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Bistability and oscillation raised by recombination between dimers

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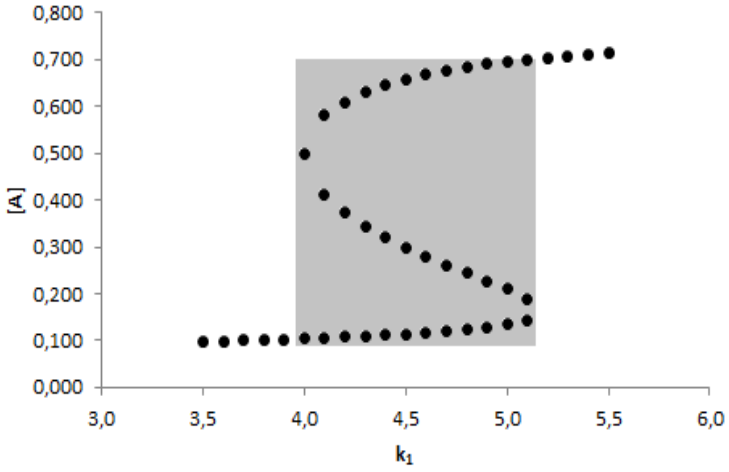
Abstract: Multistability is a phenomenon that describes a condition that a system has two or more steady states. The study of multistability is crucial to the understanding of the cell functions. Such a behavior is present in cell cycles, cell differentiation and apoptosis [1]. Chemical oscillations are rhythmic, temporal or spatial changes in the concentration of each specie in a reaction. Oscillations occurring in biochemical systems are important events for the maintenance of life. Some known examples are the glycolytic oscillations and calcium oscillations [2]. A bistable dynamic is possible during the formation of a trimer. In a hypothetical situation a *B* homodimer consists of two subunits called *A*. A second dimer *D*, a heterodimer, is composed by subunits *A* and *C*. By recombining the dimers an *E* trimer is formed as described in the following equations:

$$\begin{aligned} A + A &\overset{K_1}{\rightarrow} B \\ B &\overset{K_2}{\rightarrow} A + A \\ A + C &\overset{K_3}{\rightarrow} D \\ D &\overset{K_4}{\rightarrow} A + C \\ B + D &\overset{K_5}{\rightarrow} E + C \\ E &\overset{K_6}{\rightarrow} B + A \end{aligned} \qquad (1)$$

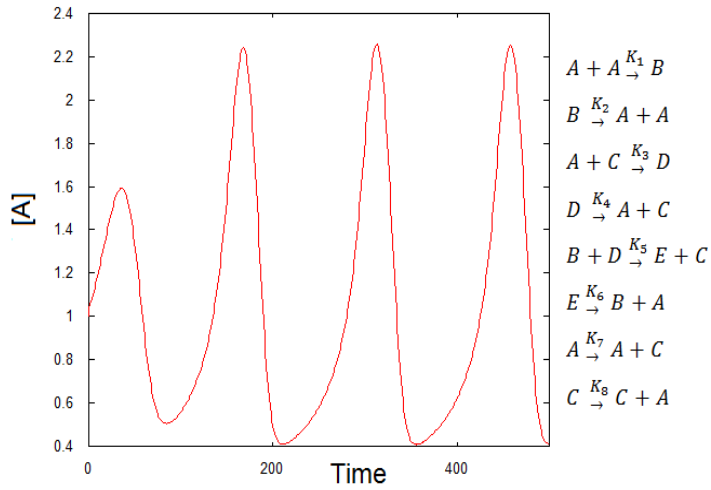
Using the Stoichiometric Network Analysis (SNA) method, a systematic approach to this hypothetical mechanism dynamics was calculated [3] The analysis begins with the determination of a set of velocity vectors from steady states in the reactions. Such set forms an array called "extreme currents" and physically has the value of a subsystem. To study instabilities in the extreme currents is equivalent to observing them in the original system. For this set, the Clarke extreme currents ensure the existence of a saddle knot bifurcation, however, the system still does not present multistability. With an adjustment in the kinetic constants it is possible to generate a sigmoidal curve graph where each point is a stable or unstable steady state.

Figure 1. Bifurcation analysis by kinetic constant k_1 and the concentration of *A* in arbitrary units (a.u.). The dark area shows in which region there are multiple stationary states.



Here the bistability is caused only by the recombination of dimers with no need for autocatalysis reaction, positive or negative feedback. The same system can be modified by adding a cross-regulation component to obtain an oscillatory dynamics.

Figure 2. Oscillations as a function of time by concentration of species A in a.u.



Key-words: Multistability, oscillations, dimers
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References:

[1] T. Wilhelm, Bmc Syst Biol, 3, 90 (2009).
[2] W. Mazala Junior, U. Schuchardt, M. Paoli, Química Nova, 1, 9 (1978).
[3] B. L. Clarke, Cell Biophysics, 12, 237 (1988).