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Prediction Algorithm for Transverse Permeability of Unidirectional Fiber Reinforced Composites with Electric-Hydraulic Analogy

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Abstract

This study suggests the prediction algorithm for transverse permeability, represented the flow resistance during the manufacturing process of composite, of unidirectional continuous fiber reinforced plastics. The cross-sectional shape of representative volume element (RVE) is considered to reflect fiber arrangement. The equivalent length is used as a factor to express the change of resin flow according to fiber arrangement. The permeability prediction algorithm is created by grafting the electric-hydraulic analogy and validity is confirmed. The code for permeability prediction was composed by means of MATLAB and Python, flow analysis was performed by using FLUENT. The algorithm was verified as the permeability results obtained through algorithm and numerical analysis were almost identical to each other, and the calculation time was reduced around 1/450 compared to the numerical analysis.

Keywords

Permeability
Manufacturing process of composite material
Representative volume element
Equivalent length
Electric-hydraulic analogy

1. Introduction

Unidirectional fiber reinforced composites are widely used in various fields due to their high specific stiffness, specific strength, fatigue strength, and excellent corrosion resistance. The market size of fiber-reinforced composites is expected to increase as the demand for light weighting increases due to stricter environmental regulations, and at the same time, research on manufacturing processes is being actively conducted. Although there are many different processes, the impregnation of composites is done by passing water through the fibers. The impregnation of composites is accomplished through the flow of resin between several micrometer-sized fibers, and voids created during the impregnation process are a major defect in composites. Therefore, minimizing voids during the process is a very important task in the composite manufacturing process, and for this purpose, it is necessary to accurately understand the flow behavior of resin inside the composite.

In the composite manufacturing process, the flow of resin through the composite is simulated by the flow of fluid through a porous material. The flow behavior through a porous material is dominated by pressure, viscosity, and material properties. Among these, the permeability coefficient, a factor that reflects the geometric characteristics of the material, is relatively inaccurate because it is essential to reflect the characteristics of the porous material at the microscopic scale. Therefore, accurate prediction of the water permeability coefficient is essential for identifying and minimizing composite defects.

The permeability coefficient was proposed to quantitatively express the resistance to fluid flow inside a porous material. Kozeny-Carman proposed an expression for the permeability coefficient in isotropic materials by combining the Navier-Stokes equation, simplified by assumptions, with Darcy's Law [1]. This was further developed by Gebert, who expressed the permeability coefficient of evenly placed reinforcement in a resin transfer formation as a first-order function of porosity and a suitable combination of constants [2]. Since then, many researchers have developed Kozeny-Carman's equation to express the water permeability coefficient as a function of porosity, but it does not reflect the geometry of the fiber arrangement, which is the geometric feature of the reinforcement, and shows a difference from the actual value. Numerical analysis has been used to derive a water permeability coefficient that reflects the fiber arrangement geometry. Bodaghi *et al.* derived the water permeability coefficients of 22,000 randomly placed representative volume elements at various porosities by simulation and identified the probability density functions [3]. This shows that the fiber arrangement affects the water permeability coefficient. Other studies have been conducted to predict the water permeability coefficient, and Zarandi *et al.* compared various studies that can derive the water permeability coefficient [4]. Each study provides different water permeability coefficient predictions under the same conditions. Therefore, it is difficult to accurately predict the water permeability coefficient using existing studies.

Recent research trends in composite manufacturing processes report that interfacial effects between materials also affect the flow properties of resins. Anastasiadis and Hatzikiriakos found that slip occurs when a force above the limit shear stress is applied at the interface with a solid during polymer flow [5]. Lim *et al.* confirmed through experiments that the lower the surface free energy and surface roughness, the faster the impregnation rate of carbon fiber reinforcement [6]. Therefore, in this study, we developed an algorithm to predict the water permeability coefficient by reflecting the porosity, internal fiber arrangement, and surface properties of the material, which are all characteristics of the composite material that determine the resin flow behavior.

