Medical Implants and Devices: Numerical modeling of galvanic corrosion problems of dental implants screws and nuts via BEM

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Introduction

- Dental implant fixtures have become an integral part of treatment for partially or fully edentulous patients since Branemark introduced the two-stage treatment protocol

- Commercially pure titanium and its alloys have been widely used for dental implants due to their mechanical properties, good corrosion resistance in biological fluids and biocompatibility

- It is widely accepted that titanium alloys are good materials for endoosseous implantation

- The choice of a suitable alloy for the suprastructure still remains an open question

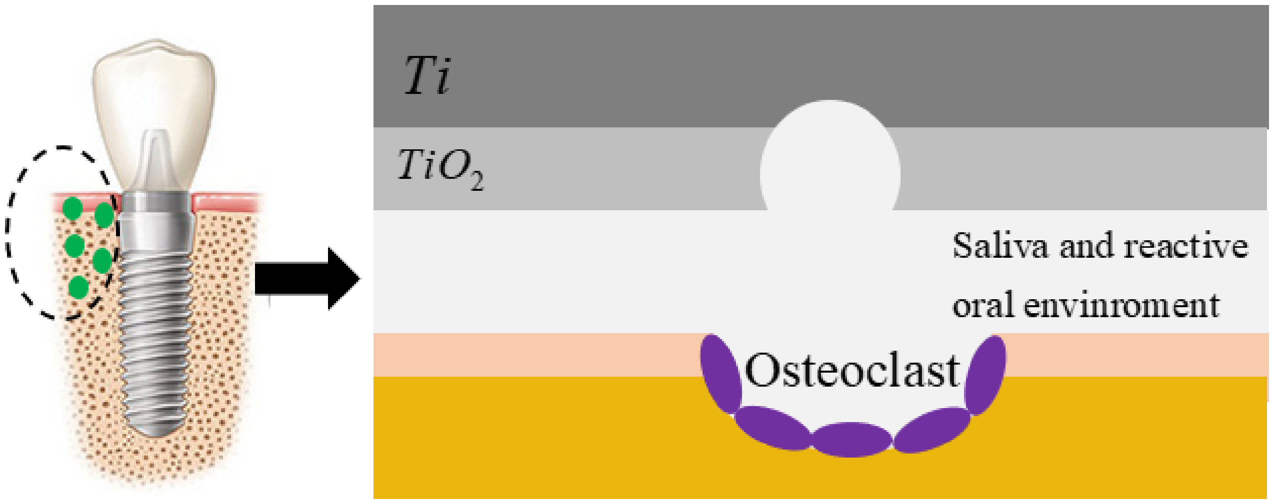
Corrosion of Dental implants

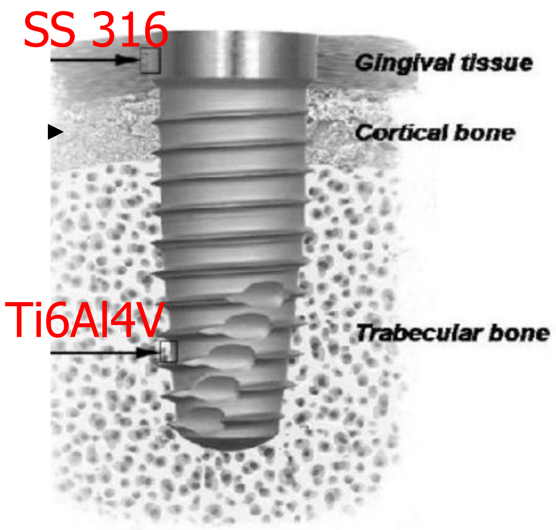
Implants corrode due their contact with saliva that disrupts the passive film, creating galvanic cells.

Galvanic corrosion is the most common corrosion type fond in dental implants.

Typical galvanic couplings:

1. SS304 and SS316
2. CoCr and Ti6Al4V
3. SS316 and Ti6Al4V
4. SS316 and CoCrMo





Clinically relevant effects of galvanic corrosion

In the case of dental implants, complicated electrochemical processes related to implant and suprastructure are linked to galvanic corrosion which leads to a clinically relevant situation due to two main reasons:

1. the biological effects that may result from the dissolution of alloy components
2. the bone destruction caused by the current flow that results from galvanic coupling

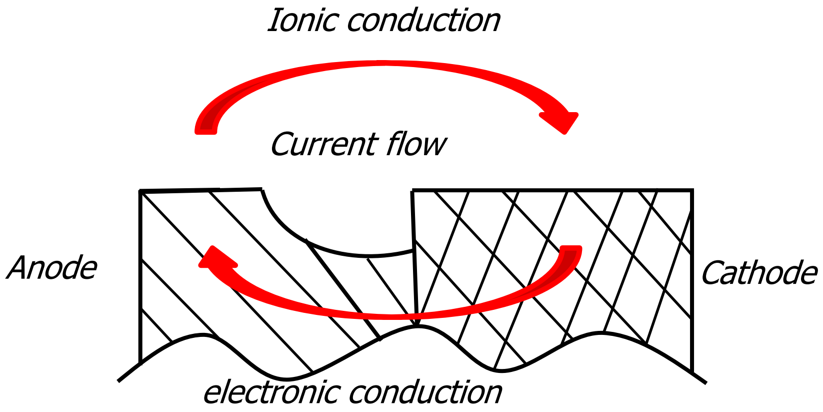
Undesirable effects of galvanic corrosion:

1. electropositive local environment along the implant interface, could directly influence bone resorption
2. ionic release induced by corrosion could be responsible for peri-implantitis and treatment failure
3. The corrosion process may limit the metal’s resistance to fatigue (corrosion fatigue)
4. The corrosion products can be distributed throughout the entire body and cause allergic reactions or a hypersensitivity reaction

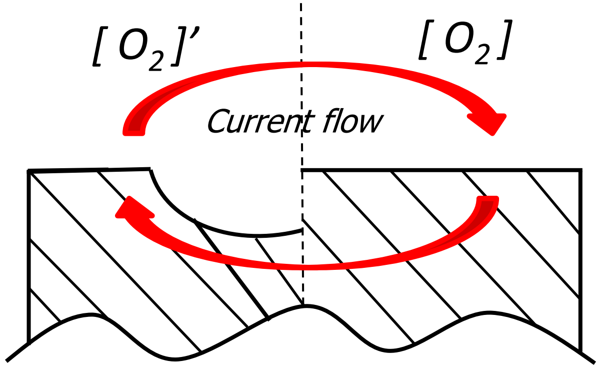
Galvanic Corrosion

The **potential difference** established when two metals (alloys) are **electrically connected** in a **conducting medium** produces electron flow and causes:

- the metal (alloy) with more negative potential to preferentially corrode (**anode**)
- the more positive metal (alloy) becomes a **cathode** and is protected by the negative metal (alloy)

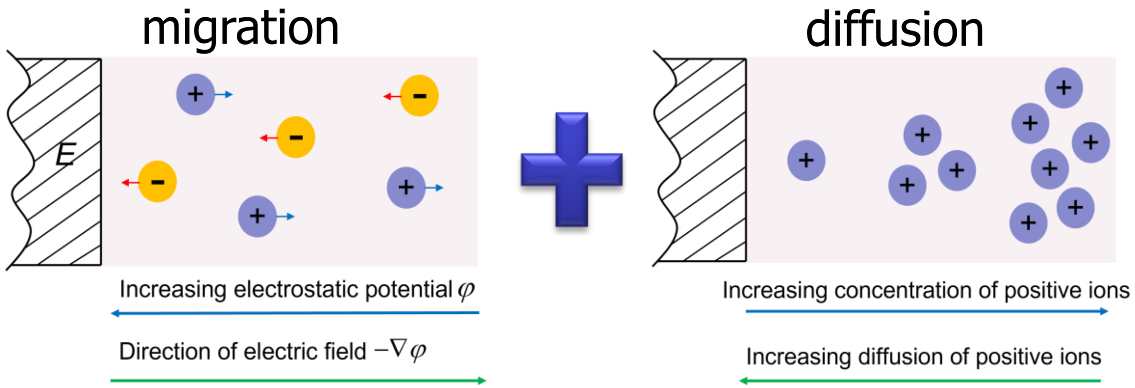


- Galvanic corrosion also occurs when the **same metal** is in contact with an electrolyte at two **different concentrations** or with **different aeration** levels (differential aeration cell).
- Electrolyte with varying pH, in contact with a structure, creates galvanic cells.



