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## Research Article

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# Gas Diffusivity in Fibrous Gas Diffusion Layers: Linking Pore Structure to Transport

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## Abstract

Gas transport through gas diffusion layers strongly influences the performance of PEM fuel cells. The effective gas diffusivity depends on microstructural characteristics, particularly pore size distribution, which conventional porosity-based models do not capture. Although numerical approaches can represent these effects, they remain computationally expensive. This study develops a new model based on effective medium theory to predict gas diffusivity in dry GDLs. A key feature of the model is the development of a pore size transformation, in which porosimetry-based pore size distributions obtained from standard porosimetry are converted from an equivalent cylindrical pore representation into an equivalent unit cell length distribution representative of the fibrous GDL structure. The transformed distribution is then used to construct a statistical three-dimensional network of unit cells for evaluating diffusive transport.

To reduce computational cost, a new compact correlation is developed using the overall porosity and the transformed pore size distribution. The correlation reproduces the numerical model with high accuracy while providing a simple form suitable for rapid estimation and implementation in larger-scale models. The proposed model predictions are validated against relative diffusivity measurements obtained using the symmetrical modified Loschmidt cell method and literature data, showing good agreement with a maximum relative difference of 8%.

Keywords: Gas diffusivity; Gas diffusion layer; Symmetrical modified Loschmidt cell; Pore size distribution

## 1. Introduction

Gas transport through the gas diffusion layer (GDL) is a key source of mass transfer resistance in proton exchange membrane fuel cells (PEMFCs), directly affecting overall cell performance. The effective diffusivity of gases through the porous structure of the GDL depends not only on porosity but also on microstructural characteristics such as pore size distribution and fiber diameter. Capturing the influence of these structural features is essential for accurately predicting transport behavior and guiding the design of GDL materials.

Several experimental techniques have been used to measure the effective gas diffusivity in porous media. Among these, the symmetrical modified Loschmidt cell (SMLC) method (Mohammadi et al. 2025), (Chan et al. 2012) provides a direct measurement of diffusivity by tracking concentration evolution under controlled conditions. Compared to alternative approaches (Yakovlev et al. 2022), the SMLC method enables measurements under well-defined conditions without additional assumptions or imposed operating constraints; for example, it allows characterization of the GDL in its uncompressed state, providing a more representative assessment of the intrinsic transport properties of the material.

From a modeling perspective, analytical approaches are attractive due to their simplicity and low computational cost. However, conventional models, often expressed solely as functions of porosity, an aggregate measure of the medium morphology, tend to overpredict gas diffusivity (Zamel et al. 2010), as porosity alone is insufficient to capture microstructural effects. To address this limitation, fractal-based models (Shi et al. 2010), (Wu et al. 2011) have been proposed in the literature, which incorporate pore size distribution (PSD) to better represent the hierarchical nature of porous media. However, these fractal models rely on empirical geometric parameters that cannot be independently determined, which limits their predictive capability. More advanced analytical models based on effective medium theory use a “unit cell” representation of the porous structure and have been developed to overcome these challenges. In particular, studies from our group on catalyst layers (Salari et al. 2018) and microporous layers (MPLs) (Andisheh-Tadbir et al. 2015), as well as a recent model for GDLs (Mohammadi et al. 2026), have demonstrated that incorporating microstructural parameters can significantly improve

prediction accuracy compared to traditional correlations. In the latter, a physically based formulation for tortuosity was developed using pore size distribution and structural parameters and subsequently used to estimate gas diffusivity with good agreement against experimental data. Although these models provide accurate estimates for dry GDLs, they are limited in their ability to predict diffusivity under partially saturated conditions because they do not explicitly account for pore interconnectivity and its impact on transport pathways.

Numerical approaches, such as pore network modeling (PNM) (Guan et al. 2023) and direct numerical simulations (DNS), including lattice Boltzmann methods (Jiang et al. 2022), (Farzaneh et al. 2021), offer a more detailed representation of transport processes in porous media. Such approaches have been applied to fibrous GDL structures to examine the relationship between pore-scale morphology, transport pathways, and effective transport properties (Tranter et al. 2018), (García-Salaberri 2022). In these approaches, the computational domain is typically constructed either from three-dimensional imaging techniques, such as X-ray computed tomography (XCT), or through algorithmic reconstruction methods that mimic the statistical properties of the microstructure. PNM simplifies the structure into a network of pores and throats, enabling efficient simulation of transport processes, while DNS resolves transport directly within the pore space, providing highly accurate results. Comparative studies in the literature (Jung et al. 2021) have shown that both approaches can capture gas transport behavior accurately. However, their computational cost and the requirement for detailed structural input limit their applicability for rapid evaluation and integration into larger-scale models. This creates a need for modeling approaches that retain key microstructural features while remaining computationally efficient. A summary of the key modeling approaches for predicting gas diffusivity in GDLs, along with their main advantages and limitations, is provided in Table 1.

Table 1 Summary of modeling approaches for predicting gas diffusivity in GDLs.

| Model type | Method                                                                | Description                                                                                                       | Advantages                                                                                          | Limitations                                                                                                                                       |
|------------|-----------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| Analytical | Porosity-based models (Bruggeman 1935)                                | Express diffusivity solely as a function of porosity.                                                             | Simple, computationally negligible, easy to implement in system-level models.                       | Consistently overpredicts diffusivity; cannot distinguish between different microstructures with the same porosity.                               |
|            | Fractal models (Shi et al. 2010), (Wu et al. 2011)                    | Represent pore space as a bundle of tortuous capillaries; incorporate pore size distribution via fractal scaling. | Include microstructural information beyond porosity; can capture effects of pore size distribution. | Require empirical fitting parameters (fractal dimension, tortuosity dimension) that cannot be determined a priori; often overpredict diffusivity. |
|            | Effective medium models (Salari et al. 2018), (Mohammadi et al. 2026) | Simplify the microstructure to a repeating geometric unit cell.                                                   | Physically grounded, low computational cost, good accuracy for dry conditions.                      | Do not explicitly capture pore interconnectivity, which limits prediction under partially saturated conditions.                                   |
| Numerical  | Pore network model (Guan et al. 2023)                                 | Simplify the microstructure to spherical pores and cylindrical interconnections.                                  | Lower computational cost than direct numerical simulations.                                         | Pore extraction artifacts near boundaries can lead to inaccurate estimates under partially saturated conditions.                                  |
|            | Direct numerical simulation (Jiang et al. 2022),                      | Solve transport directly on a voxel grid.                                                                         | Highest accuracy; captures pore geometry and tortuosity.                                            | High computational cost; requires expensive imaging; resolution limits for small pores.                                                           |

