Prediction of Permeability for Porous Materials Using a Surrogate Model

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Abstract: The computation of permeability for porous media through fluid simulation techniques is an intensive and a tedious process. Surrogate modeling of physical simulations offer a significantly cheaper alternative to computing permeability using numerical techniques. The main objective of this work is to develop a supervised learning model that approximates the physical simulations involving a single gaseous species through a porous material and capture the lengthscale dependency of the material's permeability. This length-scale dependency can be integrated into multiphase computational fluid dynamics (CFD) solvers to better simulate the physics of gas transport inside the material instead of assuming a constant value for the property. An analytical function is developed, which relates the permeability of a porous material with the thermodynamic conditions and length-scale of the microstructure. The analytical function is realized using support vector regression (SVR), which is found to be a robust technique in order to capture the complex relationship between temperature, average pressure, and length-scale of the microstructure. The predicted values are found to have a maximum relative error of about 20 percent with the majority of the relative errors being less than 7 percent. The analytical function is validated against a range of inputs beyond the scope of trained values to justify the use of the developed supervised learning model. The capability of the developed model to capture the length-scale dependency on permeability is emphasized by noting the difference in predicted permeability and it's accuracy for data points at either edges of the training domain.

Keywords: Effective permeability, Non-continuum flows, Direct simulation Monte Carlo (DSMC), Porous media, Surrogate modeling

1 Introduction

Understanding the thermal-fluid processes in porous media is scientifically attractive because of their applications in catalysis [1], adsorption and separation [2], energy [3], environment [4], high-end technologies [5], extracting shale gas [6], and molecular sieves [7]. The flow of gases and liquids through complex pores is dictated by an important property called permeability. Permeability is also relevant to spacecraft systems, when they enter the atmosphere of a planet.

Spacecrafts experience extreme aerothermal environments during re-entry because of hypersonic speeds. Thermal protection systems (TPS) act as a protective layer against the extreme heat flux developed on the surface of the spacecraft in such conditions. Specifically, ablative TPS materials are used to mitigate the heat loads during atmospheric re-entry through different processes such as absorption, heat rejection, and sacrificial removal of hot material [8]. Hence, TPS materials are an integral part of space missions and the study of their performance is an active on-going field of research. Carbon composites are low-density materials used as TPS that consist of a network of carbon fibers and phenolic resin. The carbon-fiber network in the matrix is referred to as FiberForm ,which has an overall porosity (ϕ) of approximately 0.9, and when this carbon fiber network is impregnated with a phenolic resin, it is called phenolic impregnated

carbon ablator (PICA), which has a porosity of approximately 0.8. Because of its high porosity, gases in the boundary layer are able to penetrate into the microstructure causing gas-phase and gas-surface reactions inside the material [9]. The gas-surface interactions in the TPS materials offer unique technical challenges because the flow inside the pores of the TPS composite occurs in the non-continuum regime. Permeability is an important property of a TPS material because it governs the transport of gases through a porous material. When the flow of gases occur in the continuum regime, permeability is only a function of the geometrical configuration of the pores. However, permeability also depends on pressure and temperature when gas transport occurs in the non-continuum regime. Well known correction factors have been applied over the years to compute the permeability of TPS materials in non-continuum regime with the most notable being the Klinkenberg formulation [10, 11].

Numerical simulations offer a unique, time and cost-effective alternative to recreate atmosphere re-entry conditions for the study of thermal-fluid behavior inside TPS materials. Computational flow solvers, referred to as material response solvers, have been historically used to simulate the aerothermal response of TPS materials subjected to hypersonic environments. To compute flow through TPS materials, the combined solid-gas momentum transport equations need to be solved. Numerous methods to solve these momentum transport equations have been proposed. These methods either formulate the momentum transport equations as surface models or one-dimensional volume averaged models [12, 10], and more recently as two/three-dimensional volume-averaged models [13, 11, 14, 15, 16, 17, 18, 19]. All these volume averaged approaches require model closure for momentum transport, specifically the material permeability. In extreme re-entry conditions at high altitudes, the pore size of the microstructure approaches the mean free path of the gaseous species, which leads to the flow inside the carbon composite being in the slip or transitional flow regime. This phenomenon has been verified in the analysis of Stardust trajectory [20]. Hence, analytical relations derived either in the continuum or in the free-molecular regime will be invalid to compute the permeability for re-entry conditions.

