STRUCTURE-DRIVEN FUNCTIONAL OPTIMISATION OF FIBROUS MATERIALS FOR FUEL-CELL ELECTRIC VEHICLES: ANALYTICAL AND COMPUTATIONAL APPROACHES

SIDDHARTH SHUKLA



DEPARTMENT OF TEXTILE AND FIBRE ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY DELHI
JUNE 2026

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Structure-Driven Functional Optimisation of Fibrous Materials for Fuel-Cell Electric Vehicles: Analytical and Computational Approaches

by

SIDDHARTH SHUKLA

Submitted
In fulfilment of the requirements of the degree of
Doctor of Philosophy

to the



INDIAN INSTITUTE OF TECHNOLOGY DELHI
JUNE 2026

Certificate

This is to certify that the thesis entitled "**Structure-driven Functional Optimisation of Fibrous Materials for Fuel-cell Electric Vehicles: Analytical and Computational Approaches**" being submitted by **Mr. Siddharth Shukla**, to the Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy** in the Department of Textile and Fibre Engineering, is a record of bonafide research work carried out by him. Mr. Siddharth Shukla has worked under my guidance and supervision and fulfilled all the requirements for the submission of the thesis.

The results contained in this thesis have not been submitted, in part or full, to any other university or Institute for the award of any degree or diploma.

Prof. Amit Rawal

Date

Professor
Department of Textile and Fibre Engineering
Indian Institute of Technology Delhi
Place: Hauz Khas, New Delhi -110016
India

Acknowledgement

It gives me immense pleasure to express my deepest gratitude to my Ph.D. supervisor, Prof. Amit Rawal, for his invaluable guidance, constant support, and encouragement throughout my doctoral journey. His clarity of thought, attention to detail, and commitment to excellence have consistently shaped the direction and quality of my research. His mentorship has not only contributed significantly to the successful completion of this thesis but has also played an important role in my overall academic and professional development. I shall remain forever grateful to him for his patience, trust, and guidance during the many stages of this journey.

I would also like to express my sincere gratitude to my SRC members, Prof. R. Alagirusamy, Prof. Vijaykumar N. Baheti, and Prof. B. K. Satapathy, for their valuable comments, constructive suggestions, and insightful discussions throughout my PhD. Their guidance helped me refine my research objectives and improve the overall quality of this work.

I want to acknowledge Anusandhan National Research Foundation (ANRF), Elofic Industries Limited, and Confederation of Indian Industry (CII) for supporting this research work under the "ANRF-CII Prime Minister Fellowship for Doctoral Research Program". I am particularly grateful to Mr. Kamlesh Koul from Elofic Industries Limited for his mentorship, encouragement, and support during the industrial component of this research. His practical insights and faith in the work helped me understand the relevance of my research from an application-oriented perspective. I would also like to thank Dr. Anuj Shukla, Dr. Sumit Sharma and Dr. Vijay Goud for their assistance and support during my work at Elofic Industries Limited.

I would like to extend my heartfelt gratitude to Prof. Ákos Kukovecz from the University of Szeged, Szeged, Hungary, and Prof. Rhodri Jervis from University College London, UK, for their valuable support in X-ray microCT analysis. Their expertise and cooperation significantly contributed to the structural characterisation aspects of this thesis.

I am also thankful to Prof. Vijay Kumar and Prof. Artem Kulachenko for their valuable help and guidance in the machine learning analysis carried out as part of this research. Their inputs were extremely helpful in strengthening the analytical and predictive components of the work.

I would like to specially acknowledge my colleagues, Mr Danvendra Singh and Mr Alok Kumar Maurya, for their assistance, support, and help at different stages of my research work. Further, I would like to thank the postgraduate student, Ms. Stuti Pandey who helped me during my research work.

I wish to acknowledge all the faculty and staff members of the Department of Textile and Fibre Engineering, IIT Delhi, as well as the Central Research Facility and Nanoscale Research Facility, IIT Delhi, who directly or indirectly contributed to my research work. I extend my special thanks to Mr. Manoranjan Kundu and Mr. Manjeet Singh for their technical assistance during sample characterisation, and testing.

On a personal note, I would like to remember my father, the late Mr Ashok Kumar Shukla, whose belief in me has been one of the strongest sources of strength in my life. His faith, values, and blessings have continued to guide me throughout this journey. Whatever I have been able to achieve carries the imprint of his love and confidence in me.

