

TMA4195 Mathematical Modelling Project

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1 Deriving the modelling equations

Diffusion equation

Flux J :

$$J = -D\nabla c$$

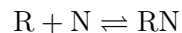
$$\begin{aligned}c_t &= \kappa \Delta c \\ \frac{dc}{dt} &= \kappa \nabla^2 c\end{aligned}$$

Neumann BC:

$$\nabla c \cdot n = g(t, c)$$

1.1 The binding process

First we look at the reversible chemical reaction



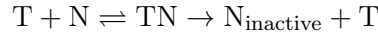
with reaction rate k_1 to the right and k_2 to the left, being respectively the probability for the reactions to occur in their direction. We get 3 ODE's from this chemical reaction:

$$\begin{aligned}\frac{d[\text{R}]}{dt} &= -k_1[\text{R}][\text{N}] + k_2[\text{RN}], \\ \frac{d[\text{N}]}{dt} &= -k_1[\text{R}][\text{N}] + k_2[\text{RN}], \\ \frac{d[\text{RN}]}{dt} &= k_1[\text{R}][\text{N}] - k_2[\text{RN}],\end{aligned}$$

where $[R]$, $[N]$ and $[RN]$ are the concentrations of the receptors, neurotransmitters and the bound product of them. We may consider $[N][R]$ the probability of a neurotransmitter meeting an unoccupied receptor, and k_1 the probability of the binding reaction happening. Likewise for k_2 . Next, we insert c for $[N]$. Introducing P^R as the probability of a receptor being unoccupied, and $(1 - P^R)$ as the probability that the neurotransmitter is attached to the receptor leads to the following simplification¹ of the above ODE's:

$$\begin{aligned}\frac{dc}{dt} &= -k_1 c P^R + k_2 (1 - P^R), \\ \frac{dP^R}{dt} &= -k_1 c P^R + k_2 (1 - P^R).\end{aligned}$$

1.2 Glia cells



Here, we define k_3, k_4, k_5 as the reaction rates of first rightward, first leftward, second rightward reactions.

Similarly to the binding process, we get the following sets of equations:

$$\begin{aligned}\kappa \nabla c \cdot n &= -k_3 c P^T + k_4 (1 - P^T), \\ \frac{dP^T}{dt} &= -k_3 c P^T + (1 - P^T)(k_4 + k_5),\end{aligned}$$

Combining these equations, we get

$$\begin{aligned}\kappa \nabla c \cdot n &= -c(k_1 P^R + k_3 P^T) + k_2 (1 - P^R) + k_4 (1 - P^T), \\ \frac{dP^R}{dt} &= -c k_1 P^R + k_2 (1 - P^R), \\ \frac{dP^T}{dt} &= -c k_3 P^T + (k_4 + k_5)(1 - P^T),\end{aligned}$$

¹Jorg Henrik Holstad. (2011). Modellering av Diffusjon av Nevrotransmittere i den Ekstracellelaere Vaesken. Retrieved from <https://www.duo.uio.no/bitstream/handle/10852/10871/MasteroppgaveHenrikHolstad.pdf>