Simulation coding for: Integrated Enzyme-Linked Immunosensor with Biofunctionalized Ion-Selective Membranes by Pulstrode Delivery of Substrate

Michaelis Menten Kinetics Equation

```
In[ ]:= v == Vmax cCh / (KM + cCh)
```

Equations for Diffusion Profile

Parameters

```
In[ ]:= n =.;
```

Distance steps in dm:

```
In[ ]:= d = 5 × 10^-5;
```

Time steps in s:

```
In[ ]:= dt = 0.01;
```

```
In[ ]:= Da = 10^-5 × 10^-2;
```

```
In[ ]:= dtaua = Da dt / d^2
```

time in s :

```
In[ ]:= tmax = 60 / dt
```

```
In[ ]:= xmax = 100;
```

```
In[ ]:= Do[c[x, t] =., {x, 0, xmax}, {t, 0, tmax}];
```

```
In[ ]:= Table[c[x, t], {x, 0, xmax}, {t, 0, tmax}];
```

```
In[ ]:= cbulk = 0;
```

Initial concentrations:

```
In[ ]:= Do[c[x, 0] = 0.00003, {x, 0, 1}]

In[ ]:= Do[c[x, 0] = 0, {x, 2, xmax}]

In[ ]:= Do[c[xmax, t] = 0, {t, 0, tmax}]

In[ ]:=

In[ ]:= c[39, 1]
```

Calculation

```
In[ ]:= For[t = 0, t < tmax,

 {c[0, t] = c[0, t - 1] + dtaua (- 2 c[0, t - 1] + 2 c[1, t - 1]),

 Do[c[x, t] =
    c[x, t - 1] + dtaua (c[x - 1, t - 1] - 2 c[x, t - 1] + c[x + 1, t - 1]),
 {x, 1, xmax - 1}]

 },

 t++]


In[ ]:= c[1, 1]
```

One second is :

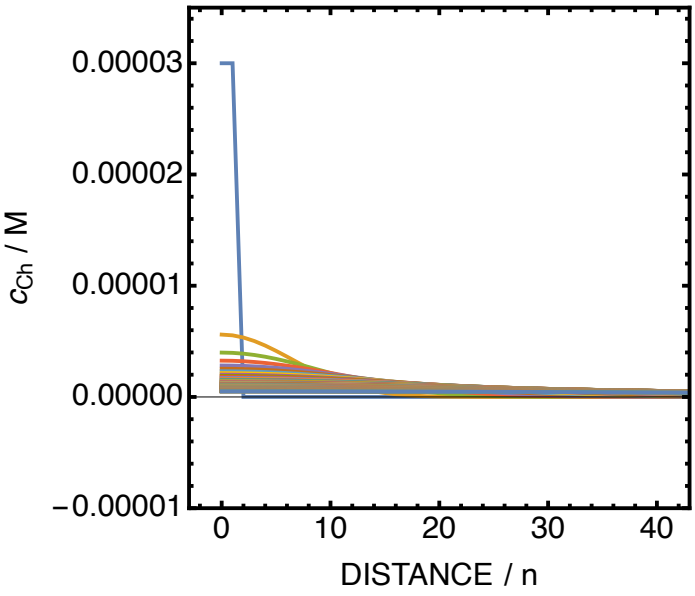
```
In[ ]:= 1 / dt
```

100.

Diffusion profile in the absence of enzyme-immunocomplex - concentration as a function of position

```
In[ ]:= ListPlot[Table[{x, c[x, u]}, {u, 0, tmax, 50}, {x, 0, xmax}],
 Joined → True, Frame → True, PlotRange → {{-3, 43}, {-0.00001, 0.000035}},
 BaseStyle → {16, FontFamily → "Helvetica"},
 LabelStyle → (FontFamily → "Helvetica"), AxesOrigin → {-10, 0},
 AspectRatio → 1, PlotStyle → {Thick}, FrameStyle → {Thick, Thick},
 FrameTicks → {{0, 10, 20, 30, 40, 50}, {0, 0.2, 0.4, 0.6, 0.8, 1}, {}, {}},
 FrameLabel → {"DISTANCE / n", "c_Ch / M"}]
```

