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ABSTRACT
We show that the permeability of periodic simply connected porous media can be reliably predicted from the Minkowski tensors (MTs) describing the pore microstructure geometry. To this end, we consider a large number of two-dimensional simulations of flow through periodic unit cells containing complex-shaped obstacles. The prediction is achieved by training a deep neural network using the simulation data with the MT elements as attributes. The obtained predictions allow for the conclusion that MTs of the pore microstructure contain sufficient information to characterize the permeability, although the functional relation between the MTs and the permeability could be complex to determine.

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I. INTRODUCTION

The characterization of the microstructure of a porous medium is an unsolved problem for nearly a century. While the influence of the porosity on the permeability is well studied,1–3 the effect of the shape of the porous microstructure itself on permeability has remained unclear. The difficulty is in identifying a shape descriptor that is concise yet relevant to the permeability of the porous microstructure. Spatial discretizations (like voxel data from tomograms or the points on a reconstructed surface) or parametric representations (such as spherical harmonics) have been used as shape descriptors, traditionally. While the first class of descriptors depends on the spatial resolution and, therefore, may require processing a large amount of data, the latter does not apply to general porous structures. Simple representations of shape, relevant to flow through porous media, such as the widely used tortuosity,4 pore constriction,5 or Euler characteristics,6 cannot fully characterize permeability even for simplified porous media. Fitting parameters, obtained experimentally, are required to relate permeability to these characterizations.7 Permeability is also predicted from a combination of tortuosity, constriction, and characteristic pore length, the combination of which is correlated with porosity in naturally occurring porous media.8 Even though porosity is correlated with pore shape characteristics in nature, it is important to separate the influence of pore shape and of porosity on the permeability. Given that porosity is a scalar quantity, isolating shape effects on the permeability can be achieved in simple porous systems and this can reveal the efficacy of the shape descriptor in characterizing permeability.

We identify Minkowski tensors (MTs)8 as shape descriptors for simply connected porous microstructure by showing that MTs can reliably characterize its permeability. Minkowski tensors, also known as valuations,9 have been introduced8,10,11 as a shape descriptor for a variety of different complex-shaped media such as cellular structures and granular media. In the latter, e.g., MTs reveal novel characteristics of the packings such as the isotropy and the angle of isotropy.12 While Minkowski functionals (MTs are a generalization of the functionals13) were proposed for the characterization of porous permeability,14 until now there is no evidence that MTs can reliably characterize the permeability of general porous media.6,15 Since a Minkowski Tensor is an additive measure, microporosity in the solid phase and surface roughness that do not influence permeability in reality, would increase the MT evaluations, making correlations difficult.15 Moreover, topological connectivity, another important aspect of pore microstructure, cannot be represented by MTs. However, MTs represent the void shape, volume, and pore connectivity,14 have the properties of uniqueness and completeness as well as contain directional information in contrast to scalar measures. Such wide-ranging features of MTs warrant...
their exploration in relating the morphology to the transport in porous media.

In this study, we simulate the flow around an obstacle of a randomly generated, two-dimensional, simply connected shape placed within a periodic cell. Data from a plethora of such flow simulations each corresponding to a random shape is used to train a deep neural network (DNN) to show that the Minkowski tensors can predict permeability to very high accuracy. Thus, we demonstrate that the MTs for a given structure are sufficient to characterize the permeability for the two-dimensional (2D) periodic porous media considered here. Previous studies (see, e.g., Ref. 15) have shown that there is no linear relationship between Minkowski functionals and the porous permeability. Since DNNs are known to capture complex non-linear relations, they can be employed to show if permeability is related to the MTs of the microstructure. In the context of realistic porous media, the use of DNNs is increasingly present, see for example Refs. 17 and 18.

In the current paper, we show that Minkowski tensors are pertinent descriptors of the permeability through a data science experiment. We generate pseudo-random 2D shapes, simulate fluid flow around these shapes in a periodic domain, and compute the permeability for each of the resulting repeating porous media. Finally, we train a DNN to show that the MTs, used as input features, can predict the computed permeabilities to a reasonable accuracy.

II. SHAPE GENERATION AND FLOW SIMULATION

We simulate the flow through representative elemental volumes (REVs) of porous media. The solid walls within the REVs need to have shapes that are complex enough such that their influence on the permeability cannot be predicted by the porosity alone.10,22 Also, the flow domain needs to be simple enough such that it is feasible to generate a large amount of data for the DNN’s training. Based on these considerations, we generate square 2D domains with periodic boundary conditions containing a simply connected arbitrary shaped obstacle of invariant area. The obstacle is assigned no-slip wall boundary conditions containing a simply connected arbitrary shaped obstacle of large amount of data for the DNN’s training. Based on these considerations, we generate square 2D domains with periodic boundary conditions containing a simply connected arbitrary shaped obstacle of invariant area. The obstacle is assigned no-slip wall boundary condition for the flow simulation. Each such domain thus forms the representative elemental volume (REV) for a separate porous medium. Shapes with regions outside the square, occurrence of sharp spikes, and self-intersections are eliminated during the data generation. Different values for \( m \), namely 1, 2, and 3, are considered, and for each of these orders \( m \), 100,000 shapes are generated. For \( m = 1 \), only ellipses are obtained, while higher values of \( m \) result in shapes with more undulations. Figure 1 shows shapes of different order generated with the same set of generator points.