The current state-of-the-art approach is to formulate permeability in the Klinkenberg formulation, which contains two constants, K_{ρ} and b. To obtain the constants, the direct simulation Monte Carlo (DSMC) method is used because it is accurate in both the continuum and non-continuum regime. The permeability computed by DSMC [21] acts as an input to the material response code to capture gas transport. The state-of-the-art DSMC technique utilized in the current work has been successfully verified to compute permeability of porous materials especially in the non-continuum regime by several groups [22, 23, 24] including current authors [25, 21, 26]. However, the constants involved in the Klinkenberg formulation needs to be determined for every combination of pressure, temperature, and length-scale, which leads to an abundance of repeated numerical simulations and a computationally intensive process of generating a lookup table when permeability as a parameter is required to evaluate macroscale material response. Further, the computational time and resources required to run DSMC simulations increases exponentially at higher pressures because of higher mesh resolution that is required to accurately compute material permeability. It is imperative to find ways to reduce the overall computational time involved in solving this multi-dimensional problem. A way to accomplish this would be to develop a supervised learning model that is capable of capturing the inherent relationship between an output parameter and a set of input parameters. Specifically, in this article, we make use of a regression technique based on support vector machines (SVM) called support vector regression (SVR). SVR uses the extensive database realized by repetitive DSMC simulations to train a supervised learning model capable of predicting the permeability of the TPS material subject to the specified set of input parameters (length-scale, pressure, and temperature). Unlike other sophisticated deep learning models, which have been used to predict permeability of porous materials [27, 28], the SVM approach can be easily integrated into a material response code to satisfy the closure problem. The analytical function developed by SVR eliminates the need for lookup tables and facilitates the computation of Jacobian matrices required in implicit material response solvers without the need for interpolation. Further, a single relationship captures the dependencies of the constants encountered in the Klinkenberg formulation with the input parameters, which saves considerable amount of computational time and effort. Along with temperature and pressure, the dependency of permeability on the length-scale of the TPS material is heavily emphasized in this work to improve the current state of the material response codes, which assume an independence of permeability with respect to length-scales. The porous nature of carbon-fiber TPS materials such as FiberForm, results in a considerable variation of their properties with respect to the size of the microstructure until a minimum representative element volume (REV) is reached. The surrogate model is designed to use both thermodynamic and material features as inputs to predict permeability of porous materials.

2 Methods

In-house python scripts are developed to automate the entire workflow involved in generating training and validating points for a wide range of inputs. The in-house python scripts leveraged the already developed and validated microstructure generation code (Fibergen) by Stern et al. [25] and the DSMC solver developed by Sandia National Laboratories [29] to determine the permeability with minimal human intervention.

2.1 Fibergen: A synthetic microstructure generating code

Fibergen is the in-house microstructure generation code used to generate the desired volumes. Note that the algorithm and its architecture have been explained and validated in detail in previous publications [21, 25, 26]. The key features used in this study are described here for completeness. Fibergen uses the domain dimensions, nominal fiber orientation, target bulk porosity, nominal fiber radius, and the variances of all the parameters to generate a volume filled with synthetic cylindrical fibers. In order for Fibergen to replicate the FiberForm microstructure, the fibers need to have a radius of 5 μ m and a standard deviation of 0.1 μ m [30]. The fiber diameters are then sampled using a Gaussian distribution using the specified mean and variance. Because of the manufacturing method to generate FiberForm, its microstructure is orthotropic in nature since fibers are pressed into billets in only one direction. Therefore, the fibers have a bias to be oriented in a plane parallel to the compression plane affecting their angle of orientation. Following the conclusion from a previously conducted parametric study [21], the angle of elevation is allowed to vary between $\pm 25^{\circ}$, which is sampled from a uniform distribution.

The current version of Fibergen allows the user to chose a convergence type based on the target bulk porosity or the target sample density of the volume. Independently of the convergence type chosen, the main algorithm of Fibergen is identical until the test for convergence step. The code chooses a random point inside the domain, an elevation angle, and a random angle of orientation in the plane of fiber generation. A fiber is generated inside the domain with a radius sampled from the Gaussian distribution and the algorithm checks if the fiber intersects another fiber or in contact with a boundary of the domain. If either condition is found to be true, the fiber is then removed and a set of three new values are generated. This procedure is repeated until the set convergence criteria is satisfied. Fibergen can export the volumes in two different formats which are stereolithography (STL) and voxels. The voxel format can be leveraged to add resin in the fibrous network to replicate a PICA-like microstructure, although, in this article we will only use the STL format and create volumes targeting FiberForm. In Fig. 1, multiple volumes generated with Fibergen can be seen for different cube lengths and porosity. The porosity of these volumes change with respect to their size. The REV for FiberForm can be estimated to be between $200 \times 200 \times 200 \ \mu m^3$ and $300 \times 300 \times 300 \ \mu m^3$ since the porosity of microstructures shown in Figs. 1(a) and 1(c) start to reach a constant value.

2.2 Sparta: DSMC Solver

The open-source DSMC solver Stochastic Parallel Rarefied-gas Time-accurate Analyzer (SPARTA) with inhouse modifications, explained previously in Ref. [26], coupled with Fibergen to generate the microstructures is used to perform the numerical simulations. The DSMC solver uses a stochastic approach to simulate the Boltzmann equation and is able to simulate all relevant physics such as convection, multi-component diffusion, gas-phase and gas-surface chemistry. DSMC is valid for all regimes from free-molecular to continuum using the same set of collision model parameters [25, 21, 31]. DSMC has the ability of decoupling the flow mesh from the surface mesh, which makes it ideal to study properties in complex microstructures such as those observed in TPS materials. A detailed description of the DSMC solver and its relevance to computing material permeability can be found in Refs. [21, 25].

Sparta uses a multi-level Cartesian mesh to track and collide particles. The microstructure generated by Fibergen is directly read by the DSMC solver where it is identified using a set of triangles, similar to an STL format, or a set of voxels that can be converted to a closed surface using the marching cube algorithm [32, 33]. The triangles are then sorted (sorting is not necessary for marching cube) and the cut-cell technique is used

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(e) 104 μm cube length with $\phi = 0.7749$.

