Transport Phenomena in Field Effect Transistors

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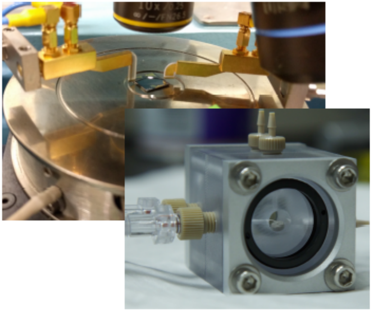
Precision Medicine

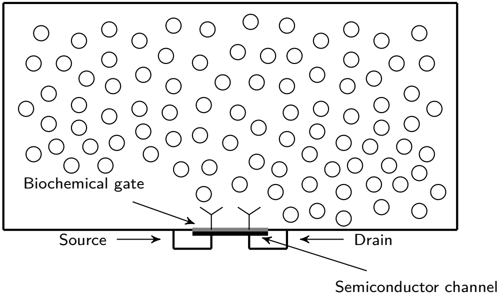
- Precision medicine–the tailoring of therapies to individuals or specific subsets of a population to deliver personalized care.
- Personalized therapies can be safer and yield better outcomes at lower doses when treating diabetes, Alzheimer's disease, or certain kinds of cancers.
- This has led to the advent of a new portable detection tool known as a *Field Effect Transistor* (FET).

Field Effect Transistor (FET)



Experimental setup

Field Effect Transistor (FET)



- Measures current: $i(t) = \frac{s}{x_{\max} - x_{\min}} \int_{x_{\min}}^{x_{\max}} B(x,t)\,\mathrm{d}x.$

Modeling FET Dynamics

- FET experiments are complex systems involve: diffusion, reaction, and semiconductor physics.
- Previous modeling efforts have been devoted to understanding semiconductor physics, and assume the system is in a steady-state [1], [2], [3].
- An accurate time-dependent mathematical model can provide theoretical predictions of the measured signal and is necessary for maximizing the sensitivity of FET-based measurements.

[1] Heitzinger, *SIAM Journal on Applied Mathematics*, 2010.
[2] Khodadadian, *Journal of Computational Electronics*, 2016.
[3] Landheer, *Journal of Applied Physics*, 2005.

Modeling FET Dynamics

- Uniform injection along top boundary.
- Sealed experiment with pulse injection at $t = 0$.

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- Uniform injection along top boundary.
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Dimensional Equations (Uniform Injection)

$$\frac{\partial \widetilde{C}}{\partial \widetilde{t}} = \widetilde{D}\ \widetilde{\nabla}^2 \widetilde{C},$$

$$\widetilde{C}(\widetilde{x}, \widetilde{y}, 0) = 0$$

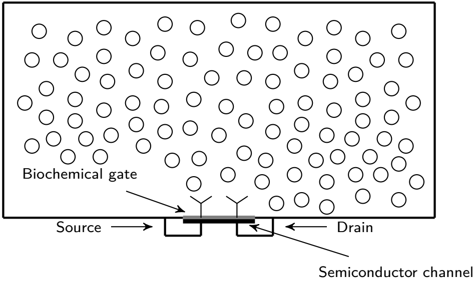
$$\frac{\partial \widetilde{C}}{\partial \widetilde{x}}(0, \widetilde{y}, \widetilde{t}) = \frac{\partial \widetilde{C}}{\partial \widetilde{x}}(\widetilde{L}, \widetilde{y}, \widetilde{t}) = 0$$

$$\widetilde{C}(\widetilde{x}, \widetilde{H}, \widetilde{t}) = \widetilde{C}_u$$

$$\widetilde{D}\frac{\partial \widetilde{C}}{\partial \widetilde{y}}(\widetilde{x}, 0, \widetilde{t}) = \frac{\partial \widetilde{B}}{\partial \widetilde{t}}\ \chi_{\mathrm{s}}(\widetilde{x}),$$

$$\frac{\partial \widetilde{B}}{\partial \widetilde{t}} = \widetilde{k}_a(\widetilde{R}_t - \widetilde{B})\widetilde{C}(\widetilde{x}, 0, \widetilde{t}) - \widetilde{k}_d \widetilde{B}$$

$$\widetilde{B}(\widetilde{x}, 0) = 0$$



Dimensionless System (Uniform Injection)