I would like to express my deepest gratitude to my mother, Mrs. Renu Shukla, for her unconditional love, sacrifices, patience, and constant support. Her strength and encouragement have been central to my personal and academic journey. I am equally thankful to my sister, Ms. Anjali Shukla, for her love, support, and belief in me. Finally, I would like to acknowledge my friends and all those people who trusted me, believed in me, and supported me in different ways during this journey. I am especially thankful to Mrs. Shashi Sony and Mrs. Mani Gupta, for their continuous support, encouragement, and faith in me. Their presence, friendship, and words of confidence have meant more to me than I can adequately express.

Siddharth Shukla

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.

सार

ईंधन-सेल चालित विद्युत वाहन (Fuel Cell Electric Vehicles, FCEVs) स्वच्छ एवं सतत परिवहन प्रणालियों के विकास में महत्वपूर्ण भूमिका निभा रहे हैं। इन वाहनों में प्रयुक्त प्रोटॉन एक्सचेंज मेम्ब्रेन ईंधन सेल (PEMFC) तथा वायु निस्पंदन प्रणालियों का प्रदर्शन काफी हद तक रेशेदार पदार्थों (Fibrous Materials) पर निर्भर करता है। PEMFC में गैस प्रसरण परतें (Gas Diffusion Layers, GDLs) अभिकारकों के परिवहन, जल प्रबंधन, विद्युत संपर्क तथा यांत्रिक समर्थन का कार्य करती हैं, जबकि रेशेदार फ़िल्टर माध्यम वायुजनित कणीय प्रदूषकों को नियंत्रित कर प्रणाली की विश्वसनीयता एवं दक्षता सुनिश्चित करते हैं। यद्यपि इन पदार्थों का प्रदर्शन उनकी त्रि-आयामी (3D) संरचना से नियंत्रित होता है, अधिकांश वर्तमान अध्ययन उन्हें केवल कुछ समष्टिगत मानदंडों, जैसे मोटाई, रंध्रता, क्षेत्रीय घनत्व तथा रेशा व्यास, के आधार पर वर्णित करते हैं। परिणामस्वरूप, संरचना एवं कार्यात्मक प्रदर्शन के मध्य संबंध पूर्णतः स्पष्ट नहीं हो पाता।

इस शोधकार्य का मुख्य उद्देश्य ईंधन-सेल चालित विद्युत वाहनों में प्रयुक्त रेशेदार पदार्थों की वास्तविक त्रि-आयामी संरचना को समझना तथा उसे उनके कार्यात्मक व्यवहार से जोड़ने हेतु एक संरचना-आधारित (Structure-Driven) कार्यप्रणाली विकसित करना है। इस उद्देश्य की पूर्ति हेतु एक्स-रे माइक्रो-कम्प्यूटेड टोमोग्राफी (X-ray Micro-Computed Tomography, MicroCT) का उपयोग कर विभिन्न बुनी (Woven) एवं अबुनी (Nonwoven) रेशेदार संरचनाओं का त्रि-आयामी पुनर्निर्माण किया गया तथा उनसे महत्वपूर्ण संरचनात्मक मानदंडों का निष्कर्षण किया गया। शोध के प्रथम भाग में बुनी हुई गैस प्रसरण परतों की सतही आर्द्रता (Wettability) का अध्ययन किया गया। बुनी हुई संरचनाएँ बहु-स्तरीय एवं पदानुक्रमिक होती हैं, जिनमें धागे स्वयं अनेक रेशों के समूह से निर्मित होते हैं। इस कार्य में एक सैद्धान्तिक मॉडल विकसित किया गया, जो वस्त्र की संरचनात्मक विशेषताओं तथा रेशों के संतुलन संपर्क कोण को वस्त्र के प्रकट जल संपर्क कोण से जोड़ता है। मॉडल द्वारा विभिन्न प्रकार की बुनी संरचनाओं में जल-बूंदों के विषमदिश (Anisotropic) व्यवहार का सफलतापूर्वक वर्णन किया गया। परिणामों से ज्ञात हुआ कि धागों की सघन पैकिंग तथा रेशों की सतही विशेषताओं का उचित संयोजन जल-विकर्षी एवं अतिजल-विकर्षी (Superhydrophobic) व्यवहार प्राप्त करने में महत्वपूर्ण भूमिका निभाता है।