(f) 53 μm cube length with $\phi = 0.6534$.

Figure 1: Multiple volumes generated with Fibergen with different length-scales. Porosity for each volume is computed using Eqn. ?? and used as input to generate the microstructure.

to compute the flow volume in each cell, where the standard ray-tracing approach is used to move the simulation particles.

The simulation setup has been discussed in one of our previous publication [26]. Figure 2 shows the

layout of the set up, which mainly consists of the microstructure placed in the centre of the domain with equal extends in the flow direction equivalent to at least one time the volume length, while symmetric boundary conditions are applied in the span-wise directions (y and z). Temperature (T_{in}) and pressure (P_{in}) are specified for the upstream boundary while inlet velocity (u) is obtained using a zeroth order extrapolation. For the downstream boundary, the pressure outlet (P_{out}) is specified and the remaining macroscopic properties are computed using the methods of characteristics of Nance et al. [34] and Fang and Liou [35] using information from the interior solution. The relevant equations used to obtain the boundary conditions can be found in Refs. [25, 34, 35] and have been validated in Ref. [21]. To make the solver more stable, one of the in-house enhancements is to use a sub-relaxation averaging approach when computing quantities from the interior cells.



Figure 2: Flow set up to compute permeability using the DSMC technique.

The simulations are run for a single gaseous species (Ar) until steady state is reached and mean flow quantities are obtained such as density, velocity, pressure, and temperature. The permeability force is computed as described by Marschall and Milos [36] (Eqn. 1).

$$F \equiv \frac{\mu \dot{m} T R L}{A M \Delta P} = K_0 (P_{avg} + b) \tag{1}$$

In Eqn. 1, F (N) is the permeability force, μ (Pa·s) is the viscosity, \dot{m} (kg·s⁻¹) is the mass flow rate, T (K) is the temperature, R (J·K⁻¹·mol⁻¹) is the universal gas constant, L (m) is the length of the sample, A (m²) is the area, M (kg·mol⁻¹) is the molecular mass, ΔP (Pa) is the pressure difference across the sample, K_0 (m²) is the permeability in the continuum limit, and b (Pa) is the Klinkenberg constant. The physical meaning and derivation of Eqn. 1 can be found in Refs. [21, 9]. A power-law viscosity model is used with the form of Eqn. 2:

$$\mu = \frac{15\sqrt{\pi m k T_{ref}}}{2(5-2\omega)(7-2\omega)\pi d_{ref}^2} \left(\frac{T}{T_{ref}}\right)^{\omega}$$
(2)

In Eqn. (2), k is the Boltzmann constant, T_{ref} is a reference temperature of 273.15 K, d_{ref} is the reference diameter with a value of 4.17×10^{-10} m for Ar, and ω is the variable hard sphere (VHS) exponent with a value of 0.81 for Ar. The Klinkenberg expression for effective permeability can be computed as shown in Eqn. 3.

$$K_{eff} = K_0 \left(1 + \frac{b}{P} \right) \tag{3}$$

In Eqn. 3, K_{eff} (m²) is the effective permeability of the sample. Note that Eqn. 3 can be obtained by dividing Eqn. 1 by P_{avg} . This relation is used to check if mass conservation is satisfied a posteriori, since DSMC does not directly enforce mass conservation. Alternatively, Darcy's law can also be used to compute the permeability (K_{Darcy}). The Darcy's law is shown in Eqn. 4:

$$K_{Darcy} = \frac{-\mu U}{\nabla P} \tag{4}$$

In Eqn. 4, K_{Darcy} (m²) is material permeability, μ (Pa·s) is viscosity obtained from Eqn. 2, ∇P (Pa·m⁻¹) is the pressure gradient in the microstructure, and U (m·s⁻¹) is the superficial velocity and can be computed from the flow field inside the pores of the sample (Eqn. 5):

$$U = \frac{1}{V} \int_{V_f} u dv \tag{5}$$

In Eqn. 5, V (m³) is the total volume of the material, V_f (m³) is the volume of fluid, u (m·s⁻¹) is the local fluid velocity within the pores, and dv (m³) is the differential fluid volume element. The comparison of results from Eqns. 3 and 4 is demonstrated in Sec. 3.1.

2.3 Support vector regression (SVR)

Figure 3 depicts the major steps involved in the development of a supervised learning model. A supervised learning model can be realized with something as simple as curve fitting or a more complex deep learning algorithm, which makes use of the data points available from the sampling stage to predict the values at the unknown region of the domain. Due to the nature of the problem involved in this work, a curve fitting regression model with a suitable kernel function is chosen as the starting point to realize the supervised learning model. Most common supervised models either use quadratic or n-th order polynomial for curve fitting following the regression process [37, 38]. However, regression models are uni-modal approaches that are best suited for simple analytical functions and fail to model the variability involved in physical processes. Most engineering applications involve multi modal functions, which require sophisticated surrogate models like SVR to approximate the process. In this work, SVR is chosen above other models owing to its robustness and flexibility to capture variability in the sampling data.

