REPRESENTATIVE DOMAIN SIZE STUDY ON SIMULATED 3D FIBER SYSTEMS

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ABSTRACT

Fibrous synthetic filter media are used for various tasks in automotive applications, in particular for filtration of air and oil. The microstructure of the filter media highly influences the macroscopic properties of the filter element such as pressure drop, efficiency, etc. Effective numerical simulation is required to examine the performance of the filter elements in the early design phase before industrial production. Numerical simulations take the microstructure model as an initial configuration. Moreover, a realistic microstructure model for a filter element is needed to analyze how the microstructure affects its physical properties. A realistic 3D stochastic model of the fiber system with fiber interaction for the non-woven filter media is developed in [1]. Since numerical simulations need extensive computation power, it is important to find the representative domain size of the generated microstructure for a required filter property. In this paper, a simulation and a statistical approach are used to estimate the representative domain size of the microstructure model from [1]. Precisely, the representative domain size with respect to the packing density, the pore size distribution, and the pressure drop are studied.

KEYWORDS

Representative volume element, Stochastic microstructure model, Fiber system model, Fiber bundle, Fibrous media
1 Introduction

Non-woven materials are widely used in automotive industry. Particularly, the importance of non-woven materials in the production of filter media is increasing. Filter properties such as pressure drop, dust holding capacity, etc. and geometric characteristics such as packing density, pore size distribution, etc. are highly influenced by the microstructure of the filter media used. For example, the fiber orientation distribution directly influences the pressure drop. Therefore, a realistic microstructure model for the filter media is required to understand how the microstructure affects their physical properties.

Moreover, there is high demand for advanced and more efficient filters in automotive industries. Designing and testing new filters through an industrial production process are tedious and cost expensive. Alternatively, virtual prototypes for new filters can be obtained by numerical simulations. Numerical simulations take the microstructure model as an initial configuration. Then, filter properties are optimized by adapting the initial microstructure model. The final microstructure model with optimized filter properties is considered as the virtual prototype of the new filter material.

Several microstructure models for fiber systems are introduced in the literature. Modeling of straight fibers using the dilated Poisson line process is introduced in [2]. It creates overlapping fiber systems. In [3, 4], the random sequential adsorption approach is used to generate non-overlapping fiber systems with straight fibers. Non-overlapping fiber systems with curved fibers are created in [5, 6]. In particular, fiber orientation distribution and fiber bending can be effectively controlled by input parameters in [5]. All approaches mentioned above generate fiber systems with individual fibers. Whereas, non-woven materials contain fiber bundles rather than individual fibers only. Thus a new microstructure model incorporating fiber bundles is developed in [1] based on the model from [5].

Numerical simulations require extensive system memory and computation time. Hence, it is important to find the representative domain size or size of the representative volume element (RVE) for a required filter property. That is, the representative domain size is the smallest domain size which represents the characteristics of domain sizes larger than this size. A purely simulation based domain size study for the non-overlapping fiber system model simulated by GeoDict2014 (www.geodict.com) is carried out in [7]. A statistical approach to compute the size of the RVE for a given physical property is proposed in [8]. In the literature, this approach has been used to compute the size of the RVE for various microstructure models and materials properties such as elasticity or thermal conductivity see [9, 10, 11].

In this paper, we use both a simulation and a statistical approach to estimate the size of the RVE for the microstructure model developed in [1]. In particular, the representative domain size for the packing density, the pore size distribution and the pressure drop are estimated using the numerical simulation. Furthermore, the statistical approach from [8] is used to compute the representative domain size for the packing density and the pressure drop. Finally, the simulation results are compared with the statistical results. It turns out that the statistical approach can be used to estimate the representative domain size for the given property more precisely and using less generated microstructures than the purely simulation based approach.
2 Microstructure generation for domain size study

2.1 Stochastic modeling of 3D fiber systems with fiber bundles

First we summarize the essential properties of the model proposed in [1]. The proposed approach is twofold. In the first step, a random walk in 3D space is used to generate an initial configuration of the fiber system. Fibers are represented by chains of spheres. Each chain of spheres is denoted as \( \{p_0, ..., p_l\} \) with \( p_i = (x_i, \mu_i, r_i) \), where \( x_i \in \mathbb{R}^3 \) is the center of the sphere, \( \mu_i \in S^2 \) (unit sphere) is the local fiber orientation, \( r_i \in \mathbb{R}^+ \) is the sphere radius, and \( l \in \mathbb{N} \) is the number of spheres in the fiber.