In this study, a new model based on effective medium theory is developed to estimate relative gas diffusivity in dry GDLs using pore size distribution as a primary structural input. A key contribution of the present work is the development of a pore size transformation that converts porosimetry-based pore size distributions, originally interpreted using an equivalent cylindrical pore geometry, into an equivalent unit cell length distribution representative of the fibrous GDL structure. The transformed distribution is then used to construct a statistical three-dimensional resistance network of unit cells, in which directional diffusive resistances are evaluated to account for the anisotropic transport behavior of GDLs. In addition, a compact correlation is developed to relate gas diffusivity to key structural parameters, enabling efficient estimation and implementation in larger-scale models. Experimental measurements of gas diffusivity are performed using the SMLC method and are used, together with literature data, to validate the proposed approach. The main contributions of this study can be summarized as follows:

- Development of a pore size transformation method to convert porosimetry-based pore size distributions into equivalent unit cell length distributions consistent with the fibrous GDL representation.
- Development of a new model based on effective medium theory to predict anisotropic gas transport in dry GDLs while incorporating pore size distribution effects.
- Development of a compact correlation for gas diffusivity as a function of overall porosity and transformed PSD parameters.

## **2. Pore size distribution characterization**

The relative diffusivity of GDLs depends not only on their porosity but also on pore size distribution. Therefore, the pore structure must be characterized before it can be incorporated into the diffusivity model. In this study, the pore structure of GDLs was quantified using standard porosimetry (Gostick et al. 2006) with octane as the wetting liquid, using a Standard Porosimeter 3.2 instrument at the Fuel Cell Research Laboratory (FCReL), Simon Fraser University.

This approach relies on establishing capillary equilibrium between the GDL and a reference sample with a known saturation–capillary pressure relationship. The measurement procedure

can be summarized as follows. A GDL is sandwiched between two reference porous media samples, and the entire assembly is fully saturated with octane. As evaporation gradually reduces the liquid content, the mass of each component is recorded at regular intervals, allowing the saturation level of each layer to be determined. Because the saturation–capillary pressure relationship is predefined for the reference sample, the corresponding capillary pressure can be obtained at each measurement point.

Since the GDL and reference samples are in capillary equilibrium, the capillary pressure within the GDL is assumed to be equal to that of the reference sample. By tracking saturation over time, the complete saturation–capillary pressure curve for the GDL is constructed. To relate the capillary pressure to an equivalent pore size, the Washburn equation (Washburn 1921) is applied, as shown schematically in Fig. 1, converting capillary pressure values into pore radius under the assumption of cylindrical pore geometry:

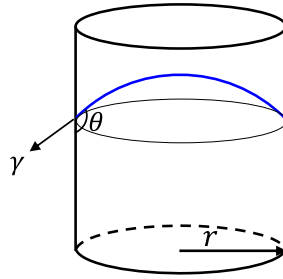


Fig. 1 Schematic representation of the capillary model used in the Washburn equation, showing the pore radius  $r$ , surface tension  $\gamma$ , and contact angle  $\theta$ .

$$p_c = \frac{2\gamma \cos \theta}{r} \quad (1)$$

where,  $p_c$  is the capillary pressure [ $kPa$ ],  $\gamma$  is the surface tension of the working fluid (octane:  $21 \text{ mN/m}$ ),  $\theta$  is the contact angle ( $0^\circ$  for octane), and  $r$  is the equivalent pore radius [ $\mu m$ ]. The resulting porosimetry-based pore size distribution is reported as cumulative pore volume versus equivalent cylindrical pore radius. Although the porosimetry-based pore size distribution provides a useful characterization of the pore structure, it is based on an equivalent cylindrical pore representation. This assumption may not accurately represent the fibrous structure of GDLs and neglects important geometric features such as fiber curvature. Therefore, a more

representative geometrical description of the GDL microstructure is required for modeling purposes.

In this study, the GDL is modeled as an assembly of cylindrical carbon fibers with a uniform diameter of 8  $\mu\text{m}$ . This value was selected as a representative mean, since experimental data show that the diameter of carbon fibers in common GDL materials typically falls within the range of 7.5–8.5  $\mu\text{m}$  (Sadeghifar et al. 2013), (Ozden et al. 2019). The fibers are also arranged orthogonal to each other, following reference (Sadeghifar et al. 2013), as shown in Fig. 2a. The present geometrical representation is developed primarily for paper-type GDLs; its application to felt- or cloth-type GDLs should therefore be interpreted as an approximate representation rather than a direct reconstruction of the fiber arrangement. Based on this representation, the complex porous structure of the GDL is reduced to a repeating unit cell (Fig. 2b). The proposed unit cell represents the local pore space formed between neighboring carbon fibers. The model captures microstructural variability by changing the cell length ( $2l$ ), while the fiber diameter ( $d$ ) remains fixed. The local porosity of the selected unit cell is given by:

$$\phi = 1 - \frac{\pi d}{8l} \quad (2)$$

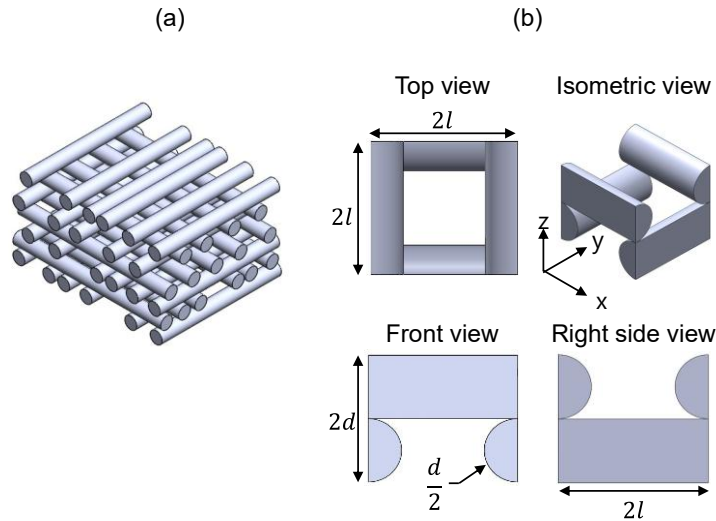


Fig. 2 a) Simplified representation of the fibrous structure of a GDL b) Selected unit cell to represent the pore space between carbon fibers. The unit cell is constructed from periodically arranged cylindrical fibers of constant diameter ( $d$ ), with a length of  $2l$ . In the proposed morphological model, variations in pore size are captured by changing  $l$ , whereas the fiber diameter  $d$  is kept constant.

The unit cell adopted in the present model has a different geometrical representation than the equivalent cylindrical pore assumption used in standard porosimetry. Therefore, the porosimetry-based pore size distribution, originally expressed in terms of equivalent pore radius, must be transformed into an equivalent distribution of unit cell lengths. This transformation allows the porosimetry-based measured pore structure to be used consistently within the selected fibrous unit cell geometry.

To perform the pore size transformation, a capillary model is developed based on the proposed unit cell geometry. The unit cell is assumed to be initially fully saturated with octane, while air gradually invades the unit cell during desaturation, consistent with the drainage process occurring in standard porosimetry measurements. Gravitational effects are neglected due to the small Bond number, and the process is assumed to be quasi-static with a constant contact angle of zero. For a unit cell with half-length  $l$  and fiber diameter  $d$ , a receding gas–liquid meniscus is formed between the parallel fibers as shown in Fig. 3.

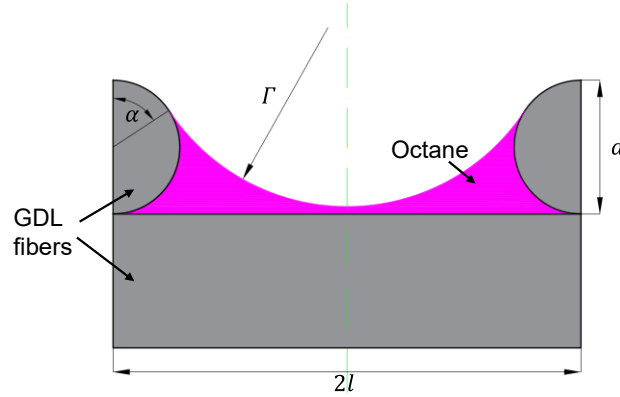


Fig. 3 Schematic of the meniscus in the unit cell.

Based on geometric considerations, the meniscus radius of curvature ( $\Gamma$ ) is expressed as:

$$\Gamma = \frac{l - 0.5d \sin \alpha}{\sin \alpha} \quad (3)$$

where,  $\alpha$  is the geometric wetting angle, describing the meniscus position in the unit cell. For a given unit cell,  $l$  and  $d$  are fixed; therefore, the radius of curvature ( $\Gamma$ ) depends only on  $\alpha$ . Taking the derivative of  $\Gamma$  with respect to  $\alpha$  shows that the minimum radius of curvature occurs

at  $\alpha = \frac{\pi}{2}$ , independent of the unit cell length. This condition represents the maximum capillary pressure that the meniscus can sustain before air invades the pore. However, this maximum-pressure condition may not always be reached. For certain unit cell sizes, the meniscus contacts the next layer of fibers before the wetting angle reaches  $\frac{\pi}{2}$ . In this case, the meniscus undergoes a geometric transition, and invasion occurs at a lower capillary pressure. The corresponding transition angle, ( $\alpha_{tr}$ ), is determined from the geometric constraint of the unit cell as:

$$\alpha_{tr} = 2\arctan\left(\frac{d}{l}\right) \quad (4)$$

Therefore, the wetting angle used to determine the capillary pressure of each unit cell is taken as the smaller of the transition angle and the angle corresponding to the minimum radius of curvature ( $\alpha = \frac{\pi}{2}$ ), as follows:

$$\alpha = \begin{cases} \alpha_{tr}, & \alpha_{tr} < \frac{\pi}{2} \\ \frac{\pi}{2}, & \alpha_{tr} \geq \frac{\pi}{2} \end{cases} \quad (5)$$

After selecting the appropriate wetting angle for each unit cell, the wetting angle is substituted into Eq. (3) to obtain the corresponding radius of curvature ( $\Gamma$ ). The capillary pressure for air invasion is then calculated using the Young–Laplace equation:

$$p_c = \frac{\gamma}{\Gamma} \quad (6)$$

where  $\gamma$  is the surface tension of octane. Repeating this calculation over a range of unit cell lengths gives the capillary pressure–unit cell length relationship, which is used to map the porosimetry-based pore radius distribution to the selected unit cell geometry. The overall PSD transformation procedure is summarized in Fig. 4. Fig. 4a shows the conceptual transformation from the porosimetry-based cylindrical pore representation to the equivalent unit cell length representation used in the present model.