Support vector machine (SVM) analysis is a popular machine learning tool for classification and regression, first identified by Vladimir Vapnik and his colleagues in 1992 [40]. SVM regression or SVR is considered a non-parametric technique because of its reliance on kernel functions. The objective is to find a function f(x) that deviates from y_n (training data value) by a value no greater than ϵ for each training point x_i , and at the same time indifferent to over-fit and under-fit. SVR further builds upon the surface objective mentioned above by including a soft margin (slack variable) in cases where the chosen kernel function is ill-equipped to handle the variability that is found in the sampling data. The slack variable (ζ) enables SVR to handle complex physics encountered in physical processes by providing additional tolerance to capture the hidden relationship between the parameters.

The general formulation of a typical SVR problem involves the determination of support vectors (x_i) and dual co-efficients $(\alpha - \alpha^*)$ by solving the first minimization problem. The underlying equation involved is given by Eqn. 6, which is constrained by Eqns. 7 and 8. A universal intercept is evaluated by solving the second minimization problem shown in Eqn. 9 constrained by Eqn. 10 in order to fit the sampling points within acceptable tolerance $(|\epsilon + \zeta_i|)$. Q_{ij} in Eqn. 6 is an $n \times n$ positive semi-definite matrix consisting of kernel functions $(G(x_i)^T G(x_j))$, y^T is the output vector associated with each training data and e is a vector of ones which facilitates the summation of slack variables defined for every training point. The dual minimization problem is setup to reduce the impact of slack variables on the overall performance of the supervised learning model.



Figure 3: Flow chart depicting various stages of supervised learning modeling [39].

$$min\left[\frac{1}{2}(\alpha - \alpha^*)^T Q(\alpha - \alpha^*) + \epsilon e^T(\alpha + \alpha^*) - y^T(\alpha - \alpha^*)\right]$$
(6)

subject to

$$\left[e^T(\alpha - \alpha^*) = 0\right] \tag{7}$$

$$[0 \le \alpha_i, \alpha_i^* \le C, i = 1, 2, ..., n]$$
(8)

$$\min[|y_i - G(x_i) - b| \le |\epsilon + \zeta_i|] \tag{9}$$

subject to

$$\zeta_i \ge 0, i = 1, 2, \dots n \tag{10}$$

SVR is formulated such that it involves a regularization parameter (C), which ultimately decides the rigidity of the predictive model. A high value of C implies greater penalty during the formulation of SVR and hence a more rigid model. On the contrary, a lower value of C allows the predictive model to be more flexible. A high value of C is generally recommended if the sampling points include a very low amount of variability since it brings down the overall error associated with the model. However, problems involving a

large amount of data are generally trained with low values of C to avoid over-fit. In such cases, the domain must be re-sampled strategically in order to bring down the overall error.

In the present work, a high value of C is chosen initially to train the surrogate model. The regularization parameter is further fine tuned by trial and error approach to obtain a supervised learning model capable of fairly accurate predictions beyond the scope of training points. A maximum relative error of 15% in the training and test data is an encouraging sign in validating the supervised learning model. The trained model is then validated against the test data generated beyond the scope of the sampling data to ensure that the predictive model is not affected by over-fit. The validation process with respective plots will be covered in greater detail in the results section.

SVR is implemented in python using sklearn library [41] for different sets of sampling points to strike a balance between underfit and overfit. The predictive function after implementing SVR on a set of training vectors x_i with corresponding values y_i is given by Eqn. 11.

$$f(x) = \sum_{i}^{n} (\alpha_i - \alpha_i^*) G(x_i, x) + b$$
(11)

where x_i is the support vector obtained from training, n is the number of support vectors, $(\alpha_i - \alpha_i^*)$ are the dual coefficients, x is the input vector, $G(x_i, x)$ is the kernel function, and b is the intercept.

By evaluating the support vectors, dual coefficient and the intercept, an analytical function can be constructed for the chosen kernel function which relates the variables in the support vectors with its corresponding output. In this work, Gaussian function given by Eqn. 12 is used as the kernel function. Equation 12 involves an additional hyper-parameter (γ) which influences the error associated with each sampling point.

$$G = \exp(-\gamma ||x_i - x||^2) \tag{12}$$

3 Results

For all results presented in this article, a nominal pressure difference of 100 Pa is used between the inlet and outlet boundaries. A nominal pressure difference of 100 Pa has been proven to be sufficient to capture the permeability in porous media using the DSMC technique from previous work [26, 21]. For example, if the average pressure (P_{avg}) is 500 Pa, then P_{in} and P_{out} are set to 550 and 450 Pa, respectively. All simulations are carried out with Argon (Ar) as the gaseous species for simplicity. After the flow is allowed to reach steady state given the boundary conditions, P_{avg} and ΔP are extracted from the flow between the inlet and outlet faces of the microstructure. Note that this values will not be identical to the values specified at the boundaries of the domains, but will be close in magnitude to them. The results from the simulations are used to perform all the necessary post-processing analysis such as calculating the values for K_{eff} and K_{Darcy} .

