processes specific for dynamic structures.

Conclusions

Developed theoretical approaches allow to present the dynamics of complex macromolecules interaction processes with water and further to assume the information transfer to natural biocapsules - cells of living organisms due to water various modular conditions realization, as well as to emphasize a dominating role of interphase spaces in the system "ice-water" in which water nanoparticles are formed providing information translation in natural capsules(cells) volume between cells in an organism, in populations and at "higher" levels of hierarchies.

References

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