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Opinion

Enhancing Performance of Polymers and Composites for Hydrogen Economy with Predictive Modelling

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Opinion

Meeting the demand for the significantly increasing world energy consumption and reducing our environmental footprint remains a challenge. Hydrogen is a promising energy carrier especially if obtained as carbon-clean from renewable resources. The transition to hydrogen economy will require significant changes to the infrastructure and materials that are used to produce, transport, distribute, store and use hydrogen in industry or in households. Polymeric materials and their composites offer promising means to play a key part in that energy transformation because of their light weight and/or ease of processability. However, their interaction with hydrogen environment (either in the gaseous or liquid form) poses several challenges, especially including their resistance to permeation, stiffening of the amorphous phase in semi-crystalline polymers, rapid gas decompression damage, low-temperature behaviour of elastomeric sealing, or microcracking caused by thermal cycling from cryogenic to ambient temperatures. These aspects have been summarised in recent papers, e.g. [1, 2].

The macroscopic response of polymers and their composites (e.g. permeation, strength) to hydrogen environments is controlled by their underlying structural and morphological characteristics (e.g. molecular weight, density, crystallinity, reinforcement content etc.) and external conditions (e.g. gas pressure, temperature etc.). While several advanced experimental techniques across the scales have been recently proposed, including in-situ Fourier transform infrared absorption spectroscopy for tracking structural changes in semi-crystalline polymers under elevated pressures up to 100 MPa [3] or growth kinetics of cavities in elastomers with 3D in-situ X-ray micro-tomography [4], the high-dimensional design space for those materials is a significant challenge for a cost- and time-effective generation of structure-property relations databases for subsequent performance enhancement and optimisation of those materials.

Computer-based prediction of those relationships holds a promise in assisting experimental efforts but needs to employ different modelling techniques from across the scales, including molecular simulations, continuum approaches, and their combinations. Examples of molecular simulations of polymers for hydrogen applications include studies on the role of amorphous phase and its confinement between crystals on the hydrogen gas sorption in semi-crystalline polymers [5], or interplay between free volume and nanoscale cavitation during rapid gas decompression in amorphous systems [6]. Despite significant efforts in modelling of hydrogen transport at given scales, no integrated multiscale modelling platform yet exists to author's best knowledge – however, recent advances in new machine learning concepts hold a promise to change that modelling landscape. For example, gas permeation in amorphous polymers was modelled in [7] by utilising molecular dynamics and Monte Carlo simulations, experimental data and machine learning – particularly, defined by the authors as the multi-task approach (e.g. multi-property, multiple-data sources) used the graph neural networks (GNNs) to predict Robeson trade-off plots (permeability vs selectivity) of the polymers for six gases (H_2, O_2, N_2, CO_2, CH_4, and He). However, some of the general challenges related to those approaches involve model training dependent on large amounts of data typically coming from traditional numerical approaches or costly experimental tests; and subsequently require even more data when the model needs further fine-tuning to fulfil and improve its predictive capability and accuracy.

Another challenge for the machine learning approaches is dealing with uncertainties which can include both *inherent* features such as randomness in polymer and composite microstructures (e.g. blend phase or reinforcement distribution) or variation in environment (e.g. temperature fluctuations); or lack of sufficient knowledge and data e.g. to identify model parameters. Bayesian modelling paradigm offers excellent means for capturing those uncertainties–recent examples include application of this approach for studying hydrogen permeation in polymer composites [8] with the help of surrogate models (e.g. Gaussian Process Regression) to carry out probabilistic inference of constituent hydrogen permeability at the microscale from macroscopic data; forward uncertainty propagation from a mesoscale to the macroscale, or simple design case study under uncertainty.

While Bayesian paradigm enables to capture uncertainties within an elegant mathematical framework, its compu-

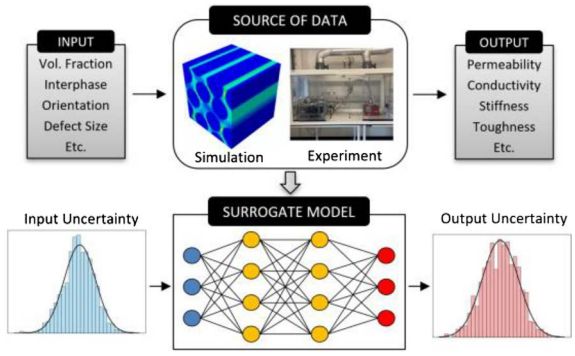

Figure 1 *Data-driven predictive modelling methodology*

tational effort increases exponentially with the increased number of design/uncertain variables (so called '*curse of dimensionality*'). A remedy may be coming from the computational power of physics-informed neural networks (PINNs) to deal with high-dimensional problems and combining them with the Bayesian methodology. The topic remains still largely unexplored, especially in the context of multiscale modelling of polymers and their composites, with major breakthroughs yet to come. Future research in that field requires a systematic comparison of computational performance of different Bayesian NNs approaches (e.g. variational, MCMC), particularly when employing this for approximation uncertainty in PINNs [9].

In summary, predictive capabilities for polymers and their composites in hydrogen economy promise to reduce time-consuming experimental and allow less conservative design through the optimisation of materials composition and infrastructure variables and reducing materials waste. However, predictive capabilities need to be validated experimentally to ensure that regulators and authorities accept the methods and to ensure larger pull from industry to be used in design, analysis and optimisation process of polymer-based materials in hydrogen energy applications. A key to that is the ability to validate models with full-scale testing that most closely mimics real-world conditions [10]–in the case of hydrogen permeation in pipes it is the ability to predict accurately the overall permeation and any leakage in a structural component, to allow time-efficient product certification, accurate assessment of allowable emission rates to alleviate potential societal/public concerns.

Biography of the author

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Dr Figiel is a Reader in Materials Engineering in the International Institute for Nanocomposites Manufacturing (IINM) in WMG at the University of Warwick, UK. He received his PhD degree from the TU Dresden (Mechanical Engineering) and then conducted his post-doctoral research at the German Aerospace Center (DLR) (Materials Research) and the University of Oxford (Solid Mechanics & Materials Engineering). He received his Habilitation from the IPPT Polish Academy of Sciences (Materials Engineering). He was a Visiting Associate in the Division of Chemistry and Chemical Engineering at the California Institute of Technology (Caltech). He has been Chair of Special Interest Group in Hydrogen in WMG, and Industry Champion in the EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems (HetSys).

Keywords

Polymers; Composites; Hydrogen Economy; Multiscale Modelling; Machine Learning, Physics-Informed Neural Networks, Bayesian Modelling

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Conflict of interest

The author declares no conflict of interest.

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