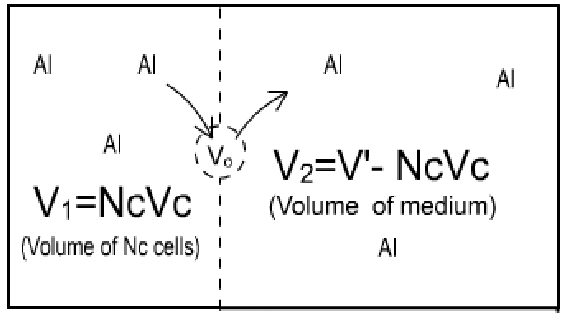
Derivation of diffusion

The variables used are as follows

- n1: number of AI molecules inside the cell.
- n2: number of AI molecules outside the cell.
- Nc: total number of cells.
- V_1: volume of left compartment which contains all the cells
- V_2: volume of right compartment whole of which contains medium.
- Vc : volume of each cell



V'=Volume of the container

The idea is that we divide our system (container) into two compartments; the left compartment contains all cells while the right compartment contains whole of medium.

So volume of left compartment V_1 = NcVc

Let V_0 be the volume of the region of the interface between the cell and the external medium through which a molecule of the autoinducer diffuses. Since there are Nc cells the total volume available for diffusion will be NcVc.

Let τ_0 be the time spent by AI molecule inside the membrane. The equation for rate of change of AI molecules would be as follows:

$$\frac{dn_1}{dt} = \frac{1}{2}\left(\frac{N_c V_o}{\tau_0}\right)\left(\frac{n_2}{V_2} - \frac{n_1}{V_1}\right)$$

The factor of ½ occurs because molecules have a 50% chance of either moving inside or outside the cell.

Solving further we get equations as follows.

$$\frac{d\phi_i}{dt} = \frac{d}{dt}\left(\frac{n_1}{V_1}\right) = \frac{1}{V_1}\frac{dn_1}{dt} + n_1\left(\frac{-1}{V_1^2}\right)\left(\frac{dV_1}{dt}\right)$$

$$\Rightarrow$$

$$\frac{d\phi_i}{dt} = \frac{1}{V_1}\left[\frac{1}{2}\left(\frac{N_c V_0}{\tau_0}\right)\left(\frac{n_2}{V_2} - \frac{n_1}{V_1}\right) - \frac{n_1}{V_1}\frac{d}{dt}\left(N_c V_c\right)\right]$$

$$N = N_o e^{\gamma ct}$$

$$\frac{d\phi_i}{dt} = \frac{1}{N_c V_c}\left[\frac{1}{2}\left(\frac{N_c V_0}{\tau_0}\right)\left(\frac{n_2}{V_2} - \frac{n_1}{V_1}\right) - \frac{n_1}{V_1} V_c\left(\gamma_c N_c\right)\right]$$

$$\phi_e = \frac{n_2}{V_2}; \phi_i = \frac{n_1}{V_1}$$

$$\frac{d\phi_i}{dt} = \left[\frac{1}{2}\left(\frac{V_0}{V_c}\right)\left(\frac{1}{\tau_o}\right)\left(\phi_e - \phi_i\right) - \phi_i\left(\gamma_c\right)\right]$$

But AI will also be created in the cell. The amount of AI produced will be proportional to concentration of LuxI. So the above equation gets transformed to…

$$\frac{d\phi_i}{dt} = K_1 Y_1 + \eta\left(\phi_e - \phi_i\right) - \gamma_c \phi_i$$

$$where,$$

$$\eta = \frac{1}{2}\left(\frac{V_o}{V_c}\right)\left(\frac{1}{\tau_o}\right)$$

But Φ_i also undergoes degradation. Let γ_i be the constant of degradation of AI inside the cell. So our final equation becomes:

$$\frac{d\phi_i}{dt} = K_1 Y_1 + \eta\left(\phi_e - \phi_i\right) - \gamma_c \phi_i - \gamma_i \phi_i$$

On similar lines equation for $\frac{d\phi_e}{dt}$ can be derived. The only important point to note is that cell division would not affect the concentration of AI external. So γ_c would not come into picture. γ_i would be replaced by γ_e, the constant for degradation of AI outside the cell.