Basic: Diffusion

Summary: Diffusion is a phenomenon in which small species such as molecules concentrated at a single spatial point at t=0 spread as time elapsed, and finally molecules are distributed all over the defined space (upper panels of Fig.1). Signal transmission by protein molecules activated at a receptor to distant downstream proteins is described by diffusion. Graphs of spreading of molecules by diffusion are shown in the bottom panel of Fig.1, where ordinate and coordinate are concentration and distance from the origin, respectively. It is clearly seen that molecules concentrated at the center spread as the increase in time. The peak concentration at the center decreases as the increase in time because molecules are gradually distributed within a space.
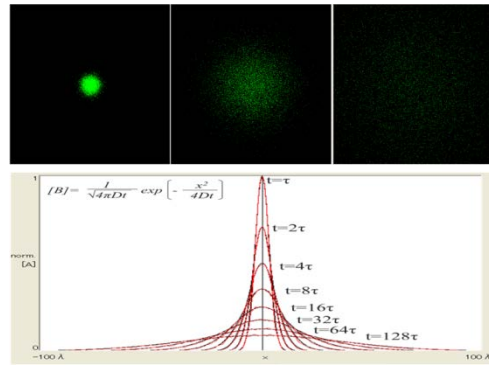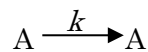

図 1 拡散の現象

Cartoon and A-Cell model: Describing diffusion in A-Cell is very simple as follows: construction of a shape→embed reaction→define diffusion constant. Although it only requires molecules to simulate diffusion, A-Cell not allows embedding only molecules. Instead, a simple dummy reaction shown below is embedded to a region where diffusion is simulated.

$$A \xrightarrow{\ k\ } A$$

Although k can be any value, let's set $k=0$. Diffusion constant was set at $10^{-11}\,m^2/s$, which is nominal value for proteins. The concentration of A was set at 1 μM at the center of the shape leaving other regions 0 M. A disk with a dimeter of 1 μm was constructed, which was divided into 51 compartments, which are small cubic, along radial direction (left panel of Fig.2). Simulation result is shown in the right panel of Fig.2. Species A spreads quickly from the center to all over the shape. The concentration at 70 μs is very low through the shape, because species A at the center at t=0 is distributed to all 2085 compartments.
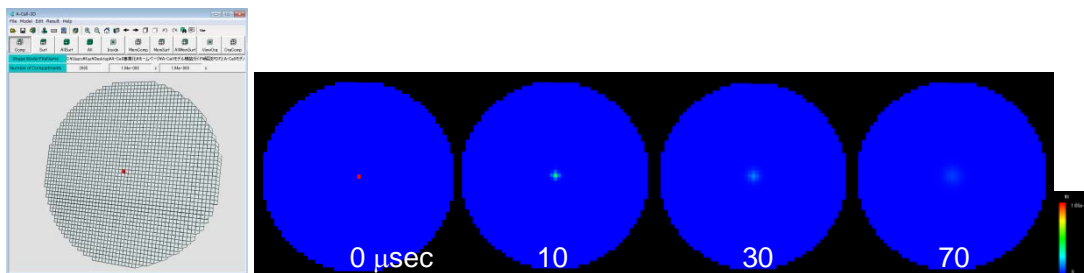

Fig.2 A-Cell model for diffusion (left) and simulation result (right)

Simulation conditions were as follows: calculation time = 0-100 μs; calculation step = 1 μs; output step = 1 μs.