Efficient Surrogate Models for Degradation Models of Biodegradable Magnesium-Based Implants

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Abstract

In silico methods to study biodegradable implants have recently received increasing attention due to their potential to reduce experimental time and cost. Various degradation models have been developed, including physical, phenomenological, analytical and machine learning-based models. No matter how sophisticated degradation models become, these computational models are inevitably characterized by uncertainties associated with different aspects of these models, such as uncertain parameters, initial and boundary conditions, validation data and model assumptions and hypotheses. Diverse uncertainty quantification methods can be used to assess the uncertainties associated with various parts of degradation models. Nevertheless, this quantification process is often computational-intensive, particularly when employing sampling-based approaches. Surrogate modelling has emerged as a promising solution to this challenge. This approach involves approximating complex degradation models with more easy-to-evaluate surrogate models. Various surrogate models have been devised to suit different problems. This study evaluated three categories of surrogate models: regression-based, integral-based and hybrid models. Specifically, we assessed the effectiveness of polynomial chaos expansion (PCE), Kriging and polynomial chaos Kriging (PCK) in capturing the degradation behaviour of various dimensionality and complexity degradation models. Kriging outperformed PCE and PCK for model parameter calibration regarding computational efficiency, sample size for training and validation data, and accuracy level in fitting degradation systems. PCE and PCK, on the other hand, demonstrated better agreement with the physical phenomena underlying degradation when performing sensitivity analyses based on the three surrogate models.

Surrogate models

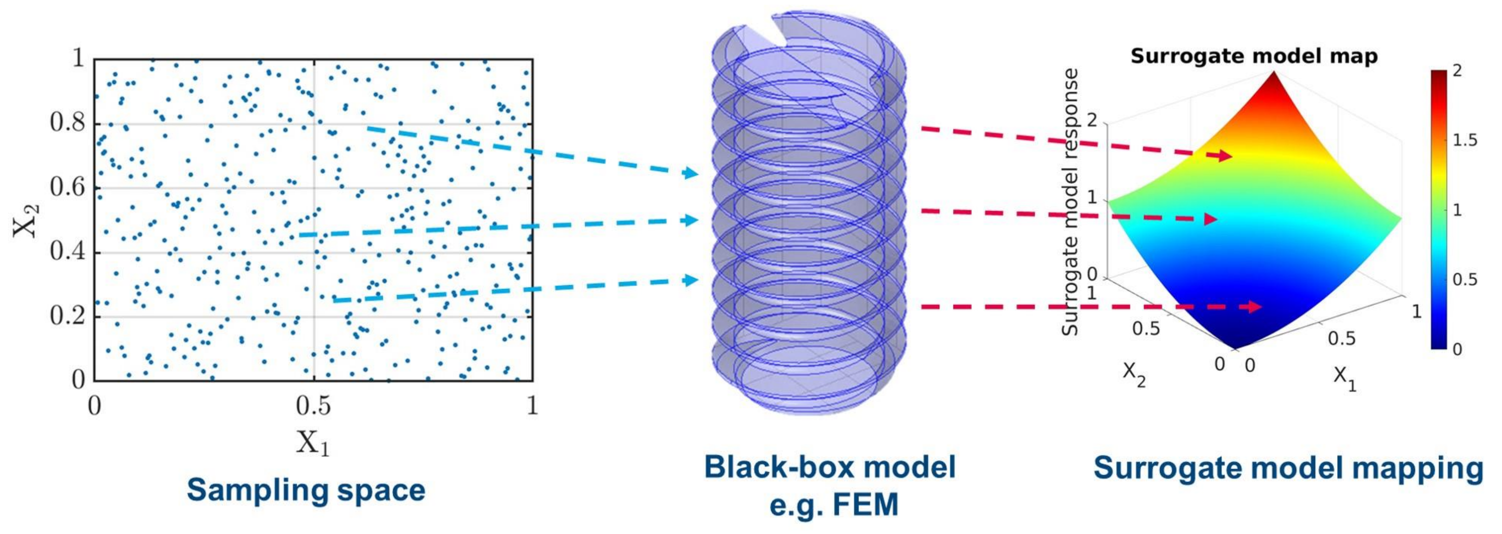

Fig. 1 : Schematic diagram of the construction of a surrogate model for a system characterised by two input parameters, denoted as X_1 and X_2 using a black-box model.