Governing Equations

Reactive species transport



$$\frac{\partial c_i}{\partial t} + \mathbf{v}\cdot\nabla c_i = \underbrace{z_i F\nabla\cdot\left(u_i c_i \nabla\varphi\right)}_{\textit{migration}} + \underbrace{\nabla\cdot\left(D_i\nabla c_i\right)}_{\textit{diffusion}} + A_i$$

$$\mathbf{J} = F\sum z_i \mathbf{N}_i$$

$$\mathbf{N}_i = -D_i\nabla c_i - z_i F u_i c_i \nabla\varphi$$

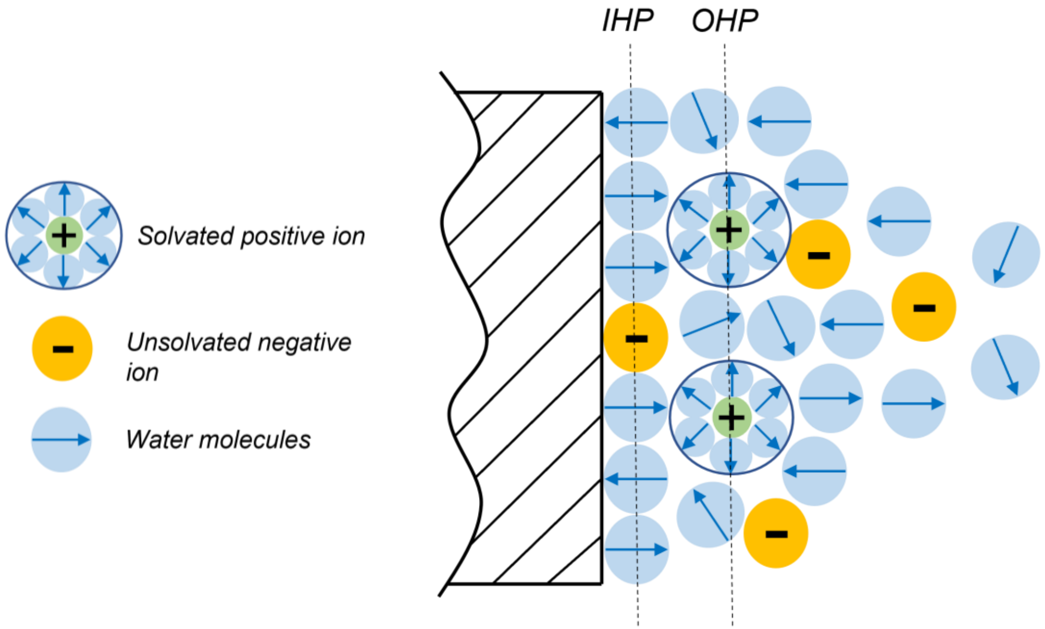
Electrolyte flow

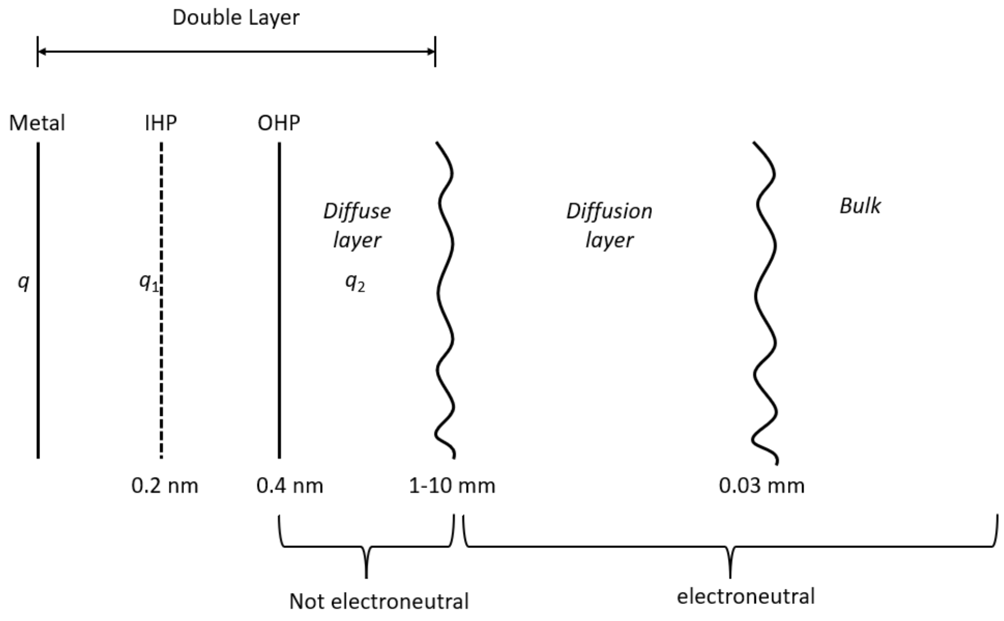
$$\nabla\cdot\mathbf{v} = 0$$

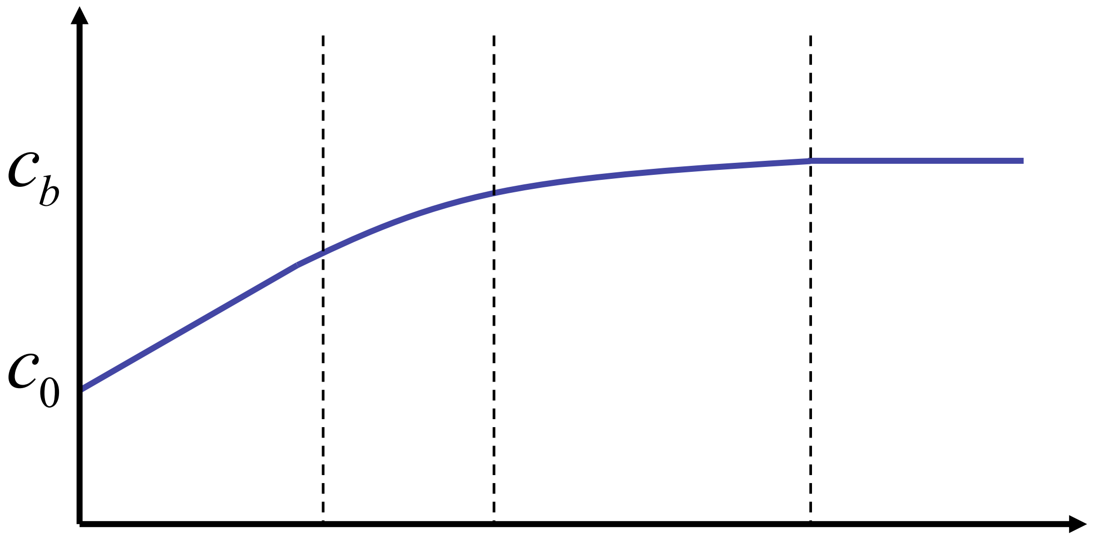
$$\rho\left(\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = \mu\nabla^2\mathbf{v} - \nabla p - \rho\mathbf{g}$$

