

Basic: 2nd order reaction

Summary: In 2nd order reaction, molecules A and B bind forming complex C, which is a fundamental reaction of protein complex formation. For example, the binding reaction of ligand L to cell surface receptor R is 2nd order reaction, and the binding of substrate S to enzyme E in Michaelis-Menten enzymatic reaction is also a 2nd order reaction.

Cartoon and A-Cell model: Cartoon and A-Cell model are shown on the left panel of Fig.1.

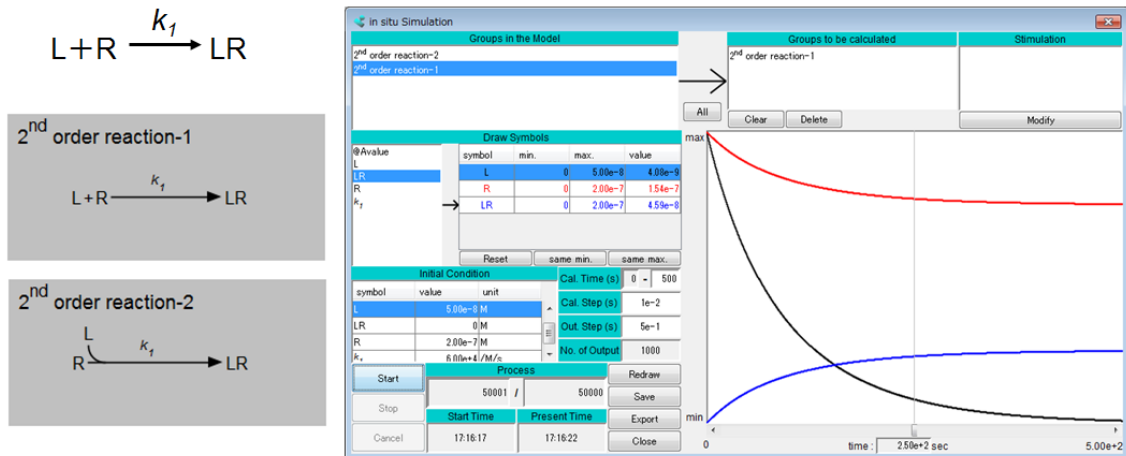


Fig.1 Cartoon and A-Cell model (left) and simulation result (right)

There are two ways in modeling 2nd order reaction by A-Cell (two gray boxes of Fig.1). These two expressions give the same simulation results, and either is used in your model. However, the expression on the bottom left is useful for consecutive ligand binding, where L binds to R forming LR, and another L binds to LR forming LRL. Simulation results by “In situ calculation” menu of A-Cell are shown on the right of Fig.1 with simulation condition as follows: calculation time = 0-500 s; calculation step = 10 ms; output step = 0.5 s.

Next, let’s consider the ligand application with constant concentration during t=0-300 s (Fig.2). Ligand application is modeled by “Stimulation” function of A-Cell. Simulation conditions are the same as in Fig.1, but the results are different. Try to find the reason for the difference.

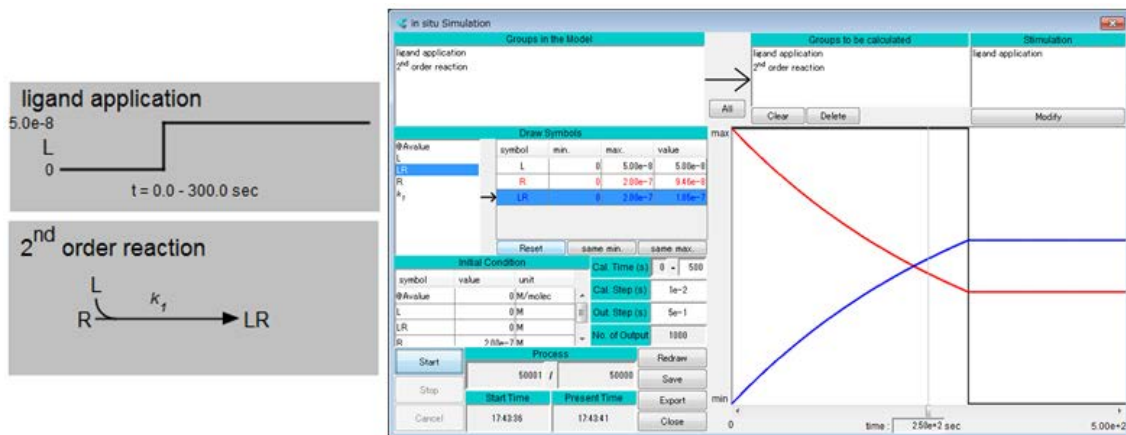


Fig.2 Model and simulation result of ligand application during 300 s.