Surrogate models are easy-to-evaluate approximation of the complex mathematical models, which reduces the computational cost and evaluation time. The general mathematical presentation of surrogate models is given by:

$$y = \mathcal{M}^{s}(x) \quad (1)$$

where $\mathcal{M}$ is the surrogate mapping function, s is the respected surrogate model; Kriging (Krg), polynomial chaos expansion (PCE) or polynomial chaos Kriging (PCK). y is the QoI and x is the input parameter vector.

$$y = \mathcal{M}^{Krg}(x) = \beta^T f(x) + \sigma^2 Z(x,\omega) \quad (2)$$

$$y = \mathcal{M}^{PCE}(x) = \sum_{\substack{\alpha\in N^M \\ 0\le|\alpha|\le p}} y_\alpha \Psi_\alpha(x) \quad (3)$$

$$y = \mathcal{M}^{PCK}(x) = \sum_{\substack{\alpha\in N^M \\ 0\le|\alpha|\le p}} y_\alpha \Psi_\alpha(x) + \sigma^2 Z(x,\omega) \quad (4)$$

Degradation models

The surrogate model presentation of QoI (y), and the input parameter vector (x) for the three case studies of the degradation models of Mg-based alloys:

Case study	x	y
Degradation of Mg	k_{deg}, t_{ini}	Mean degradation depth (MDD)
Formation of precipitation on implant surface	k_{deg}, t_{ini}, k_j $J: Mg, P, O, Ca, C$	Elemental weight percentage (wt%)
Diffusion of Mg^{2+} ions	$D_{Mg^{2+}}$	Volume loss (VL%)