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)$$

$$C(x, y, 0) = 0$$

$$\frac{\partial C}{\partial x}(\pm 1/(2l_s), y, t) = 0$$

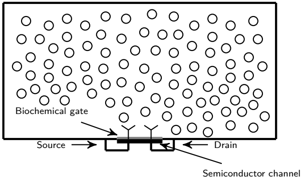
$$C(x, \epsilon/l_s, t) = 1$$

$$\frac{\partial C}{\partial y}(x, 0, t) = \mathrm{Da}\frac{\partial B}{\partial t}\ \chi_{\mathrm{s}}(x)$$

$$\frac{\partial B}{\partial t} = (1 - B)C(x, 0, t) - KB$$

$$B(x, 0) = 0$$

$$D = \frac{\widetilde{D}/\widetilde{l}_s^2}{\widetilde{k}_a\widetilde{C}_u}, l_s = \frac{\widetilde{l}_s}{\widetilde{L}}, \epsilon = \frac{\widetilde{H}}{\widetilde{L}}, \mathrm{Da} = \frac{\widetilde{k}_a\widetilde{R}_t}{\widetilde{D}/\widetilde{l}_s}, K = \frac{\widetilde{k}_d}{\widetilde{k}_a\widetilde{C}_u}$$



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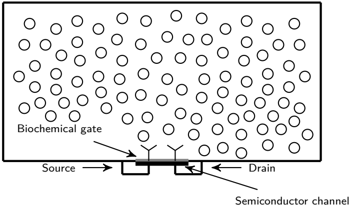
$$\frac{\partial B}{\partial t} = (1-B)C(x,0,t) - KB$$

$$B(x,0) = 0$$

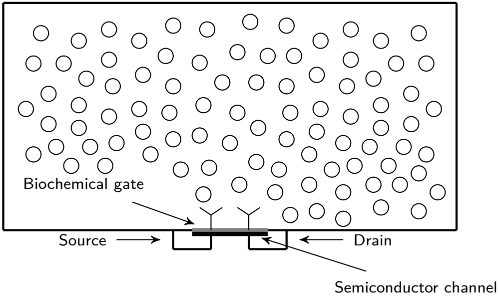
$$D \gg 1,\ \ l_s \ll 1,\ \ \epsilon = O(1),\ \ \mathrm{Da} = O(1),$$

$$K \ll 1,\ \ K = O(1),\quad \text{or } K \gg 1$$



Quasi-Steady Approximation

$$0 = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}$$
$$C(x, \epsilon/l_s, t) = 1$$
$$\frac{\partial C}{\partial y}(x, 0, t) = \mathrm{Da}\frac{\partial B}{\partial t}\ \chi_{\mathrm{s}}(x)$$
$$\frac{\partial B}{\partial t} = (1 - B)C(x, 0, t) - KB$$
$$B(x, 0) = 0$$



- Search for solutions of the form $C = 1 + C_b$.
- Only need $C(x, 0, t)$ in equation for B, so it is sufficient to solve for $C(x, y, t)|_{y=0}$.

Quasi-Steady Approximation

- This reduces the problem to

$$
\begin{aligned}
0 &= \left(\frac{\partial^2 C_b}{\partial x^2} + \frac{\partial^2 C_b}{\partial y^2}\right) \\
C_b(\overline{x}, \epsilon/l_{\mathrm{s}}, t) &= 0 \\
\frac{\partial C_b}{\partial y}(x, 0, t) &= \mathrm{Da}\frac{\partial B}{\partial t} \cdot \chi_s
\end{aligned}
$$

Take a Fourier transform in x, and evaluate at the surface to show:

$$
\widehat{C}_b(\omega, 0, t) = -\mathrm{Da}\frac{\tanh(\epsilon l_{\mathrm{s}}\omega)}{\omega}\frac{\partial \widehat{B}}{\partial t}(\omega, t) \star \left(\frac{\sin(\omega/2)}{\omega/2}\right).
$$

How to go back?

- Applying convolution theorem to

$$\widehat{C}_{\mathrm{b}}(\omega,0,t) = -\mathrm{Da}\,\underbrace{\frac{\tanh(\epsilon l_{\mathrm{s}}\omega)}{\omega}}_{\mathcal{F}(\omega)}\frac{\partial \widehat{B}}{\partial t}(\omega,t) \star \left(\frac{\sin(\omega/2)}{\omega/2}\right)$$

shows

$$C_b(x,0,t) = -\mathrm{Da}\int_{-\infty}^{\infty}\mathcal{F}^{-1}(x-\nu)\frac{\partial B}{\partial t}(\nu,t)\chi_{\mathrm{s}}(\nu)\,\mathrm{d}\nu$$

$$\Rightarrow C_b(x,0,t) = -\mathrm{Da}\int_{-1/2}^{1/2}\mathcal{F}^{-1}(x-\nu)\frac{\partial B}{\partial t}(\nu,t)\,\mathrm{d}\nu,$$

