**Title**: Computational modeling of in-vitro biodegradation of metallic scaffolds and bone implants

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**Introduction**: Biodegradable metals, including magnesium (Mg), zinc (Zn), and iron (Fe), are gaining interest for bone repair applications in last decades. This is due to their acceptable mechanical properties and their non-toxic contribution to body metabolism. Despite these advantages, their fast degradation rate and uncontrolled release remain a challenge in practical orthopedic applications. 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 and situations. In this study, we have developed a mathematical model to predict the biodegradation behavior of biodegradable metallic materials, which makes it possible to study the corrosion of implants and scaffolds in a simulated environment.

**Methodology**: The biodegradation process is modeled as a set of partial differential equations, which are formulating the mass transfer phenomena as well as tracking the location of the surface of the implant during degradation. For the mass transfer model, the equations are derived from the chemistry of biodegradation of the metallic scaffolds in saline and buffered solutions, which usually includes the oxidation of the metallic part, reduction of water and oxygen, changes in pH, and formation of a protective film on the surface of the scaffold, slowing down the rate of degradation. Besides these aspects, it is also crucial to consider the effect of different ions in the medium on the rate of degradation. Additionally, investigating the structural changes of the scaffolds and implants in practical applications requires tracking the movement of the surface. This has been done by constructing an equation based on the Level Set principle, which captures the movement of the medium-scaffold interface by defining an implicit surface. Aforementioned equations are coupled and solved by the Finite Element method, mainly implemented in FreeFem++ and open source solvers. Degradation data to validate the models are collected from immersion tests of simple scaffolds made of Commercial Pure Mg, Zn, and Fe. Different models are being developed for different materials.

**Results and Discussion**: Postprocessed results of the solution of the equations clearly show the formation of a protective film on the surface of the implant. In addition to this, experimental corrosion graphs, which show the mass loss of the scaffold over time, were compared with the simulation predicted ones. Instead of direct mass loss measurement, we measured the volume of formed side chemical components (such as hydrogen gas in Mg corrosion, shown in figure 1), which can be converted to mass loss by considering the stoichiometry of the reactions. 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.

**Conclusion**: Currently, validation, benchmarking, and calibration of the models are taking place. Once fully validated, the models will serve as an important tool to find the biodegradable metal properties and predict the biodegradation behavior of metallic implants for bone repair applications, that improve current workflows of designing biomedical implants.

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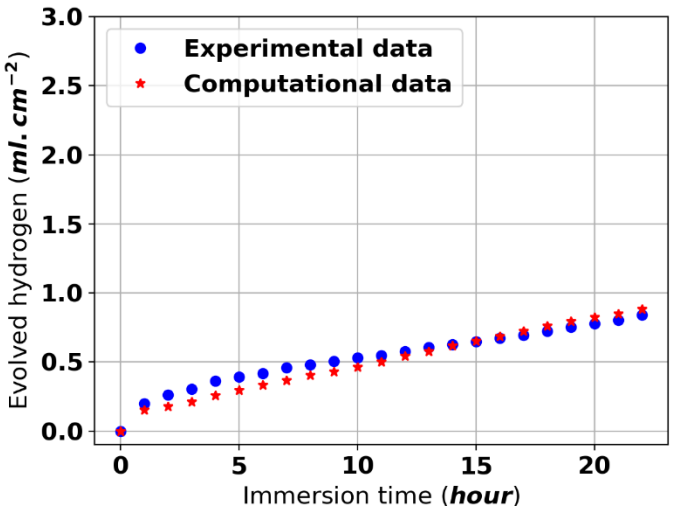
**Figure**:




Formed hydrogen as a criterion for mass loss of a Mg scaffold over time, plotted for both simulation output and extracted experimental data (Experimental data from Mei et al., 2019)

**Reference**: Mei, D.; Lamaka, S. V.; Gonzalez, J.; Feyerabend, F.; Willumeit-Römer, R. & Zheludkevich, M. L. The role of individual components of simulated body fluid on the corrosion behavior of commercially pure Mg, Corrosion Science, 2019, 147, 81-93