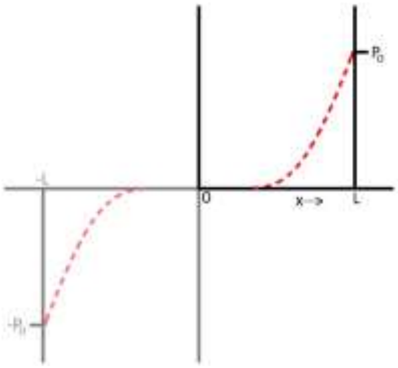
File Dif_Exp.docx

Diffusion through a flat layer - non-steady-state - approach with exponential functions.

Layer runs from x=0 to x=L;

At x=0 the O_2 pressure P is kept (virtually) zero; the O_2 streaming into the adjacent gas chamber is measured by following the increasing but negligibly low P.

On x=L at time t=0 the pressure is increased from 0 to P_0. This will induce a 'moving front' of O_2 from x=L towards x=0, which ultimately will approach a steady-state straight line for P within the layer, $P \rightarrow P_0\, x/L$ for 0<x<L.



For solving the time-dependent profile in the layer the Fourier method will be applied. The easiest way is, to solve for a (virtual) layer that runs from x=–L to x=L where the profile is antisymmetric: this means, that P(–x)=–P(x). Then, there indeed is a precondition P=0 at x=0, as required; and an additional precondition will be at the virtual opposite boundary $P=-P_0$ at x= –L, all for t>0.

Because of the antisymmetry, the solution can be written as Fourier series in x with only sine terms:

$$P = P_0\, x + \sum_{n=1}^{\infty} f_n(t) \sin\left(n\pi \frac{x}{L}\right)$$

which must satisfy the differential equation:

$$D\frac{\partial^2 P}{\partial x^2} = \frac{\partial P}{\partial t}$$

applied on the nth sine term, we find for the nth time function $f_n()$, dropping the sin():

$$-D\, f_n(t)\left(\frac{n\pi}{L}\right)^2 = \frac{df_n}{dt}(t)$$

which is easily solved as an exponential function so that:

$$P = P_0\, x + \sum_{n=1}^{\infty} g_n \exp\left(-n^2\pi^2\frac{Dt}{L^2}\right)\sin\left(n\pi\frac{x}{L}\right)$$

The coefficients g_k can be found in a standard Fourier way by multiplying P on t=0 – which is zero everywhere - by the kth sine term and integrating from –L to L:

$$0 = \int_{x=-L}^{L} dx\, P_0\, x \sin\left(k\pi\frac{x}{L}\right) + \sum_{n=1}^{\infty} g_n \int_{x=-L}^{L} dx \sin\left(n\pi\frac{x}{L}\right)\sin\left(k\pi\frac{x}{L}\right)$$

The first term is integrated easily:

$$\int_{x=-L}^{L} dx\, P_0\, x \sin\left(k\pi\frac{x}{L}\right) = P_0\left[-x\frac{L}{k\pi}\cos\left(k\pi\frac{x}{L}\right) + \frac{L^2}{k^2\pi^2}\sin\left(k\pi\frac{x}{L}\right)\right]_{-L}^{L} = -2P_0\frac{L^2}{k\pi}(-)^k$$

and for the second term, all elements of the sum are zero except for n=k:

$$g_k \int_{x=-L}^{L} dx \sin\left(k\pi \frac{x}{L}\right) \sin\left(k\pi \frac{x}{L}\right) = g_k L$$

from which the g_k can be solved:

$$g_k = = 2P_0 \frac{L}{k\pi} (-)^k$$

which in turn can be substituted into the equation for P:

$$\frac{P}{P_0} = x + \sum_{n=1}^{\infty} \frac{(-)^n 2L}{n\pi} \exp\left(-n^2\pi^2 \frac{Dt}{L^2}\right) \sin\left(n\pi \frac{x}{L}\right)$$

Note, that this solution is derived for the 'virtual' layer –L<x<L but in reality is valid only for the 'real' layer 0<x<L. The oxygen flux J into the gas chamber next to x=0 is directly proportional to ∂P/∂x at x=0:

$$J \propto \frac{1}{P_0} \frac{\partial P}{\partial x}\bigg|_{x=0} = 1 + \sum_{n=1}^{\infty} (-)^n 2 \exp\left(-n^2\pi^2 \frac{Dt}{L^2}\right)$$

and the build-up of pressure by integrating J over time:

$$P_{GAS} \propto \int_0^t dt\, J \propto \int_0^t dt \left\{ 1 + \sum_{n=1}^{\infty} (-)^n\ 2 \exp\left(-n^2\pi^2 \frac{Dt}{L^2}\right) \right\}$$

easily solved as:

$$P_{GAS} \propto \left[t - \frac{L^2}{D} \sum_{n=1}^{\infty} \frac{(-)^n 2}{n^2\pi^2} \exp\left(-n^2\pi^2 \frac{Dt}{L^2}\right) \right]_0^t$$

$$= t + \frac{L^2}{D} \left\{ \sum_{n=1}^{\infty} \frac{(-)^n 2}{n^2\pi^2} - \sum_{n=1}^{\infty} \frac{(-)^n 2}{n^2\pi^2} \exp\left(-n^2\pi^2 \frac{Dt}{L^2}\right) \right\}$$

$$= t - \frac{L^2}{6D} - \frac{L^2}{D} \sum_{n=1}^{\infty} \frac{(-)^n 2}{n^2\pi^2} \exp\left(-n^2\pi^2 \frac{Dt}{L^2}\right))$$

For increasing time, the exponential terms disappear and the increase of gas pressure will follow a straight line;

$$P_{GAS} \propto => t - \frac{L^2}{6D}$$

with an apparent starting time t_L:

$$t_L = \frac{L^2}{6D}$$