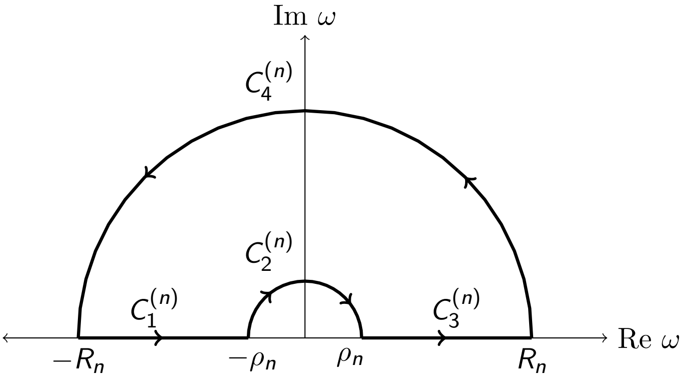
where

$$\mathcal{F}^{-1}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\tanh(\epsilon l_{\mathrm{s}}\omega)}{\omega}\mathrm{e}^{-i\omega x}\,\mathrm{d}\omega.$$

Residue Theorem

Apply residue theorem to show

$$\mathcal{F}^{-1}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\tanh(\epsilon l_s \omega)}{\omega} \mathrm{e}^{-i\omega x}\,\mathrm{d}\omega = \tanh^{-1}(\mathrm{e}^{-|x|\pi l_s/(2\epsilon)}).$$



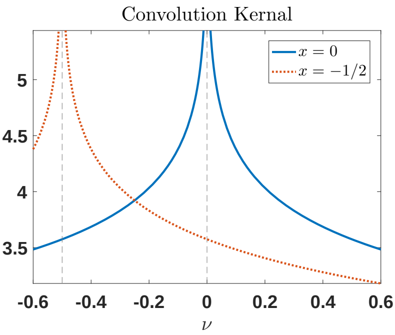
Integral Equation for $C(x, 0, t)$

- Putting these facts together leads to the conclusion:

$$C(x,0,t) = 1 - \frac{2\ \mathrm{Da}}{\pi} \int_{-1/2}^{1/2} \tanh^{-1}(\mathrm{e}^{-|x-\nu|\pi l_{\mathrm{s}}/(2\epsilon)}) \frac{\partial B}{\partial t}(\nu, t)\ \mathrm{d}\nu.$$

- First term 1 is the uniform injection concentration.
- Second term captures the effect of diffusion into the surface.

Convolution Kernel



- Convolution kernal $\tanh^{-1}(\mathrm{e}^{-|x-\nu|\pi l_s/(2\epsilon)})$ centered at $x = 0$, and $x = -1/2$.
- Kernal captures the effect of ligand molecules spreading out and diffusing into the surface.

Integrodifferential Equation (IDE)

- Substituting our formula for C into the equation for B we find:

$$\frac{\partial B}{\partial t} = (1 - B) \underbrace{\left(1 - \frac{2\ \mathrm{Da}}{\pi} \int_{-1/2}^{1/2} \tanh^{-1}(\mathrm{e}^{-|x-\nu|\pi l_{\mathrm{s}}/(2\epsilon)}) \frac{\partial B}{\partial t}(\nu, t)\ \mathrm{d}\nu\right)}_{C(x,0,t)} - KB,$$

$$B(x, 0) = 0.$$

Numerical Solution

- How to solve

$$\frac{\partial B}{\partial t} = (1-B)\left(1 - \frac{2\ \mathrm{Da}}{\pi}\int_{-1/2}^{1/2} \tanh^{-1}(\mathrm{e}^{-|x-\nu|\pi l_{\mathrm{s}}/(2\epsilon)})\frac{\partial B}{\partial t}(\nu,t)\ \mathrm{d}\nu\right) - KB,$$

$B(x,0) = 0$?

- Since $\tanh^{-1}(x) = (\ln(x+1) - \ln(x-1))/2$, kernal is singular at $x = \nu$.
- Use method of lines $B(x,t) \approx \sum_{i=1}^{N} \phi_i(x) h_i(t)$, where $\phi_i(x)$ are locally-defined hat functions.

