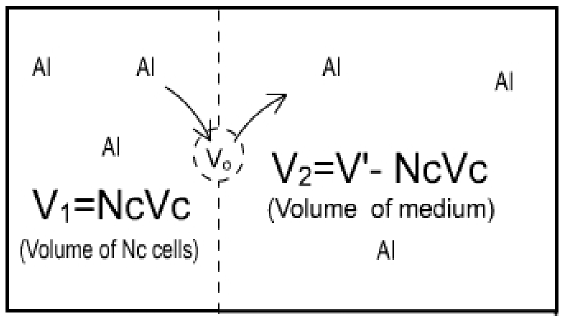
Derivation of expression for [AI]

The autoinducer (AI) is a chemical species that passively diffuses across the cell membrane. Its concentration inside the cell is hence dependent both on its creation in the cell and its diffusion across the membrane. As the density of cells increases, more and more AI collects in the medium, and this in turn increases its concentration inside the cell.

We use basic principles in diffusion to arrive at an expression for the concentration of AI.
The following figure is a schematic representation of this system.



V'=Volume of the container

Here, we represent the diffusion process by considering the cells and the medium to form two compartments of a container, separated from each other by a semi-permeable membrane. AI passively diffuses across this membrane. N_C stands for the number of cells and V_C stands for the volume of an individual cell. As the cells grow in size and divide, they take in the surrounding medium. In our diagram, this corresponds to a gradual movement of the membrane from left to right.

Let n_1 be the total number of AI molecules inside the cells and n_2 the number of AI molecules in the surrounding medium. Let τ_0 be the time spent by an AI molecule in a region of volume V_0 at the interface of the cell membrane and the surrounding medium. Since there are N_C cells, the effective volume of this interface between the left and right compartments is N_cV_c. Once present at the interface, the AI molecule has an equal probability of moving into or out of the cell.

Thus, the differential equation representing the change in the number of AI molecules inside the cells with time is:

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

We now use this equation to derive an expression for the concentration of AI inside the cells.

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

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

$$N_c = N_o e^{\gamma_c t} \Rightarrow$$

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

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

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

The above treatment only takes into account the effects of diffusion and dilution. In addition, AI is also produced in the cell by the activity of the LuxI (Y_I) enzyme, and degraded at a certain rate (γ_i). Incorporating these terms, the final expression becomes,

$$\frac{d\phi_i}{dt} = k_1 Y_I + \eta\left(\phi_e - \phi_i\right) - \gamma_c \phi_i - \gamma_i \phi_i \qquad [1]$$

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

Similarly, one can derive an expression for φ_e.

$$\frac{dn_2}{dt} = -\frac{1}{2}\left(\frac{N_c V_o}{\tau_0}\right)\left(\frac{n_2}{V_2} - \frac{n_1}{V_1}\right)$$

$$\frac{d\phi_e}{dt} = \frac{d}{dt}\left(\frac{n_2}{V_2}\right) = \frac{1}{V_2}\frac{dn_2}{dt} + n_2\left(\frac{-1}{V_2^{\,2}}\right)\left(\frac{dV_2}{dt}\right)$$

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

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

$$\frac{d\phi_e}{dt} = \frac{V_1}{V_2}\left[\frac{1}{2}\left(\frac{V_0}{V_c}\right)\left(\frac{1}{\tau_o}\right)\left(\phi_i - \phi_e\right) + \gamma_c \phi_e\right]$$

$$V' >> N_c V_c \Rightarrow V_2 \sim V'; \frac{V_1}{V_2} = \frac{N_c V_c}{V'} = \rho V_c \Rightarrow$$

$$\frac{d\phi_e}{dt} = \rho V_c\left[\eta\left(\phi_i - \phi_e\right) + \gamma_c \phi_e\right]$$

After taking into account the degradation of AI outside the cell, the final expression becomes,

$$\frac{d\phi_e}{dt} = \rho V_c\left[\eta\left(\phi_i - \phi_e\right) + \gamma_c \phi_e\right] - \gamma_e \phi_e \qquad [2]$$