Computational Modeling of Biodegradation of Metallic Biomaterials

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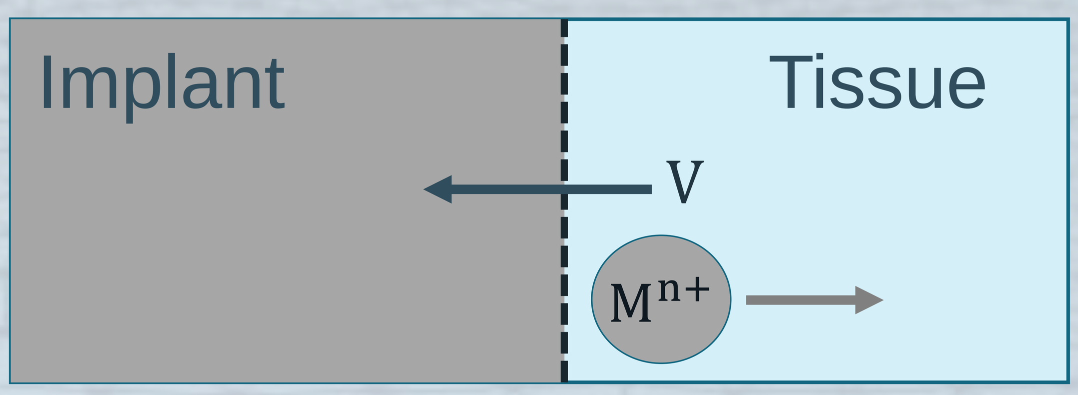
Background

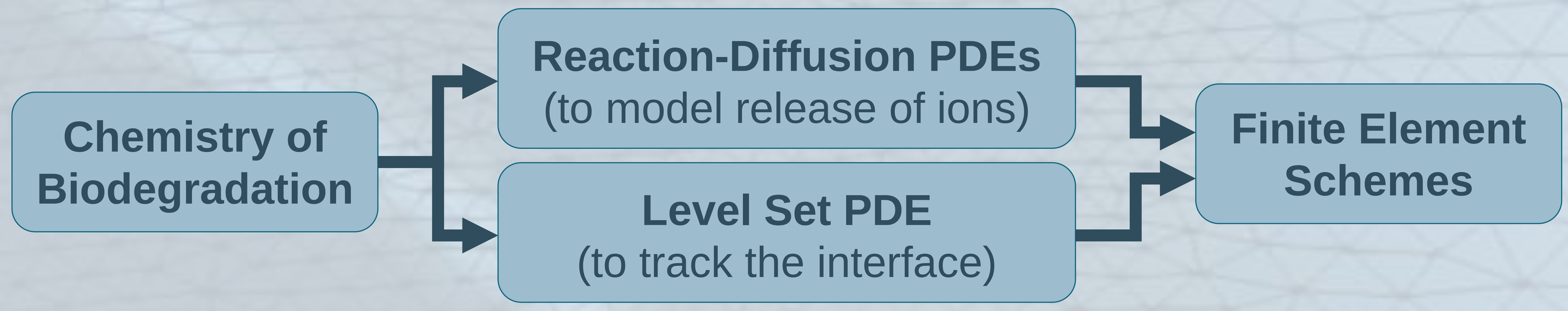
- Bio-inert materials remain in the body forever or require additional surgery to remove.
- But, taking advantage of biodegradable materials requires tuning the degradation parameters to the rate of regeneration of new tissue.
- A quantitative mathematical model of degradation process is a solution to this issue.
- Magnesium (Mg) has been selected to start with due to its acceptable mechanical properties, biocompatibility, and contribution in osteoinductivity [1].