3.1 Convergence test and comparison of permeabilities

A numerical convergence test for DSMC simulations is initially performed with a microstructural volume of $300 \ \mu m^3$ generated using the Fibergen code at 500 K with an average pressure of 2,000 Pa to find optimal cell resolution (Δx), timestep (Δt), and number of timesteps required to reach steady state and compute average flow properties. The microstructure size, temperature, and average pressure is chosen for the convergence test since it is the most computationally intensive case in the training domain, ensuring that the rest of the cases converge to the desired accuracy. The number of timesteps are divided equally between the timesteps to reach steady state and the timesteps to collect the statistics to compute mean flow quantities. If a simulation is run for 30,000 timesteps, the first 15,000 timesteps is used to reach steady state, and the remaining 15,000 steps are used to calculate mean flow quantities.

The results from the convergence test can be seen in Table 1. All values of K_{Darcy} are compared against the baseline case of $\frac{\Delta x}{\lambda} = 0.50$, $\frac{\Delta t}{\tau} = 1/20$, and number of timesteps=10,000. A convergence test is initially performed by varying the number of timesteps from 10,000 to 50,000. The change in permeability with increased statistics for mean flow quantities is only 0.87%. A convergence test in timestep is performed by performing a simulation with a timestep of $\frac{\Delta t}{\tau} = 1/25$. The number of timesteps is adjusted to keep the total time of the simulation equivalent to the baseline case. A difference of 1.61% against the baseline case

is observed as the timestep is lowered. Finally, a simulation is performed with $\frac{\Delta x}{\lambda}$ of 0.33 and the percent difference against the baseline is found to be 1.87%. From this analysis, a cell resolution of $\frac{\Delta x}{\lambda} = 0.33$, timestep of $\frac{\Delta t}{\tau} = 1/20$, and number of timesteps=10,000 are chosen for all cases presented in the following sections. Care must be taken with the timestep and number of steps taken to reach steady state. The simulations are performed by initializing particles in the domain and allowing collisions with replacement that allows a much higher timestep to be used, as well as significantly reduces the number of steps required to reach steady state. This effect is discussed at length in our previous publication [26].

Δx	Δt	Number of	K_{Darcy}	Percent
$\overline{\lambda}$	$\overline{\tau}$	timesteps	(m^2)	difference
0.50	1/20	10,000	1.53E-10	0.00%
0.50	1/20	30,000	1.52 E- 10	0.73%
0.50	1/20	50,000	1.52E-10	0.87%
0.50	1/25	25,000	1.51E-10	1.61%
0.33	1/20	10,000	1.56E-10	1.87%

Table 1: Convergence of DSMC simulations using the microstructure obtained from Fibergen with a volume of 300 μm^3 at 500 K and 2000 Pa.

In our previous publication [42], the equivalence of K_{eff} (Eqn. 3) and K_{Darcy} (4) is demonstrated. This is accomplished by performing simulations at three different average pressures at a given temperature, and repeating the set of simulations for three different temperatures. The results from this comparison can be seen in Table 2. The surface is obtained from a X-ray computed tomography (XRCT) scan of FiberFrom with a volume of $399.52 \times 399.52 \times 399.52 \ \mu m^3$ and Ar is used as the gaseous species transporting through the microstructure. For each set of temperature and pressure, the permeability is computed with both Eqns. 3 and 4. As explained in our previous publication [42], this is an important equivalency to demonstrate because the derivation for the permeability force (Eqn. 1) does not consider Darcy's law, but material response solvers use this law for the momentum transport. In addition, the equivalence of K_{eff} and K_{Darcy} further demonstrates that the DSMC solver is valid for all flow regimes. As observed from Table 2, the maximum error observed between K_{eff} and K_{Darcy} for the different pairs of temperature and pressure is 2.34%, which demonstrates good agreement between the two methods for calculating permeability. For the remainder of the article, we have directly calculated K_{Darcy} and refer to it as the permeability (K) of the microstructure. The numerical convergence of the simulations and the equivalency of K_{eff} and K_{Darcy} demonstrates the ability of the DSMC technique to generate reliable true data to build a supervised learning model to predict permeability of porous materials.

Table 2: Equivalence of permeability ((K_{Darcy}) and	l permeability for	rce (K_{eff}) .	Percent difference	is calculated
as $\frac{ K_{Darcy} - K_{Force} }{K_{Darcy}} \times 100.$	-				

T (K)	\mathbf{P}_{avg} (Pa)	F (N)	K_{eff}	K_{Darcy}	Percent Differ-
				(111)	ence
300	300	1.53E-07	5.09E-10	5.05E-10	0.97%
300	900	1.84 E-07	2.04 E- 10	2.09E-10	2.34%
300	1500	2.20E-07	1.47E-10	1.51E-10	2.43%
900	300	5.91E-07	1.97E-09	1.94E-09	1.64%
900	900	6.20E-07	6.89E-10	6.82E-10	1.04%
900	1500	6.52 E- 07	4.35E-10	4.35E-10	0.05%
1500	300	1.14E-06	3.80E-09	3.73E-09	1.90%
1500	900	1.15 E-06	1.28E-09	1.26E-09	1.58%
1500	1500	1.17E-06	7.83E-10	7.75E-10	1.00%

3.2 Training the SVR model

The permeability of the material is captured by developing a learning function that depends on three input parameters. The input parameters are the length of the sample, average temperature, and average pressure. To build a supervised learning model, the training data for the machine learning model needs to be generated, which is referred to as sampling. In the LHS sampling approach, a point in the multi-dimensional space is chosen that corresponds to a given pressure and temperature. The chosen pressure and temperature are considered the input average pressure and temperature in the DSMC simulations. The pressure boundary conditions are set such that the pressure gradient across the sample is 100 Pa with the mean of the upstream and downstream pressure equaling the chosen input pressure. The input length is used to compute a value for porosity, which is used as in input into the Fibergen code to generate the microstructure of the porous TPS material.

