Abstract

Fibrous materials are the “unsung heroes” of fuel-cell electric vehicles (FCEVs). Inside the proton exchange membrane fuel cell (PEMFC) stack, the gas diffusion layers (GDLs), made of fibrous materials, regulate reactant transport, water removal, electrical contact, and mechanical support. Beyond the stack, fibrous materials-based filter media protect the system from airborne particulate contaminants while controlling pressure drop and energy demand. Despite these critical roles, the structural complexity of these materials is often reduced to bulk descriptors, such as thickness, mass per unit area, porosity, and fibre diameter. While useful for comparison and quality control, these parameters do not capture the three-dimensional (3D) architecture that governs functional behaviour. GDLs are typically composed of woven or nonwoven fibrous materials, each with distinct structural features and design challenges. Woven GDLs are multiscale, hierarchical structures composed of interlaced yarns, which are themselves assemblies of individual fibres. Although fabric construction parameters are readily apparent, hidden structural details such as yarn packing fraction, yarn cross-sectional geometry, and yarn curvature strongly influence their performance in PEMFCs. On the contrary, the nonwoven GDLs and filter media pose distinct challenges. They are often treated as isotropic porous materials in simulations of gas diffusion and filtration, even though their fibre networks can exhibit pronounced structural anisotropy arising from preferential fibre orientation and spatial heterogeneity. This thesis addresses these gaps by treating GDLs and filter media as true 3D fibrous architectures, rather than simplified porous continua.

This work employed X-ray micro-computed tomography (microCT) to deconstruct realistic 3D geometries and extract key structural descriptors that are otherwise difficult to access. These descriptors formed the basis of a structure-driven framework for linking the fibrous architecture to functional performance across woven GDLs, nonwoven GDLs, and filter media. For woven systems, a structure-property relationship was established between the apparent water contact angle, the equilibrium contact angle of the constituent fibres, and the multiscale hierarchy of the fabric. The model successfully captured anisotropic droplet behaviour and identified that tightly packed weaves with moderately hydrophilic fibres undergo the fastest Cassie-Baxter-to-Wenzel wetting transition. Parametric analysis further demonstrated that tuning yarn packing and fibre-level equilibrium contact angles can achieve superhydrophobic behaviour. In the case of nonwoven systems, a stereological approach was developed to connect 3-D descriptors to lower-dimensional measurements. The findings revealed that standard isotropic

assumptions are inadequate; incorporating orientation-dependent correction terms significantly improves the accuracy of structural estimates. Furthermore, the analysis indicates that recycled carbon fibre nonwovens can form viable structures for GDL applications, given that their anisotropic characteristics are explicitly quantified.

A further contribution of this thesis is the comparison of two complementary routes for nonwoven filter design: machine learning (ML) using experimental datasets, and physics-based simulation using realistic 3D geometry. Three ML models, Gaussian process regression (GPR), artificial neural network (ANN), and decision tree (DT), were trained using literature-derived datasets comprising key structural and operating parameters of fibrous filter media, with an aim to develop a rapid screening tool for selecting suitable filter media for cathode air filtration in FCEVs. Herein, GPR emerged as the most reliable predictor for both filtration efficiency (FE) and pressure drop (PD), showing the highest coefficient of determination (R^2) and the lowest root mean squared error (RMSE) during training and testing. The robustness of the GPR model was further confirmed through validation using commercially available filter media. Furthermore, the GPR model also captured established filtration behaviour, including the characteristic drop in filtration efficiency at the most penetrating particle size (MPPS).

In contrast to the data-driven ML framework, FE and PD simulations based on particle momentum and stokes flow were performed directly on X-ray microCT-reconstructed geometries. After validation against experimental data, the simulations were extended to investigate the change in filtration performance in layered and compressed filter media. Digital twins of compressed filter media were developed using X-ray microCT data and analytically derived structural parameters. Compression levels of as high as 80% revealed a significant increase in FE, while a non-linear response in PD was observed. These findings were used to tailor a stainless-steel fibre filter media for a brake-dust collection device for FCEVs. Consequently, this thesis establishes a unified structure-aware methodology for analysing fibrous materials in FCEV systems. By combining X-ray microCT, stereology, analytical modelling, realistic-geometry simulation, and machine learning, it demonstrates that the performance of both GDLs and filter media is governed by a common principle: function emerges from 3D fibrous architecture. This structure-driven perspective provides a pathway for designing more efficient, durable, sustainable, and application-specific fibrous materials for FCEVs.