Double Layer

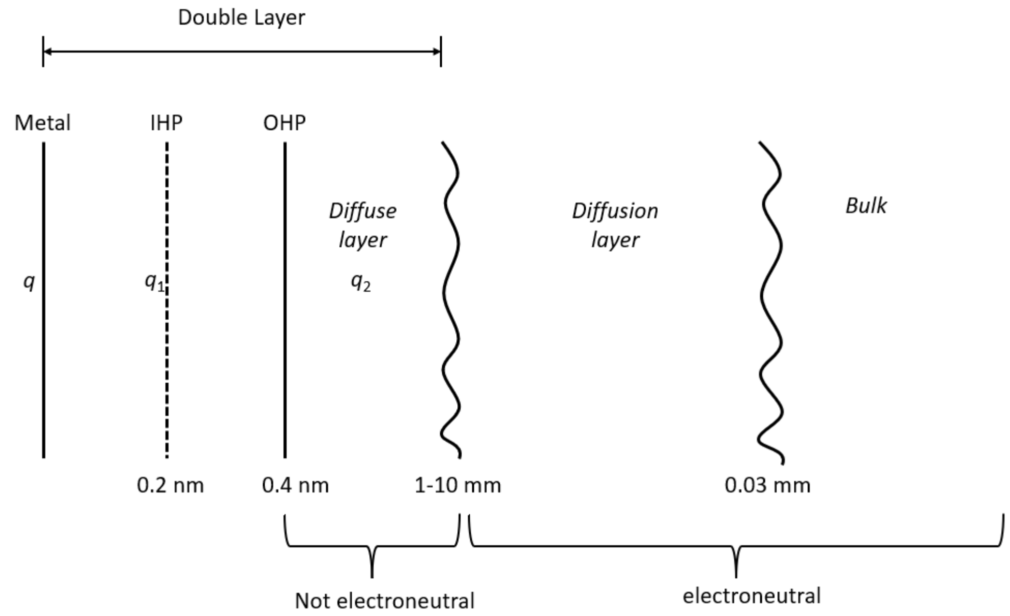
- The movement of ions is due to forces from ion-ion interaction
- Molecular Dynamics simulation







Electroneutrality



- Electroneutral electrolyte $\sum z_i c_i = 0$
- Electrically balanced reactions $\sum z_i A_i = 0$

$$\left.\begin{aligned}
&\frac{\partial c_i}{\partial t} + \mathbf{v}\cdot\nabla c_i = z_i F\nabla\cdot\left(u_i c_i \nabla\varphi\right) + \nabla\cdot\left(D_i \nabla c_i\right) + A_i \\
&\nabla^2\varphi = -\frac{1}{\varepsilon} F\sum z_i c_i \\
&\mathbf{J} = -F\sum z_i D_i \nabla c_i - F\nabla\varphi\sum z_i^2 u_i c_i
\end{aligned}\right\}$$

$$\frac{\partial}{\partial t}\left(F\sum z_i c_i\right) = -\nabla\cdot\left(F\sum z_i \mathbf{N}_i\right) + F\sum z_i A_i$$

$$\Downarrow$$

$$\nabla\cdot\left(F\sum z_i \mathbf{N}_i\right) = 0 \Rightarrow \boxed{\nabla\cdot\mathbf{J} = 0}$$

Potential Model

$$\nabla \cdot \mathbf{J} = 0$$

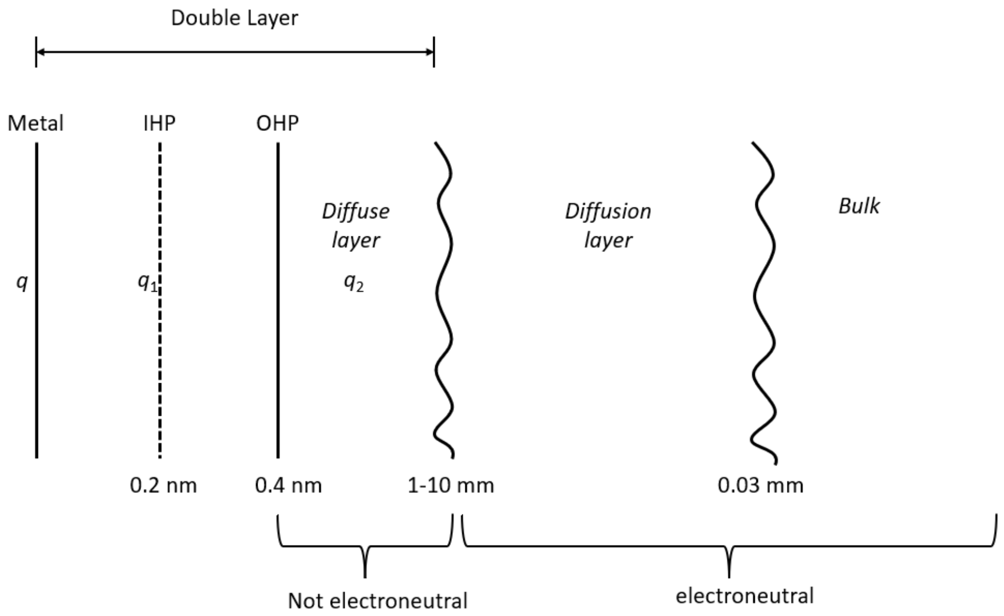
$$\nabla \cdot \left(F^2 \sum z_i^2 u_i c_i \nabla \varphi \right) - F \sum z_i \nabla \cdot \left(D_i \nabla c_i \right) = 0$$