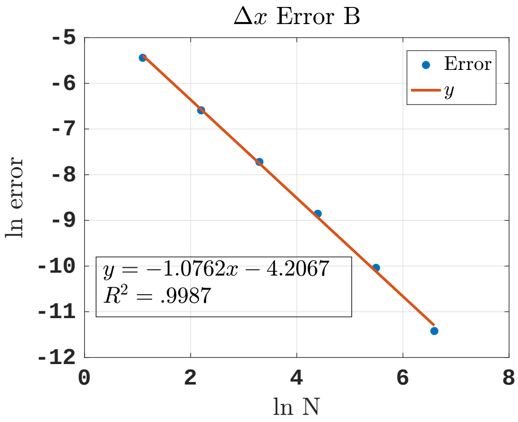
Numerical Solution

- This requires computing

$$\int_{-1/2}^{1/2} \mathsf{tanh}^{-1}(\mathrm{e}^{-|x_j-\nu|\pi l_\mathrm{s}/(2\epsilon)})\phi_i(\nu)\ \mathrm{d}\nu$$

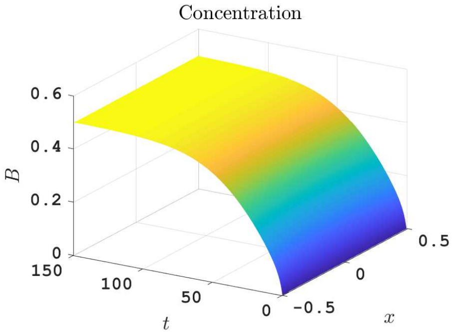
where x_j is one of our discretization nodes. Fortunately, we are able to compute the exact value of this integral in terms of polylogarithms.

Convergence



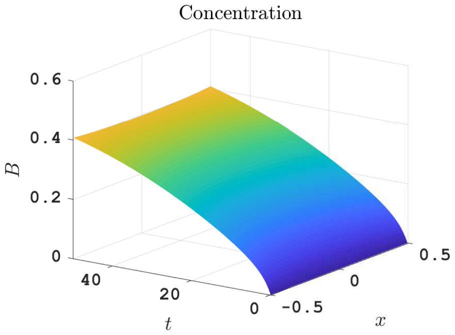
- Error $||\ ||B_{\mathrm{ref}}(x,t) - B(x,t)||_{2,x}||_{\infty,t}$. We get first-order convergence, despite logarithmic singularity.

Results



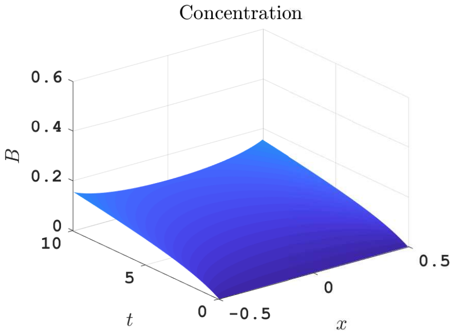
- Evolution of $B(x,t)$. Here we took $\mathrm{Da} = 66$, $l_{\mathrm{s}} = 10^{-3}$, $\epsilon = 1$, and $K = 1$.

Results



- Evolution of $B(x,t)$. Here we took $\mathrm{Da} = 66$, $l_\mathrm{s} = 10^{-3}$, $\epsilon = 1$, and $K = 1$.

Results: Depletion Region for Small t



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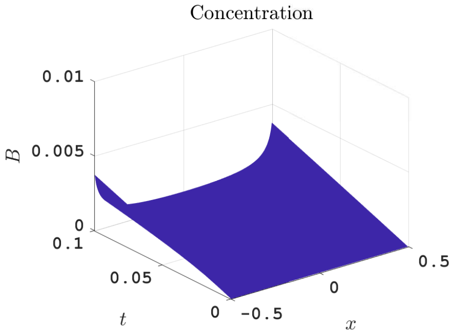
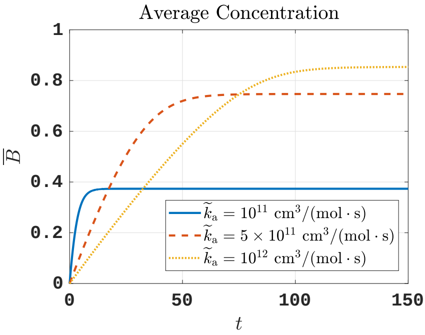


- Evolution of $B(x, t)$. Here we took $\mathrm{Da} = 66$, $l_s = 10^{-3}$, $\epsilon = 1$, and $K = 1$.

Results: Measured Signal Prediction



- Depicted: average concentration $\overline{B}(t) = \int_{-1/2}^{1/2} B(x,t)\,\mathrm{d}x$ (which is proportional to measured signal) for $\widetilde{k}_{\mathrm{a}} = 10^{11},\ 5\times 10^{11},\ 10^{12}\ \mathrm{mol}/(\mathrm{cm}^3\cdot\mathrm{s})$
- This corresponded to $\mathrm{Da} = 6.64,\ 33.21,$ and 66.42; and $K = 1.67,\ 0.33$ and 0.17.

Modeling FET Dynamics

- Uniform injection along top boundary.
- Sealed experiment with pulse injection at $t = 0$.