For each fiber, an initial sphere \( p_0 = (x_0, \mu_0, r_0) \) is generated at first. Here, \( \mu_0 \) represents the main orientation of the fiber. The main fiber orientation \( \mu_0 \) is assumed to follow the spherical distribution described in [12], which represents a special case of the angular central Gaussian distribution [13]. The probability density function of this distribution is defined as:

\[
p(\theta, \phi | \beta) = \frac{\beta \sin \theta}{4\pi(1 + (\beta^2 - 1)\cos^2 \theta)^{\frac{3}{2}}}
\]

where \( \beta > 0 \) and \( (\theta, \phi) \in [0, \pi) \times [0, 2\pi) \) are the polar coordinates of the orientation. For \( \beta \to 0 \), the orientations concentrate on the z-axis, for \( \beta = 1 \), the orientations are uniformly distributed on the sphere and for \( \beta \to \infty \), the orientations are isotropically distributed in the \( xy \)-plane.

The new local orientation \( \mu_{i+1} \) for the sphere \( p_{i+1} \) during a random walk is generated from the multivariate von Mises-Fischer distribution [5]. The probability density function of this distribution is:

\[
f_{mvMF}(\mu_{i+1}|\mu_0, \kappa_1, \mu_i, \kappa_2) = \frac{|\kappa_1 \mu_0 + \kappa_2 \mu_i|}{2\pi \left(e^{\kappa_1 |\mu_0 + \kappa_2 \mu_i|} - e^{-|\kappa_1 |\mu_0 + \kappa_2 \mu_i|}\right)} e^{\kappa_1 \mu_0^T \mu_{i+1} + \kappa_2 \mu_i^T \mu_{i+1}}
\]

where \( \mu_{i+1} \in S^2 \), \( \mu_0 \in S^2 \) is the main fiber orientation, \( \mu_i \in S^2 \) is the local orientation of the previous sphere, \( \kappa_1 > 0 \) is the reliability parameter towards \( \mu_0 \), and \( \kappa_2 > 0 \) is the reliability parameter towards \( \mu_i \). Thus, \( \kappa_1 \) and \( \kappa_2 \) control fiber bending.

The new center \( x_{i+1} \) for the sphere \( p_{i+1} \) is computed as \( x_{i+1} = x_i + \frac{r_{i+1}}{2} \mu_{i+1} \), where \( r_{i+1} \) is a newly generated radius. Refer to [1] for more details about the model.

The initial configuration may contain overlapping fibers. In the second step, the force biased fiber packing approach is used to render this initial configuration with overlapping fibers into non-overlapping fibers while keeping the fibers intact.

The input parameters for the model are the packing density, distributions of fiber diameter, orientation and length, the parameters for fiber bending, the frequency of fiber bundles and the number of fibers in each bundle.

2.2 Sample simulation

Due to the stochasticity of our model, each model simulation run with fixed input parameters generates a different realization of the geometric structure. For our domain size
study, we consider 10 independent realizations of the fiber model for four different domain sizes 1,500 µm × 1,500 µm × 512 µm, 750 µm × 750 µm × 512 µm, 500 µm × 500 µm × 512 µm and 250 µm × 250 µm × 512 µm as in Figure 1. Totally, we have 40 realizations. All input parameters are fixed for all realizations as in the following. Fiber thickness = 10 µm, fiber length = 5, 200 µm, β = 10, κ₁ = 10 and κ₂ = 100. In these realizations, 40% of the given fibers form bundles of four fibers, 30% of fibers form bundles of three fibers, 20% of fibers are paired and the remaining fibers are modeled as individual fibers.

Furthermore, we observe that due to the fiber length exceeding even the largest considered domain size, there are some edge effects in the stochastic model proposed in [1]. In order to avoid these edge effects, domain sizes larger than the required sizes are generated and boundary regions of side length at least 100 µm are removed. For example, the realization of domain size 750 µm × 750 µm × 512 µm is cropped from a microstructure generated in a domain size of 1200 µm × 1200 µm × 712 µm.