The actual shape of the carbon fiber composite was simulated inside the volume element, and the fibers were placed to create a representative volume element that represents the whole on a microscopic scale. The space inside the representative volume element was then divided into polygons by setting the effective distance and effective space. The process was implemented through MATLAB (MATLAB R2020b, Mathworks, USA) code. The electric-hydraulic similarity was then applied to calculate the flow resistance of the representative volume element under anti-slip conditions, and the algorithm was implemented in Python (Python 3.10.0, Python Software Foundation, USA).

The equivalent length was introduced as a factor to reflect the flow variation due to the fiber volume fraction and arrangement in the composite and the surface properties of the material, and numerical analysis was performed using a commercial program to derive the equivalent length. The numerical analysis was performed with the same representative volume element and was performed with FLUENT (FLUENT 2020 R1, Ansys Inc., USA). The velocity field in the representative volume element was applied to Darcy's law to calculate the permeability coefficient.

To validate the algorithm, the algorithm and commercial simulation results were compared on five different representative volumetric elements.

2. Theory development

2.1. Representative volume elements

Composites are mixtures of two or more materials at the macroscopic scale. As a result, they exhibit different physical behaviors at the macroscopic and microscopic scales. The macroscopic behavior of a composite with evenly distributed constituent materials is the same in all parts, but at the microscopic scale, a randomly selected part cannot be representative of the whole because the fiber diameters are in the micrometer range.

It is self-evident that the most accurate results can be obtained by considering all the fibers inside the composite, but this is very inefficient due to the large number of fibers inside. Therefore, it is essential to select a representative volume element of appropriate size to represent the whole. In this study, the validity of the representative volume element was determined based on the number of fibers contained in the volume element [7].

2.2. Resin flow between fibers

Due to the high viscosity of the resin, a flow with a Reynolds number less than 1 is formed inside the composite. Therefore, the flow of resin perpendicular to the fibers can be treated as a stable laminar flow through the cylinder. The flow can be described by a quadratic function of the velocity field of the flow in a plane parallel to the fiber direction, including a straight line through the fiber centers, as a flow caused by a pressure gradient, with stable non-slip conditions in the boundary layer while passing through the cylinder. By simplifying the continuity and Navier-Stokes equations, the velocity field and average velocity of the resin flow passing between the fibers are given below.

$$v = -\frac{h^2}{2\mu}\frac{dp}{dx}\left(1-\frac{y^2}{h^2}\right) \quad (1)$$

$$v_{average} = -\frac{h^2}{3\mu}\frac{dp}{dx} \quad (2)$$

In the above equation, h is the shortest distance between fibers, μ is the viscosity of the resin, v is the flow velocity, and p is the pressure.

2.3. Permeability coefficient and Darcy's law

The flow of resin through a composite material can be treated as fluid flow through a porous material. Darcy expressed the velocity v of the fluid in such a flow as a function of the pressure gradient ∇P, the viscosity μ of the resin, and the permeability coefficient K, as shown in the equation below.

$$v = -\frac{\mathbf{K}}{\mu}\nabla P \quad (3)$$

From the equation above, the permeability coefficient represents the smoothness of the flow and it is a factor that is affected by the structural features of the porous material.

2.4. Electric-hydraulic similarities and the analysis of a nodal circuit

The movement of water in a hydraulic circuit and the movement of electrons in an electrical circuit are very similar, and the relationship of physical quantities in each circuit can be expressed by Darcy's law and Ohm's law. In both equations, the physical quantity corresponding to the linear velocity density is expressed as the product of flow resistance and potential energy.

The similarity of the two circuits makes it possible to calculate flow in hydraulic circuits through electrical circuit analysis.

Nordahl circuit analysis is a method of electrical circuit analysis that analyses the electrical features of a circuit through relationships between physical quantities. The potential energy of an electron passing between nodes with constant potential is reduced by resistance, and this can be applied to hydraulic circuits to calculate the flow rate corresponding to the linear velocity density.