Dimensionless System (Pulse Injection)

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)$$

$$C(x,y,0) = f(x,y)$$

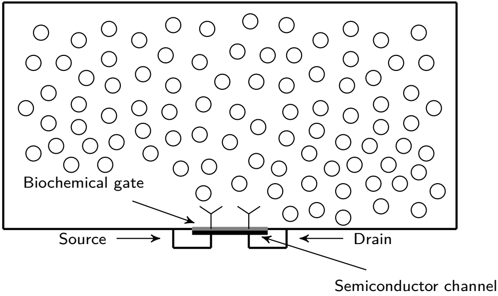
$$\frac{\partial C}{\partial x}(\pm 1/(2l_s), y, t) = 0$$

$$\frac{\partial C}{\partial y}(x, \epsilon/l_s, t) = 0$$

$$\frac{\partial C}{\partial y}(x,0,t) = \mathrm{Da}\frac{\partial B}{\partial t}\ \chi_{\mathrm{s}}(x),$$

$$\frac{\partial B}{\partial t} = (1-B)C(x,0,t) - KB$$

$$B(x,0) = 0$$



Quasi-Steady Approximation?

$$
\begin{aligned}
&0 = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\\
&\frac{\partial C}{\partial x}(\pm 1/(2l_s), y, t) = 0\\
&\frac{\partial C}{\partial y}(x, \epsilon/l_s, t) = 0\\
&\frac{\partial C}{\partial y}(x, 0, t) = \mathrm{Da}\frac{\partial B}{\partial t}\ \chi_{\mathrm{s}}(x),\\
&\frac{\partial B}{\partial t} = (1 - B)C(x, 0, t) - KB\\
&B(x, 0) = 0
\end{aligned}
$$

- The equation for C is now elliptic, and we can't enforce the initial condition.

Existence issues?

- It is not clear whether a solution to this set of equations even exists.

$$
\begin{aligned}
0 &= \nabla^2 C \\
\Rightarrow 0 &= \int_\Omega \nabla \cdot (\nabla C)\, \mathrm{d}\mathbf{x} \\
\Rightarrow 0 &= \int_{\partial\Omega} \nabla C \cdot \mathbf{n}\, \mathrm{d}\sigma \\
\Rightarrow 0 &= \int_{-1/2}^{1/2} \frac{\partial B}{\partial t}(x, t)\, \mathrm{d}x
\end{aligned}
$$

- Physically, we expect $\frac{\partial B}{\partial t}$ to be positive for all x and t.
- Must deal with full parabolic system.

Dimensionless System (Pulse Injection)

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)$$

$$C(x, y, 0) = f(x, y)$$

$$\frac{\partial C}{\partial x}(\pm 1/(2l_s), y, t) = 0$$

$$\frac{\partial C}{\partial y}(x, \epsilon/l_s, t) = 0$$

$$\frac{\partial C}{\partial y}(x, 0, t) = \mathrm{Da}\frac{\partial B}{\partial t}\ \chi_{\mathrm{s}}(x),$$

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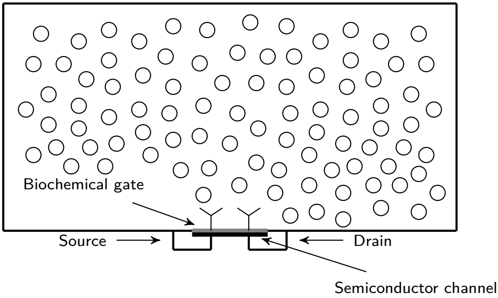
$$B(x, 0) = 0$$



How to solve for $C(x, 0, t)$?

- Decompose C into $C = C_i + C_b$.
- C_i–satisfies associated system with homogeneous boundary conditions.
- C_b–satisfies associated system with homogeneous initial condition.
- Once we find C_i and C_b, it follows that $C(x, 0, t) = C_i(x, 0, t) + C_b(x, 0, t)$.

Equation for C_i

- The function C_i is governed by:

$$\frac{\partial C_i}{\partial t} = D \nabla^2 C_i,$$
$$C_i(x, y, 0) = f(x, y),$$
$$\nabla C_i \cdot \mathbf{n} = 0 \qquad \text{on } \partial\Omega.$$

- One can find the Green's function via separation of variables to show:

$$C_i(x, 0, t) = \int_\Omega \mathcal{G}(x, 0, t; \mathbf{w}) f(\mathbf{w}) \, \mathrm{d}\mathbf{w}.$$

Equation for C_b

- The function C_b is governed by:

$$\frac{\partial C_b}{\partial t} = D\,\nabla^2 C_b,$$
$$C_b(x,0,t) = 0,$$
$$\frac{\partial C_b}{\partial y}(-1/(2l_\mathrm{s}), y, t) = \frac{\partial C_b}{\partial y}(1/(2l_\mathrm{s}), 0, t) = \frac{\partial C_b}{\partial y}(x, \epsilon/l_\mathrm{s}, t) = 0,$$
$$\frac{\partial C_b}{\partial y}(x,0,t) = \mathrm{Da}\,\frac{\partial B}{\partial t}\,\chi_\mathrm{s}.$$

- One can find $C_b(x,y,t)$ via a Laplace transform.