Figure 1: Realizations of our stochastic geometry model in different domain sizes 1,500 µm × 1,500 µm × 512 µm, 750 µm × 750 µm × 512 µm, 500 µm × 500 µm × 512 µm and 250 µm × 250 µm × 512 µm. Packing density ≈ 10%, fiber thickness = 10 µm and fibers are oriented in the xy-plane.

3 Simulation study regarding domain size

In this section, we estimate the representative domain size for the packing density and the pore size distribution which are geometric characteristics of the fiber system and the pressure drop which is a macroscopic property of the resulting filter.
The packing density, the pore size distribution and the pressure drop are calculated for the 10 realizations of each domain size using GeoDict2015. Mean and standard deviation are computed for all domains. Corresponding results for the packing density, the pore size distribution and the pressure drop are plotted in Figures 2 - 4, respectively.

The mean value of the packing density, the pore size distribution and the pressure drop stabilize from domain size $750 \, \mu m \times 750 \, \mu m \times 512 \, \mu m$ (see Figures 2 - 4). That is, the representative domain size for the packing density, the pore size distribution and the pressure drop is $750 \, \mu m \times 750 \, \mu m \times 512 \, \mu m$.

Furthermore, the standard deviation of all studied characteristics from Figures 2 - 4 shows that the estimated physical properties at the representative domain size do not vary too much for different realizations with fixed parameters. Therefore, using our model, only a few realizations of the representative domain sizes are required to achieve the needed virtual prototype for filter materials.

Figure 2: Mean and standard deviation of the packing density computed for 10 realizations of each domain size
Figure 3: Mean and standard deviation of three different quantiles of the pore size distribution computed for 10 realizations of each domain size.

Figure 4: Mean and standard deviation of pressure drop computed for 10 realizations of each domain size.
4 Statistical study regarding domain size

The statistical approach to estimate the size of the RVE for a given physical property $Z$, for a given relative precision in the estimation of $Z$, and given number of realizations that one is ready to simulate is defined in [8].

We summarize this approach in the following. Let $\bar{Z}$ be the mean of the given property $Z$ estimated on $m$ independent realizations of domain $V_s$ of volume $v$. Here, independent realizations are the realizations that are generated from different random seeds. The sub-domains $V_{s1}, V_{s2}, ..., V_{sm}$ of equal volume $s < v$ are cropped from $m$ independent realizations. The mean squared error of the given property $Z$ in $m$ sub-domains of equal volume $s$ to the target property $\bar{Z}$ is defined as

$$D^2_Z(V) = \frac{1}{m} \sum_{i=1}^{m} (Z_i - \bar{Z})^2$$

where $Z_i$ is the calculated value of the given property $Z$ on sub-domain $V_{si}$.

For an ergodic stationary random function $Z(x)$, the mean squared error $D^2_Z(V)$ of its mean value $\bar{Z}$ over the volume $V$ is defined as

$$D^2_Z(V) = D^2_Z A_3^3 V$$

$D^2_Z$ is the point variance of $Z(x)$ and $A_3$ is so-called the integral range. The integral range provides information on the domain size of the structure for which the parameters measured in this volume have a proper statistical representativity.

Equation (4) is only valid for an additive combination of the variable $Z$ over the volume $V$. The following power law is proposed for non-additive combination of the variable $Z$:

$$D^2_Z(V) = D^2_Z A_3^a V^a$$

The above equation can be rewritten as follows, compare [11]:

$$D^2_Z(V) = \frac{K}{V^a}$$

where $K = D^2_Z A_3^a$.

The variables $K$ and $\alpha$ can be numerically approximated by fitting a straight line to the logarithmic version of Equation (5):

$$\log D^2_Z(V) = \log K - \alpha \log V$$

The absolute error $\epsilon_{abs}$ on the mean value of the given property obtained with $n$ independent realizations of volume $V$ is deduced from the interval of confidence (95%) by

$$\epsilon_{abs} = \frac{2D_Z(V)}{\sqrt{n}}$$
The relative error $\epsilon_{rel}$ is given as

$$\epsilon_{rel} = \frac{\epsilon_{abs}}{Z} \Rightarrow \epsilon_{rel}^2 = \frac{4D_n^2(V)}{nZ^2} \tag{7}$$