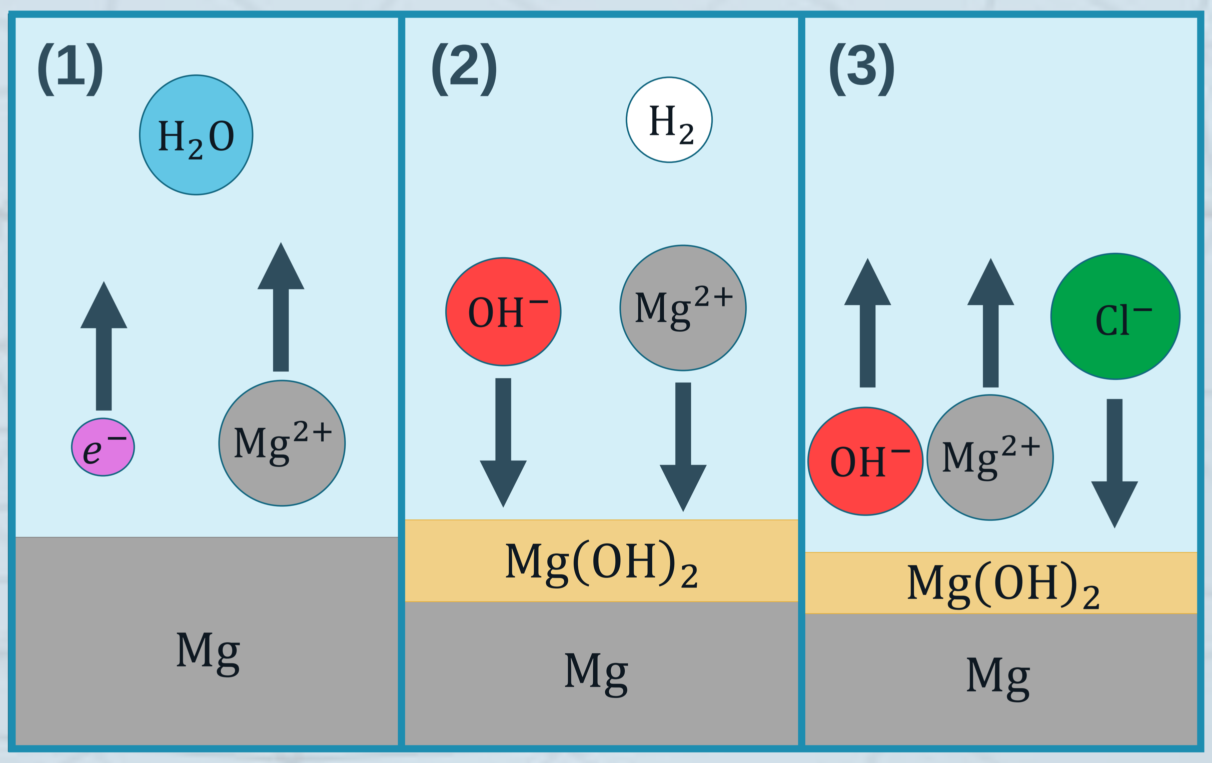
Schematic representation of degradation of a metallic biomaterial and the growth of the tissue

Methodology

- Biodegradation is modeled as a set of reaction-diffusion PDEs.
- The model captures:
  - The chemistry of dissolution of metallic implant (here Mg)
  - Formation of a protective film
  - Effect of ions in the medium (currently Chloride ions -Cl-)
- Derived PDEs are solved using finite element schemes.