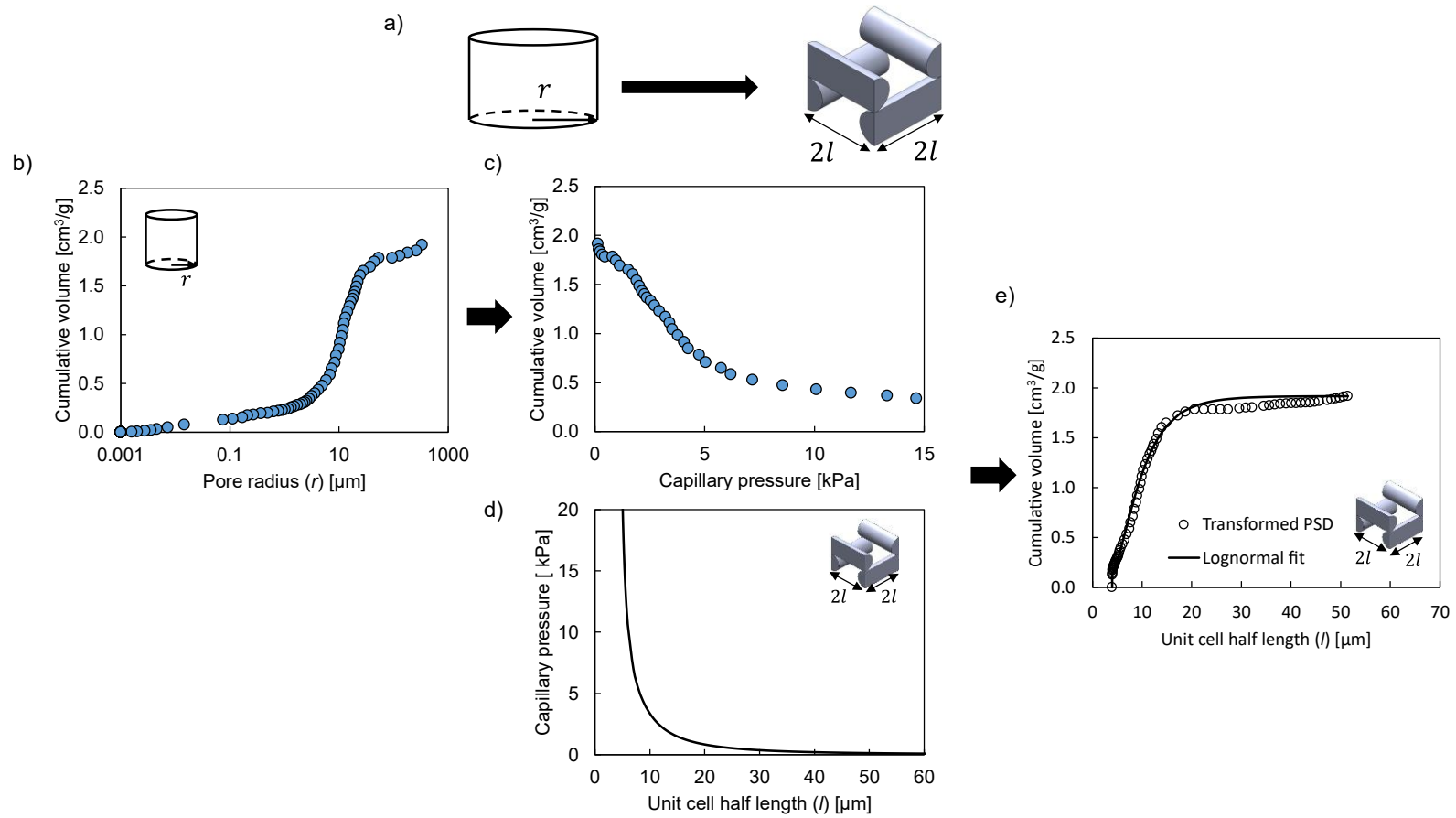


Fig. 4 Schematic representation of the PSD transformation procedure. (a) Conceptual transformation from the porosimetry-based cylindrical pore representation to the equivalent unit cell length representation used in the present model. (b) Original porosimetry-based pore size distribution, reported as cumulative pore volume versus equivalent cylindrical pore radius. (c) Conversion of equivalent pore radius to capillary pressure using the Washburn equation. (d) Capillary pressure–unit cell length relationship obtained from the capillary model developed for the selected fibrous unit cell. (e) Transformed pore size distribution obtained by combining the mappings in (c) and (d), where the cumulative pore volume is expressed as a function of the equivalent unit cell length, along with the fitted log-normal distribution.

The porosimetry-based PSD is originally reported as cumulative pore volume versus equivalent cylindrical pore radius (Fig. 4b). Using the Washburn equation (Eq. (1)), each pore radius is first converted to the corresponding capillary pressure (Fig. 4c). Then, using the capillary model developed in this study, the capillary pressure corresponding to each unit cell length is calculated, as shown in Fig. 4d. This relationship shows the inverse dependence between unit cell size and capillary pressure: smaller unit cells require higher pressures for air invasion, while larger unit cells are associated with lower invasion pressures. By combining the mappings in Fig. 4c and Fig. 4d, the PSD is transformed into an equivalent unit cell length distribution, where the cumulative pore volume is expressed as a function of  $l$ .

The resulting PSDs for three commercially available GDLs are shown in Fig. 5. All samples are based on Toray carbon paper (TGP-060) with different PTFE contents and were selected because they are widely used in the literature and have well-documented structural and transport properties, enabling comparison with previously reported data. Fig. 5a shows the porosimetry-based PSDs interpreted using the equivalent cylindrical pore assumption, and Fig. 5b shows the corresponding transformed PSDs, where the cumulative pore volume is expressed as a function of the unit cell length  $l$ .

