

### Basic: 1<sup>st</sup> order Reaction

**Summary:** There are many examples of 1<sup>st</sup> order reaction in a cell. For example, dissociation of ligands from cell surface receptor is a 1<sup>st</sup> order reaction, and the decomposition of enzyme-substrate complex producing product and enzyme in Michaelis-Menten enzymatic reaction are two well-known examples. Here we show generalized two examples: one is a change in the molecular conformation from A to B, and another is a dissociation of ligand L from ligand-receptor complex LR.

**Cartoon and A-Cell model:** Cartoon of reaction schemes is quite helpful for constructing A-Cell model even if reactions are complex. In simple examples shown here, cartoon and A-Cell model are exactly the same (left panel in Fig.1).

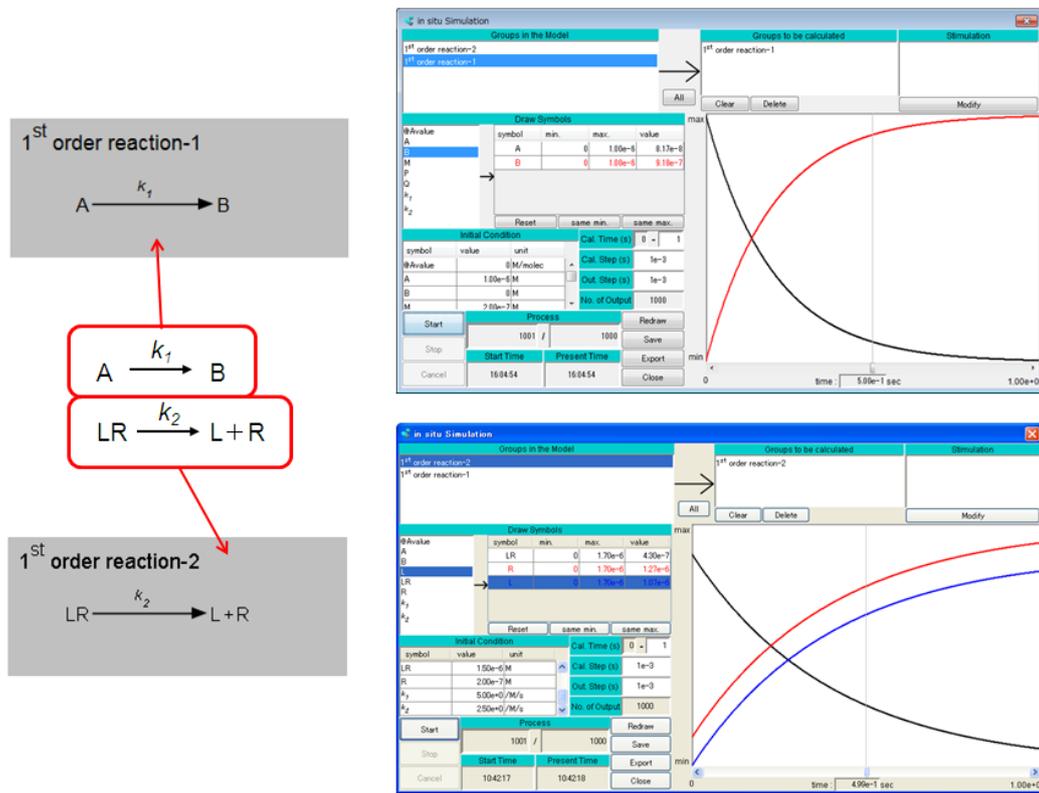


Fig.1 Cartoons (red boxes) and A-Cell models (gray boxes) and simulation results (right)

These simulations were run by “In situ calculation” menu of A-Cell. In the simulation of 1<sup>st</sup>-order reaction, A (black line on the top right panel of Fig.1) and B (red line) simply decays and increases, respectively. In the example of dissociation of L from LR, LR (black line on the bottom right panel) decays, and L (blue line) and R (red line) increase. Initial concentration of R was 0.2  $\mu\text{M}$  to avoid overlap between L and R. Simulation condition was as follows: calculation time = 0-1 s; calculation step = 1 ms (1e-3 s); output step = 1 ms (1e-3 s). These models are easily constructed and simulated by free edition of A-Cell.