Computational Modeling of the Electrochemical Microenvironment Adjacent to Cathodically Stimulated Orthopedic Implants

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Introduction: Previous studies have shown that cathodic voltage-controlled electrical stimulation (CVCES) of titanium (Ti) implants is an effective and broad-spectrum antimicrobial treatment for implant-associated infections[1,2]. We have recently developed and validated a computational model of the electrochemical modifications that occur in the microenvironment adjacent to cathodically polarized, planar coupons of Ti [3]. The purpose of this study was to utilize computational modeling to generate temporal and spatial mapping of the electrochemical changes in the microenvironment adjacent to cathodically polarized total knee arthroplasty implants composed of cobalt-chromium-molybdenum (CoCrMo).

Methods: Human-sized, CoCrMo, femoral and tibial components of a total knee replacement system were subjected to potentiodynamic polarization tests within a custom test chamber filled with saline. An Ag/AgCl reference electrode was used and a custom flexible counter electrode was wrapped around the perimeter of the electrochemical cell. Fig. 1 describes the cell orientation, with the blue shaded region as the counter electrode and the femoral component as the working electrode. Curve-fitting is done on the polarization scan data (Fig. 2) using Matlab to evaluate the charge transfer coefficients and exchange current densities for the two dominant reduction reactions taking place on the implant's surface, namely oxygen reduction reaction and hydrogen evolution reaction. Charge transfer coefficients and exchange current density serve as the input parameters for the Butler-Volmer equation. Computational models are developed using COMSOL Multiphysics (v 5.6). CAD import feature of COMSOL enables us to import human-sized knee implant structures. The analysis is done for saline electrolyte (0.154 M) with a graphite counter electrode. Cathodic voltage of -1.9 V is applied vs Ag/AgCl. Mathematical models are developed with Tertiary Current Distribution, Nernst-Planck physics interface of the Electrochemistry module in COMSOL. The model simulates the electrode surface reactions using Butler-Volmer kinetics. The Nernst-Planck equation and the condition of electroneutrality govern the mass transport of species through the electrolyte. The 3D computational models simulate a period of 10 mins and the measurable outcomes include spatial and temporal distribution of current density and pH.

Results: Fig. 3 displays the spatial distribution of the current density and pH values along the surface of the femoral and tibial components after 10 mins of CVCES at -1.9V has been applied. Fig.4 displays plots of the surface averaged current density and surface averaged pH values.

Conclusion: A novel computational model has been developed to simulate the electrochemical modifications associated with CVCES applied to human-sized, CoCrMo total knee replacement components. This model will be used to optimize parameters for clinical translation of CVCES therapy to prevent/ eradicate implant infections.

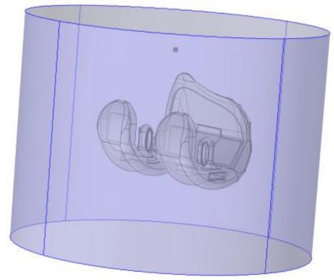

Fig. 1: Cell orientation and electrode positioning used for experimental polarization tests and computational modeling

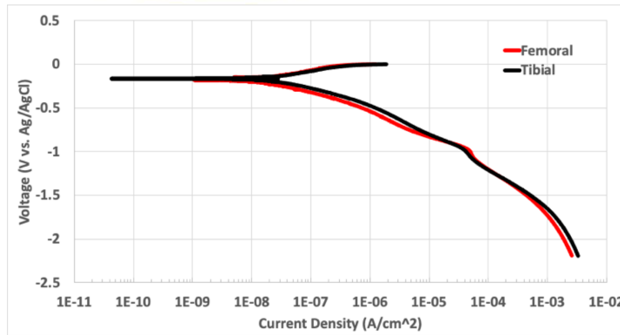

Fig. 2: Potentiodynamic polarization plots of the implants.

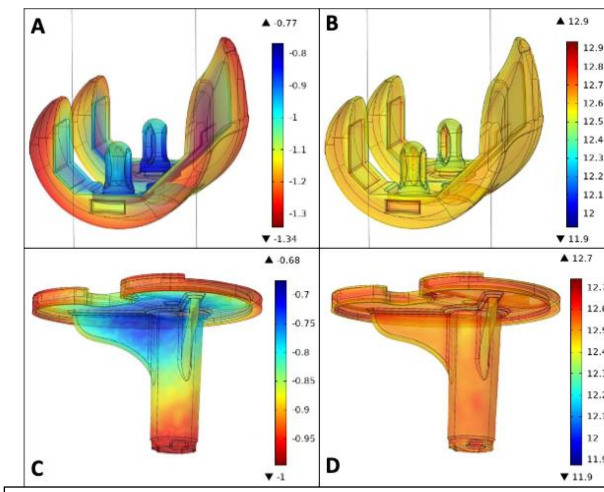

Fig. 3: Spatial distribution of the current density (mA/cm^2) (A,C) and pH (B,D) values along the surface of the femoral (A,B) and tibial (C,D) components.

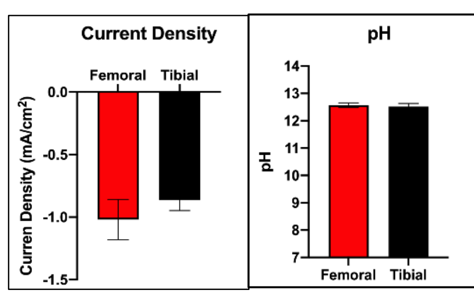

Fig.4 displays plots of the surface averaged current density and surface averaged pH values.

References:

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3.Clark,C et al. Electrochimica Acta, 2021 393:138853