Developing a mathematical model of biodegradable metallic scaffolds for bone tissue engineering applications

Mojtaba Barzegari[1], Liesbet Geris[1,2]

[1] Biomechanics Section, Department of Mechanical Engineering, KU Leuven, Leuven, Belgium

[2] Biomechanics Research Unit, GIGA in Silico Medicine, University of Liège, Liège, Belgium

Biodegradable metallic materials are gaining more attention as promising candidates for bone implants in the recent decade. For tissue engineering applications, these biodegradable materials are magnesium (Mg), zinc (Zn), and (Iron), each of which has its own positive and negative features. They have been widely used in orthopedics and cardiovascular applications, both in commercially pure (CP) and alloyed form. They possess acceptable biocompatibility and bioabsorption properties, as well as sufficient mechanical stability.

Among these biodegradable metallic materials, Mg is gaining interest for use in bone repair applications. Despite its high degradation rate, pure Mg and Mg alloys have similar physical and mechanical properties as the natural bone, making them a perfect choice to prevent stress shielding, which is the one of the main causes of implant failure. For this reason, Mg-based alloys are called revolutionary metals in biomedical applications [1].

In order to take advantage of these materials in bone tissue engineering applications, their degradation parameters should be tuned to the rate of regeneration of the bone. One approach for investigating biodegradation behavior is to construct computational models to assess the biodegradation properties prior to conducting any in-vitro or in-vivo tests. In addition to degradation tuning, these models can be used for tuning controlled release of ions, which can be considered as an example of applications in biological processes.

We have developed a quantitative mathematical model to simulate the degradation of Mg-based orthopedic implants in silico (in the computer). To model the corrosion of the implant, a set of reaction-diffusion partial differential equations were derived from the underlying oxidation-reduction reactions, which reflect the behavior of the Mg scaffold in the presence of Chloride (Cl^-) ions in the medium. The model captures the formation of a protective film that slows down the degradation, as well as taking into account the role of Cl- ions on the dissolution of the formed film. The equations are solved numerically using the finite element method.

Currently, the model has been validated with experimental data and simple scaffold shapes, so it can be used as an important tool to find the appropriate design and degradation properties of the Mg-based implants for bone repair applications. In the future, the model will be also extended to include the biodegradation behavior of iron and zinc. Moreover, by adding a (bone) tissue formation model, the whole process of replacing the implant with the newly formed bone will be simulated.

References:

1. Shuai, C.; Li, S.; Peng, S.; Feng, P.; Lai, Y. & Gao, C., Biodegradable metallic bone implants, *Materials Chemistry Frontiers, Royal Society of Chemistry (RSC)*, **2019**, 3, 544-562