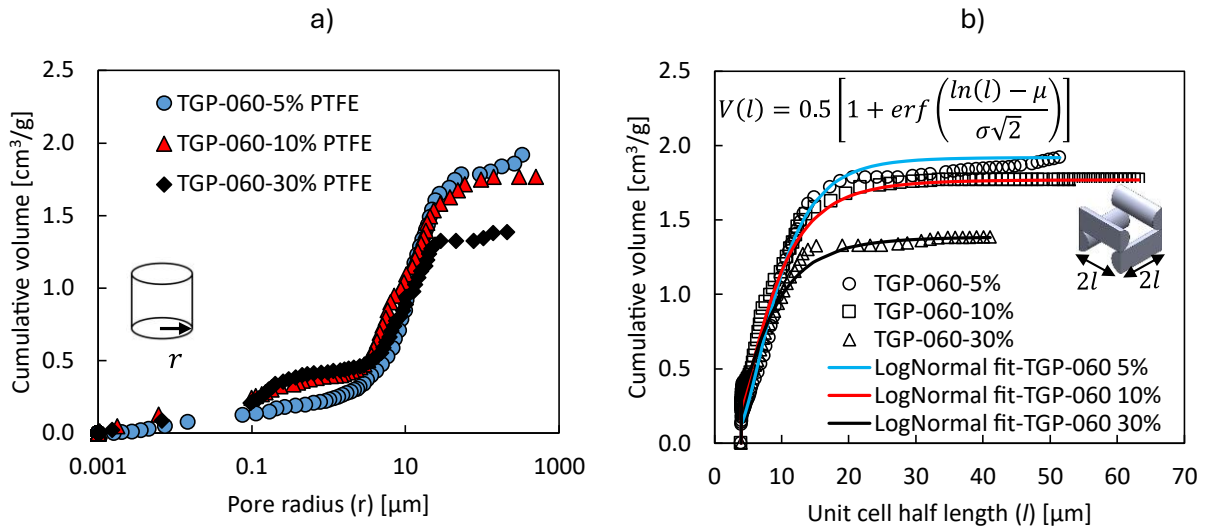


Fig. 5 Transformation of the measured pore size distribution into the unit cell length distribution. (a) Original cumulative pore volume distribution reported in terms of cylindrical

pore radius, as obtained from standard porosimetry measurements for TGP-060 GDLs with different PTFE loadings. The cylindrical inset represents the pore geometry assumed in the experimental PSD interpretation. (b) Transformed cumulative distribution expressed in terms of the unit cell half-length  $l$ . The inset shows the selected unit cell, where the unit cell size variation is represented by changing  $l$ , while the fiber diameter  $d$  is kept constant.

To provide a concise statistical representation of the transformed pore structure, the transformed PSDs were fitted using a cumulative lognormal distribution:

$$V(l) = 0.5 \left[ 1 + \operatorname{erf} \left( \frac{\ln(l) - \mu}{\sigma\sqrt{2}} \right) \right] \quad (7)$$

where,  $\mu$  and  $\sigma$  are the logarithmic mean and standard deviation of the distribution, respectively. The fitted values of  $\mu$ ,  $\sigma$  and  $R^2$  for the three GDL samples are reported in Table 2. As shown in Fig. 5b, the fitted curves closely follow the transformed distributions over the full range of unit cell length, confirming that the lognormal function provides an accurate representation of the transformed PSDs. As the PTFE content increases from 5% to 30%,  $\mu$  decreases from 2.18 to 1.93, while  $\sigma$  increases from 0.52 to 0.66. This trend indicates that higher PTFE loading shifts the distribution toward smaller unit cell sizes and broadens the pore size distribution, which is consistent with non-uniform PTFE deposition within the fibrous network.

Table 2 Log-normal distribution parameters ( $\mu$  and  $\sigma$ ) and corresponding coefficient of determination ( $R^2$ ) for the transformed pore size distributions of the selected GDL samples.

| GDL              | $\mu$ | $\sigma$ | $R^2$ |
|------------------|-------|----------|-------|
| TGP-060-5% PTFE  | 2.18  | 0.52     | 0.99  |
| TGP-060-10% PTFE | 2.07  | 0.61     | 0.99  |
| TGP-060-30% PTFE | 1.93  | 0.66     | 0.99  |

The transformed distribution forms the basis for constructing the unit cell network used in the subsequent diffusivity modeling.

### 3. Diffusivity model development

Following the transformation of the pore size distribution, a three-dimensional network of unit cells is constructed. The network consists of 30×30×30 unit cells arranged in a regular cubic

lattice. The length of each unit cell is assigned by random sampling from the transformed distribution according to its corresponding volume fraction. In this way, the generated network preserves the statistical characteristics of the pore structure while introducing spatial variation across the domain, with no assumed correlation between neighboring cells. Each unit cell is connected to its six adjacent neighbors (in the  $\pm x$ ,  $\pm y$ , and  $\pm z$  directions). The total solid and pore volumes of all unit cells are then calculated to determine the overall network porosity and verify that the generated structure is representative of the actual material.

Gas transport through a porous medium can be characterized using Fick's law, from which a diffusive resistance can be defined to quantify the opposition to diffusive flux. For a medium of transport length  $\delta$  [m], cross-sectional area  $A$  [m<sup>2</sup>], and bulk diffusivity  $D_b$  [ $\frac{m^2}{s}$ ], the diffusive resistance  $R$  [ $\frac{s}{m^3}$ ] is defined as:

$$R = \frac{\delta}{AD_b} \quad (8)$$

In the present model, each unit cell is assigned directional resistances based on its geometry. Due to geometric symmetry (Fig. 2b), the in-plane resistances are identical ( $R_x = R_y$ ), while the through-plane resistance ( $R_z$ ) is evaluated separately to account for the spatial variation in cross-sectional area.

For transport in the  $x$  direction, the cross-sectional area remains constant along the path. The resistance is therefore:

$$R_{IP_x} = \int_0^{2l} \frac{dx}{AD_b} = \frac{8l}{D_b(8dl - \pi d^2)} \quad (9)$$

The same expression holds for  $R_{IP_y}$ . Substituting Eq. (2) into Eq. (9) and nondimensionalizing the resistance yields the dimensionless in-plane resistance:

$$R_{IP}^* = R_{IP} d D_b = \frac{1}{\phi} \quad (10)$$

Equation (10) shows that the dimensionless in-plane resistance depends only on the local porosity of the unit cell.