- Uniform concentration

$$\mathbf{J} = -\sigma \nabla \varphi \qquad \sigma = F^2 \sum z_i^2 u_i c_i$$

- Constant electrical conductivity

$$\nabla^2 \varphi = 0$$



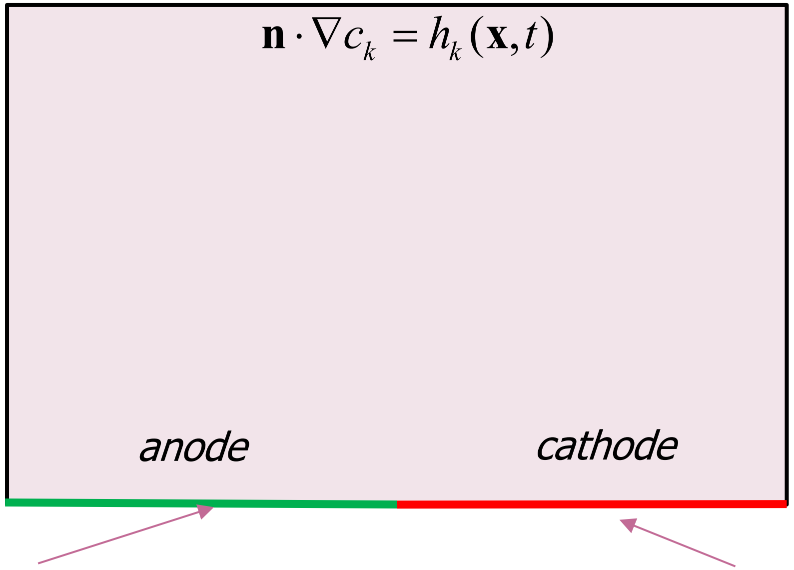
Boundary conditions assignment

Nernst-Planck equations

$$c_k = c_k^b \text{ or}$$

$$\mathbf{n}\cdot\nabla c_k = p_k \text{ or}$$

$$\mathbf{n}\cdot\nabla c_k = h_k(\mathbf{x},t)$$

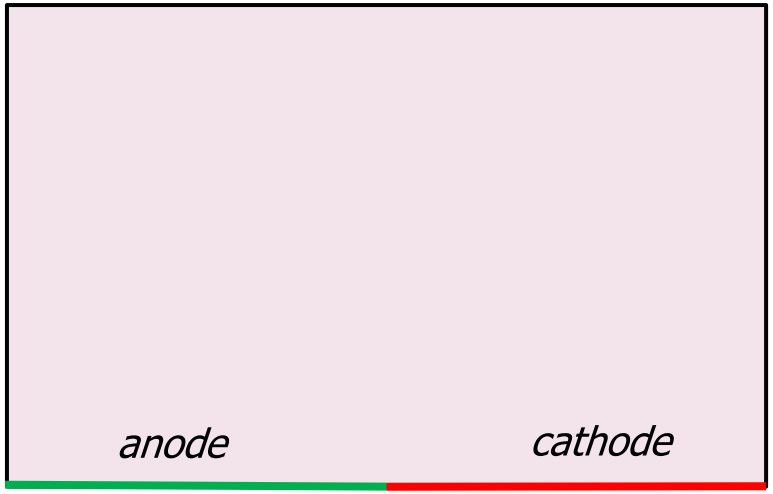


$$-Fz_kD_k\mathbf{n}\cdot\nabla c_k - F^2z_k^2u_kc_k\,\mathbf{n}\cdot\nabla\varphi = f_k(c_k,\varphi)$$

$$-Fz_kD_k\mathbf{n}\cdot\nabla c_k - F^2z_k^2u_kc_k\,\mathbf{n}\cdot\nabla\varphi = g_k(c_k,\varphi)$$

Poisson / Laplace equation

$$-\sigma\,\mathbf{n}\cdot\nabla\varphi = 0$$



$$-\sigma\,\mathbf{n}\cdot\nabla\varphi = f(\varphi)$$

$$-\sigma\,\mathbf{n}\cdot\nabla\varphi = g(\varphi)$$

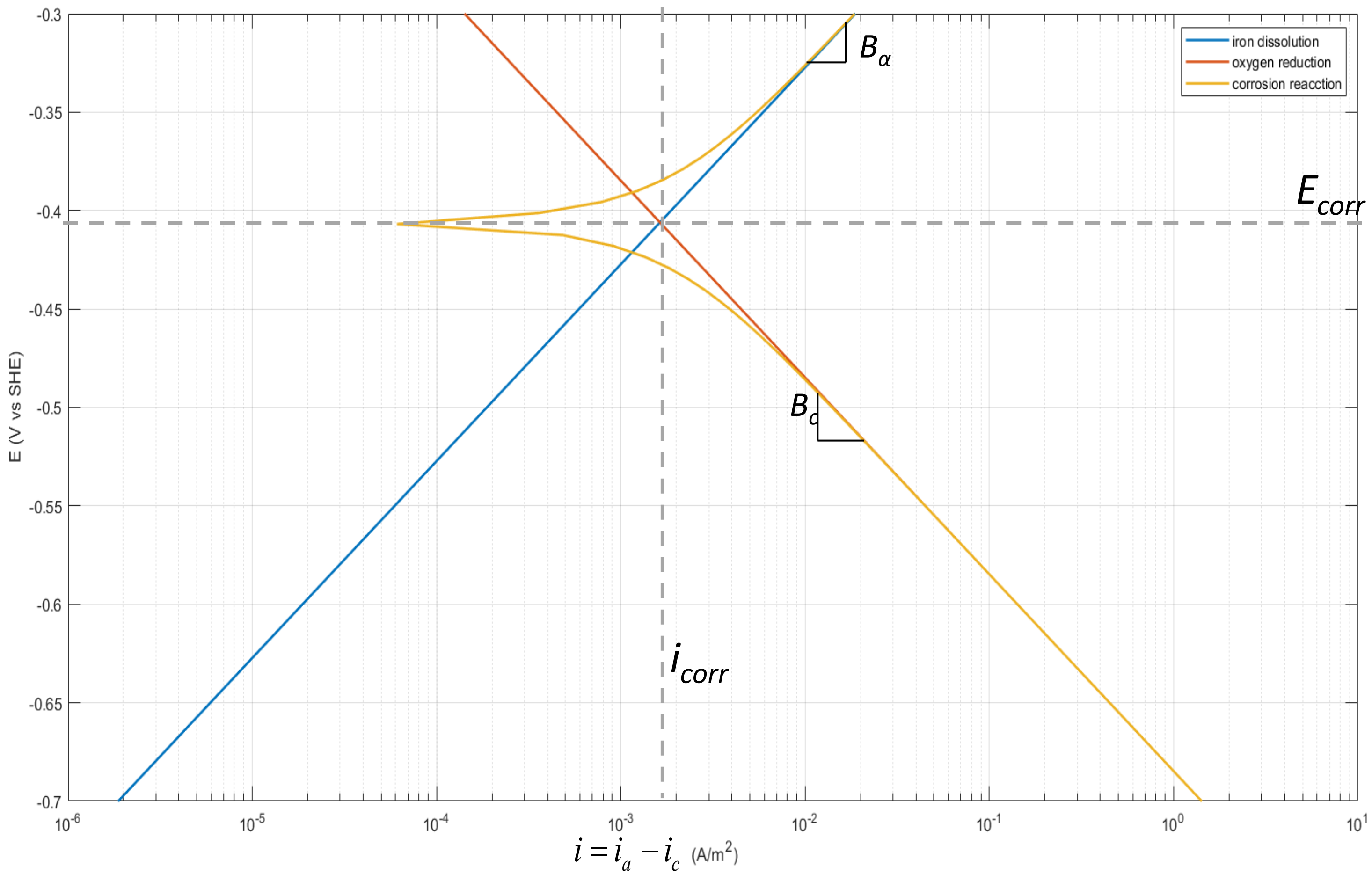
Overall reaction rate

The overall rate of the corrosion reaction is the given by the summation of the anodic and cathodic rates:

$$i = i_a - \sum_j i_{c,j}$$

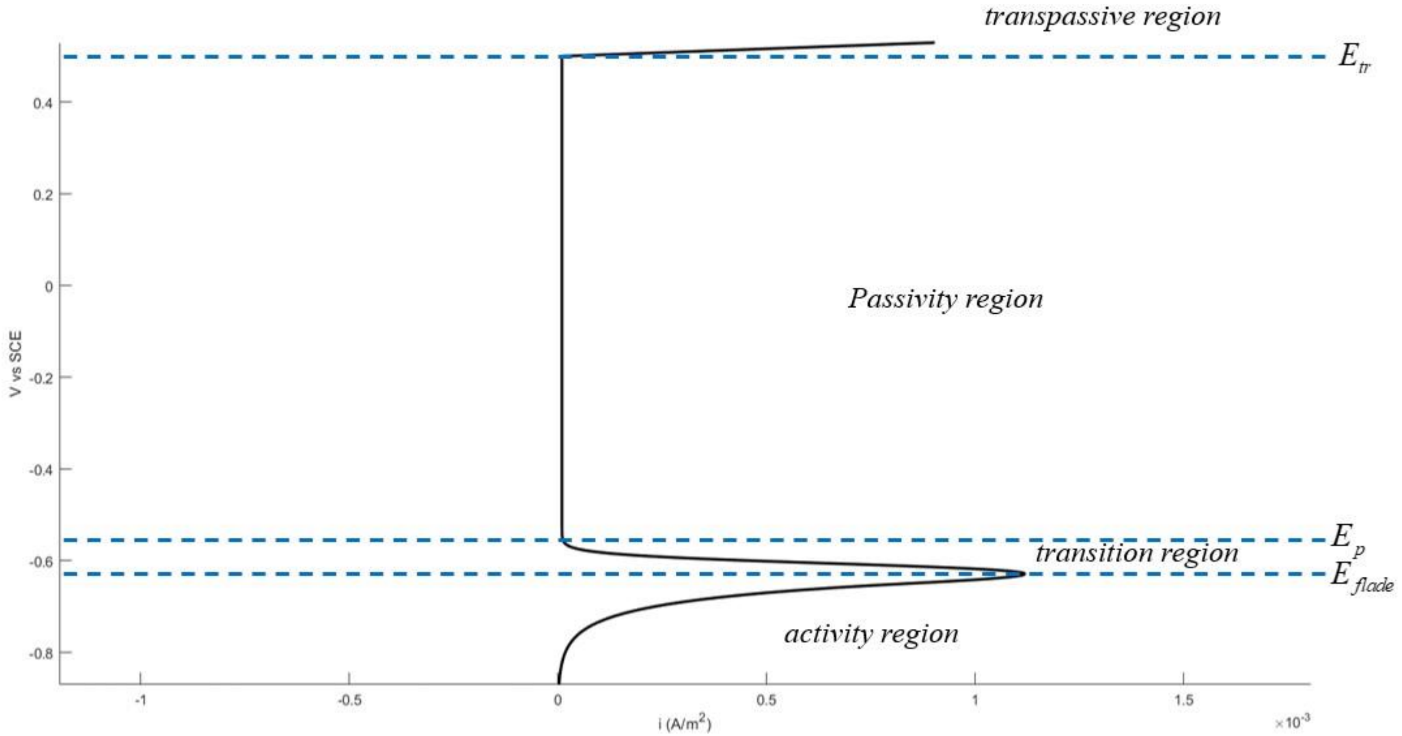
Factors that influence corrosion rate:

1. presence of fluoride ion,
2. difference in oxygen concentration
3. dental plaque
4. microorganisms
5. Mechanical stress



Active-passive behavior of metals and alloys

- **Activity region**: Active dissolution of steel.
- **Transition region**: Unstable region, eventually steel will become either active or passive.
- **Passivity region**: A protective barrier film is sustained.
- **Transpasive region**: Pitting corrosion occurs.



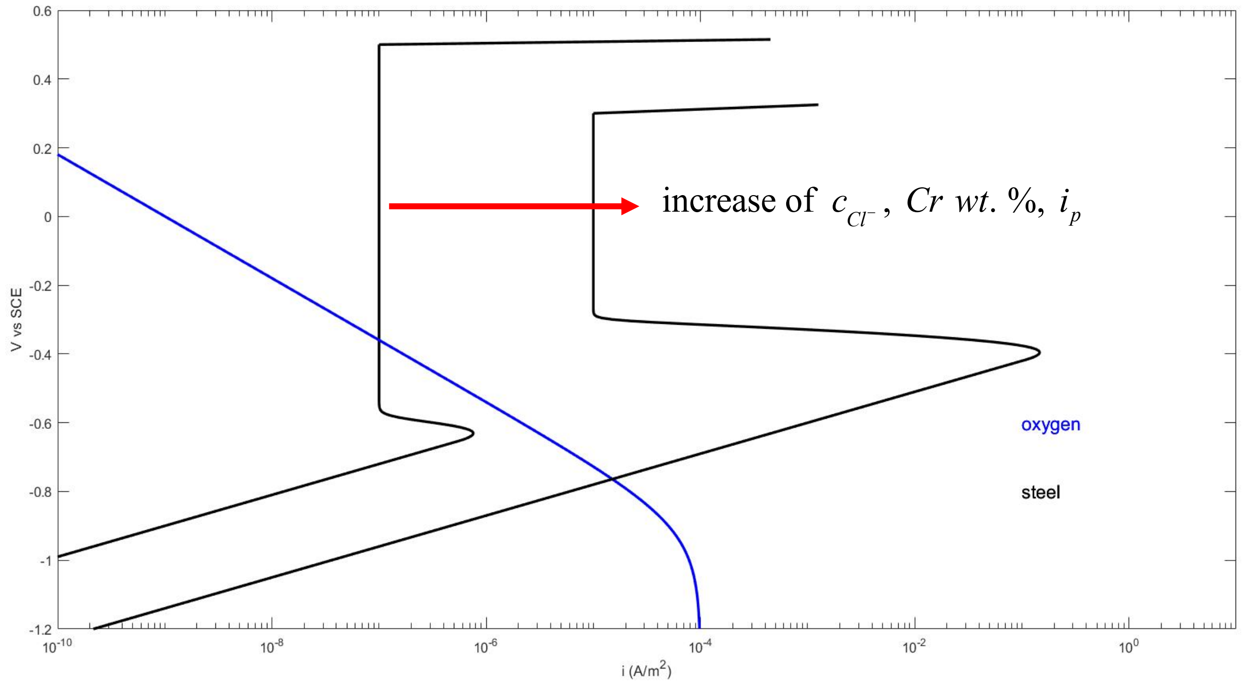
Passive region

$$E_{tr} = a - b\log([Cl^-]/[OH^-])$$

$$Ep \simeq E_{flade} + 100mV$$

$$E_{flade} = E^0_{flade}([Cr]) - 0.059\,pH$$

$$i_{Fe,p}(\varphi) = i_p$$



increase of c_{Cl^-}, $Cr\ wt.\ \%$, i_p

$$i_p(T,pH,[Cl^-]) = a_0\; i_p(298.15,13.5,0)\; e^{-a_1\left(\frac{1}{T}-\frac{1}{298.15}\right)}\; e^{a_2(pH-13.5)}\; e^{a_3[Cl^-]}$$