Equation for $\widehat{C}_b$

- Introducing a Laplace transform, we have:

$$s\widehat{C}_b = D\ \nabla^2 \widehat{C}_b,$$
$$\frac{\partial \widehat{C}_b}{\partial y}(-1/(2l_\mathrm{s}), y, t) = \frac{\partial \widehat{C}_b}{\partial y}(1/(2l_\mathrm{s}), 0, t) = \frac{\partial \widehat{C}_b}{\partial y}(x, \epsilon/l_\mathrm{s}, t) = 0,$$
$$\frac{\partial \widehat{C}_b}{\partial y}(x, 0, t) = \mathrm{Da}\ (s\widehat{B})\ \chi_\mathrm{s}.$$

- Search for separable solutions $\widehat{C}_b(x, y; s) = \phi(x)h(y; s)$.
- This yields

$$\widehat{C}_b(x, y, t) = \sum_{n\geq 0} \alpha_n(s) \cos\left(\lambda_n \left(x + \frac{1}{2l_s}\right)\right) \cosh((y-\epsilon/l_s)\sqrt{s/D + \lambda_n})$$

Determining $\alpha_n(s)$

- How to determine $\alpha_n(s)$? Use the relations

$$\widehat{C}_b(x,y,t) = \sum_{n\geq 0} \alpha_n(s) \cos\left(\lambda_n\left(x + \frac{1}{2l_s}\right)\right) \cosh((y-\epsilon/l_s)\sqrt{s/D+\lambda_n}),$$

$$\frac{\partial \widehat{C}_b}{\partial y}(x,0,t) = \mathrm{Da}(s\widehat{B})\chi_s,$$

and orthogonality of the cosines to show

$$\alpha_n(s) = -\mathrm{Da}\ b_n \frac{\int_{-1/2}^{1/2}(s\widehat{B})\cos(\lambda_n(\nu+1/(2l_s)))\ \mathrm{d}\nu}{\sqrt{s/D+\lambda_n}\sinh(\epsilon/l_s\sqrt{s/D+\lambda_n})},$$

where $b_0 = l_s$, and $b_n = 1/(2l_s)$ for $n \geq 1$.

Putting it Together

- Putting this information together we have.

$$\widehat{C}_b(x,0,t) = \sum_{n\geq 0} -\mathrm{Da} b_n \int_{-1/2}^{1/2} \frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})(s\widehat{B})}{\sqrt{s/D+\lambda_n}} \cos(\lambda_n(\nu+1/(2l_s)))\mathrm{d}\nu$$
$$\times \cos(\lambda_n(x+1/(2l_s)))$$

- How to invert?

Putting it Together

- Putting this information together we have.

$$\widehat{C}_b(x,0,t) = \sum_{n\geq 0} -\mathrm{Da}\, b_n \int_{-1/2}^{1/2} \frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})(s\widehat{B})}{\sqrt{s/D+\lambda_n}} \cos(\lambda_n(\nu+1/(2l_s)))\mathrm{d}\nu$$
$$\times \cos(\lambda_n(x+1/(2l_s)))$$

- How to invert?

Mapping Back

- Apply the convolution theorem

$$\mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})(s\widehat{B})}{\sqrt{s/D+\lambda_n}}\right\} = \mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})}{\sqrt{s/D+\lambda_n}}\right\}\star\mathcal{L}^{-1}\{s\widehat{B}\}$$
$$= \mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})}{\sqrt{s/D+\lambda_n}}\right\}\star\frac{\partial B}{\partial t}(x,t)$$

- Must evaluate

$$\mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})}{\sqrt{s/D+\lambda_n}}\right\} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})e^{st}}{\sqrt{s/D+\lambda_n}}\,\mathrm{d}s$$

Mapping Back

- Applying residue theorem shows

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})e^{st}}{\sqrt{s/D+\lambda_n}}\,\mathrm{d}s=\frac{Dl_s e^{-\lambda_n Dt}}{\epsilon}\theta_3(\mathrm{e}^{-(\pi l_s/\epsilon)^2 Dt})$$