Out[ ]=



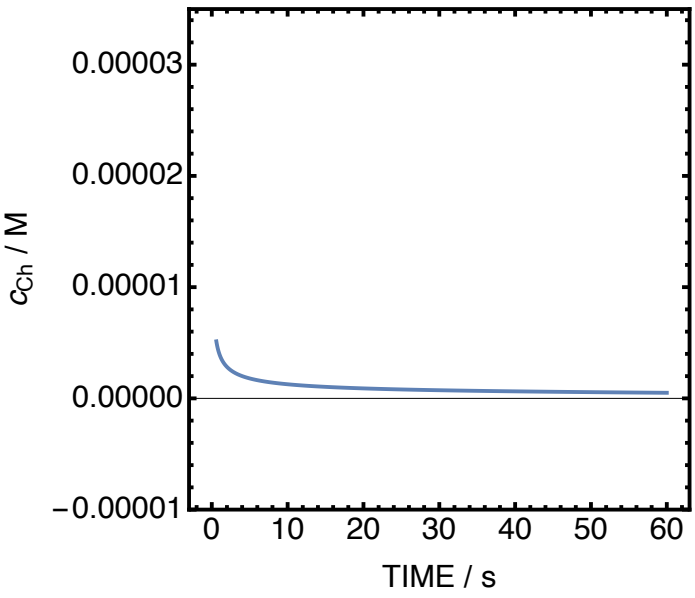

```
In[ ]:= c[1, 100]
```

```
In[ ]:= dt
```

```
In[ ]:= listc0 = Table[{u dt, c[0, u]}, {u, 60, tmax}];
```

```
In[ ]:= ListPlot[listc0, Joined → True, Frame → True,
 PlotRange → {{-3, 63}, {-0.00001, 0.000035}},
 BaseStyle → {16, FontFamily → "Helvetica"},
 LabelStyle → (FontFamily → "Helvetica"), AxesOrigin → {-10, 0},
 AspectRatio → 1, PlotStyle → {Thick}, FrameStyle → {Thick, Thick},
 FrameTicks → {{0, 10, 20, 30, 40, 50}, {0, 0.2, 0.4, 0.6, 0.8, 1}, {}, {}},
 FrameLabel → {"TIME / s", "cCh / M"}]
```

Out[ ]=



Equations for Diffusion Profile with Enzyme Kinetics

```
In[ ]:= cCh Vmax / (cCh + KM)
```

Parameters

```
In[ ]:= n = .;
```

Distance steps in dm:

```
In[ ]:= d = 5 × 10^-5;
```

Time steps in s:

```
In[ ]:= dt = 0.01;
```

```
In[ ]:= Da = 10^-5 × 10^-2;
```

```
In[ ]:= dtaua = Da dt / d^2
```

time in s :

```
In[ ]:= tmax = 60 / dt
```

```
In[ ]:= xmax = 100;
```

In[ ]:=

In[ ]:= `Do[ce[x, t] =., {x, 0, xmax}, {t, 0, tmax}];`

In[ ]:= `Table[ce[x, t], {x, 0, xmax}, {t, 0, tmax}];`

In[ ]:= `cbulk = 0;`

Initial concentrations:

In[ ]:= `Do[ce[x, 0] = 0.00003, {x, 0, 1}]`

In[ ]:= `Do[ce[x, 0] = 0, {x, 2, xmax}]`

In[ ]:= `Do[ce[xmax, t] = 0, {t, 0, tmax}]`

In[ ]:=

In[ ]:= `c[39, 1]`

Calculation

In[ ]:=
```
For[t = 0, t < tmax,

 {ce[0, t] = ce[0, t - 1] +
     dtaua (- 2 ce[0, t - 1] + 2 ce[1, t - 1]) - ce[0, t - 1] *2.3*10^-6 / ce[0, t - 1] +0.2×10^-3,

  Do[ce[x, t] =
     ce[x, t - 1] + dtaua (ce[x - 1, t - 1] - 2 ce[x, t - 1] + ce[x + 1, t - 1]),
  {x, 1, xmax - 1}]

 },

 t++]
```