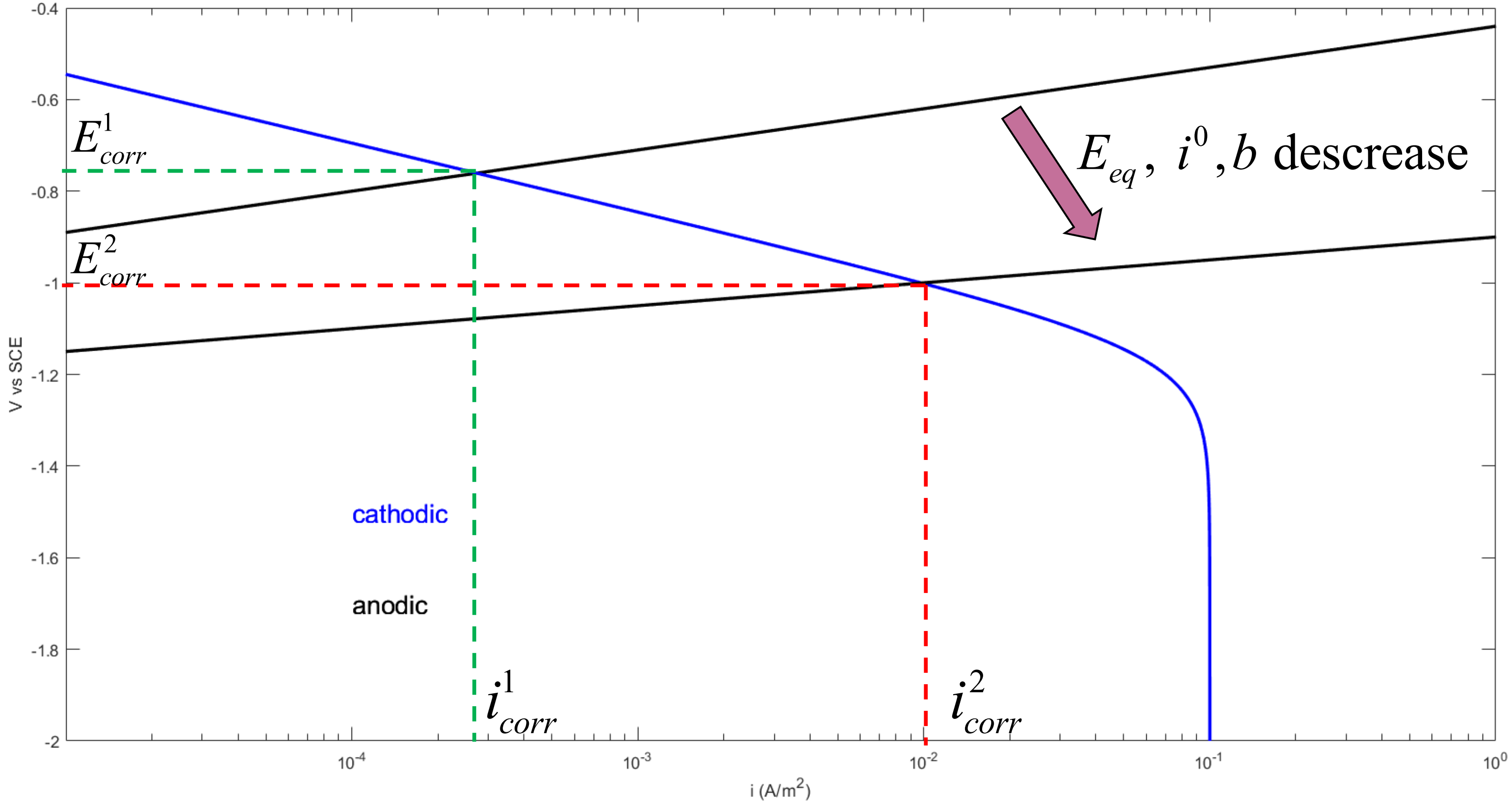
Active region: steel dissolution

$$E_{eq,Fe} = E_{0,Fe}(T) - \frac{RT}{2F}\log([Fe^{2+}])$$

$$i_{Fe,act}\left(\varphi\right) = i^0_{Fe} e^{\frac{\varphi - E_{eq,Fe}}{b_{Fe}}}$$

$$b_{Fe} = \frac{RT}{a_{FE}2F}$$

$$i^0_{Fe} = FAk_0C^b_{Fe}e^{\frac{E_{eq,Fe}-E_{0,Fe}}{b_{Fe}}}$$



Active region: oxygen reduction reaction

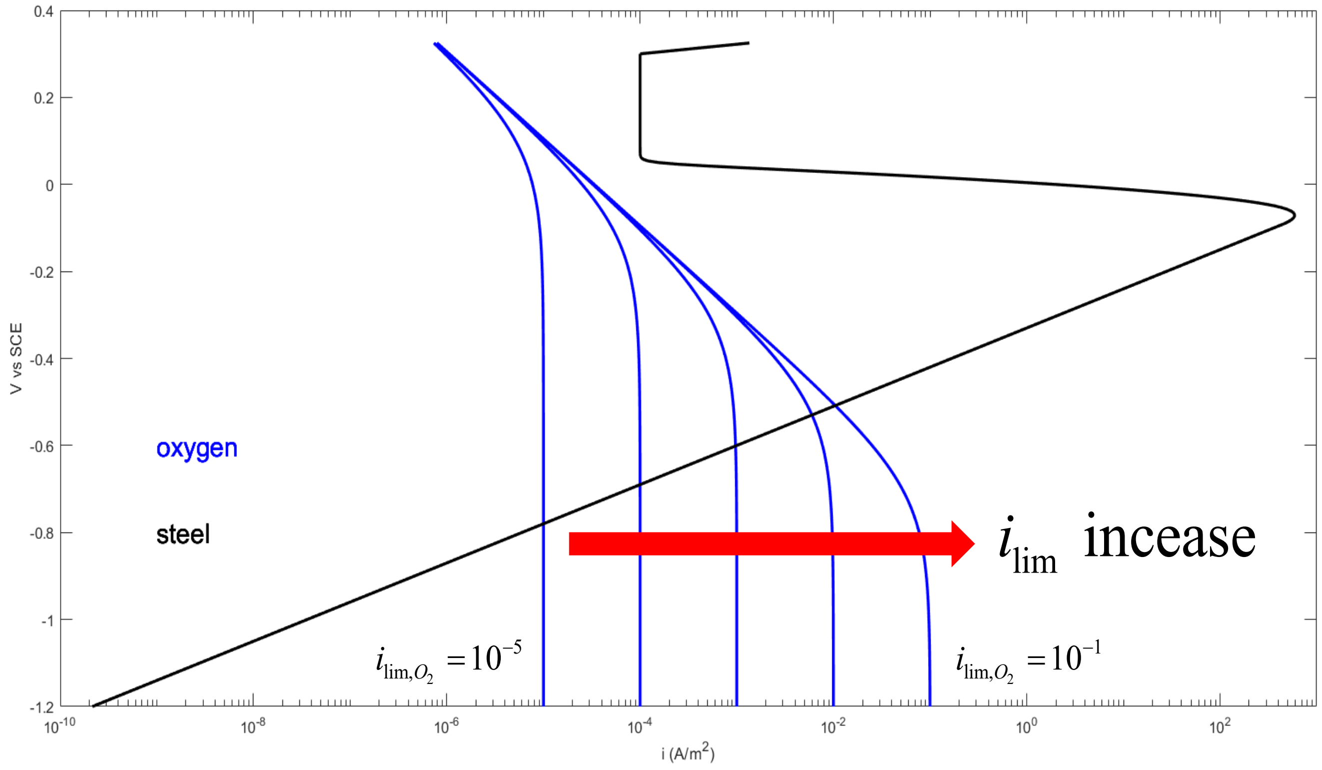
$$i_{O_2}(\varphi) = \frac{i^0_{O_2} e^{\frac{\varphi - E_{eq,O_2}}{b_{O_2}}}}{1 + \left(\frac{i^0_{O_2}}{i_{\lim,O_2}}\right) e^{\frac{\varphi - E_{eq,O_2}}{b_{O_2}}}}$$

$$E_{eq,O_2} = E_{0,O_2}(T) + \frac{RT}{zF}(14 - pH)$$

$$b_{O_2} = \frac{RT}{a_{O_2} zF}$$

$$i^0_{O_2} = FAk_0 C^b_{O_2} e^{\frac{E_{eq,O_2} - E_{0,O_2}}{b_{O_2}}}$$

$$i_{\lim,O_2} = \frac{zFD}{1-\tau}\left(n \cdot \nabla c_{O_2}\right) \qquad \text{when } c_{O_2} = 0$$