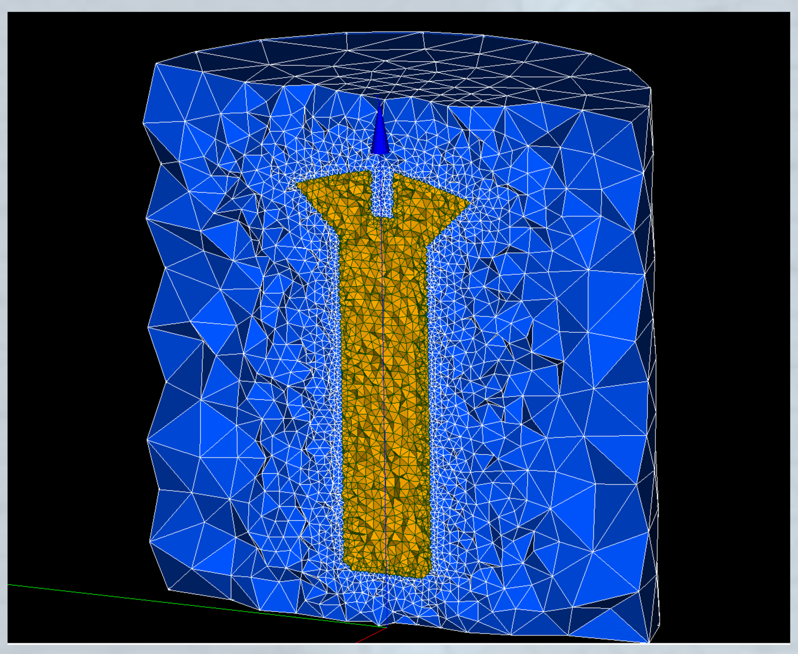
The overall workflow of biodegradation model

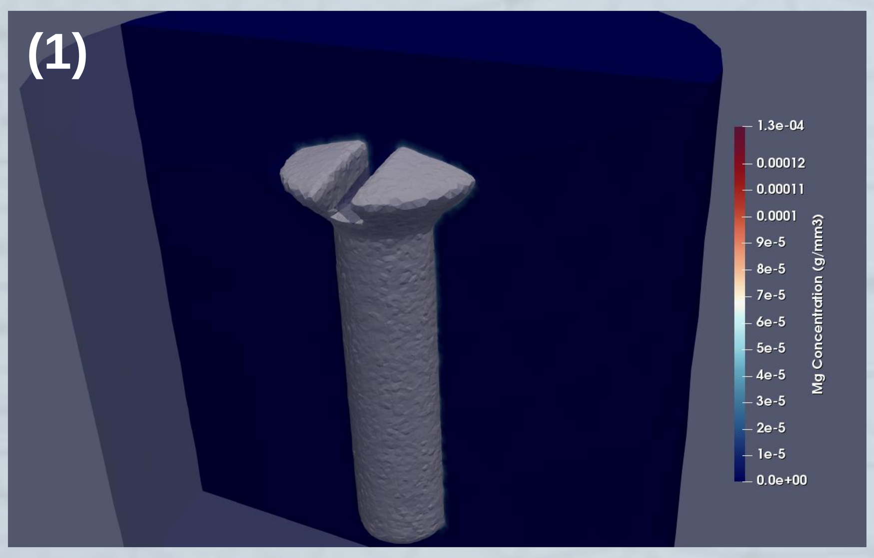


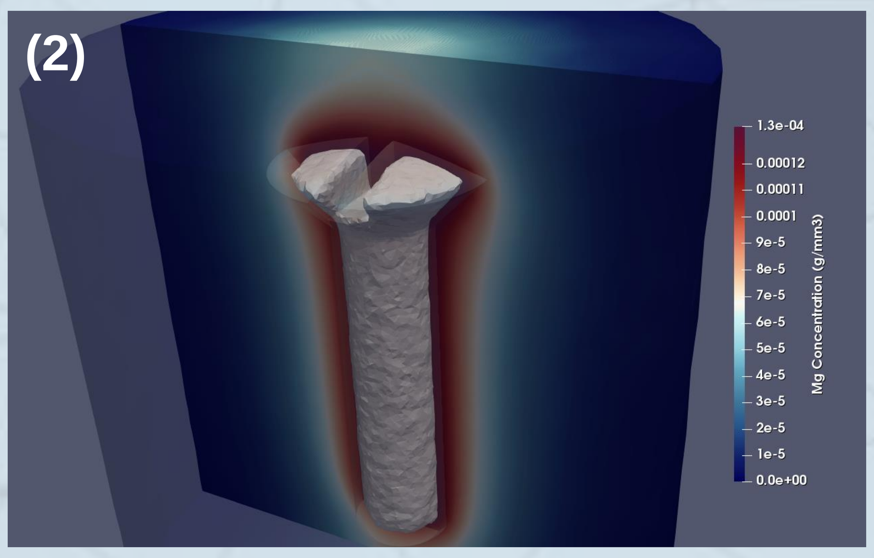
The chemistry of biodegradation of Mg comprises the release of Mg^{2+} ions, formation of a protective film, and the dissolution of this film due to the effect of Cl^- ions

