The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

Mathematical investigation of corrosion behavior of bioabsorbable metals on the biodegradation interface

Mojtaba Barzegari[1] and Liesbet Geris[1]

[1] Biomechanics Section, Department of Mechanical Engineering, KU Leuven, Leuven, Belgium
{mojtaba.barzegari , liesbet.geris}@kuleuven.be

Key Words: *Multiphysics Problems, Biomedical Applications, Finite Element, Level Set.*

Taking advantage of biodegradable metals is gaining more attention for various kinds of biomedical applications in recent decades, but controlling their functionality and behavior inside the body has remained a challenge [1]. Computational modeling of the materials' interaction with the body can help avoid part of the expensive experimental works required to characterize the degradation properties and provide an integrated spatiotemporal view on the whole process.

One of the most challenging parts of performing such a modeling study is capturing the chemical interactions and the dynamics and kinetics of the reactions occurring on the material-environment interface. Taking advantage of mechanistic modeling principles of mass transfer coupled with free boundary and moving interface formulations seems to be a promising solution to this complex problem. By doing so, one can model the degradation process by a set of equations capturing the interaction of various chemical components while tracking the moving corrosion front, which changes the location where the dynamic is taking place.

In this study, we have developed a mathematical and computational model to predict the biodegradation behavior of biodegradable metallic biomaterials. This model enables us to investigate the chemical, and later on biological, phenomena occurring on the corrosion interface of these biomaterials. Our developed model captures the release of metallic ions, changes in pH, the formation of a protective film, the effect of different ions in the environment, and the effect of perfusion of the surrounding fluid, if applicable. This has been accomplished by deriving a system of time-dependent reaction-diffusion-convection partial differential equations from the underlying oxidation-reduction reactions and solving them using the finite element method. The level set formalism was employed to track the biodegradation interface between the biomaterial and its surroundings [2]. In this approach, a signed distance function defines the distance of each point in space (within the domain of interest) to the interface. Such a definition implies that the zero iso-contour of the function belongs to the interface, making it possible to define various modeling parameters and boundary conditions on this interface using penalization techniques. The model was validated by comparing the predicted and experimentally obtained values of global pH changes in corrosion tests, for which a good agreement was observed [2].

Additionally, coupling the model with other existing cell and tissue growth models leads to a multi-physics model combining the chemistry of biodegradation, the physics of the electrolytes and body fluids flow, and the biology of tissue growth/regeneration. Building such a model requires dealing with several challenges, one of which is to couple various functions used to track the moving boundary of different sub-problems. Moreover, adding the effect of convection imposed by the fluid flow increases the complexity of the system. Elaborating these challenges from a mathematical point of view will facilitate future contributions to the construction of such models.

REFERENCES

[1] S. Agarwal et al. (2016) Biodegradable magnesium alloys for orthopedic applications. Material Science and Engineering C 68: 948-963.

[2] M. Barzegari et al. (2021) Computational modeling of degradation process of biodegradable magnesium biomaterials. Corrosion Science 190.