शोध के द्वितीय भाग में अबुनी गैस प्रसरण परतों की संरचनात्मक विशेषताओं के विश्लेषण हेतु एक नवीन स्टीरियोलॉजिकल (Stereological) कार्यप्रणाली विकसित की गई। वर्तमान साहित्य में अधिकांश विश्लेषण समदिश (Isotropic) संरचना की धारणा पर आधारित हैं, जबकि वास्तविक

अबुनी रेशेदार पदार्थों में रेशों का अभिविन्यास प्रायः विषमदिश (Anisotropic) होता है। विकसित पद्धति द्वारा यह प्रदर्शित किया गया कि संरचनात्मक मापदंडों के सटीक निर्धारण के लिए अभिविन्यास-निर्भर सुधार कारकों को सम्मिलित करना आवश्यक है। अध्ययन से यह भी स्पष्ट हुआ कि पुनर्चक्रित कार्बन रेशा आधारित अबुनी संरचनाएँ गैस प्रसरण परतों के लिए संभावित विकल्प बन सकती हैं, बशर्ते उनकी विषमदिश संरचनात्मक विशेषताओं का उचित परिमाणीकरण किया जाए।

शोध के तृतीय भाग में ईंधन-सेल वायु निस्पंदन हेतु प्रयुक्त रेशेदार फ़िल्टर माध्यमों के डिज़ाइन के लिए मशीन लर्निंग (Machine Learning, ML) आधारित दृष्टिकोण विकसित किया गया। साहित्य से संकलित प्रायोगिक आँकड़ों के आधार पर Gaussian Process Regression (GPR), Artificial Neural Network (ANN) तथा Decision Tree (DT) मॉडल प्रशिक्षित किए गए। इन मॉडलों का उपयोग निस्पंदन दक्षता (Filtration Efficiency, FE) तथा दाब-पतन (Pressure Drop, PD) के पूर्वानुमान हेतु किया गया। परिणामों से ज्ञात हुआ कि GPR मॉडल ने सर्वोत्तम प्रदर्शन प्रदर्शित किया तथा प्रशिक्षण, परीक्षण एवं स्वतंत्र सत्यापन के दौरान उच्च सटीकता बनाए रखी। इसके अतिरिक्त, मॉडल ने सर्वाधिक प्रवेशी कण आकार (Most Penetrating Particle Size, MPPS) पर निस्पंदन दक्षता में होने वाले विशिष्ट परिवर्तन को भी सफलतापूर्वक निरूपित किया। शोध के चतुर्थ भाग में भौतिकी-आधारित अनुकरण (Physics-Based Simulation) का उपयोग कर रेशेदार फ़िल्टर माध्यमों के निस्पंदन व्यवहार का अध्ययन किया गया। एक्स-रे माइक्रोCT से प्राप्त यथार्थवादी त्रि-आयामी संरचनाओं पर आधारित डिजिटल मॉडल विकसित किए गए तथा कण गतिकी एवं स्टोक्स प्रवाह सिद्धांतों का उपयोग करते हुए निस्पंदन दक्षता एवं दाब-पतन का अनुकरण किया गया। प्रयोगात्मक सत्यापन के पश्चात इस पद्धति का उपयोग परतदार तथा संपीडित फ़िल्टर माध्यमों के अध्ययन के लिए किया गया। परिणामों से ज्ञात हुआ कि संपीड़न बढ़ने पर निस्पंदन दक्षता में उल्लेखनीय वृद्धि होती है, जबकि दाब-पतन का परिवर्तन गैर-रैखिक प्रकृति का होता है। इन निष्कर्षों के आधार पर ईंधन-सेल चालित वाहनों हेतु ब्रेक-धूल संग्रहण उपकरण के लिए स्टेनलेस स्टील रेशा आधारित फ़िल्टर माध्यम का डिज़ाइन किया गया।

समग्र रूप से यह शोधप्रबंध रेशेदार पदार्थों के विश्लेषण एवं डिज़ाइन के लिए एक एकीकृत संरचना-सजग (Structure-Aware) दृष्टिकोण प्रस्तुत करता है, जिसमें एक्स-रे माइक्रोCT, स्टीरियोलॉजी, विश्लेषणात्मक मॉडलिंग, यथार्थवादी ज्यामिति-आधारित अनुकरण तथा मशीन लर्निंग का समन्वित उपयोग किया गया है। अध्ययन से यह सिद्ध होता है कि गैस प्रसरण परतों तथा फ़िल्टर माध्यमों का कार्यात्मक प्रदर्शन उनकी त्रि-आयामी रेशेदार संरचना द्वारा नियंत्रित होता है।

