Problem Statement: Microscale Modeling

This system consists of one unit cell, where a spherical active particle (anode) is surrounded by the electrolyte.

The governing equations in the anode spherical particle are as follows:

$$\frac{\partial c_2}{\partial t} - \nabla \cdot [D^s \nabla c_2] = 0$$

$$-\nabla \cdot [K^s \nabla \varphi_2] = 0$$

The boundary flux equations in the anode spherical particle are as follows:

$$-n_s \cdot [D^s \nabla c_2] = \frac{2k}{F} \cdot \sqrt{c_{max}} \cdot \sqrt{c_1 . c_2 . (1 - c_2)} \cdot [\sinh(\varphi_2 - \varphi_1 - U_0(c_2))]$$

$$-n_s \cdot [K^s \nabla \varphi_2] = \frac{k \cdot F}{R \cdot T} \cdot c_{max} \cdot \sqrt{c_{max}} \cdot \sqrt{c_1 . c_2 . (1 - c_2)} \cdot [\sinh(\varphi_2 - \varphi_1 - U_0(c_2))]$$

The governing equations in the electrolyte are as follows:

$$\frac{\partial c_1}{\partial t} - \nabla \cdot \left[\left(D^e + \frac{R \cdot T \cdot t_+^2 \cdot K^e}{F^2 \cdot c_1 \cdot c_{max}} \right) \nabla c_1 + \left(\frac{2 \cdot t_+ \cdot K^e \cdot R \cdot T}{F^2 \cdot c_{max}} \right) \nabla \varphi_1 \right] = 0$$

$$-\nabla \cdot \left[\left(\frac{R \cdot T \cdot t_+ \cdot K^e}{F \cdot c_1} \right) \nabla c_1 + \frac{2 \cdot K^e \cdot R \cdot T}{F} \nabla \varphi_1 \right] = 0$$

The boundary flux equations in the electrolyte are as follows:

$$-n_s \cdot \left[\left(D^e + \frac{R \cdot T \cdot t_+^2 \cdot K^e}{F^2 \cdot c_1 \cdot c_{max}} \right) \nabla c_1 + \left(\frac{2 \cdot t_+ \cdot K^e \cdot R \cdot T}{F^2 \cdot c_{max}} \right) \nabla \varphi_1 \right] = -\frac{2k}{F} \cdot \sqrt{c_{max}} \cdot \sqrt{c_1 . c_2 . (1 - c_2)} \cdot [\sinh(\varphi_2 - \varphi_1 - U_0(c_2))]$$

$$-n_s \cdot \left[\left(\frac{R \cdot T \cdot t_+ \cdot K^e}{F \cdot c_1} \right) \nabla c_1 + K^e \nabla \varphi_1 \right] = -2k \cdot c_{max} \cdot \sqrt{c_{max}} \cdot \sqrt{c_1 . c_2 . (1 - c_2)} \cdot [\sinh(\varphi_2 - \varphi_1 - U_0(c_2))]$$

Parameter	Value	Notation in COMSOL
Universal Gas Constant, R	8.314 J/mol.K	R
Temperature, T	298 K	T
Maximum concentration, c_{max}	30540 mol/m^3	c_max
Faraday's constant, F	96485 C/mol	F
Electrolyte Diffusion Coefficient, D^e	$8.39*10^{-11}$ m^2/s	D_e
Transference Coefficient, t_+	0.363	T_plus
Electrolyte Conductivity, K^e	1.3 S/m	K_e
Reaction Rate Constant, k	$4.63*10^{-6}$	k
Anode Conductivity, K^s	100 S/m	K_neg
Anode Diffusion Coefficient, D^s	$5*10^{-13}$ m^2/s	D_neg
Initial Electrolyte Concentration	2000 mol/m^3	ce_ini
Initial Anode Concentration	12000 mol/m^3	cs_ini
Anode Open Circuit Potential (non-dimensional) $U_0(c_2)$	Interpolation Values	E_neg(c_2)

$$c_1 = \frac{c_e}{c_{max}}, c_2 = \frac{c_s}{c_{max}}, \varphi_1 = \frac{\varphi_e \cdot F}{2RT}, \varphi_2 = \frac{\varphi_s \cdot F}{2RT}$$