The through-plane diffusive resistance is obtained by integrating the differential resistance along the through-plane direction:

$$R_{TP} = \int_0^{2d} \frac{dz}{A_z D_b} \quad (11)$$

where,  $A_z$  is the local cross-sectional area normal to the through-plane diffusion direction. The through-plane direction presents a more complex geometry since cross-sectional area varies along the transport path due to fiber curvature (see Fig. 2b). Substituting the corresponding expression for  $A_z$  into Eq. (11) and non-dimensionalizing using Eq. (2) leads to the following closed-form expression for the dimensionless through-plane resistance (Eq. (12)), where  $\beta$  is a geometric parameter defined in Eq. (13):

$$R_{TP}^* = \frac{4(\phi - 1)\sqrt{\beta^2 - 1} + 4 \arctan\left(\frac{\beta - 1}{\sqrt{\beta^2 - 1}}\right) + 4 \arctan\left(\frac{1}{\sqrt{\beta^2 - 1}}\right)}{\sqrt{\beta^2 - 1}} \quad (12)$$

$$\beta = \frac{\pi}{4(1 - \phi)} \quad (13)$$

To examine the behavior of the derived resistance expressions, the dimensionless in-plane and through-plane resistances are plotted as functions of local porosity of the unit cell in Fig. 6. At low porosity values (corresponding to smaller unit cells), the through-plane resistance is significantly higher than the in-plane resistance. This indicates that transport in the through-plane direction is strongly hindered in small unit cells, and gas transport preferentially occurs through in-plane pathways. As the porosity increases, the through-plane resistance decreases rapidly and approaches values comparable to the in-plane resistance. This behavior reflects the reduced obstruction to transport in larger pores, where gas molecules can more easily diffuse in the through-plane direction. These trends highlight the anisotropic nature of gas diffusivity in GDLs.

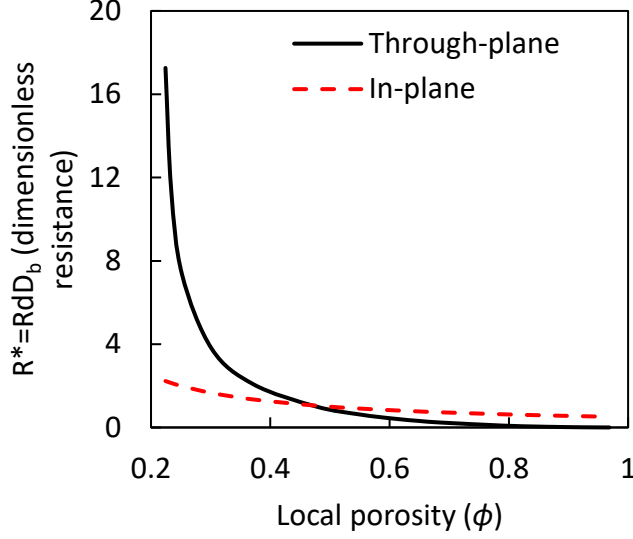


Fig. 6 Dimensionless in-plane and through-plane diffusive resistances ( $R_{IP}^*$  and  $R_{TP}^*$ ) as functions of local porosity ( $\phi$ ) for a unit cell, based on Eqs. (10) and (12).

With the directional resistances defined for each unit cell, a global resistance matrix is assembled. At the network level, fixed dimensionless concentrations are assigned to the bottom and top boundary layers, while the side boundaries are treated as zero-flux boundaries. The resulting linear system is solved for the nodal concentrations. The total flux is then computed, and the equivalent resistance of the entire network is obtained.

The equivalent resistance of the network can be related to that of an equivalent medium with an effective diffusivity. The total thickness of the network is  $n_z(2d)$ , and the total cross-sectional area is  $n_x n_y (4l_{ave}^2)$ , where  $l_{ave}$  is the mean unit cell length obtained from the transformed distribution. Accordingly, the equivalent resistance can be written as:

$$R_{eq} = \frac{n_z(2d)}{n_x n_y (4l_{ave}^2) D_{eff}} \quad (14)$$

Equating the resistance obtained from the network solution to Eq. (14) gives the effective diffusivity, which is then normalized by the bulk diffusivity to obtain the relative diffusivity ( $D^* = \frac{D_{eff}}{D_b}$ ).

A sensitivity analysis was performed to ensure that the predicted relative diffusivity was independent of the selected network size. The network dimension was increased from

$30 \times 30 \times 30$  to  $40 \times 40 \times 40$  unit cells, while using the same transformed pore size distribution. The resulting change in the predicted relative diffusivity was less than 0.2%. Therefore, a  $30 \times 30 \times 30$  network was used in the present study to provide network-size-independent results while maintaining computational efficiency.

To show the ability of the proposed model to capture pore size distribution effects beyond porosity, two synthetic transformed PSDs were generated with similar overall porosity but different distributions of unit cell length. The first distribution was generated using  $\mu = 2.2$  and  $\sigma = 0.5$ , while the second was generated using  $\mu = 1.9$  and  $\sigma = 0.7$ . These parameters were selected so that the generated networks have nearly the same overall porosity while maintaining different pore size distributions. The first distribution contains a larger fraction of relatively large unit cells, whereas the second distribution is broader and contains a higher fraction of smaller unit cells. These synthetic cases do not correspond to specific commercial GDL materials; they are used only as a controlled comparison.

The network model predicts different relative diffusivities for these two cases, even though their porosities are nearly the same. Specifically, the relative diffusivity of the second case is approximately half that of the first case because the second distribution contains a higher fraction of smaller unit cells that introduce greater local diffusive resistance and restrict transport pathways. In contrast, a conventional porosity-based model, such as the Bruggeman relation, would predict identical diffusivity values for the two cases because it depends only on porosity and does not account for pore size distribution. This comparison shows that the proposed model captures microstructural effects that cannot be represented by porosity alone.

#### **4. Compact Correlation**

Although the resistance-network model provides a physics-based prediction of relative diffusivity, solving the full network for each GDL microstructure may not be convenient for rapid estimation or implementation in larger-scale models. Therefore, a compact correlation is developed to relate the relative diffusivity to the main structural parameters obtained from the transformed pore size distribution.