The flow through each of the REVs then modeled using the Navier–Stokes equation and simulated using the finite volume method solver called Gerris.24 This solver uses an adaptive quadtree mesh which eliminates the need for additional meshing and pre-processing difficulties. The boundary conditions for velocity and pressure are set to be periodic in both the horizontal and vertical directions. For each REV, three different pressure gradient values are applied to drive the flow in the horizontal direction. The largest pressure gradient magnitude is chosen such that the corresponding Reynolds number is about 1 (Rey = \( \rho U r / \mu \), where \( r \) is the radius of the circle of equal area as the obstacle, \( U \) is the superficial velocity and \( \rho \) and \( \mu \) are the density and viscosity of the fluid). Therefore, we expect the flow regime to not deviate substantially from the regime where the Darcy’s equation is applicable, at least at the smallest pressure gradient magnitude considered. Darcy’s equation for porosity reads:

\[
\frac{dp}{dx} = -\frac{\mu}{K} U.
\]

where \( x' = dx/d\theta \). The shapes are scaled such that the area is maintained to an invariant value of 0.5 for all shapes (to keep the porosity fixed: \( \phi = 0.5 \)) and the centroid \((X_0/2, Y_0/2)\) is translated to the center of the unit square (side length of 1m) domain. Shapes with regions outside the square, occurrence of sharp spikes, and self-intersections are eliminated during the data generation. Different values for \( m \), namely 1, 2, and 3, are considered, and for each of these orders \( m \), 100,000 shapes are generated. For \( m = 1 \), only ellipses are obtained, while higher values of \( m \) result in shapes with more undulations. Figure 1 shows shapes of different order generated with the same set of generator points.

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\]
assuming an isotropic porous medium. For each REV, we fit the pressure gradient, \( \frac{dp}{dx} \), to a 2nd order polynomial function of the superficial velocity, using a least squares fit. The 2nd order fit is performed in order to minimize errors when the flow regime is beyond the Darcy regime. Moreover, the second-order polynomial in \( U \) is the Forchheimer permeability\(^{25} \) which includes inertial effects:

\[
\frac{dp}{dx} = -\frac{\mu}{K} U - \frac{\rho}{K_1} U^2, \tag{5}
\]

where \( \rho \) is the density of the fluid and \( K_1 \) is the inertial permeability. The slope of this curve at the origin (\( U = 0 \)), gives the coefficient of the linear term in \( U \), namely \( \mu/K \). For a given viscosity, \( \mu \), the value of \( K \) can be thus computed for each REV from the simulated flow field.

In a stricter sense, the permeability is anisotropic and is represented as a tensor.\(^{26} \) However, we assume the off diagonal element of the permeability tensor to be small due to the array structure of the porous medium and also because the flow is expected to be in a non-inertial (low Reynolds number) regime. Making the approximation that the permeability tensor is diagonal, the scalar \( K \) in Eq. (4) becomes the diagonal element of the tensor corresponding to the \( x \)-direction.

Figure 2(a) shows four example shapes from the dataset including the extreme cases, i.e., the most permeable REV (A) as well as the least permeable REV (D) among the shapes with \( m = 2 \). The other two cases (B) and (C) were picked at random from the dataset to correspond to permeability values below and above that of a circle, respectively. The plot in Fig. 2(b) shows the Reynolds number against the pressure gradient for each of these example shapes and the polynomial fit to these data.

Figure 3 shows the distribution of the permeability values for each set of shapes with the corresponding values of \( m \). As \( m \) increases, we observe that an increasing number of shapes in the dataset has permeability zero. This is because the probability of a shape blocking the flow increases as the number of free parameters determining the shape increases. The permeability values with a circular obstacle (\( \phi = 0.5 \)) in the periodic domain, calculated analytically\(^{19} \) and obtained from simulations are marked using a dash-dot line and a solid line, respectively. The permeability of the circular obstacle is close to the value corresponding to the peak probability density of our dataset.

