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

$$\mathrm{R} + \mathrm{N} \rightleftharpoons \mathrm{RN}$$

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:

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

where [R], [N] and [RN] are the concentratinos 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 attatched to the receptor leads to the following simplification[1] 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

$$\mathrm{T} + \mathrm{N} \rightleftharpoons \mathrm{TN} \rightarrow \mathrm{N}_{\text{inactive}} + \mathrm{T}$$

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

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

[1] Jorg 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