3. Water permeability coefficient prediction algorithm

3.1. Generating representative volume elements

In this study, representative volume elements with different fiber volume fractions were generated using the nearest neighbor algorithm [8]. As shown in **Figure 1**, the placement of new fibers satisfied the periodic boundary conditions and did not overlap with the already generated fibers.

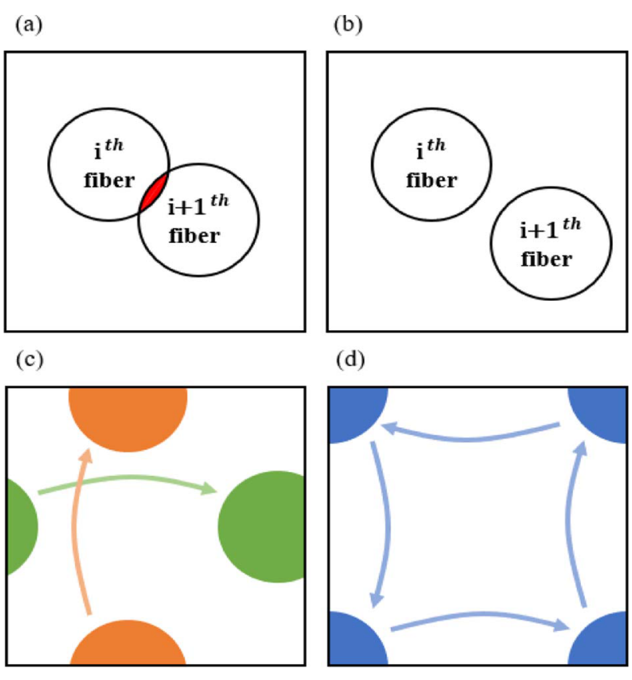

Figure 1. Mechanism for generating RVE (a) not allowed (b) allowed (c) periodic boundary condition for fibers on edge (d) periodic boundary condition for fiber on corner

The diameters of the fibers inside the generated representative volume element follow an exponential distribution with a diameter of 8 μm, which is the diameter of a typical carbon fiber, and an average inter-fiber spacing of 3 μm. The minimum distance between fibers was set to 0.1 μm, as it is impossible to generate a mesh for numerical analysis if the distance between fibers is too close. The generation angle of the fibers follows a continuous uniform distribution with a minimum value of 0 rad and a maximum value of 2π rad. The generation of representative volume elements stops immediately after the target volume fraction is exceeded.

3.2. Selecting effective fiber pairs and deriving effective distances

Among the fibers in the interior of a representative volumetric element, the fiber pairs with flow resistance are selected and the distance between them is called the effective distance. Flow in the direction perpendicular to the fibers passes through the fibers and the smaller the distance between the fibers, the greater the flow resistance. In addition, if there are other fibers between the fiber pairs or the gap between the fibers is very large, the gap formed by the fiber pair cannot be judged as effective.

To select effective fiber pairs, two criteria were applied as shown in **Figure 2**. First, when a peripheral fiber is drawn from the center of the reference fiber to the peripheral fiber, the area between them and the fiber that is wholly or partially enclosed is considered invalid. Secondly, when a common perimeter line was

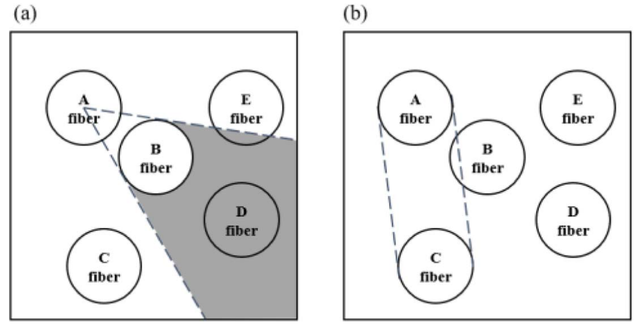

Figure 2. Valid fiber based on (a) angle, (b) outer common tangent

drawn between two fibers, fibers that included all or part of the other fiber were considered invalid.