### III. MINKOWSKI TENSORS

Minkowski tensors are generalizations of the Minkowski functionals and can characterize a shape using translation covariant and translation invariant tensors. Four linearly independent Minkowski tensors can be defined for two spatial dimensions and six for three spatial dimensions. Our study includes only two spatial dimensions. The MTs are integrals over a compact set \( \Omega \) with non-empty interior bounded by a sufficiently smooth surface \( \partial \Omega \):

\[
W_{0,0}^{2,0} = \int_{\Omega} r \otimes r \, dA, \tag{6}
\]

\[
W_{1,0}^{2,0} = \frac{1}{2} \int_{\partial \Omega} r \otimes r \, dr, \tag{7}
\]

\[
W_{2,0}^{2,0} = \frac{1}{2} \int_{\partial \Omega} x(r) r \otimes r \, dr, \tag{8}
\]

\[
W_{0,2}^{2,0} = \frac{1}{2} \int_{\partial \Omega} n \otimes n \, dr. \tag{9}
\]
Here, the vectors \( \mathbf{r} \) and \( \mathbf{n} \) are the position and the unit normal vector at the surface, respectively, \( \kappa \) is the local curvature, \( dr \) is the infinitesimal line element and \( dA \) is the infinitesimal area element in 2D. We use an open-source software called “Papaya,” which is described in Ref. 13, to numerically compute the MTs.

Each MT is a symmetric, two-dimensional, second-order tensor and, thus, contains three independent scalar values. For the purpose of building the DNN model we use the Eigenvectors as well as the elements of the Eigenvectors as training features. This results in six features (scalar values) for each MT, making a total of 24 features.

IV. THE DNN MODEL

The features (Eigenvectors and Eigenvector elements) are provided as input nodes to a DNN comprised of seven hidden layers and an output layer with a single node representing the permeability value. We have chosen the \( \tanh \) function as the activation function. We have used the Keras\textsuperscript{12} library with a TensorFlow backend for the purpose of setting up the DNN and training it. Further details of the neural network architecture used in our study are provided in Table I. The \( L_2 \) norm of the difference between the predicted and the actual \( K \) value is used as the \textit{loss function} for the training. The DNN is trained by optimizing the weights and biases of each node (neuron) of the network for minimizing the loss function through several iterations (also known as epochs).

The available dataset is split into a \textit{training set} containing 95\% of the data selected at random and a \textit{validation set} containing the rest of the data. While the training set is used to optimize the nodal weights, the validation set is used to establish the accuracy of the prediction and to check for overfitting. A higher rate of decrease in error for the training set than that for the validation set would mean overfitting of the training data. We stop the training process either when the error stops decreasing simultaneously for both the training and validation sets or when overfitting sets in. The training parameters were chosen by experimenting with the training process.

We show, in Fig. 4, that the model we trained predicts \( K \) within 6\% mean squared error (both training and validation dataset) relative to the total variance in the permeability values for each of the set of shapes. It may be possible to improve the parameters of the DNN and achieve better prediction of \( K \). We believe that the achieved accuracy of prediction is sufficient to show that MTs effectively characterize the permeability. This is because, the porosity, which has a major influence on permeability,\textsuperscript{14} is invariant in the data set and the MTs are able to expose the effect of shape (excluding porosity) in isolation. The accuracy achieved with a linear regression fit is also provided in Fig. 4. The considerable difference in accuracy of prediction shows that the MT–permeability relationship is indeed non-linear in nature, and justifies the use of DNNs for this exploration.

V. RESULTS AND DISCUSSION

Beyond the obvious dependence of permeability on porosity,\textsuperscript{1} a comprehensive dependence of permeability on shape has been a subject of intense research.\textsuperscript{28–32} Previous studies that used simple fit functions were unable to conclude that the permeability is dependent on MTs.\textsuperscript{33,34} A DNN, on the other hand, is able to learn non-linear relationships, and therefore, can reveal if Minkowski tensors characterize the permeability.

Figure 4 shows the convergence of the mean squared error (MSE) normalized by the total variance of the permeability values of all the shapes, with increasing epochs. While the training converges for \( m = 1 \), the DNN starts overfitting for the shapes with \( m = 2 \) and \( m = 3 \), and hence the training was terminated when the error in the training set started deviating from the error in the validation set. The training parameters used were kept constant across these data sets and the same parameters do not result in same accuracy across the data sets. We show that training accuracy is the highest (MSE/\( \sigma^2 < 1\% \)) for shapes with \( m = 1 \) (ellipses) and the error increases with increasing \( m \). Nevertheless, we believe that the overall accuracy is still high enough for practical purposes, given that the porosity is invariant across the data set.

