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In silico design of magnesium implants: macroscopic modelling

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Abstract

Magnesium-based biomedical implants offer many advantages versus traditional ones although some challenges are still present. In this context, mathematical modeling and computational simulation may be a useful and complementary tool to evaluate *in silico* the performance of magnesium biomaterials under different conditions. In this paper, a phenomenologically-based model to simulate magnesium corrosion is developed. The model describes the physico-chemical interactions and evolution of species present in this phenomenon. A set of 7 species is considered in the model, which allows to simulate hydrogen release, pH evolution, corrosion products formation as well as degradation of magnesium. The model is developed under the continuum media theory and is implemented in a finite element framework. In the results section, the effect of model parameters on outcomes is firstly explored. Second, model results are qualitative validated versus two examples of application found in the literature. Two main conclusions are derived from this work: (i) the model captures well the experimental trends and allows to analyze the main vari-

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