3.3. Partitioning effective space by effective distance

When all effective distances are represented, the space inside the representative volume element is partitioned into polygons of various shapes. The interior space of the polygons corresponds to the nodes of the Nodal circuit analysis and the sides of the polygons are treated as resistors. In order to satisfy the periodic boundary condition, each side of the polygon located at the left and right ends is treated equally. **Figure 3** shows the result of the effective space division of a representative volume element with a length of 100 µm on one side.

3.4. Water permeability coefficient calculation

In order to quantitatively express the flow resistance of the complex fiber arrangement inside the representative volume element, the Kirchhoff current law of Nodal circuit analysis is used. The effective space inside the polygon is the node corresponding to the equipotential in the Nodal circuit analysis, and the effective distance can be expressed as a resistance, which allows the flow resistance to be calculated in the same way as the equivalent resistance is calculated in a current circuit.

4. Deriving the equivalent length through numerical analysis

As shown by Stokes' paradox, there is no solution to Stokes' equation around the cylinder, so it is necessary to derive the equivalent length by experiment or numerical analysis. In this study, a numerical analysis was performed to derive the equivalent length under the condition that the fiber with circular cross-section satisfies the anti-slip condition.

To derive the water permeability coefficient in the direction perpendicular to the fiber, a representative volume element of a two-dimensional shape was generated by an algorithm. Periodic boundary conditions were imposed on the left and right sides, and no-slip conditions were imposed on the fiber surface. A pressure difference of 10 Pa was applied between the top and bottom to generate a flow with a Reynolds number less than 1. The density and viscosity of the fluid were given as 1000 kg/m^3 and 1 Pa·s, similar to those for epoxy resin flow.

The size of one side of the mesh for the numerical simulation was created to allow for a fiber to fiber spacing of 0.1 µm. The size of one side of the mesh at the fiber surface was set to 0.05 µm, and the inflation was set so that the anti-slip condition was limited to the area adjacent to the fiber surface, and the second layer was placed with a thickness of 0.025 µm. For computational convenience, the mesh size was set to increase with distance from the fiber surface, while the growth rate was kept at the default setting of 1.2.

The velocity field obtained through numerical analysis was substituted for the velocity of Darcy's law to calculate the permeability coefficient, and the equivalent length was derived by comparing with the results obtained through the algorithm.

5. Results and discussion

5.1. Algorithm results with arbitrary equivalent lengths

In this study, 10 different representative elements with fiber volume fractions of 0.4, 0.5, and 0.6 were generated by the nearest neighbor algorithm as shown in **Figure 3**.

The effective fiber pairs were then selected to derive the effective distance information. Based on the effective distance information, the interior of the representative volume element was divided into effective spaces as shown in **Figure 4**.

The partitioned effective space provides information about the nodes and resistances in the space inside the representative volume element, and the permeability coefficient can be calculated using the Kirchhoff current law.

The mean values of the permeability coefficients of the representative volume elements with fiber volume fractions of 0.4, 0.5, and 0.6 calculated by this algorithm are 3.40×10^{-13} m^2, 1.24×10^{-13} m^2, and 0.37×10^{-13} m^2, with standard deviations of 4.59×10^{-14} m^2, 2.27×10^{-14} m^2, and 0.21×10^{-14} m^2.

5.2. Deriving equivalent lengths

The equivalent length was derived by comparing the results of the numerical analysis with the results of the algorithm applying an arbitrary equivalent length. As shown in **Figure 5**, the velocity field of the resin is higher for wider fiber-to-fiber spacing, and it can be seen that the flow characteristics change rapidly as it passes between adjacent fibers. The mean values of the water permeability coefficients of representative volume elements with fiber volume fractions of 0.4, 0.5, and 0.6 calculated by numerical analysis are 9.77×10^{-13} m^2, 3.16×10^{-13} m^2, 0.48×10^{-13} m^2, with standard deviations of 1.54×10^{-13} m^2, 2.30×10^{-13} m^2, and 0.06×10^{-13} m^2. The equivalent lengths calculated by the harmonic mean are 0.363 m, 0.391 m, and 0.495 m.

