**INTRODUCTION**

- In a surface-volume reaction, one reactant (the unbound ligand) is convected in a fluid over a surface to which another reactant (the receptor) is confined.
- These reactions are quite common and occur in antigen-antibody interactions, drug absorption, and blood clotting, among others.\(^1,2,3\)
- Mathematical models exist for single component reactions, but there is little quantitative information regarding multi-component reactions. Here we analyze a mathematical model multi-component surface volume reactions.
- Below is a schematic for ligand flow through a channel.\(^4\)

**MATHEMATICAL MODEL**

- It is the reactions occurring at the boundary that are of primary interest:

\[
E \begin{pmatrix}
\frac{k_1}{k_{d1}} & B_1 & \frac{k_2}{k_{d2}} & B_2 \\
\end{pmatrix}
\]

- By the mass-action principle the governing equations for \(B_1, B_{12}, B_2\) are:

\[
\frac{\partial B_1}{\partial t} = (1 - B_{22})C_1 + \frac{1}{2}K_d B_1 B_2 - \frac{1}{2}K_d B_1 C_2 (1) \\
\frac{\partial B_{12}}{\partial t} = \frac{1}{2}K_d B_1 C_2 + \frac{1}{2}K_d B_2 C_1 - \frac{1}{2}K_d B_{12} (2) \\
\frac{\partial B_2}{\partial t} = 2K_a(1 - B_{22})C_2 + \frac{1}{2}K_d B_2 C_1 - \frac{1}{2}K_d B_2 (3)
\]

Here \(C_i(x, \eta, t)\) denotes the unbound ligand concentration. It can be shown that at the boundary \(C_i(x, 0, t)\) is given by the formula:

\[
C_i(x, 0, t) = 1 - \frac{\text{Da}}{3^2 + D_{a1}^2 + D_{a2}^2} \int_0^x \left( \frac{\partial B_1}{\partial t} + \frac{\partial B_{12}}{\partial t} \right) (x - v)^{-2} dv (4) \\
C_i(x, 0, t) = 1 - \frac{\text{Da}}{3^2 + D_{a1}^2 + D_{a2}^2} \int_0^x \left( \frac{\partial B_{12}}{\partial t} + \frac{\partial B_2}{\partial t} \right) (x - v)^{-2} dv (5)
\]

Here \(B_{22} := B_1 + B_{12} + B_2, \text{Da} - \text{Damköhler number}, \text{key perturbation parameter and is very small. Represents the ratio of reaction to diffusion. Also }D_r = \frac{D_{a1}}{D_{a2}}, \text{the ratio of the diffusivities of the two ligands.}\)

- The integral terms in (4), (5) represent upstream ligand depletion.

**Perturbation Analysis**

- Experimentalists are interested in an approximation to the average of \(\vec{B}\):

\[
\bar{B}(t) = \frac{1}{x_{max} - x_{min}} \int_{x_{min}}^{x_{max}} \vec{B}(x, t) dx
\]

A regular expansion of the form

\[
\vec{B} = \vec{B}_0 + \text{Da}\vec{B}_1 + \mathcal{O}(\text{Da}^2)
\]

has a secular term.

- By manipulating the average of equations (1)-(3), together with (4) and (5), we obtain a simple set of ODE’s:

\[
\frac{d\vec{B}}{dt} = M^{-1}(t)(A\vec{B} + \vec{f}) + \mathcal{O}(\text{Da}^2) (6)
\]

Here we have eliminated the secularity without the aid of a multiple scale expansion. Also we don’t have to manipulate the data to obtain the average.

**Numerical Verification**

- In order to test the accuracy of our approximation (6) we developed a semi-implicit finite difference scheme. The results are depicted for \(B_1\) below. Similar results for \(B_{12}, B_2\) hold.

Left: \(B_1\)

Middle: Error in (6) for \(\text{Da} = .01\)

Right: Error in (6) for different \(\text{Da}\)

- Our approximation (6) does quite well, giving five digits of accuracy for \(\text{Da} = .01\).
- Motivated by previous results\(^5\) and (6) we asked: how well does our approximation - that is only formally valid for \(\text{Da} \ll 1\) - do for moderate and large \(\text{Da}\)?
- Error remains small, and reaches an asymptote corresponding to about a one percent error.

**REFERENCES**


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