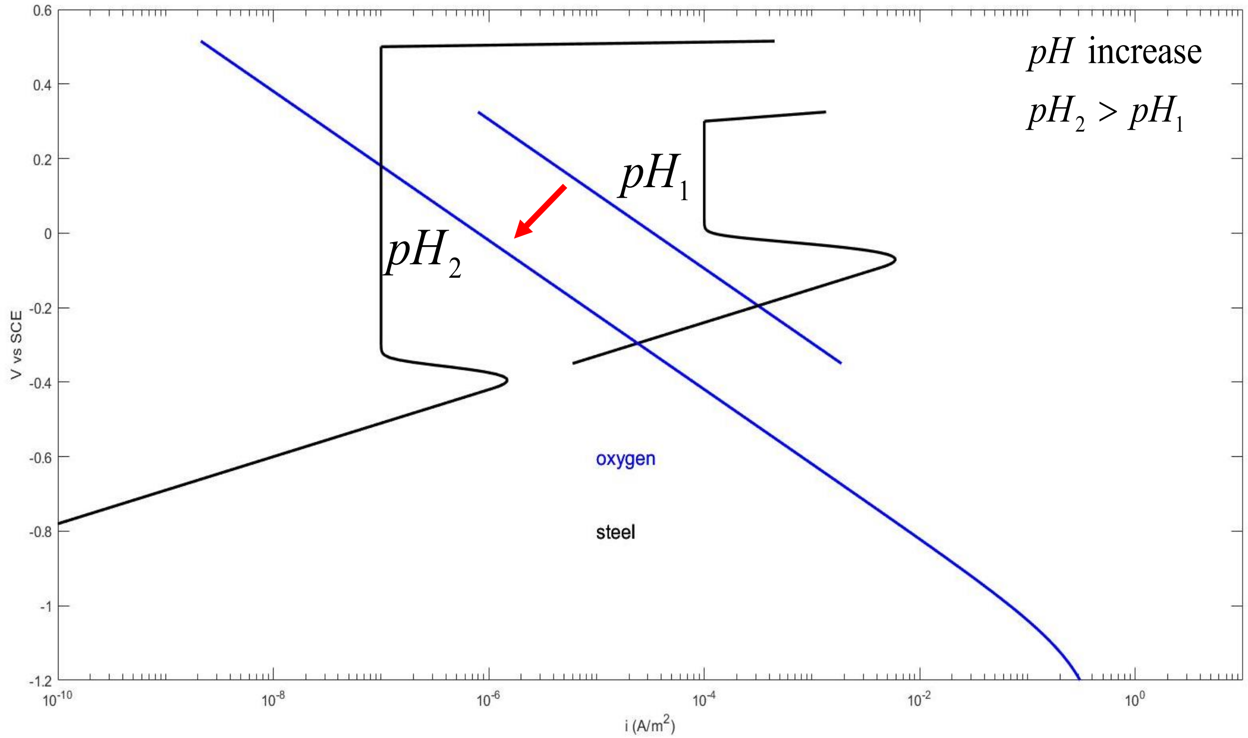


Effect of pH on polarization

$$pH = -\log\left([H^+]\right)$$

or

$$pH = pK_w + \log\left([OH^-]\right)$$



BEM formulation

The integral form of Laplace Equation reads[1,2]:

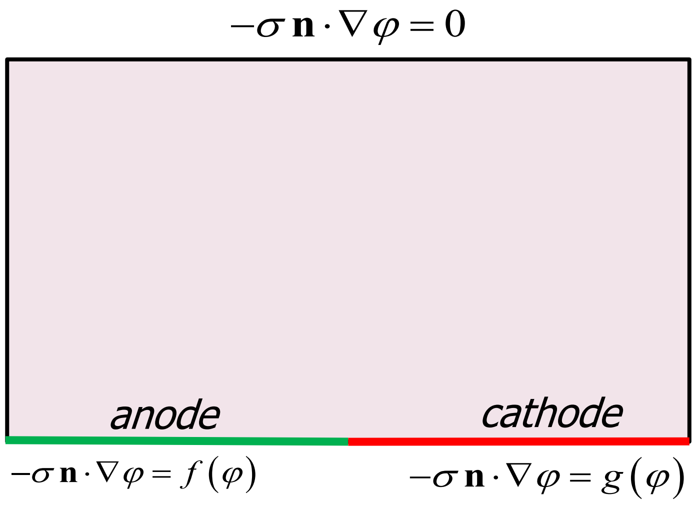
$$\alpha(\mathbf{x})\varphi(\mathbf{x})+\int_S \partial_n G(\mathbf{x},\mathbf{y})\varphi(\mathbf{y})\,dS_y=-\frac{1}{\sigma}\int_S G(\mathbf{x},\mathbf{y})\,i(\mathbf{y})\,dS_y$$

$$G(\mathbf{x},\mathbf{y})=\frac{1}{4\pi r}$$

$$\partial_n G(\mathbf{x},\mathbf{y})=-\frac{1}{4\pi r^3}\mathbf{r}\cdot\hat{\mathbf{n}}$$

$$c(\mathbf{x})=\begin{cases}0.5, & \mathbf{x}\in S\\ 1, & \mathbf{x}\in V\\ 0, & \mathbf{x}\notin V\end{cases}$$

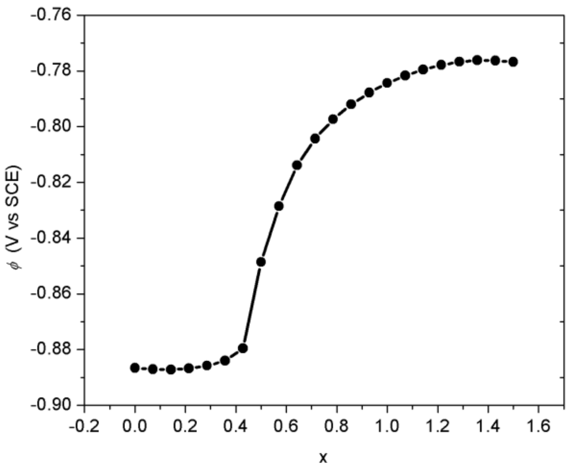
$$r=|\mathbf{y}-\mathbf{x}|$$

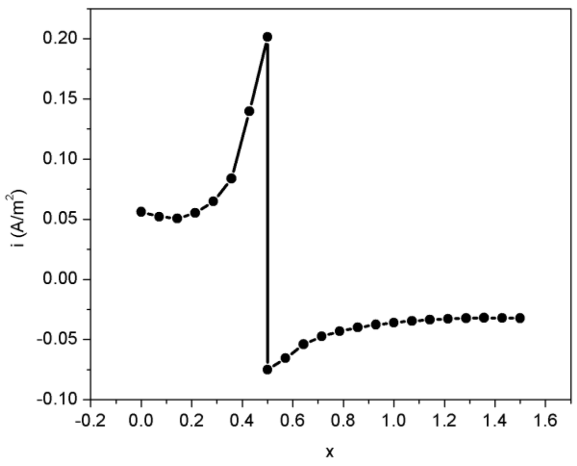


$$-\sigma\,\mathbf{n}\cdot\nabla\varphi=0$$

$$-\sigma\,\mathbf{n}\cdot\nabla\varphi=f(\varphi)$$

$$-\sigma\,\mathbf{n}\cdot\nabla\varphi=g(\varphi)$$





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[1] Becker, A. A. (1992). *The boundary element method in engineering: a complet* *course*. McGraw-Hill Companies, UK.

