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INVESTIGATING THE BIODEGRADATION OF METALLIC BIOMATERIALS USING HPC-BASED SIMULATION TECHNIQUES

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Biodegradable metals are gaining interest for biomedical applications in last decades. This is due to their acceptable mechanical properties and their non-toxic contribution to body metabolism [1]. Despite these advantages, their fast degradation rate and uncontrolled release remain a challenge in practical biomedical 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.

The developed model captures the release of metallic ions, the formation of a protective film on the surface of the material, the effect of presented ions in the surrounding environment on the thickness of this protection layer, and tracking of the movement of the corrosion front. The corresponding computational model was constructed using the finite element method. Tracking the moving front at the diffusion interface requires high numerical accuracy of the diffusive state variables, which was achieved using a refined computational grid. This made the model computationally intensive and in need of parallelization. Thus, an easy-to-implement approach for parallelization was also developed to enable the model to simulate large scale systems with higher performance and efficiency in high-performance computing (HPC) environments. The weak-scaling and strong-scaling tests were performed to evaluate the performance of the parallelized algorithm.

After calibrating the model with the data of magnesium degradation tests, results showed a good agreement between the predicted biodegradation rates and the experimental data. The model will be extended to include the chemistry of other metallic materials, and once fully validated, it can serve as an efficient tool to assess the biodegradation behavior of metallic biomaterials. In a wider scope, the developed model can be used for the high-performance simulation of large-scale systems in which the movement of the system boundaries is controlled by reaction-diffusion phenomena.

REFERENCES

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