UQ workflow

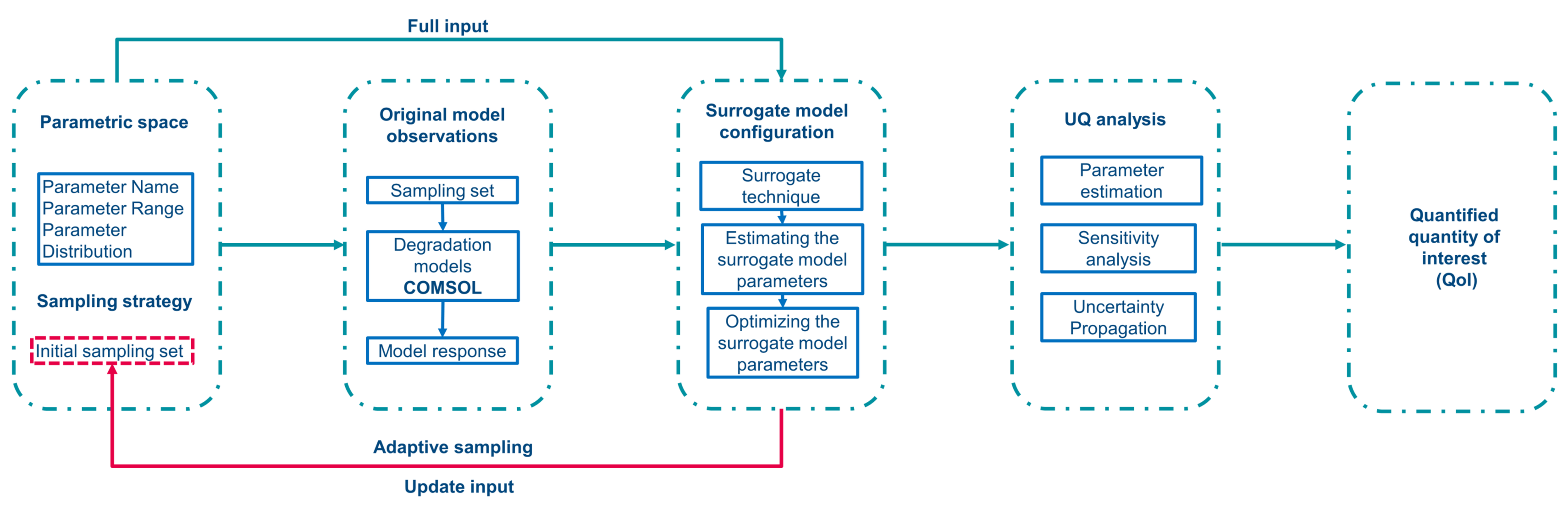

Fig. 2: Workflow of quantifying the uncertainty associated with degradation models of Mg-based biodegradable implants using the surrogate modelling approach

Design of computer experiment

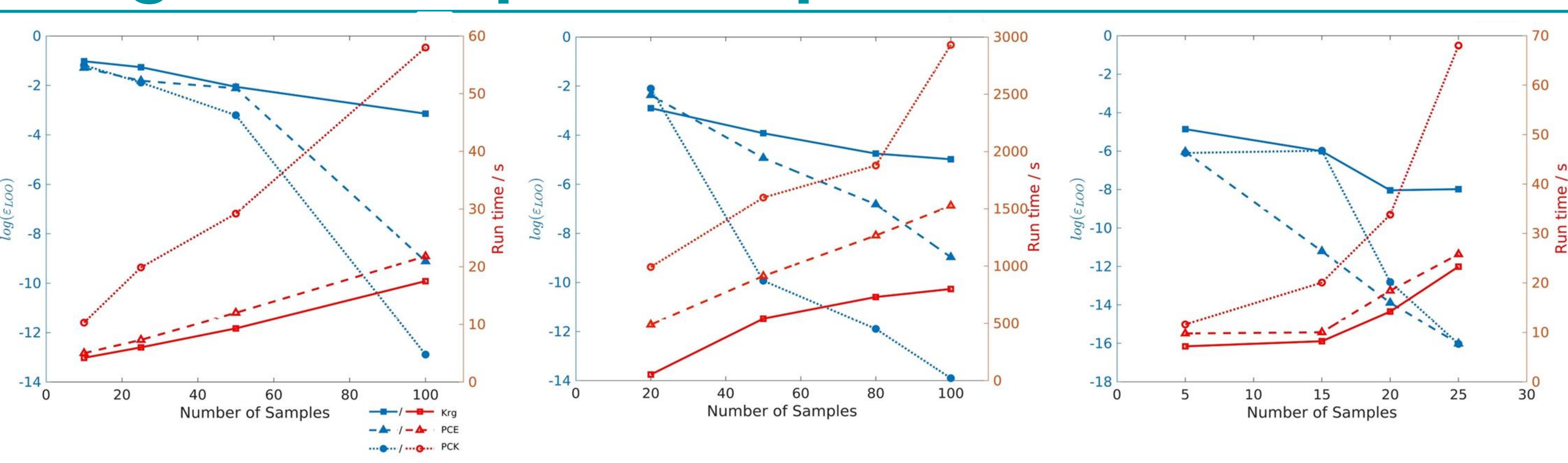

Fig. 3: Illustrate the number of adaptive samples as functions of accuracy (ε_{LOO}), training time, and type of surrogate model for three degradation models.