[2] Wrobel, L.C. (2002). *The Boundary Element Method, Volume 1: Application in Thermo-Fluids and Acoustics.* Wiley, UK.

Local Domain Boundary Element Method (LD-BEM)

Convection-diffusion with constant velocity: $\frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \nabla c_i - D_i \nabla^2 c_i - k_i c_i = 0$

BIE:

$$\alpha(\mathbf{x})c(\mathbf{x},t) = \int_{\partial V_i} \Phi(\mathbf{x},\mathbf{y})q(\mathbf{y})dS - \int_{\partial V_i} Q(\mathbf{x},\mathbf{y})c(\mathbf{y},t)dS - \frac{1}{D_1}\int_{V_i} \Phi(\mathbf{x},\mathbf{y})\dot{c}(\mathbf{y},t)dV$$

$$\Phi(\mathbf{x},\mathbf{y}) = G(\mathbf{x},\mathbf{y})e^{-\frac{\mathbf{v}_t \cdot (\mathbf{y}-\mathbf{x})}{2D_1}} = \frac{1}{2\pi}\mathrm{K}_0(sr)e^{-\frac{\mathbf{v}_t \cdot \mathbf{r}}{2D_1}}$$

$$s = \sqrt{\frac{k}{D_1} + \frac{(v_{t_x})^2 + (v_{t_y})^2}{4D_1^2}}$$

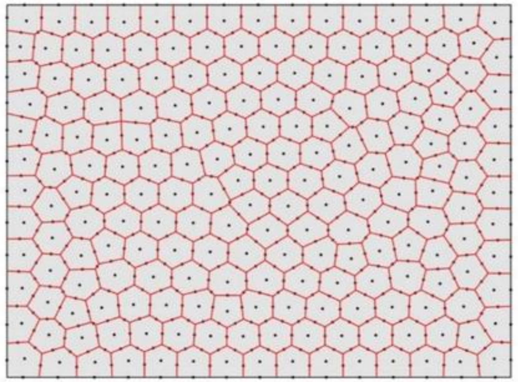
$$P(\mathbf{x},\mathbf{y}) = \frac{\partial G(\mathbf{x},\mathbf{y})}{\partial \mathbf{n}_\mathbf{y}} e^{-\frac{\mathbf{v}_t \cdot (\mathbf{y}-\mathbf{x})}{2D_1}} = -\frac{s}{2\pi}\mathrm{K}_1(sr)(\hat{\mathbf{r}} \cdot \mathbf{n}_\mathbf{y})e^{-\frac{\mathbf{v}_t \cdot \mathbf{r}}{2D_1}}$$

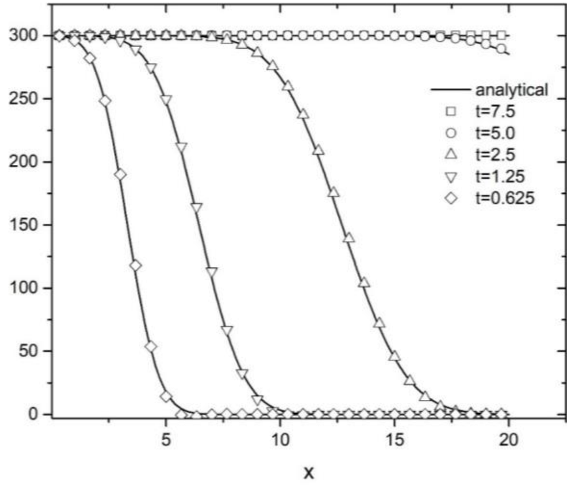
Applying the BIE in all domain nodes the flux term is eliminated:

$$[\mathbf{A}]\{\mathbf{c}_{n+1}\} = \{\mathbf{b}_{n+1}\} - \{\mathbf{F}_n\}$$

Previous time step contribution

Boundary conditions





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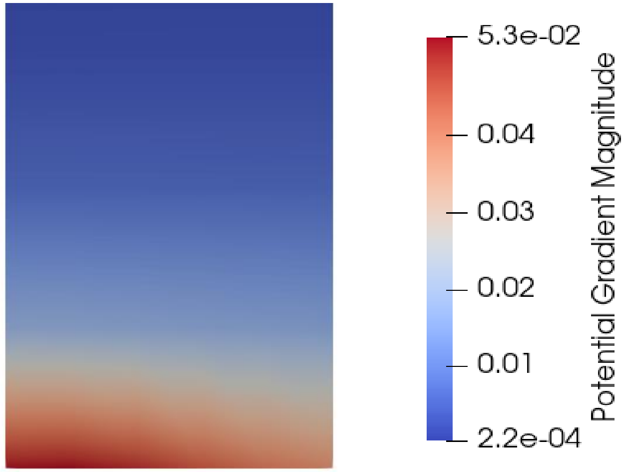
LD-BEM for electrically neutral electrolytes

$$\boxed{\begin{gathered}\nabla^2\varphi = 0\\ \frac{\partial c_i}{\partial t} + \mathbf{v}\cdot\nabla c_i + \nabla\cdot\mathbf{N}_i = R_i\\ \mathbf{N}_i = -D_i\nabla c_i - z_i F u_i c_i \nabla\varphi\\ R_i = k_i c_i\end{gathered}}$$



$$\frac{\partial c_1}{\partial t} + \mathbf{v}\cdot\nabla c_1 + (-Fz_1u_1\nabla\varphi)\cdot\nabla c_1 \cancel{-(Fz_1u_1\nabla^2\varphi)c_1} - D_1\nabla^2 c_1 = kc_1 \Rightarrow$$

$$\boxed{\begin{gathered}\frac{\partial c_1}{\partial t} + \mathbf{v}_t\cdot\nabla c_1 - D_1\nabla^2 c_1 - kc_1 = 0\\ \mathbf{v}_t = \mathbf{v} + \mathbf{v}_e\\ \mathbf{v}_e = -Fz_1u_1\nabla\varphi\end{gathered}}$$

$$\Downarrow$$

$$\boxed{\begin{gathered}c(\mathbf{x})c_1(\mathbf{x}) + \int_\Gamma P(\mathbf{x},\mathbf{y})c_1(\mathbf{y})d\Gamma = \int_\Gamma \Phi(\mathbf{x},\mathbf{y})\mathbf{n}\cdot\nabla c_1(\mathbf{y})d\Gamma - \frac{1}{D_1}\int_\Omega \Phi(\mathbf{x},\mathbf{y})\boldsymbol{\Delta}\mathbf{v}_t\cdot\nabla c_1(\mathbf{y})d\Omega - \frac{1}{D_1}\int_\Omega \Phi\left(\mathbf{x},\mathbf{y}\right)\dot{c}\left(\mathbf{y},t\right)d\Omega\\ \mathbf{v}_t = \bar{\mathbf{v}}_t + \boldsymbol{\Delta}\mathbf{v}_t\end{gathered}}$$

Conclusions

- Dental implants corrode due their contact with saliva that disrupts the passive film, creating galvanic cells.
- Bone destruction is caused by the current flow that results from galvanic coupling
- The dissolution of alloy components may have adverse biological effects
- BEM is ideal for solving corrosion problems
- Factors that influence corrosion rate should be incorporated in the robin boundary conditions