LHS sampling is employed to generate 150 samples of training data. LHS method ensures that the samples are distributed uniformly along the sampling domain given their parameter bounds. The maximum and minimum values for the length of the sample, temperature, and pressure is set to 50-300 μm , 500-2,000 K, and 500-2,000 Pa, respectively. All simulations are performed with the parameters discussed in Sec. 3.1 and permeability is computed using Eqns. 4 and 5. All simulations are performed with Ar as the gaseous species. After the simulations are completed, the average temperature and average pressure are updated from the flow bounded by the microstructure and the computed permeability is used as the training data for the prediction model as discussed in Sec. 2.3. The training data points are then used to check the accuracy of the prediction model by using the same length of the sample, updated average temperature and updated average pressure as the inputs for the prediction model and comparing the predicted permeability against the value obtained from the simulations. The results from this comparison can be seen in Fig. 4, where the spheres in Fig. 4(a) are colored to represent the relative error at that point and Fig. 4(b) shows a histogram of the relative error distribution for all the training points, following the same color scheme. The error is computed by comparing the permeability obtained from the DSMC simulations (true data) and the permeability predicted by the SVR model at the given data point (predicted value). The relative error is computed as $\frac{|DSMC value - predicted value|}{DSMC value}$. From Fig. 4(b), it can be seen that 83% of the training points have a relative error below 7% with only one point being above 11%, demonstrating overall good agreement against the training data with a root mean square error (RMSE) of 0.0497.

3.3 Testing and validating the SVR model

To further validate the model, 48 more sampling points are generated following the same procedure used to generate the training data. These 48 new points are then used as inputs in the SVR model and the predicted permeability is compared with the computed value from the simulation. This comparison is shown in Fig. 5 and it helps evaluate the performance of the predictor model for data different than its training data since the predictor function is expected to perform well when comparing to the training data. For this new set of data, the RMSE is 0.0627, which is slightly higher than that for the training data , but 83% of the point have a relative error that is less than 10%, with only one point above 13%. The low relative errors demonstrates that the trained model is performing with a good level of accuracy with data inside its training scope.

To study the relationship between relative error and both average pressure and temperature, a slice of the training domain is taken for a cube length of 200 μm . Keeping the cube length constant, 12 new points are generated with pressures ranging from 300 Pa to 1,500 Pa with 300 Pa increments and an extra point at 2,000 Pa and temperature ranging from 300 K to 1,500 K with 300 K increments. These 12 new points are then compared against the predictor function following the same process as for the training and testing data and the results from the comparison are used to generate a relative error contour plot shown in Fig.6(a). From Fig. 6(a), it can seen that the majority of the domain has a relative error below 10% and maximum errors are concentrated at the corners of the domain for the combination of high pressure, low temperature and low pressure, high temperature. To better evaluate the relative error in the boundaries of the training domain, two more length-scales are selected to generate similar contour plots for 46 μm and 300 μm depicted in Figs. 6(b) and 6(c), respectively. Note that the length-scales selected to plot Figs. 6(b) and 6(c) are the lower and upper limits of the training data with respect to length-scale. The main purpose of this comparison is to evaluate the relative error at the boundary of the training domain. As expected, the higher relative



(a) Relative error with training points used to develop the SVR model.



(b) Histogram of the relative error for the 150 training points.

Figure 4: Relative error distribution of the predictive model on the trained data points for Fibergen with Ar as the gaseous species. Each data point corresponds to a length-scale, pressure, and temperature that is used to compute permeability.

errors can be seen closer to the corners of the domain because of a lack of sampling points in the corner of the domain when using LHS to generate the training points.

To better depict the dependency of the relative error with respect to temperature and average pressure, Figs. 7(a) and 7(b) are plotted for constant temperatures and average pressures, respectively. In Fig. 7(a), three constant temperatures are selected and the relative error is plotted against a range of average pressures going from 250 Pa to about 2000 Pa. Following the same configuration, Fig. 7(b) is plotted at four constant average pressures against the relative error for a range of temperatures going from 300 K to 2000 K. As seen in both figures, the lower relative errors in the domain tend to be in the middle range of both temperature and and average pressure since the number of sampling points is higher in those regions. On the other hand, as already explained, the highest error is close to the boundaries of the training data due to the lack of points to train the model in those specific areas. Figure 7(c) is created to depict the relative error



(a) Relative error with training points used to develop the SVR model.



(b) Histogram of the relative error for the 48 training points.

Figure 5: Relative error distribution for the predicted values against the result from the simulations of the testing data points for Fibergen with Ar as the gaseous species.

distribution with respect to length-scale. In Fig. 7(c), three sets of temperatures and average pressures are plotted for different length-scale in a range of 50 μm to 300 μm against the relative error at each point. A similar distribution can be seen where the maximum relative error is in the corner of the domain. The highest relative error is observed close to one of the corners of the training domain for a cube length, temperature and average pressure of 300 μm , 294 K and 305 Pa, respectively. A higher error can be expected in that region as compared to other regions in the training domain since it is close to the bounds of the three input parameters for the model.

