Comparing different methods of sensitivity analysis for computational modelling of magnesium-based implant biodegradation

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Background

- Degradation of magnesium is a multiphysics process that is **complex** and. **computationally expensive** to model.
- Model **key** parameters (e.g. reaction rate constants, diffusion coefficients, etc) cannot be found in literature and some cannot be measured using experiments.
- **Sensitivity analysis** approaches are computationally expensive and limited in the case of complex models.
- The **surrogate models** reduce the complexity of the degradation models without compromising their accuracy.
- Model **predictions** are strongly influenced by parameter **uncertainty**.

$$Mg_{(s)} \rightarrow Mg^{2+}_{(aq)} + 2e^-$$

$$2H^+_{(aq)} + 2e^- \rightarrow H_2$$

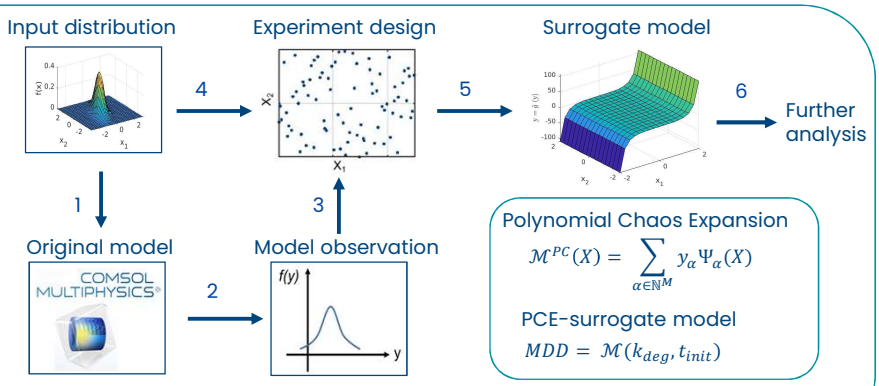
$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(D_i \nabla c_i - z_i \frac{D_i}{RT} F c_i \nabla V \right) = R_i$$

$$\frac{\partial c_{Mg}}{\partial t} = \frac{\epsilon k_{deg}}{1 + \exp(-(t - t_{init}))}$$

Degradation reaction and its corresponding kinetic mathematical model

Methodology

- Creating the surrogate model required a minim observations of the original model ($\cong 2N_p$) (steps 1 and 2).
  * N_p : Number of Parameters
- After creating a surrogate model (steps 3-5) and validating it, further analysis and testing can be performed; e.g. uncertainty propagation and sensitivity analysis (step 6).
- The surrogate model is able to cover the entire input distribution of parameters (step 4).
- The sensitivity analysis reflect the impact of each parameter over the model output.



Polynomial Chaos Expansion

$$\mathcal{M}^{PC}(X) = \sum_{\alpha \in \mathbb{N}^M} y_\alpha \Psi_\alpha(X)$$

PCE-surrogate model

$$MDD = \mathcal{M}(k_{deg}, t_{init})$$

Fig. 1: Schematic diagram of implementing the surrogate modeling approach to model the degradation of magnesium-based implants.

Results

PCE Surrogate model

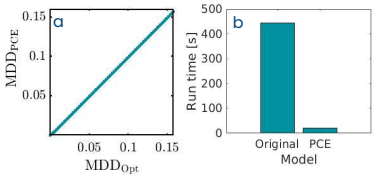


Fig. 2: a) The estimated mean degradation depth distribution by PCE model vs optimized model. **b)** The run time of surrogate vs. original model

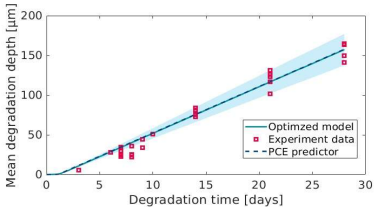
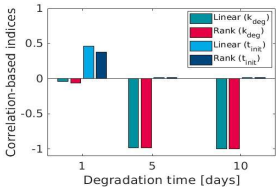


Fig. 3: The validation of the PCE surrogate model of mean degradation depth *vs.* Optimized model and experimental data obtained using µCT.

Surrogate model based sensitivity analysis

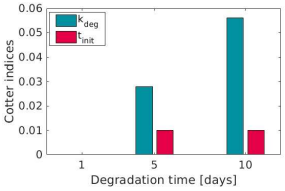
Sample–based methods



$$\rho_i = \rho(X_i, Y) = \frac{\mathbb{E}[(X_i - \mu_i)(Y - \mu_Y)]}{\sigma_i \sigma_Y}$$

ρ_i: correlation based indices

Linearization methods

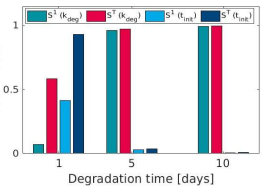


$$C_o(i) = \frac{1}{4}[(y_{2M+1} - y_{M+1}) + (y_i - y_0)]$$

$$C_e(i) = \frac{1}{4}[(y_{2M+1} - y_{M+1}) - (y_i - y_0)]$$

$$I_{Cotter}(i) = |C_o(i)| + |C_e(i)|$$

Sobol' Indices



$$S^1 = \frac{Var(\mathcal{M}_u(X_u))}{Var(\mathcal{M}(X))}$$

$$S^T_k = \sum_{k \in u} S_u$$

Fig. 4: PCE-based sensitivity analysis for the first 10 days of the degradation. The influence of the key parameters k_{deg} and t_{init} on the mean degradation depth of magnesium-based implants

Conclusions

- **Surrogate modelling** approach reduces the computation time and simplifies the simulation of the degradation process without compromising the accuracy of the complex degradation model.
- A **PCE-Surrogate model** enables us to carry out the sensitivity analysis for the **full range** of input parameter distributions.
- We implemented **global sensitivity analyses** in order to quantify the influence of the variation in model key parameters k_{deg} and t_{init} on the estimations of the degradation rate for magnesium-based implants.
- Sample-based and linearization methods provide **an overview** of the system especially in the case of **limited** computing power.

References

Zeller-Plumhoff, B., Albaraghtheh, T., et al., 2021. Computational modelling of magnesium degradation in simulated body fluid under physiological conditions Journal of Magnesium and Alloys, 10(4), pp.965-978

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