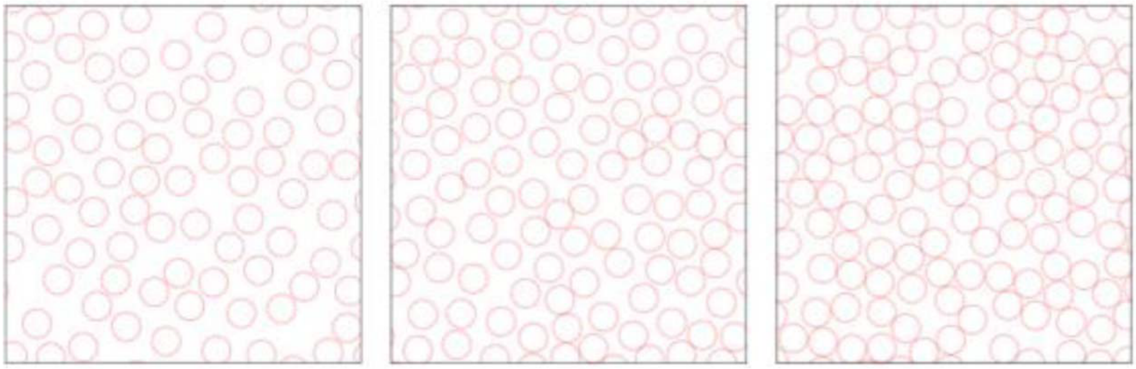

Figure 3. Generated RVE

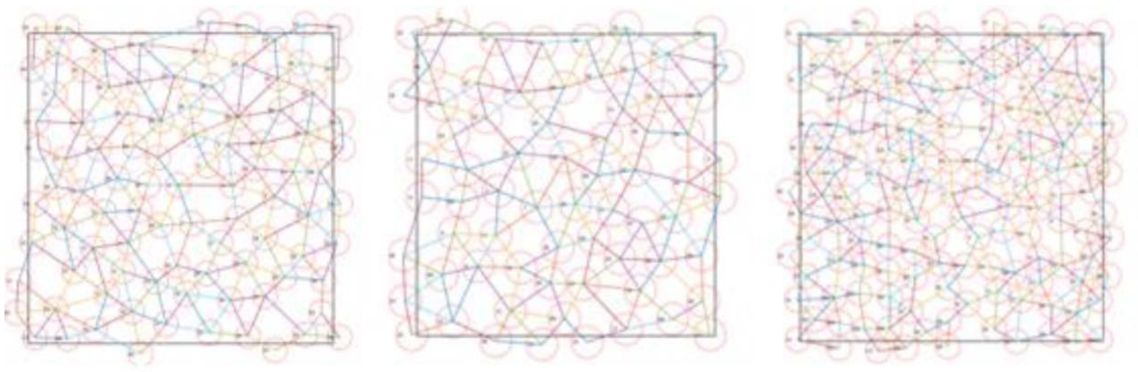

Figure 4. Divided valid space

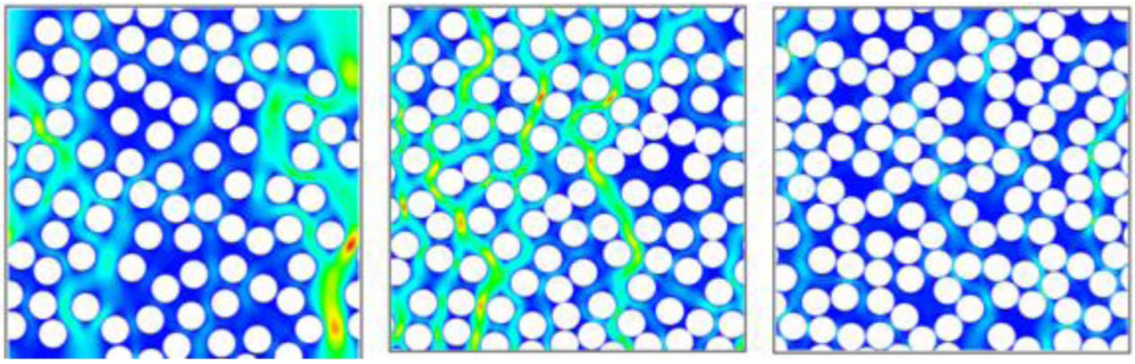

Figure 5. Velocity field of resin flow through RVE

5.3. Predicting pitch coefficients

For the validity of the algorithm, the derived equivalent lengths were applied to predict the water permeability coefficient. Five additional representative volumetric elements with the same size and fiber volume fraction were generated, and the average values of the water permeability coefficients of the representative volumetric elements with volume fractions of 0.4, 0.5, and 0.6 were predicted to be 9.37×10^{-13} m^2, 3.24×10^{-13} m^2, and 0.48×10^{-13} m^2, with standard deviations of 1.26×10^{-13} m^2, 0.59×10^{-13} m^2, and 0.04×10^{-13} m^2, confirming the validity of the algorithm.

5.4. Algorithm and numerical solution time

The time required to derive the water permeability coefficient in FLUENT and the algorithm was checked. As shown in **Table 1**, the algorithm did not show a significant difference in the effective space division and water permeability coefficient calculation time, but FLUENT took longer to generate the mesh than to run the solver. It can also be seen that the time required for each representative volume element varies greatly.

As shown in **Figure 6**, the absolute running time of the two methods is significantly different. While the algorithm's effective spatial partitioning and water permeability coefficient calculations were completed within seconds, FLENT required several hours to generate the mesh.

6. Conclusion

In this study, an algorithm for the prediction of the water permeability coefficient in the vertical direction of continuous fiber reinforced composites is proposed when the fibers with circular cross-section satisfy the anti-slip condition. For accurate prediction of the water permeability coefficient, a