- A change of variables and term-by-term series inversion shows

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})e^{st}}{\sqrt{s/D+\lambda_n}}\,\mathrm{d}s=\frac{\sqrt{D}e^{-\lambda_n Dt}}{\sqrt{\pi t}}\theta_3(\mathrm{e}^{-\epsilon^2/(l_s^2 Dt)})$$

where

$$\theta_3(q)=1+2\sum_{n=1}^{\infty}q^{n^2}$$

Mapping back

- Thus since

$$\mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})}{\sqrt{s/D+\lambda_n}}\right\} = \frac{\sqrt{D}e^{-\lambda_n Dt}}{\sqrt{\pi t}}\theta_3(\mathrm{e}^{-\epsilon^2/(l_s^2 Dt)})$$

we have

$$\mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})(s\widehat{B})}{\sqrt{s/D+\lambda_n}}\right\} = \frac{\sqrt{D}e^{-\lambda_n Dt}}{\sqrt{\pi t}}\theta_3(\mathrm{e}^{-\epsilon^2/(l_s^2 Dt)})\star\frac{\partial B}{\partial t}(x,t)$$

Putting it Together

- Thus since

$$\widehat{C}_b(x,0,t) = \sum_{n\geq 0} -\mathrm{Da} b_n \int_{-1/2}^{1/2} \frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})(s\widehat{B})}{\sqrt{s/D+\lambda_n}} \cos(\lambda_n(\nu+1/(2l_s)))\mathrm{d}\nu \times \cos(\lambda_n(x+1/(2l_s)))$$

and

$$\mathcal{L}^{-1}\left\{\frac{\coth(\epsilon/l_s\sqrt{s/D+\lambda_n})(s\widehat{B})}{\sqrt{s/D+\lambda_n}}\right\} = \frac{\sqrt{D}e^{-\lambda_n Dt}}{\sqrt{\pi t}}\theta_3(\mathrm{e}^{-\epsilon^2/(l_s^2 Dt)}) \star \frac{\partial B}{\partial t}(x,t)$$

we have

$$C_b(x,0,t) = \sum_{n\geq 0} -\frac{\sqrt{D}\mathrm{Da} b_n}{\sqrt{\pi}} \int_{-1/2}^{1/2} \frac{e^{-\lambda_n Dt}\theta_3(\mathrm{e}^{-\epsilon^2/(l_s^2 Dt)})}{\sqrt{t}} \star \frac{\partial B}{\partial t}(\nu,t)\cos(\lambda_n(\nu+1/(2l_s)))\mathrm{d}\nu \times \cos(\lambda_n(x+1/(2l_s)))$$

Integrodifferential Equation Reduction

- Laplace transform → eigenvalue problem → separable solutions → inversion → integrodifferential equation

$$\frac{\partial B}{\partial t} = (1 - B)C(x, 0, t) - KB$$

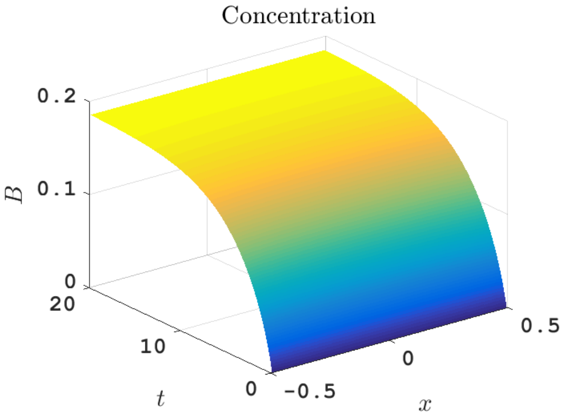
where

$$C(x, 0, t) = \int_\Omega \mathcal{G}(x, 0, t; \mathbf{w}) f(\mathbf{w}) \, \mathrm{d}\mathbf{w}$$
$$- \sum_{n=0}^{\infty} \frac{\alpha_n \mathrm{Da} \sqrt{D}}{\sqrt{\pi}} \int_{-1/2}^{1/2} \int_0^t \frac{\mathrm{e}^{-\lambda_n D\tau} \theta_3(0, \mathrm{e}^{-(\epsilon^2 / l_\mathrm{s}^2 D\tau)})}{\sqrt{\tau}} \frac{\partial B}{\partial \tau}(\nu, t - \tau) \mathrm{d}\tau \cos(n\pi l_s(\nu + 1/2l_s)) \mathrm{d}\nu$$
$$\times \cos(n\pi l_s(x + 1/(2l_\mathrm{s})))$$