In the present formulation, the transformed PSD is represented by the lognormal parameters  $\mu$  and  $\sigma$ , while the overall porosity of the GDL is denoted by  $\varepsilon$ . Therefore, the relative diffusivity is expressed as a function of these three parameters:

$$D^* = f(\varepsilon, \mu, \sigma) \quad (15)$$

Since porosimetry-based PSD data were available for only three GDL samples, a parametric dataset was generated to cover a broader range of representative pore structures. The lognormal parameters  $\mu$  and  $\sigma$  were varied within physically relevant ranges, and for each generated PSD, the corresponding network porosity was calculated from the total pore and solid volumes of the generated unit cells. The full resistance-network model was then solved for each case to obtain the corresponding relative diffusivity. The resulting dataset was used to fit a compact correlation for  $D^*$ . Several functional forms were tested, and the following expression was selected because it provides high accuracy while maintaining a simple and physically interpretable form:

$$D^* = 0.60\varepsilon^{1.14}\exp(0.37\mu - 2.03\sigma) \quad (16)$$

The quality of the fit was evaluated by comparing the compact-correlation predictions with the full resistance-network model results. The selected correlation gives  $R^2 = 0.985$  and  $RMSE = 0.014$ , indicating that it accurately reproduces the resistance-network model over the range of parameters considered in this study.

The form of the correlation is also physically consistent. The positive exponent of  $\varepsilon$  indicates that higher porosity increases relative diffusivity by increasing the available pore volume for gas transport. The positive coefficient of  $\mu$  shows that larger characteristic unit cell sizes increase diffusivity by reducing local transport resistance. In contrast, the negative coefficient of  $\sigma$  indicates that broader pore size distributions reduce diffusivity, since they contain a larger fraction of small unit cells that introduce higher local resistance and restrict transport pathways.

A sensitivity analysis was performed to examine the effect of the transformed PSD parameters on the predicted relative diffusivity. In this analysis,  $\mu$  and  $\sigma$  were varied over representative ranges, and for each  $\mu$  and  $\sigma$  pair, the corresponding overall porosity was recalculated from the transformed unit cell distribution before evaluating the compact correlation. Therefore, the results reflect the coupled effect of the PSD parameters and the resulting porosity. As shown in

Fig. 7, increasing  $\sigma$  decreases the relative diffusivity for all values of  $\mu$ , indicating that broader transformed PSDs reduce gas transport by increasing the contribution of smaller, high-resistance unit cells. In contrast, increasing  $\mu$  increases the relative diffusivity at a given  $\sigma$ , since the distribution shifts toward larger unit cell sizes with lower local diffusive resistance. These trends are consistent with the physical interpretation of the resistance-network model and confirm that the compact correlation preserves the main microstructural dependencies captured by the full model.

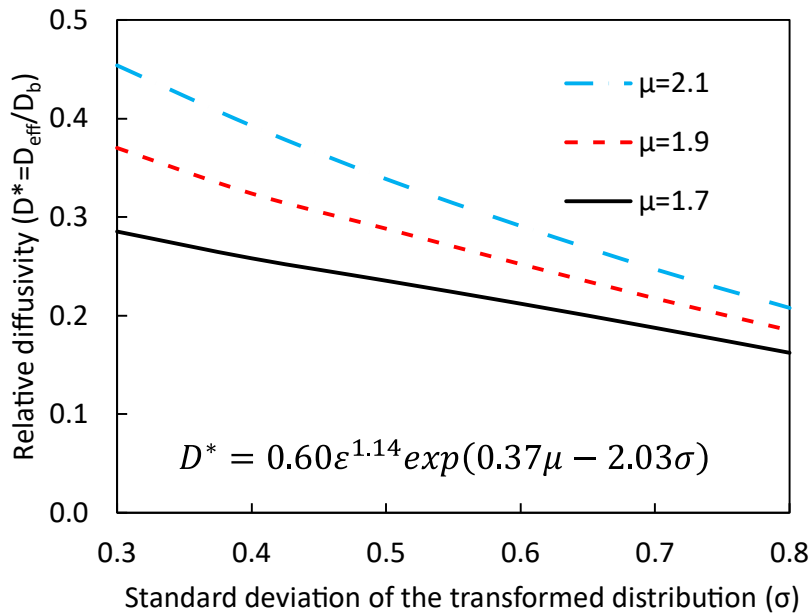


Fig. 7 Sensitivity of the compact correlation to the transformed PSD parameters.

## 5. Model validation

The predictive capability of the proposed compact correlation developed in Section 4 is evaluated by comparing its predictions with relative diffusivity values for five GDL samples, as shown in Fig. 8. The validation dataset includes TGP-060-5%, TGP-060-10%, TGP-060-30%, TGP-090-0%, and SGL 10 BA. For the TGP-060 series, both the pore size distributions (PSD) and relative diffusivity values were obtained in the present work. For TGP-090-0%, the porosimetry-based PSD was taken from the literature (Gostick et al. 2007), while the relative diffusivity was measured in the present work. For SGL 10 BA, the PSD was also taken from the literature (Gostick

et al. 2007), whereas the relative diffusivity was obtained from a separate study (Hwang and Weber 2012). For each validation sample, the porosimetry-based PSD was transformed into the corresponding unit cell length distribution and fitted using the lognormal function to obtain  $\mu$  and  $\sigma$ . The overall porosity  $\varepsilon$  was then calculated from the transformed PSD and used, together with  $\mu$  and  $\sigma$ , as inputs to the compact correlation.