prediction technique has been developed that can take into account the porosity, internal fiber arrangement, and surface properties of the material, which are all factors affecting the impregnation properties of continuous fiber composites. Porosity and fiber arrangement are reflected in the algorithm through the geometry of the fibers located within a representative volume element, while the surface properties of the material are reflected through the equivalent length.

The algorithm was used to predict the permeability coefficient of a representative volume element with different fiber volume fractions. The prediction results were found to be in good agreement with the results of a conventional prediction technique that calculates the permeability coefficient by substituting the results of numerical analysis into Darcy's law.

The algorithm calculates the permeability coefficient by expressing the flow resistance of a representative volume element as a function of distance. This allows

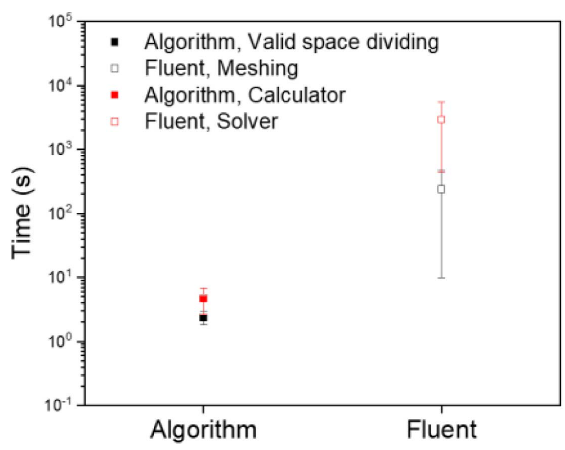

Figure 6. Taken time of Algorithm and FLUENT

Table 1. Taken time of Algorithm and FLUENT

	Algorithm		FLUENT	
	Valid space dividing	Calculator	Meshing	Solver
Taken time	4.72	2.38	2949.9	239.8
Standard deviation	2.03	0.57	2500	230

for the prediction of the permeability coefficient of a representative volume element containing two fibers in contact, which is not possible with conventional finite element techniques.

The algorithm has a very short running time compared to commercial simulation programs, thus it is expected to have high economic efficiency when applied to actual processes, and it is expected to be highly useful in analyzing composite processes through data-driven research such as machine learning.

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Disclosure statement

The authors declare no conflict of interest.

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