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Nomenclature

Symbol	Description
α_f	Inclination angle formed by liquid meniscus on filament
α_f^{max}	Maximum inclination angle formed by liquid meniscus on filament
α_{lr}	Learning rate
α_{wf}	Inclination angle formed by liquid meniscus on weft yarn
α_{wp}	Inclination angle formed by liquid meniscus on warp yarn
α_{wp}^{max}	Maximum inclination angle formed by liquid meniscus on warp yarn
β	Associated coefficients of basis functions
$\hat{\beta}$	Optimised β
γ_{LV}	Surface tension of liquid
δ	Acute angle between the two neighbouring filaments
δ_c	Constrictivity
ΔG^o	Gibbs free energy
$\Delta\varepsilon$	Compressive strain
ϵ	Porosity
ε	Noise in the observations
ϵ_g	Gravimetric porosity
ϵ_X	Porosity obtained from X-ray microCT
ζ	Out-of-plane fibre orientation angle
ζ'	Out-of-plane orientation angle after compression
ζ_X	Polar angle of fibre with X axis
ζ_Y	Polar angle of fibre with Y axis
η	Dynamic viscosity
$\boldsymbol{\theta}$	Set of hyperparameters
$\widehat{\boldsymbol{\theta}}$	Optimised $\boldsymbol{\theta}$
θ^*	Apparent contact angle
$\theta^*_{(wf,WF)}$	Apparent contact angle on the weft-rich face (weft-axis view)
$\theta^*_{(wf,WP)}$	Apparent contact angle on the warp-rich face (weft-axis view)
$\theta^*_{(wp,WF)}$	Apparent contact angle on the weft-rich face (warp-axis view)
$\theta^*_{(wp,WP)}$	Apparent contact angle on the warp-rich face (warp-axis view)
θ_a	Advancing contact angle of filament
θ_a^{wf}	Advancing contact angle of weft yarn
θ_a^{wp}	Advancing contact angle of warp yarn
θ_d	Dynamic contact angle
θ_{eq}	Equilibrium contact angle
θ_{eq}^{wf}	Equilibrium contact angle of weft yarn
θ_{eq}^{wp}	Equilibrium contact angle of warp yarn
θ_{LV}	Equilibrium contact angle between air and the liquid
θ_r	Receding contact angle of filament
θ_r^{wf}	Receding contact angle of weft yarn
θ_r^{wp}	Receding contact angle of warp yarn
θ^*_{wf}	Apparent contact angle of a weft yarn
θ^*_{wp}	Apparent contact angle of a warp yarn
θ^*_y	Apparent contact angle of yarn
κ	Helical angle of the fibres
λ	Eigenvalue
λ_{reg}	Regularisation strength

λ_w	The number of water molecules per sulfonic acid group
μ	Friction coefficient
ν_t	Out-of-plane Poisson's ratio of the nonwoven
ξ	Ratio of particle diameter to fibre diameter
ρ_f	Density of fibre
ρ_g	Density of fluid
ρ_p	Density of particle
ρ_w	Density of water
σ^2	Variance
$\hat{\sigma}^2$	Optimised σ^2
τ	Tortuosity
φ	In-plane fibre orientation angle
ϕ_{wp}	Angle of lenticular arc in warp yarn
χ	Spacing ratio
χ^*	Spacing ratio
χ_1^*	Spacing ratio at fabric level
χ_2^*	Spacing ratio at yarn level
χ_3^*	Spacing ratio at fibre level
χ_f	Angle between the axis of two fibres
$\psi_{d,adv}$	Liquid-solid area fraction during droplet displacement while advancing
$\psi_{d,rec}$	Liquid-solid area fraction during droplet displacement while receding
ω	Coverage parameter
$\Omega(\zeta, \varphi)$	Probability density function for fibre orientation distribution
$\Omega(\zeta\text{^}', \varphi)$	Modified fibre orientation distribution function after compression
$\Omega(\varphi)$	In-plane fibre orientation distribution function
Ω_o	Orientation distribution function for an isotropic structure
$\langle \boldsymbol{A} \rangle$	Second-order orientation tensor of nonwoven
$\bar{A}$	Average areal intercept, A_A/N_A
$\boldsymbol{A}$	Second-order tensor of a single fibre
A_A	Area fraction. Area of intercepted features per unit test area
A_{app}	Total apparent contact length
A_f	Fibre area fraction
A_t	Planar area of intercepted features or test area
a_{wf}	Major diameter of weft yarn
a_{wp}	Major diameter of warp yarn
a_y	Major diameter of yarn
$b^{(out)}$	Bias for the neuron in the output layer
b_j^l	Bias for the neuron j
b_{wf}	Minor diameter of weft yarn
b_{wp}	Minor diameter of warp yarn
b_y	Minor diameter of yarn
C	Concentration
C_c	Cunningham correction factor
c_t	Empirical twist parameter
$\bar{d}_{TCL}$	Average diameter of the TCL
$D_{o,g}$	Intrinsic diffusivity of gas
$D_{o,p}$	Intrinsic diffusivity of particle
D_{eff}	Effective diffusivity
d_f	Fibre diameter
d_{max}	Major diameter of the elliptical fibre cut end
d_p	Particle diameter