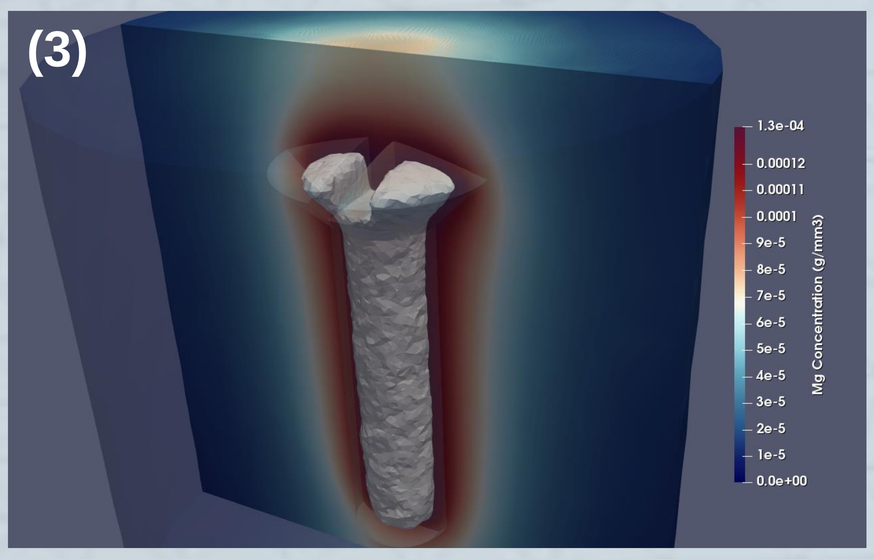
Results for Magnesium

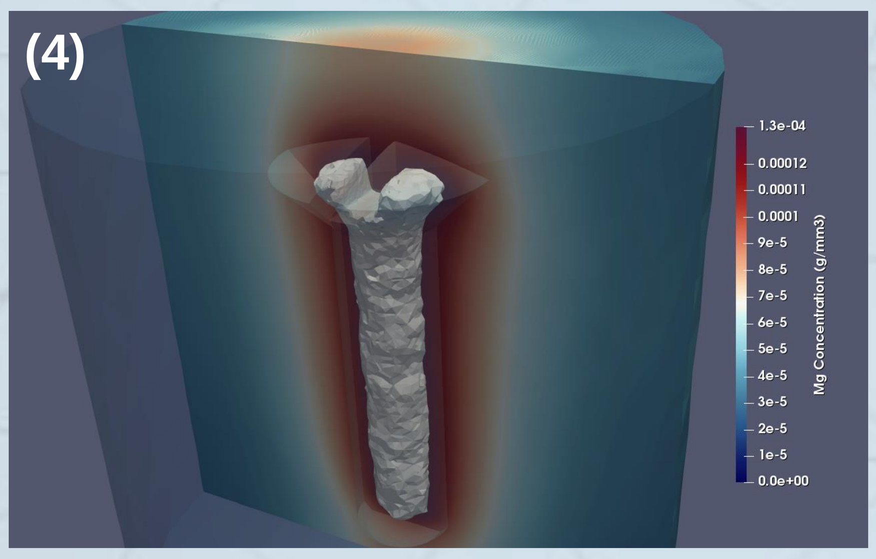
Numerical reproduction of the initial shape of a simple 3D screw geometry. The mesh is refined at the medium-implant interface to increase the accuracy of the biodegradation simulation.







