Mathematical modeling of degradation process of biodegradable metallic biomaterials in immersion and perfusion setups

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Summary

Despite the advantages of using biodegradable metals in implant design, their uncontrolled degradation and release remain a challenge in practical applications. A validated computational model of the degradation process can facilitate the tuning of implant biodegradation by changing design properties. In this study, a physicochemical model was developed by deriving a mathematical description of the chemistry of magnesium biodegradation and implementing it in a 3D computational model. The model was validated by comparing the predicted and experimentally obtained hydrogen evolution and change of pH during the corrosion tests in both immersion and perfusion setups, showing a good agreement between the results.

Introduction

Due to their bio-friendly properties and non-toxic contribution to body metabolism, biodegradable metallic biomaterials, including magnesium (Mg), iron (Fe), and zinc (Zn), are regaining attention in recent years for fixation applications [1]. Despite these advantages, their fast degradation rate and uncontrolled release have always been a challenge. These issues are usually investigated by conducting *in vitro* and *in vivo* tests of biodegradable metallic scaffolds and implants, which requires conducting multiple experiments for different scenarios. In this research, we have developed a mathematical model to predict the degradation behavior of biodegradable metallic materials *in silico*, which makes it possible to study their corrosion in a simulated environment.

Methods

In this study, a mathematical model of the biodegradation process of commercially-pure Mg was developed by deriving a set of partial differential equations (PDE), formulating the mass transfer and fluid flow phenomena as well as tracking the location of the moving corrosion surface during degradation. The equations were derived from the chemistry of biodegradation of Mg in saline (NaCl) and buffered (SBF) solutions, which includes the oxidation of the metallic part, reduction of water, changes in pH, formation of a protective film on the surface, the effect of different ions in the medium, and the effect of a perfusion setup. Tracking the movement of the surface was done by constructing a PDE based on the level set method, which captures the movement of the medium-scaffold interface by defining an implicit surface. The derived equations were coupled and solved using finite element methods. The degradation data to validate the models was collected from corrosion tests performed by using circulating media for simple scaffolds made of Mg. The model parameters were calibrated using a Bayesian optimization approach, and the obtained parameters were used to simulate the pH changes in NaCl and SBF solutions.

Results and Discussion

In order to obtain the degradation rate over time, instead of direct mass loss measurement, we measured the volume of formed hydrogen gas in Mg corrosion, which can be converted to mass loss by considering the stoichiometry of the reactions. Figure 1 shows the model output for the predicted produced hydrogen and the pH changes in immersion tests. The graph of the evolved hydrogen is used as input during the parameter calibration process, but the pH results are produced by the simulations using the optimized parameters to demonstrate the validation of the developed mathematical and computational models. The predicted pH result shows a difference of 5.35% for the simulation in NaCl and 1.03% for SBF simulation. Although the pH simulations are insufficient in terms of experimental input to call the model fully validated, the obtained validation results show that the developed mathematical and computational models give a correct *in silico* representation of the studied process.

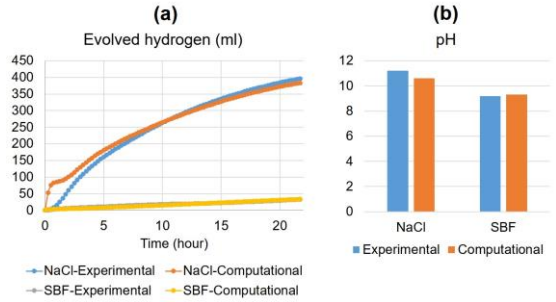

Figure 1: Comparing the quantitative output of the model for the rate of degradation (a) and the pH changes (b) in NaCl and SBF solutions with experimentally measured values.

Conclusions

Once fully validated, the models will serve as an important tool to find the biodegradable metal properties and predict their biodegradation behavior for improving the current workflows of designing biomedical implants and scaffolds.

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References

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