In[ ]:= `listce0 = Table[{u dt, ce[0, u]}, {u, 60, tmax}];`

In[ ]:= `c[1, 1]`

One second is :

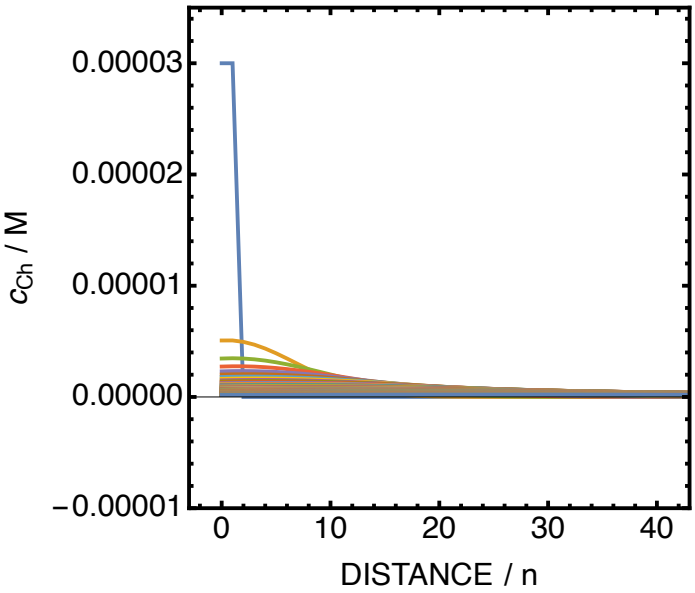
In[ ]:= `1 / dt`

100.

Diffusion profile in the presence of enzyme-immunocomplex - concentration as a function of position

In[ ]:=
```
ListLinePlot[Table[{x, ce[x, u]}, {u, 0, tmax, 50}, {x, 0, xmax}],
 Joined → True, Frame → True, PlotRange → {{-3, 43}, {-0.00001, 0.000035}},
 BaseStyle → {16, FontFamily → "Helvetica"},
 LabelStyle → (FontFamily → "Helvetica"), AxesOrigin → {-10, 0},
 AspectRatio → 1, PlotStyle → {Thick}, FrameStyle → {Thick, Thick},
 FrameTicks → {{0, 10, 20, 30, 40, 50}, {0, 0.2, 0.4, 0.6, 0.8, 1}, {}, {}},
 FrameLabel → {"DISTANCE / n", "cCh / M"}]
```

Out[ ]=

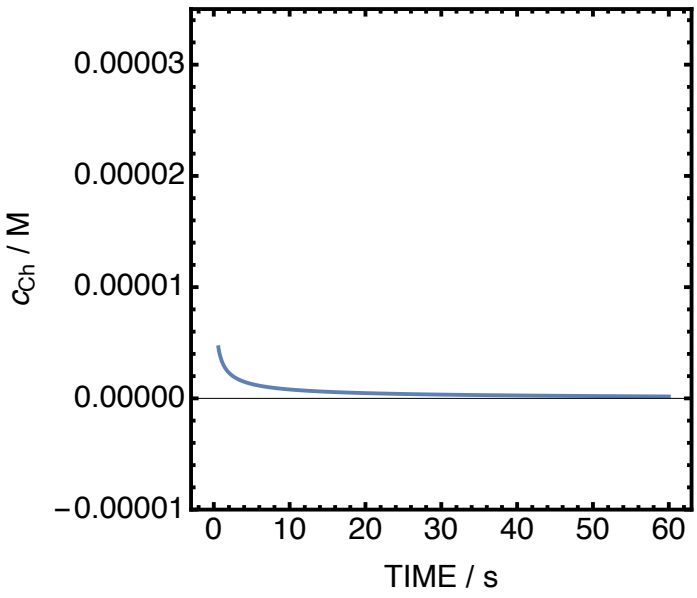


In[ ]:=
```
c[1, 100]
```

In[ ]:=
```
dt
```

```
In[ ]:= ListLinePlot[listce0, Frame → True,
 PlotRange → {{-3, 63}, {-0.00001, 0.000035}},
 BaseStyle → {16, FontFamily → "Helvetica"},
 LabelStyle → (FontFamily → "Helvetica"), AxesOrigin → {-10, 0},
 AspectRatio → 1, PlotStyle → {Thick}, FrameStyle → {Thick, Thick},
 FrameTicks → {{0, 10, 20, 30, 40, 50}, {0, 0.2, 0.4, 0.6, 0.8, 1}, {}, {}},
 FrameLabel → {"TIME / s", "cCh / M"}]
```

