2nd grade: Closed loop reaction

Summary: Closed loop reaction is a kind of chain reaction. In closed loop reaction, however, the last product of a chain reaction is connected to the first molecule activating it again. An example is shown in Fig.1, where the reaction in each step is 1st order reaction. Chain reaction shown here is a basis for the feedback in Calcium Induced Calcium Release (CICR) and circadian rhythms.

Cartoon and A-Cell model: Cartoon and the A-Cell model is the same as shown in Fig.1.

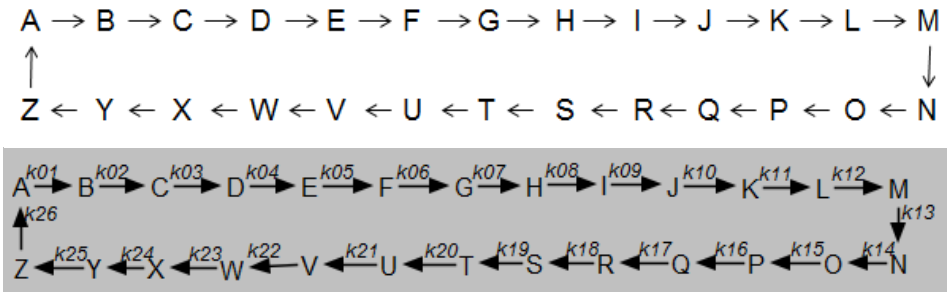

Fig.1 Cartoon (top) and A-Cell model (bottom) for a closed loop reaction.

Here, molecule A activates B, B activates C, and chain activations are cascaded to Z, which finally activates A again. The initial concentration for A was 1 μM and all others were 0 μM. All rate constants k_{01}-k_{26} were 0.1 /s, and simulation condition was as follows: simulation time = 0-1,000 s; calculation step = 10 ms; output step = 1 s. Simulation results are shown in Fig.2. The time of peaks is in sequence to the activation step of molecules from A to Z as in the chain reaction. However, there are at least two peaks in each species (e.g. F in Fig.2). Thus, molecules are oscillating. These results might be unexpected. A delay in the activation of the next species is the cause of the oscillation seen in Fig.2.

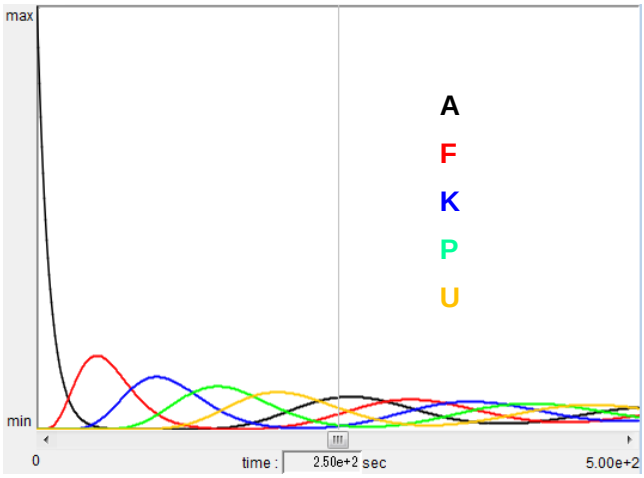

Fig.2 Simulation results for closed loop reaction.