In other applications using MTs such as in the structure of sphere packings, the higher order MTs have not revealed additional insights about the structures than those by the lower order MTs,\textsuperscript{35} raising the question whether these higher order measures are significant for characterization of the permeability. The volume moment tensor \( W_0^m \) is equivalent to the area moment of inertia tensor and could thus capture effects such as blocking of the flow due to orientation of shapes as is evident from several other studies.\textsuperscript{33,34} In order to show that all the

### Table I. Training parameters used in training the DNN. For details of implementation, refer to the scripts in the supplementary material.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
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<tr>
<td>Activation function</td>
<td>Tanh</td>
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<td>Hidden layer type</td>
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<td>Number of layers</td>
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<tr>
<td>Hidden layer sizes</td>
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<tr>
<td>Loss function</td>
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<td>Optimizer</td>
<td>Stochastic gradient descent</td>
</tr>
<tr>
<td>Initial learning rate</td>
<td>0.005</td>
</tr>
<tr>
<td>Feature normalization</td>
<td>Min – max</td>
</tr>
</tbody>
</table>
MTs contribute to the prediction of the permeability, we present training results where only one MT is used at a time (six features) considering the dataset for \( m = 2 \), in Fig. 5. For the Y-axis in Fig. 5, the same data and normalization approach were used as in Fig. 4(b). Clearly, all four MTs are independently able to predict the permeability to great accuracy (MSE/\( \sigma^2 \) < 10%) and, thus, contribute to the model.\textsuperscript{35,36} Moreover, there seems to be not much difference in the convergence behavior (note that the Y-axis in these plots is in logarithmic scale).

FIG. 4. Training and validation of the DNN model for shapes of different complexity (\( m \)): (a) \( m = 1 \), (b) \( m = 2 \) and (c) \( m = 3 \). Results of linear regression is also provided for comparison (black lines). The Y-axis in each of the plots shows the mean-squared error (MSE) of the model prediction normalized by the variance in the permeability values in each case. As test set we randomly take about 10% out of the total data set in each case. The X-axis shows the number of training epochs (iterations).

FIG. 5. Training and validation of the DNN with different Minkowski tensors: (a) \( W_0^2 \), (b) \( W_1^2 \), (c) \( W_2^0 \), and (d) \( W_1^0 \), used exclusively as features.
between the different tensors. Thus MTs embody much more information about the shape, relevant to the permeability, than simple scalar descriptions such as tortuosity and porosity.

It is a worthwhile question to ask whether a large amount of data may always be required for a successful permeability prediction model based on the MTs. To answer this question we perform the training process with different training data set sizes and juxtapose these results in Fig. 6. Here we plot the minimum error achieved against the size of the training data \( m = 2 \). Remarkably, only a very small number of samples, namely 100, is required to predict the permeability \( \text{MSE}/\sigma^2 < 10\% \). This suggests that a similar exercise using three-dimensional domains can be achieved with computationally feasible data size.

VI. CONCLUSION

We have demonstrated that the answer to the titular question whether Minkowski tensors of simply connected porous microstructure can be related exclusively to the permeability of the medium is in the affirmative. We have generated a large enough dataset of complex shapes of constant porosity with different orders of complexity and performed CFD simulations of flows through the REVs containing these non-convex simply connected shapes. We trained a DNN using these simulated data, validated the model, and demonstrated its predictive accuracy for different shape complexity and for different data set sizes. We also show that all the different MTs considered have equivalent predictive ability. Reasonably accurate prediction results from even a small number (\( \approx 100 \)) of data points for training the model. This indicates that computationally more challenging systems can be investigated following the procedure outlined above.

The above approach of generating data from simulations and mapping morphology description using MTs to the permeability motivates several new directions of enquiry. Certain Minkowski tensors may have greater relevance for a particular class of porous media. Also the undulations on surfaces will stop having an effect on the transport properties as the length scale of undulations approach the scale of roughness on the wall while increasing (additively) certain MT measures. How well individual MTs contribute to separate aspects of this morphology–function relationship can be studied further by further deep learning explorations.

Physically, these unit cells with obstacles represent cross Sections of uni-directional regular fibrous porous media and may seem limited in application. However, the motivation to the above exercise has been to identify a simple system where a data experiment relating the MTs to the permeability may be conducted. Our results show that Minkowski tensors are adequate descriptors of the pore microstructure. This observation motivates the hypothesis that the same may be true for non-uniform porous microstructure. Prediction of the full permeability tensor for the same system as well as other anisotropic systems is a natural extension to the present work.

SUPPLEMENTARY MATERIAL

See the supplementary material for Python scripts for machine learning from the data, the input files for the CFD simulations, the automation script for generating the shapes, for executing the CFD simulation and the data used in this paper are provided as supplementary material. The material is also openly available in Zenodo at https://doi.org/10.5281/zenodo.4017111, Ref. 37.

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The authors report no conflict of interest.

DATA AVAILABILITY

The data that supports the findings of this study are available within the article and its supplementary material.

REFERENCES