Based on the relative errors for all points inside the training domain, the predictive model does not exhibit under-fitting. In machine-learning under-fit happens when the the model is not able to low relative errors inside its training domain and this can happen for two reasons: The model parameters explained in Sec. 2.3 are not set correctly or there are not enough training in the training domain for the model to accurately capture the behavior of the target process. To arrive at a balance between under-fit and over-fit, the model



(a) $L = 200 \ \mu m$ and $\phi = 0.8591$.



Figure 6: Relative error distribution for 3 different cube lengths with respect to pressure and temperature.

needs to be tested for points outside its training range which is 300 K to 2,000 K for temperature, 250 Pa to 2,000 Pa for average pressure, and 50 μm to 500 μm for length-scale of the microstructure.

To accomplish this, a comparison with two points out of the training range can be seen in Table 3. From Table 3, it can be seen that the maximum relative error between simulated and predicted permeability for the two points out of the training range is 8.85% for the case with temperature and average pressure of 1,500 K and 4,000 Pa, respectively. Note that 4,000 Pa is twice the upper bound for the average pressure in the training data and, therefore, a relative error of 8.85% demonstrates that the prediction model has the capability of maintaining a good level of accuracy outside its training range. The prediction model is then compared against two even higher pressure cases, 10,000 and 15,000 Pa with a temperature of 1,500 K temperature and a length-scale of 200 μm . The maximum error is observed for a mean pressure of 10,000 Pa with an error of 24.85%. Although an error of 24.85% is high, a value of 10,000 Pa is five times higher than the upper limit of the training data. Therefore, an error of ~25% can be considered to be reasonably accurate.

An REV of 300 μm^3 is necessary for permeability to be invariant to the size of the microstructure. The



(a) Relative error with respect to P_{avg} for L = 200 μm and $\phi = 0.8591.$



(b) Relative error with respect to T_{avg} for L = 200 μm and (c) Relative error with respect to cube length for a set of tem- $\phi = 0.8591.$ peratures and average pressures.

Figure 7: Relative error plotted against average pressure, temperature and cube length.

Table 3: Testing the model with data outside its training range for 200 μm cube length microstructure. Relative error is calculated as $\frac{|K_{eff} - K_{predicted}|}{K_{eff}} \times 100$.

T (K)	P_{avg} (Pa)	$ \begin{array}{c} K_{eff} \\ (\mathrm{m}^2) \end{array} $	$K_{predicted} (\mathrm{m}^2)$	Relative Error
1,500	3,500	2.65E-10	2.84E-10	7.27%
1,500	4,000	2.37 E-10	2.58E-10	8.85%

permeability at an REV of 300 μm^3 and 100 μm^3 at various pressures and temperature have been listed in Table 4 to demonstrate the importance of capturing the length-scale dependency when computing values for permeability. Table 4 is constructed by following the same distribution of temperature and average pressure that is used in Fig. 6(a), where pressure varies from 300 Pa to 1,500 Pa with 300 Pa increments and an

additional data at 2,000 Pa. Temperature is varied from 300 K to 1,500 K with 300 K increments. The permeability values are computed from the supervised learning model described in Eqn. 13. It is observed that the change in permeability is at least 40% as the length of the REV is modified. Permeability is used as a closure term for momentum transport in material response simulations. Typically, mesh sizes in material response solvers are in the order of 100 μm^3 . Using permeability values computed at converged REVs will introduce errors in the material response simulations.

Table 4: Comparison of permeability for 100 μm and 300 μm length-scales. K_{100} and K_{300} are the permeability values for the 100 μm cube length and the 300 μm cube length, respectively. Absolute difference is calculated as $\frac{|K_{100} - K_{300}|}{K_{300}} \times 100$.

T (K)	P _{avg} (Pa)	$ \begin{array}{c} K_{100} \\ (m^2) \end{array} $	$ \begin{array}{c} K_{300} \\ (m^2) \end{array} $	Absolute Differ-
300	300	2.02F 10	5.26F 10	43 50%
300	900	9.05E-10	$1.86E_{-10}$	45.5970
300	1500	6.36E-11	1.00E-10 1 21E-10	47 25%
300	2000	5.06E-11	9.65E-11	47.58%
900	300	1.05E-09	1.83E-09	42.30%
900	900	3.41E-10	6.21E-10	45.18%
900	1500	2.12E-10	3.93E-10	46.04%
900	2000	1.66E-10	3.10E-10	46.38%
1500	300	1.93E-09	3.28E-09	41.28%
1500	900	6.26E-10	1.12E-09	44.17%
1500	1500	3.88E-10	7.06E-10	45.04%
1500	2000	3.02E-10	5.53E-10	45.39%