d_{po}	Pore diameter
d_{wf}	Diameter of the parametric circle of warp yarn
d_y	Diameter of yarn with circular cross-section
E	Electric field
E^o	Cell potential
E_d	Filtration efficiency from diffusion
E_f	Single-fibre filtration efficiency
E_{icp}	Filtration efficiency from interception
E_{imp}	Filtration efficiency from inertial impaction
$\mathcal{F}$	Faraday's constant
f	Activation function
F	Forces acting on the particle
$f(x)$	Latent function
f_1	Liquid-solid fractional contact area
$f_1^{(wf,WF)}$	Area fraction of liquid-solid (weft yarn) on weft face
$f_1^{(wf,WP)}$	Area fraction of liquid-solid (weft yarn) on warp face
$f_1^{(wp,WF)}$	Area fraction of liquid-solid (warp yarn) on weft face
$f_1^{(wp,WP)}$	Area fraction of liquid-solid (warp yarn) on warp face
f_1^f	Area fraction of liquid-solid (yarn tow)
f_1^{wf}	Area fraction of liquid-solid (weft yarn)
f_1^{wp}	Area fraction of liquid-solid (warp yarn)
f_{11}^{wf}	Area fraction of liquid-solid (weft yarn) in yarn configuration I
f_{11}^{wp}	Area fraction of liquid-solid (warp yarn) in yarn configuration I
f_{12}^{wf}	Area fraction of liquid-solid (weft yarn) in yarn configuration II
f_{12}^{wp}	Area fraction of liquid-solid (warp yarn) in yarn configuration II
f_{13}^{wf}	Area fraction of liquid-solid (weft yarn) in yarn configuration III
f_{13}^{wp}	Area fraction of liquid-solid (warp yarn) in yarn configuration III
f_2	Liquid-air fractional contact area
f_2^f	Area fraction of liquid-air contact on yarn tow
f_{21}	Area fraction of liquid-air in yarn configuration I
f_{22}	Area fraction of liquid-air in yarn configuration II
f_{23}	Area fraction of liquid-air in yarn configuration III
F_f	Force applied by the fibre in Wilhelmy's method
f_p	Second-order orientation parameter
F_T	Other external forces on the particle
f_x, f_y, f_z	External body-force components in X, Y and Z direction
FE	Filtration efficiency
FE_{train}	Transformed filtration efficiency
g	Acceleration due to gravity
g_p	Fourth-order orientation parameter
h	Thickness of nonwoven material/ filter media
$\boldsymbol{H}$	Set of basis function
$h(x)^T$	Transpose of a matrix of basis functions
h_c	Reduced thickness after compression
$\boldsymbol{I}$	Identity matrix
J	Diffusional flux
$k(x, x')$	Covariance function between two set of inputs x and x'
$k(x, x'\|\boldsymbol{\theta})$	Covariance function between two set of inputs x and x' at specific $\boldsymbol{\theta}$
$\boldsymbol{K}(X, X\|\boldsymbol{\theta})$	Covariance function at specific $\boldsymbol{\theta}$
k_B	Boltzmann's constant