Numerics Overview

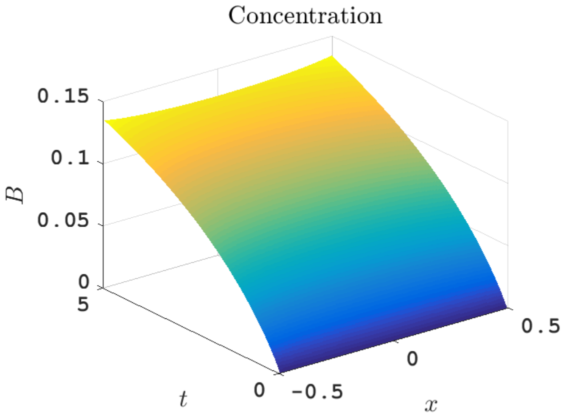
1. consider semi-implicit system
$$\frac{\partial B}{\partial t}(x, t_{n+1}) = (1 - B(x, t_n))C(x, 0, t_{n+1}) - KB(x, t_n)$$
2. singularity handling
3. method of lines discretization $B(x,t) \approx \sum_{i=1}^{n} \phi_i(x) h_i(t)$
4. discretize temporal integral with the trapezoidal rule
5. write $h_i'(t_m) \approx \Delta h_i^{(m)} / \Delta t$
6. solve resulting linear system for $\Delta h_i^{(m)}$
7. update h_i with $h_i^{(m+1)} = h_i^{(m)} + \frac{3}{2}\Delta h_i^{(m+1)} - \frac{1}{2}\Delta h_i^{(m)}$

Results



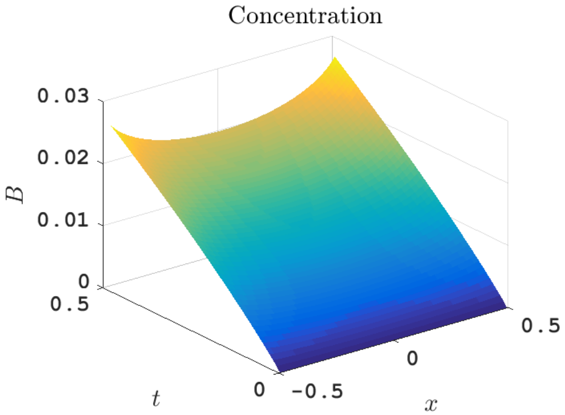
- Evolution of $B(x, t)$. Parameter values of $D = 8 \times 10^4$, $\mathrm{Da} = 3.3210$, $l_s = 10^{-3}$, $\epsilon = 0.4$, and $K = 1$ were used.

Results



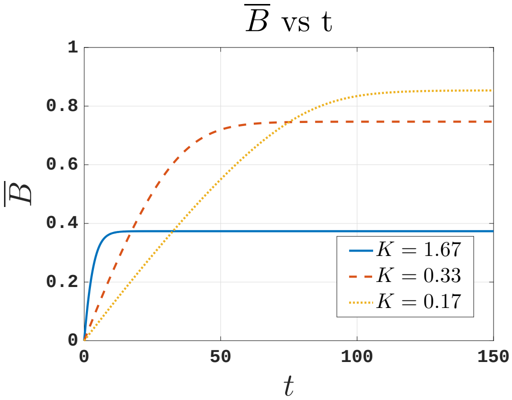
- Evolution of $B(x,t)$. Parameter values of $D = 8 \times 10^4$, $\mathrm{Da} = 3.3210$, $l_s = 10^{-3}$, $\epsilon = 0.4$, and $K = 1$ were used.

Results: Depletion Region for Small t



- Evolution of $B(x,t)$. Parameter values of $D = 8 \times 10^4$, $\mathrm{Da} = 3.3210$, $l_s = 10^{-3}$, $\epsilon = 0.4$, and $K = 1$ were used.

Results: Measured Signal Prediction



- Depicted: average concentration $\overline{B}(t) = \int_{-1/2}^{1/2} B(x,t)\,\mathrm{d}x$ (proportional to signal) for $D = 4 \times 10^4,\ 8 \times 10^4$ and 4×10^5.
- Correspondingly $\mathrm{Da} = 6.6420,\ 3.321,\ 0.6642$.

Conclusions

- Personalized therapies have the potential to fundamentally improve treatment of diseases such as diabetes, Alzheimer's disease, and certain kinds of cancers.
- This has led to the development of FETs, and we have developed the first time-dependent model for FET experiments.
- Our model predicts an unexpected depletion region. This effect is not directly observable experimentally and provide insight into the origin of the measured signal.

Future Work

- Develop small time asymptotic approximation.
- Separate signal from noise in experimental data using stochastic regression techniques.
- Identify key model parameters, such as the dissociation rate constant.