Surrogate models performance

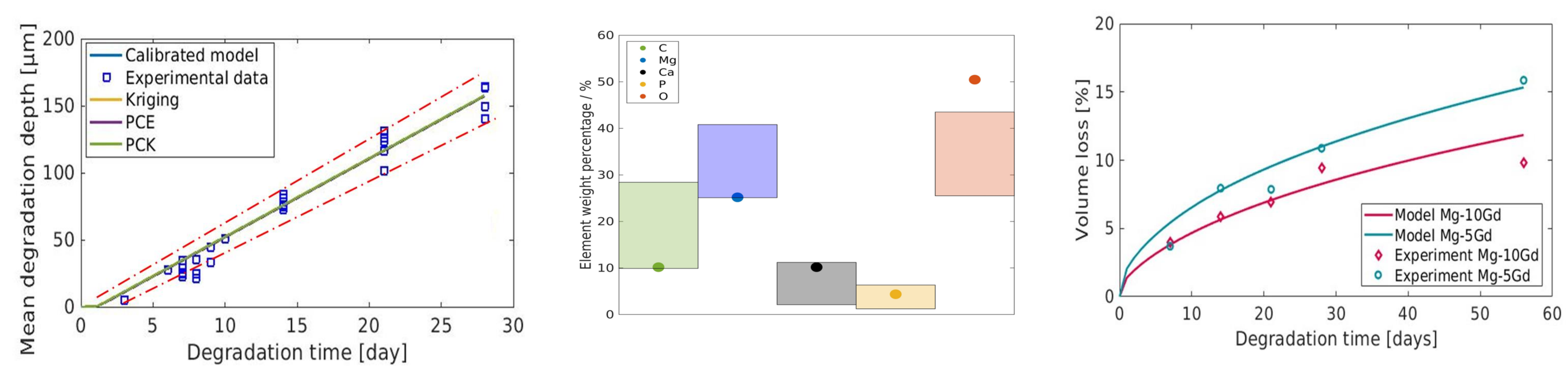

Fig. 4: Comparison of the performance of the calibrated surrogate models for the three degradation models

Uncertainty propagation

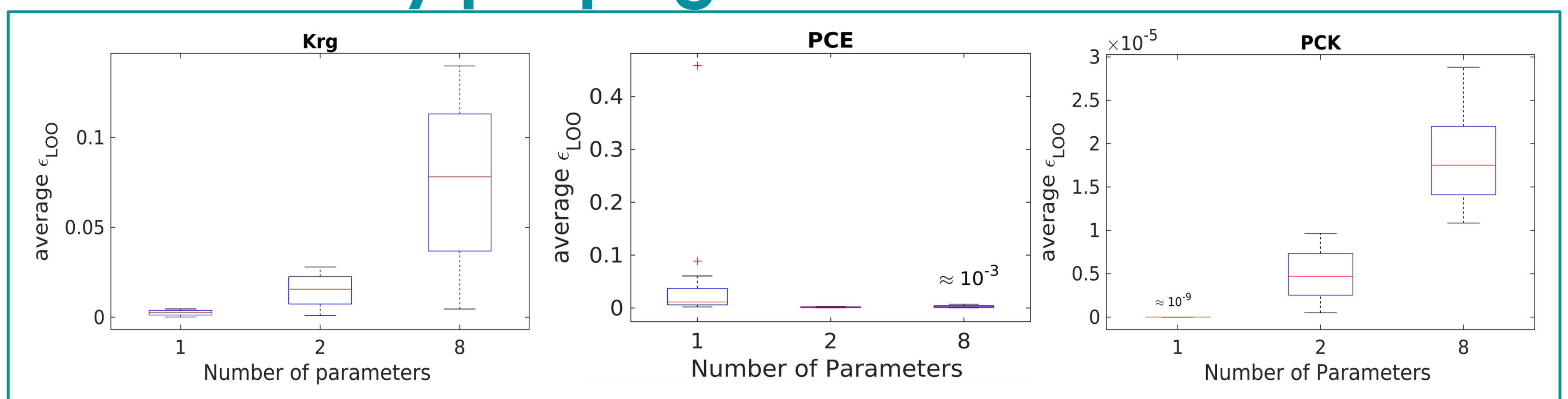

Fig. 5: Propagation of uncertainty as a function of changing number of parameters in terms of ε_{LOO}

Conclusions

- In parameter estimation problems, Kriging surrogate models provide accurate estimation with the least amount of samples and computational effort.
- Accordingly, PCE and PCK are more practical for further UQ analysis. The propagation of uncertainty within the surrogate model is less than for Kriging, regardless of the mathematical and computational complexity of the degradation model.
- Using surrogate modeling can reduce the computational burden of calibrating and quantifying degradation models without compromising their accuracy.

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