Gaussian Process Framework for Bayesian Inference of Hydrogen Permeation in Polymer Composites

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Reliable modelling and prediction of hydrogen permeation in fibre-reinforced polymer composites are essential for the safe and efficient design of hydrogen infrastructure. However, key material parameters — such as in-situ matrix, fibre, and fibre–matrix interphase permeabilities — remain extremely challenging to determine and are inherently uncertain [1]. Furthermore, high-fidelity three-dimensional (3D) microstructure-resolved finite element (FE) simulations required to capture transport mechanisms are computationally expensive, limiting their direct use in design optimisation and inverse parameter identification.

This work introduces data-driven probabilistic framework that integrates Gaussian Process (GP)-based surrogate modelling with three-dimensional Representative Volume Element (RVE) mass transport simulations and hydrogen permeation experiments on composites to enable efficient Bayesian inference of constituent parameters, including interphase [2]. The likelihood entering Bayes' theorem is formulated as a joint GP marginal likelihood of an augmented dataset, combining high-fidelity simulation outputs with experimental observations through the GP covariance structure. In this formulation, both forward-model responses and experimental measurements are treated as noisy observations of a shared latent function, allowing uncertainty to be naturally propagated via the GP covariance matrix.

Hydrogen permeation tests are conducted on the neat polymer specimens, and the measured permeabilities are used to define the prior distribution for the in-situ matrix permeability within the Bayesian framework. For the fibre–matrix interphase permeability, two physically motivated prior regimes are considered: (i) reduced molecular mobility near the fibre surface leading to decreased local transport, and (ii) microvoid-induced enhancement of local permeability. The prior distribution for interphase thickness is constructed using experimentally measured interface dimensions reported in the literature.

Posterior sampling of the uncertain parameters is performed using Hamiltonian Monte Carlo via the No-U-Turn Sampler (NUTS), enabling efficient exploration of the high-dimensional parameter space [3]. Owing to the GP-based probabilistic emulator, thousands of Markov Chain Monte Carlo (MCMC) evaluations can be carried out at negligible computational cost compared to direct finite element simulations. The joint GP marginal likelihood formulation ensures that forward-model uncertainty, surrogate (GP) uncertainty, and experimental measurement noise are consistently incorporated within the Bayesian inference process. The resulting posterior parameter distributions are subsequently propagated through the GP forward model, yielding uncertainty-aware predictions of composite hydrogen permeability which can be used to derive confidence-based permeability limits for design specification. The framework is readily transferable beyond mass transport (e.g., hydrogen permeability in here), enabling solution of other multi-parameter inverse problems in data-driven composite material design.

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