Ku	Kuwabara hydrodynamic factor
$\mathcal{L}$	Loss function / Mean squared error
$\bar{L}$	Average lineal intercept, L_L/N_L
$\mathcal{L}_1$	L1 loss
$\mathcal{L}_2$	L2 loss
L_A	Length of lineal elements per unit test area
L_c	Characteristic length scale
L_f	Length of fibre segment
L_L	Lineal fraction. Length of lineal intercepts per unit length of test line
L_{po}	Length of pore path
$\mathcal{L}_{reg}$	Regularisation penalty
L_t	Length of test line
L_T	Total loss signal
L_V	Length of lineal elements (fibres) per unit test volume
L_X	Dimension of cuboidal nonwoven material along the X-direction
L_Y	Dimension of cuboidal nonwoven material along the Y-direction
L_Z	Dimension of cuboidal nonwoven material along the Z-direction
m_A	Mass per unit area
m_p	Particle mass
MSE_{left}	Mean squared error of data points in the left subsets
MSE_{parent}	Mean squared error of data points in the parent subsets
MSE_{right}	Mean squared error of data points in the right subsets
n	Number of observations
$N(0,\sigma^2)$	Normal distribution
$N(\varphi)$	Number of fibres that fall within a bin of width $\Delta\varphi$
$n_{\|\|}$	Number of parallel test planes
n_1	Repeats of yarn configuration I in a weave unit
n_2	Repeats of yarn configuration II in a weave unit
n_3	Repeats of yarn configuration III in a weave unit
N_A	Number of interceptions of features per unit test area
N_a	Number of fibre segments intersecting a single test plane
n_e	Number of electrons transferred in a reaction
N_f	Number of features (as opposed to points)
N_L	Number of interceptions of features per unit length of test line
N_n	Total number of neuron
N_P	Number of point elements or test points
N_{rep}	Total yarn configuration repeats in a weave unit
N_t	Number of vertical test lines intersecting a single fibre segment
n_t	Total number of vertical test lines
N_V	Number of features per unit test volume
$\boldsymbol{P}$	Unit vector along fibre axis
P_x, P_y, P_z	Component of $\boldsymbol{P}$ along the X, Y and Z axes, respectively
$\langle P_x^2 \rangle, \langle P_y^2 \rangle, \langle P_z^2 \rangle$	Principal diagonal elements of $\langle \boldsymbol{A} \rangle$
p	Pressure
$P(d_p)$	Probability of occurrence of a pore with a diameter $\leq d_p$
$P(y_i \| f(x_i), x_i)$	Likelihood
$P(y\|X)$	Probability of observed data
P_5	5th percentile
P_{95}	95th percentile
P_A	Number of feature intersections per unit area of the test plane
P_A^X	Fibre intersections per unit area of the sectioning planes perpendicular to the X-axes
P_A^Y	Fibre intersections per unit area of the sectioning planes perpendicular to the Y-axes

P_L	Number of intersections per unit length of a test line
P_L^X	Point intersections of fibre per unit length of test lines drawn along the X direction
P_L^Y	Point intersections of fibre per unit length of test lines drawn along the Y direction
P_P	Point fraction. Number of points (in areal feature) per test point
P_V	Number of particles per unit volume
PD	Pressure drop
Pe	Peclet number
Q	Charge on the particle
R^2	Coefficient of determination
r_f	Radius of fibres/filaments
R_f	Radius of curvature of the liquid meniscus between filaments
r_{np}	Radius of nanoparticles
r_p	Radius of spherical particle
r_{wf}	Radius of filament in weft yarn
r_{wp}	Radius of filament in warp yarn
R_{wp}	Radius of curvature of the liquid meniscus between warp yarns
r_y	Radius of yarns
r_ψ	Roughness of wetted solid-liquid interface
Re	Reynolds number
S	Surface or interface area (not necessarily planar)
$\bar{S}$	Average surface area, S_V/N_V
s_f	Half-spacing between two neighbouring filaments
S_f	Wetted perimeter of the fibre
s_{leaf}	Leaf size
s_{np}	Half-spacing between two neighbouring nanoparticles
S_T	Total surface area of all cylindrical fibres within the test volume
S_V	Surface area of an interface per unit volume
s_{wf}	Weft yarn spacing
s_{wf}	Inter-yarn distance between weft yarn
s_{wp}	Warp yarn spacing
s_{wp}	Inter-yarn distance between warp yarn
s_y	Inter-yarn distance
s_y	Half of edge-to-edge spacing between yarns
stk	Stokes number
T	Absolute temperature
T_y	Twist per unit length
T_y^{wf}	Twist per unit length in weft yarn
T_y^{wp}	Twist per unit length in warp yarn
$\mathbf{u}$	Fluid velocity
U	Superficial/Face velocity
u_x	Component of $\mathbf{u}$ in X-direction
u_y	Component of $\mathbf{u}$ in Y-direction
u_z	Component of $\mathbf{u}$ in Z-direction
v	Eigen vector corresponding to eigenvalue
$\bar{V}$	Average volume, V_V/N_V
$V(\bar{y}_*)$	Predictive variance
V_{y_m}	Maximum possible yarn packing fraction of a twisted yarn
V_{y_o}	Minimum yarn packing fraction of the twisted yarn
V_{drop}	Volume of droplet
V_f	Fibre volume fraction