Out[ ]=



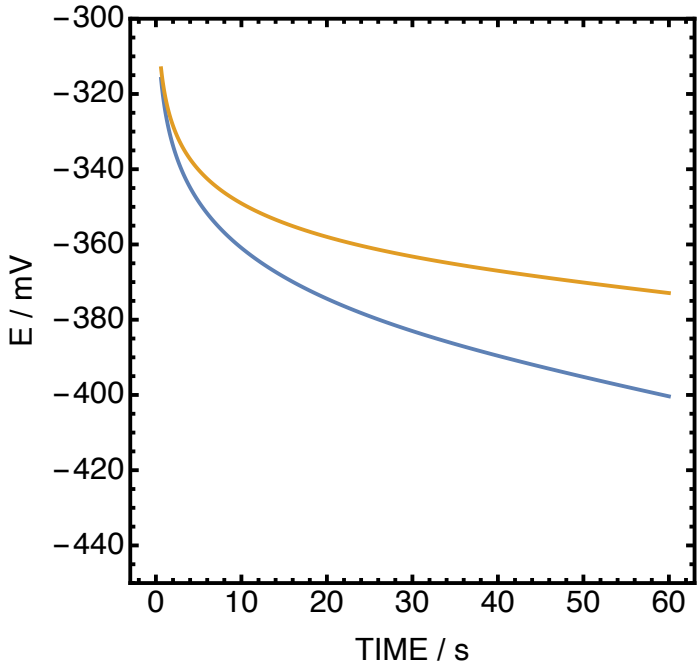

```
In[ ]:= listce[[-1]] - listc0[[-1]]
```

Potential measurement over time by inserting concentration at position zero in the Nernst equation in the absance and presence of enzyme-immunocomplex

```
In[ ]:= Ec = Table[{u dt, 59.2 Log10[c[0, u]]}, {u, 60, tmax, 10}];

In[ ]:= Ee = Table[{u dt, 59.2 Log10[ce[0, u]]}, {u, 60, tmax, 10}];

deltaE =
  Table[{u dt, 59.2 Log10[ce[0, u]] - 59.2 Log10[c[0, u]]}, {u, 60, tmax, 10}];
```

In[ ]:=
```
ListLinePlot[{Ee, Ec},

 Frame → True, PlotRange → {{-3, 63}, {-300, -450}},
 BaseStyle → {16, FontFamily → "Helvetica"},
 LabelStyle → (FontFamily → "Helvetica"), AxesOrigin → {-10, 0},
 AspectRatio → 1, PlotStyle → {Thick}, FrameStyle → {Thick, Thick},
 FrameTicks → {{0, 10, 20, 30, 40, 50}, {0, 0.2, 0.4, 0.6, 0.8, 1}, {}, {}},
 FrameLabel → {"TIME / s", "E / mV"}]
```

Out[ ]=



Potential change over time by subtracting the potential response in the absence of enzyme-immunocomplex from the potential measured in the presence of an enzyme-immunocomplex

In[ ]:=
```
ListLinePlot[deltaE,

 Frame → True, PlotRange → {{-3, 63}, {-35, 0}},
 BaseStyle → {16, FontFamily → "Helvetica"},
 LabelStyle → (FontFamily → "Helvetica"), AxesOrigin → {-10, 0},
 AspectRatio → 1, PlotStyle → {Thick}, FrameStyle → {Thick, Thick},
 FrameTicks → {{0, 10, 20, 30, 40, 50}, {0, 0.2, 0.4, 0.6, 0.8, 1}, {}, {}},
 FrameLabel → {"TIME / s", "ΔE / mV"}]
```

Out[ ]=