Title: Mathematical modeling of biodegradation of metallic biomaterials using reaction-diffusion equations and level set method

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Abstract: In order to take advantage of biodegradable metallic materials (magnesium, zinc, and iron) in tissue engineering applications, their degradation parameters should be tuned to the rate of regeneration of new tissue. One approach for investigating biodegradation behavior is to construct computational models to assess the biodegradation properties prior to conducting experiments. Our developed model captures the release of metallic ions, changes in pH, the formation of a protective film, and the dissolution of this film due to the effect of different ions in the surrounding fluid. This has been accomplished by deriving a system of time-dependent reaction-diffusion partial differential equations from the underlying oxidation-reduction reactions. The level set formalism has been employed to track the biodegradation interface between the biomaterial and its surroundings. The equations were solved implicitly using the finite element method for spatial terms (with a 1st order Lagrange polynomial as the shape function) and backward-Euler finite difference method for temporal terms on an Eulerian mesh. The general predicted degradation behavior was qualitatively similar to the behavior observed in experiments. A Bayesian optimization routine was used to calibrate the models by minimizing the difference between simulation output and experimental data.

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