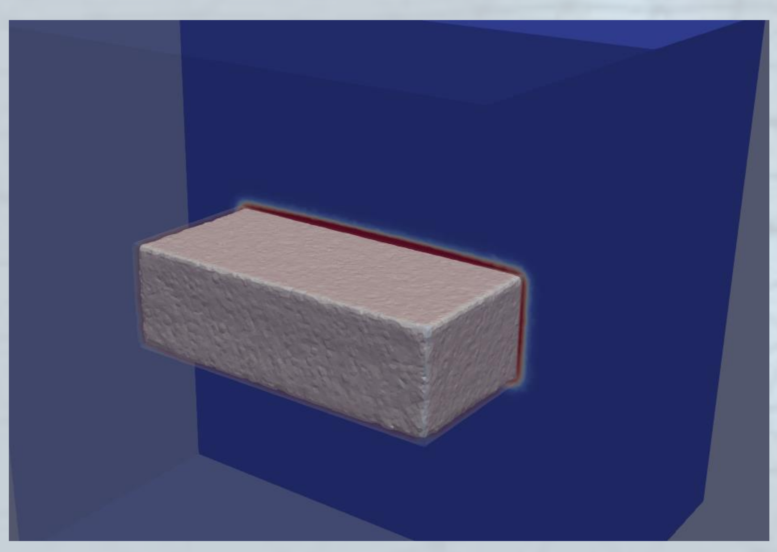




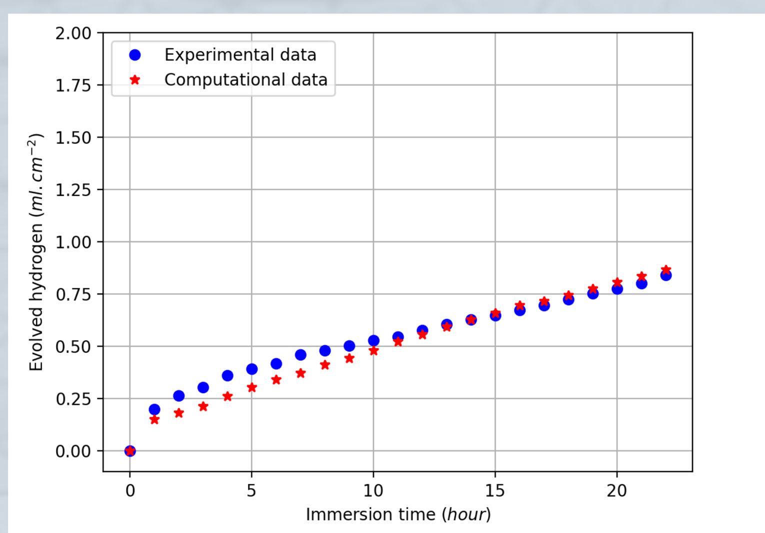
Comparison of the degraded shape of the screw (white body) with its initial shape (transparent surface) over time. The color contour shows the concentration of Mg^{2+} that is increasing as it releases to the surrounding media.

Time Calibration & Validation

- Reference data and initial conditions are extracted from Mei et al [2].
- Parameter estimation (chemical coefficients) has been performed using a Bayesian optimization algorithm.



Reference geometry for the parameter estimation as well as the formed protective film (red region)



Time calibration using the produced hydrogen as the criterion to compare the output with experimental data

References

1. B. Luthringer, et al. (2014) *Magnesium-based implants: a mini-review*, Magnesium Research; 27:142-54
2. D. Mei, et al. (2019) *The role of individual components of simulated body fluid on the corrosion behavior of commercially pure Mg*, Corrosion Science, 147: 81-93

This research is financially supported by the PROSPEROS project, funded by the Interreg VA Flanders - The Netherlands program, CCI grant no. 2014TC16RFCB046.

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