V_f'	Modified fibre volume fraction after compression
$\mathbf{v}_p$	Particle velocity
V_t	Test volume
V_V	Volume fraction
V_y	Yarn packing fraction
V_y^{wf}	Weft yarn packing fraction
V_y^{wp}	Warp yarn packing fraction
$W(t)$	Brownian motion
w_{it}	Weight in the iteration, it
$w_j^{(out)}$	Weight of the output layer
w_{jk}^l	weight of the connecting neuron k in layer $l-1$ to neuron j in layer l
wf	Weft yarn
WF	Weft-rich face of the fabric
wp	Warp yarn
WP	Warp-rich face of the fabric
X	Input data
x	An element of X
x'	An element of X other than x
x_*	New input (to be predicted)
X_{FE}	Matrix of input data for FE
X_{PD}	Matrix of input data for PD
y	Response variable
$\bar{y}_*$	Predictive mean response from GPR model
$\bar{y}_i$	Predicted response from ANN model
$\bar{y}_{leaf}$	Mean output from the final leaf or subset
$y_{(FE,PD)}$	Response variable FE or PD
y_{left}	Number of data points in the left subsets
y_{parent}	Number of data points in the parent subsets
y_{right}	Number of data points in the right subsets
z_j^l	Intermediate output
z_j^Γ	Output from the last hidden layer Γ
z_k^{l-1}	input from the previous layer $l-1$

List of Acronyms

Abbreviation	Description
3D	Three-dimensional
1D	One-dimensional
2D	Two-dimensional
BP	Bipolar plates
CC	Carbon cloth
CCM	Catalyst-coated membrane
CL	Catalyst layer
CO	Carbon monoxide
Co	Cobalt
EJ	Explicit Jump
FC	Fuel cell
FE	Filtration efficiency
FCEVs	Fuel cell electric vehicles
FCEVs	Fuel cell electric vehicles
GDLs	Gas diffusion layers
GE	General Electric
HOR	Hydrogen oxidation reaction
ICEs	Internal combustion engine
LBM	Lattice Boltzmann method
MEA	Membrane electrode assembly
microCT	Micro-computed tomography
MIL	Mean intercept length
ML	Machine learning
Mn	Manganese
MPL	Microporous layer
MPPS	Most penetrating particle size
OCP	Open circuit potential
ODF	Orientation distribution function
ORR	Oxygen reduction reaction
PAAM	Polyacrylamide
PBI	Polybenzimidazole
PEI	PEI
PEK	Polyetherketone
PEM	Proton exchange membrane
PEMFCs	Proton-exchange membrane fuel cells
PESF	Polyether sulfone
PET	Polyethylene terephthalate
PFCA	Perfluorocarboxylic acid
PFSA	Perfluorosulfonic acid
PI	Polyimide
Pt/C	Carbon black supported platinum
PTFE	Polytetrafluoroethylene
PTFE-g-TFS	Polytetrafluoroethylene-grafted trifluorostyrene
PtRh	Platinum-rhodium
PtRu	Platinum-ruthenium
PVA	Polyvinyl alcohol
PVDF-g-PSSA	Polyvinylidene fluoride-grafted polystyrene sulfonic acid

rCFs	Recycled carbon fibres
SEM	Scanning electron microscopy
SPEEK	Sulfonated poly (ether-ether-ketone
SPPBP	Sulfonated poly(4-phenoxybenzoyl-1,4-phenylene)
SPSU	Sulfonated polysulfone
vCFs	Virgin carbon fibres
VOCs	Volatile organic compounds
VOF	Volume-of-fluid
VOI	Volume of interest