3.4 Predictive model for FiberForm with length-scale dependency

The final analytical expression developed by the supervised learning model to evaluate the permeability of the TPS material is given by Eq. 13 in conjunction with Table 5, which represent the elements of the support vectors (x_i) . As evident from Table 5, six support vectors with their respective dual coefficients $(\alpha - \alpha^*)$ are found to be sufficient to maintain the prediction errors within an acceptable range as explained in section 3.3. The simplicity of the analytical expression with six terms points towards an exponential reduction in the computational time required to predict the permeability when compared to DSMC simulations. The final expression given by Eq. 13 is a function of length-scale (L), pressure (P), and temperature (T). The term X represents the input vector containing the input parameters in logarithmic scale required to predict permeability. For example, if the permeability of a TPS material at 500 Pa and 1,000 K with a length-scale of 100 μm needs to be evaluated, then the corresponding input vector for Eq. 13 is $X = \{ln(L), ln(T), ln(P)\} =$ $\{4.605, 6.907, 6.215\}$ resulting in a permeability of 6.966×10^{-10} m². As explained in the previous sections, the single relationship given by Eq. 13 is capable of completely eliminating the need to find the constants involved in Klinkenberg correction for each combination of inputs. The capability of the supervised learning model to solve the multi-dimensional problem by utilising a very small number of support vectors indicates a linear relationship of the length-scale with permeability when the REV is below the target size.

$$K = exp\left[-19.94950563 + \sum_{i=1}^{6} (\alpha_i - \alpha_i^*)exp(-0.015||x_i - X||^2)\right]$$
(13)

Another key feature to highlight in both original and extended length-scale model is the ability to converge to the permeability in the continuum limit (K_o) as the pressure average is increased for a given temperature. This behavior can be seen in Fig. 8 for two different length scales, 75 μm and 200 μm , and it follows the expected trends from Eqn. 3. Note in Eqn. 3, if P_{avg} approaches infinity then K_{eff} approaches K_o .

Table 5: Support vectors and dual coefficients used to compute the effective permeability of FiberForm using Eqn. 13.

$\ln(L)$	$\ln(T)$	$\ln(P)$	$\alpha_i - \alpha_i^*$
4.16846	6.9222	7.48814	63.894
4.20277	6.79578	5.63757	41.792
5.70364	5.75391	6.65682	-24.648
5.22808	5.90183	7.20845	56.174
4.33733	6.54071	7.03018	-160.000
5.08209	7.46652	6.01977	22.788



(a) Permeability with respect to P_{avg} for L = 75 μm and $\phi = 0.7277.$



(b) Permeability with respect to P_{avg} for L = 200 μm and $\phi = 0.8591.$

Figure 8: Predicted permeability for extended range of length-scales against pressure average for different sets of temperatures.

The permeability of a TPS material was calculated using the DSMC technique through a digital microstructure generated with Fibergen. A function relating the porosity of FiberForm and the sample length was derived to use as input in the Fibergen algorithm to study the dependence of length-scale on the permeability of the microstructure. By noting the good agreement of K_{eff} and K_{Darcy} , Darcy's law was verified and the capability of DSMC simulations to accurately model the permeability through porous media in all flow regimes was validated. Grid and time independent study were performed to determine the optimal values for mesh and time resolution. The ability of the DSMC simulations to reproduce similar results was considered as the major criteria for grid and time independent study. A good agreement of results from simulations using XRCT scans of FiberForm and the digital microstructure obtained from Fibergen was presented and discussed in great detail in our previous work [42]. The validation of digital microstructure generated from Fibergen with respect to the simulations using XRCT scans allowed us to use the synthetic microstructure generation code for training the supervised learning model. Fibergen enabled us to significantly reduce the supervised learning model set-up and training time since it was seamlessly integrated into the in-house python scripts developed to automate the data generation process. LHS sampling was integral in ensuring a uniform spread of training data which is essential to develop a robust and flexible supervised learning model.

uniform spread of training data which is essential to develop a robust and flexible supervised learning model. The results from the DSMC simulations evaluated for the data points in the domain were used as training points to develop a supervised learning model based on support vector machine to predict the REV dependence on the permeability of porous media for a wide range of length sample, temperature, and average pressure. The model was trained to target permeability of FiberForm, and it was found to be fairly accurate with a relative RMSE of 0.0627 and maximum error of $\sim 25\%$ on the edge of the training domain. Two extra runs were conducted to study the performance of the model on the external domain close to its training data. A similar spread of values for relative error and RMSE was obtained for extra runs which helped in validating the capability of the supervised learning model to remain indifferent to over-fit and under-fit. The second run of data points specifically consisted of length-scales at either edge of the chosen training range to underscore the effect of length-scale on permeability. To accurately capture the plateau in permeability after the 300 μm length-scale, a new set of points with extended length-scale domain were generated. With the extended number of samples and larger range for the length-scale, both the plateau and the relative error for the model were improved. The extended length-scale model is currently being tested and optimized to produce the lowest relative error possible while maintaining the plateau and the final model will be published in a future article.

The model allows the prediction of the permeability of FiberForm for an arbitrary length-scale, temperature and average pressure while exponentially saving time and computational power when compared to high fidelity simulations like the DSMC technique. In addition to this, the analytical function derived in this article allows for a simple integration into a material response code to serve the purpose of augmenting the underlying CFD problem, which uses permeability as a closure parameter in the momentum transport equation for flows through porous materials. To conclude, the analytical function developed through SVR satisfied the primary goal of developing an alternative time and cost-efficient way to compute the permeability of a TPS material given its length-scale for a range of pressures and temperatures.

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