The relative diffusivity measurements in the present work were performed using the symmetrical modified Loschmidt cell (SMLC) method (Waterloo Technical Instrument Inc.) at the Laboratory for Alternative Energy Conversion (LAEC), Simon Fraser University. In this method, the porous sample is placed between two chambers containing gases of different compositions, and the transient concentration evolution is monitored to determine the effective diffusivity. Further details regarding the SMLC setup, data reduction procedure, and validation of the method are available in our previous studies (Mohammadi et al. 2025), (Mohammadi et al. 2026). For the TGP-060 substrates and TGP-090-0%, the experimentally measured diffusivity values were found to be consistent with previously reported data for similar materials in the literature (Chan et al. 2012), (Unsworth et al. 2013), (Kramer et al. 2008), supporting the reliability of the present SMLC measurements. For SGL 10 BA, the diffusivity value used for validation was taken directly from the literature and was measured using the limiting current method (Hwang and Weber 2012).

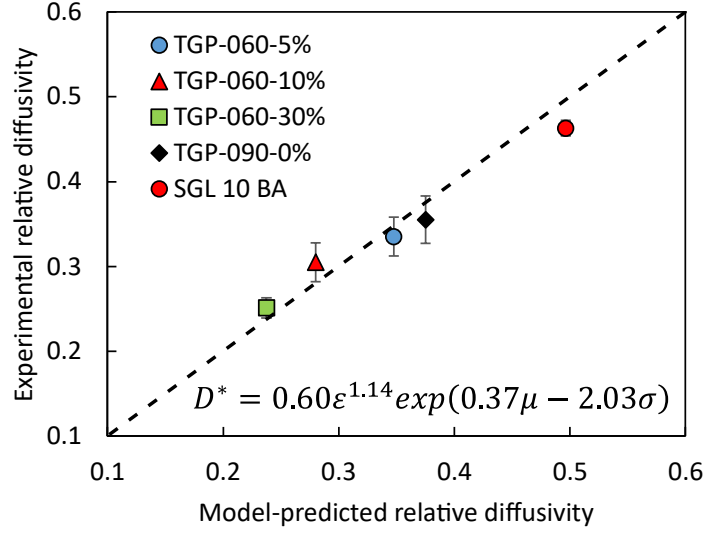


Fig. 8 Comparison between model-predicted and experimentally measured relative diffusivity for various GDL substrates. The dashed line represents perfect agreement ( $y = x$ ), and error bars indicate experimental uncertainty.

As shown in Fig. 8, the model predictions are in good agreement with the experimental data, with a maximum relative difference of 8%. The deviations can be attributed to uncertainties in PSD characterization, differences in experimental measurement techniques, and inherent material variability. Overall, the results show that the proposed compact correlation provides a reliable and computationally efficient method to estimate the gas diffusivity of GDLs.

## Conclusions

In this study, a model based on effective medium theory was developed to predict gas diffusivity in dry gas diffusion layers (GDLs). A pore size transformation method was developed to convert porosimetry-based pore size distributions, originally interpreted using an equivalent cylindrical pore geometry, into equivalent unit cell length distributions representative of the fibrous GDL structure. This transformation allowed the experimentally obtained pore size distribution to be incorporated consistently into the selected unit cell geometry. A statistical three-dimensional resistance network of unit cells was then constructed to evaluate diffusive transport by assigning directional resistances to each unit cell.

The results demonstrate that pore size distribution has a significant influence on gas diffusivity and cannot be represented by porosity alone. The proposed resistance-network model predicts different diffusivity values for GDL structures with nearly identical porosity but different unit cell length distributions. This comparison confirms that the proposed model captures microstructural effects that conventional porosity-based correlations cannot distinguish.

To improve computational efficiency, a compact correlation for relative diffusivity was developed based on the overall porosity and the lognormal parameters of the transformed pore size distribution. The correlation reproduces the predictions of the resistance-network model with high accuracy. A sensitivity analysis further showed that increasing the logarithmic mean of the transformed distribution increases relative diffusivity, while increasing the distribution broadness reduces relative diffusivity when the corresponding porosity is recalculated consistently.

The compact correlation was validated against experimental relative diffusivity data obtained using the symmetrical modified Loschmidt cell method and literature data for multiple GDL substrates. The compact correlation predictions showed good agreement with the experimental data, with a maximum relative difference of approximately 8%. Overall, the results demonstrate that incorporating the transformed pore size distribution enables more accurate prediction of gas diffusivity in GDLs than models based on porosity alone.

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## Nomenclature

|       |                                        |
|-------|----------------------------------------|
| $A$   | Cross-sectional area [m <sup>2</sup> ] |
| $d$   | Fiber diameter [μm]                    |
| $D^*$ | Relative diffusivity [-]               |
| $D_b$ | Binary diffusivity [m <sup>2</sup> /s] |

|                      |                                                                         |
|----------------------|-------------------------------------------------------------------------|
| $D_{eff}$            | Effective diffusivity [ $\text{m}^2/\text{s}$ ]                         |
| $l$                  | Unit cell half length [ $\mu\text{m}$ ]                                 |
| $p_c$                | Capillary pressure [kPa]                                                |
| $r$                  | Pore size in standard porosimetry [ $\mu\text{m}$ ]                     |
| $R$                  | Diffusive resistance [ $\text{s}/\text{m}^3$ ]                          |
| $R^*$                | Nondimensional diffusive resistance                                     |
| $V$                  | Volume [ $\text{m}^3$ ]                                                 |
| <b>Greek letters</b> |                                                                         |
| $\Gamma$             | Radius of curvature [ $\mu\text{m}$ ]                                   |
| $\alpha$             | Wetting angle [ $^\circ$ ]                                              |
| $\gamma$             | Surface tension [ $\text{mN}/\text{m}$ ]                                |
| $\delta$             | Thickness [ $\mu\text{m}$ ]                                             |
| $\varepsilon$        | GDL Porosity [-]                                                        |
| $\theta$             | Contact angle [ $^\circ$ ]                                              |
| $\mu$                | Logarithmic mean of unit cell half-length log-normal distribution [-]   |
| $\sigma$             | Standard deviation of unit cell half-length log-normal distribution [-] |
| $\phi$               | Local porosity of the unit cell                                         |
| <b>Subscripts</b>    |                                                                         |
| IP                   | In-plane                                                                |
| TP                   | Through-plane                                                           |

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