Spatio-temporal change of BZ gel

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The Belovsov-Zhabotinsky reaction is well-known as one of the oscillatory chemical reactions to understand rhythmic phenomena under non-equilibrium conditions including living matter and living cell. On the other hand, living body is made from various biopolymers. In particular, motor proteins (myosin, kinesin) and their scaffolds (actin, microtubule) generate motion under the hydrolysis of adenosine triphosphate (ATP), a kind of non-equilibrium conditions. Here, we present a theoretical scenario for the BZ gel, which is a gel containing the BZ reaction field, based on free-energy arguments of volume-phase transition of cross-linked polymer gel and the Oregonator (2 parameter version), a simple model of the BZ reaction.

The essence is that polymer chain elongates in good solvent, while it collapses in poor solvent, where the BZ reaction switches the solvent quality (good or poor solvents) spontaneously. Addition to this, we roughly assume that the volume of polymer gel reflect the size of a sub-chain, which is the short polymer chain between cross-linking points. Free energy of the gel, F_{gel}, can be described as [1]

$$F_{gel} \sim (3/2\,N_{sub})\left(\alpha^2+\alpha^{-2}\right)+C*\alpha^{-6}/N_{sub}-\ln\left[1-\lambda/(N_{sub}^{-1/2}\alpha^{-2})\right] \quad (1)$$

where N_{sub} is the length of a sub-chain, α is the normalized size of a polymer chain ($\alpha \sim 0$; collapse, $\alpha \sim 1$; elongate), $-C^*$ is the solvent quality (smaller: good solvent, larger: poo solvent), the aspect ratio of a sub-chain λ. The BZ reaction changes $-C^*$, which is obtained from the Oregonator. The Oregonator is

$$\varepsilon\frac{dx}{dt} = x(1-x) - fz\frac{x-q}{x+q} \quad (2)$$

$$\frac{dz}{dt} = x - z \quad (3)$$

where x, y, z are the concentrations of chemical species, and $1 - z = -C^*$ although we skip the explanation of the parameters. From the calculations of the Oregonator, we obtain oscillating $-C^*$. We thus succeed to describe the oscillatory volume change of the BZ gel. Based on this scenario, we succeeded to explain other experimental results of polymer system under the BZ reaction.

[1] Mayama, H., Nakai, T., Takushi, E., Tsujii, K., and Yoshikawa, K., Marked differences in volume phase-transitions between gel and single molecule in DNA, *J. Chem. Phys.*, 127:034901, 2007.