

A PHASE FIELD MODEL TO SIMULATE TRANSPORT AT THE ELECTRODE/ELECTROLYTE INTERFACE

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The present work seeks to investigate the effect of varying electrochemical conditions (both static and dynamic) on material transport in a model system. The overall purpose is to predict corrosion in implant materials (for example nitinol or magnesium alloys) in physiological environments.

The electrochemical system comprises of two “phases”, namely the electrode (phase 1) and the electrolyte (phase 2) as shown in Figure 1. Each phase comprises of four species (e^- , M^+ , A^- and N^+). The reference species (N) can be charged or neutral to represent a molten slag or an aqueous electrolyte respectively^{1,2}.

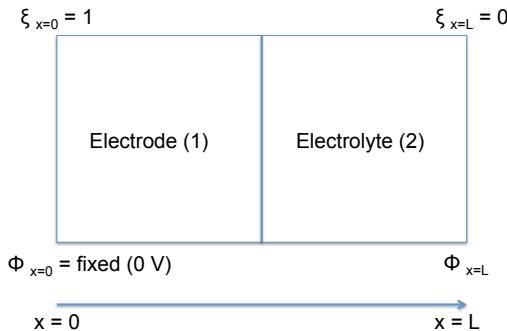


Figure 1: Schematic of model electrochemical system.

The initial bulk concentrations of each species are given in Table 1. Under static conditions no voltage is applied across the simulation domain and concentration variation for the different species and charge distribution across the interface are extracted at steady state. Sufficient points are required to represent the diffuse interface and to maintain numerical stability for bulk concentrations varying by orders of magnitude across the interface. Also the domain size should be sufficiently larger than the interface width to ensure that the interface is far from the boundaries.

Species (j)	$\ln\left(\frac{X_j^2}{X_j^1}\right)$
e^-	-10.82
M^+	-3.91
A^-	10.82
N^+	10.80

Table 1: Initial bulk concentrations in electrode (phase 1) and electrolyte (phase 2).

For static conditions, both the steady-state concentrations and the charge distribution across the interface depend on the boundary conditions. In Figure 2 these quantities are plotted for the case where the concentrations are fixed at the boundaries and the electrolyte is grounded. This should be compared to Figure 3 where a ‘no flux’ condition is enforced at the boundaries and the electrolyte is not grounded.

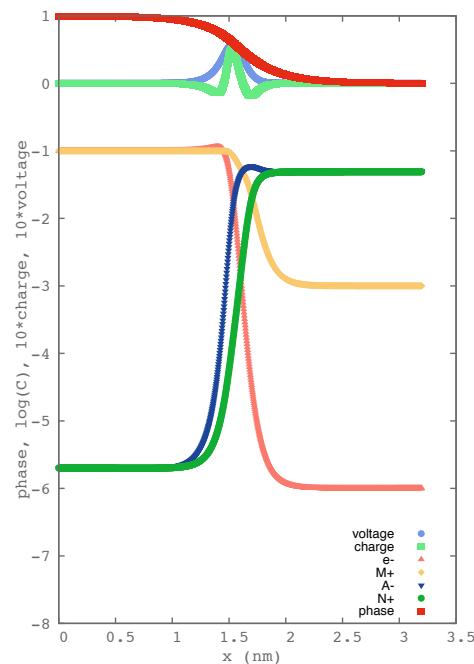


Figure 2: Concentration and charge profiles for fixed concentration boundary condition. The electrolyte end is grounded.

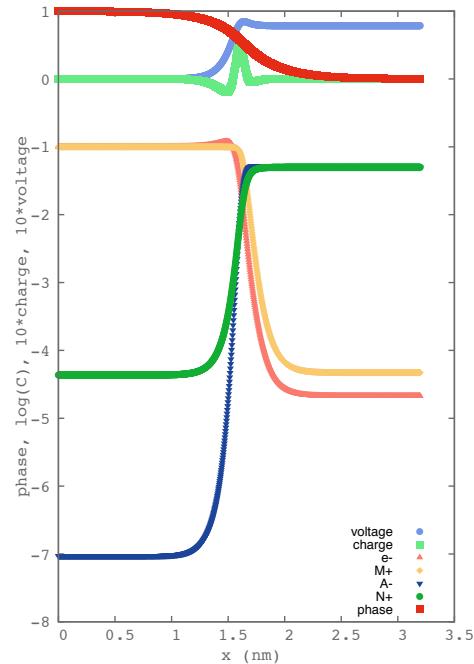


Figure 3: Concentration and charge profiles for 'no-flux' boundary condition. The electrolyte end is not grounded.

Under dynamic conditions the voltage across the domain (which is few nanometers long) is varied at intervals of a few millivolts and steady-state currents are extracted. The effect of varying kinetic parameters on the current-potential correlation will also be investigated. These parameters need to be close to physical values such that the model can better predict the response of implant materials to electrochemical stimuli in simulated environments.

REFERENCES

1. J.E. Guyer, W.J. Boettiger, J.A. Warren and G.B. Fadden, *Phys. Rev. E*, **69**, 021603 (2004).
2. J.E. Guyer, W.J. Boettiger, J.A. Warren and G.B. Fadden, *Phys. Rev. E*, **69**, 021604 (2004).