Substitute Equation (5) in Equation (7),

$$\epsilon_{rel}^2 = \frac{4K}{nZ^2V^\alpha} \tag{8}$$

The size of the RVE for effective property $Z$ with a given relative error $\epsilon_{rel}$ and $n$ realizations is defined as

$$V_{RVE} = \left( \frac{4K}{\epsilon_{rel}^2nZ} \right)^{\frac{1}{\alpha}} \tag{9}$$

**Packing density**

![Fitted straight line for the mean squared error of packing density](image)

Figure 5: Fitted straight line for the mean squared error of packing density

We apply the above mentioned statistical approach to estimate the size of the RVE of our generated microstructure for the packing density and the pressure drop. The target packing density and pressure drop are assumed as the mean of the corresponding properties measured on domain size $1,500 \mu m \times 1,500 \mu m \times 512 \mu m$ from 10 independent realizations. Here, the target packing density is 10.3 % and the target pressure drop is 7.05 $Pa$. In order to estimate the size of the RVE from Equation (9), the constants $\alpha$ and $K$ need to be estimated. These values can be estimated by fitting a straight line to the logarithmic version of the mean squared error curve (see Equation (6)).

Samples of 5 different sub-domains with cross sections $1,400 \mu m \times 1,400 \mu m$, $1,200 \mu m \times 1,200 \mu m$, $1,000 \mu m \times 1,000 \mu m$, $800 \mu m \times 800 \mu m$ and $600 \mu m \times 600 \mu m$ are cropped from each realization. The thickness of all samples is $512 \mu m$. The squared deviation from the target packing density is computed for these samples as in Equation (3). The logarithmic plot
The values of $\alpha$ and $K$ are also displayed in this figure.

Similarly, the mean squared error for the pressure drop is measured and corresponding straight line fitting is given in Figure 6.

From Equation (9), the size of the RVE for the target packing density $10.3\%$ with relative error $5\%$ and 10 realizations is $656\ \mu m \times 656\ \mu m \times 512\ \mu m$. In other words, a packing density of $10.3\%$ from our microstructure model can be achieved with a relative error of $5\%$ by taking the mean over 10 realizations of medium domain size $656\ \mu m \times 656\ \mu m \times 512\ \mu m$. Whereas, if we reduce the number of realizations to 1, we need a larger domain size of $1,809\ \mu m \times 1,809\ \mu m \times 512\ \mu m$ to attain the targeted packing density $10.3\%$ with relative error $5\%$.

Similarly, the representative domain size for the target pressure drop $7.05\ Pa$ with relative error $5\%$ and 10 realizations is $904\ \mu m \times 904\ \mu m \times 512\ \mu m$. Whereas, for single realization, the representative domain size for the target pressure drop $7.05\ Pa$ with relative error $5\%$ is $1,744\ \mu m \times 1,744\ \mu m \times 512\ \mu m$.

In Section 3, the simulation study finds out that the packing density gets stable after $750\ \mu m \times 750\ \mu m \times 512\ \mu m$ and the pressure drop stabilizes after $750\ \mu m \times 750\ \mu m \times 512\ \mu m$. The statistical approach computes the exact representative domain size for the packing density as $656\ \mu m \times 656\ \mu m \times 512\ \mu m$ and the pressure drop as $904\ \mu m \times 904\ \mu m \times 512\ \mu m$. Therefore, the statistical approach can be used to estimate the precise representative domain size from simulation measurements.
5 Conclusion

The determination of a representative domain size for virtual filter media is crucial for effective numerical filter simulations. In this work, the representative domain size is estimated for the simulated microstructure model developed in [1]. A simulation and a statistical approach are used for the study. The simulation study is performed for the packing density, the pore size distribution and the pressure drop. The statistical approach proposed in [8] is used to calculate the representative domain size for the packing density and the pressure drop. Both the simulation and the statistical domain size study yield similar results. Since the statistical domain size study is carried out in cropped sub-samples of larger domains, this approach requires less computational resources than the simulation approach. In this paper, we generated 40 realizations for the simulation study, whereas only 10 generated microstructures are needed for the statistical study. Moreover, the statistical study estimates the precise representative domain size. In addition, the simulation study shows that our microstructure model is reliable for the representative domain size. In future work, this study will be extended to other geometric and physical properties.

Acknowledgment

This work was partially funded by the German Federal Ministry of Education and Research through project 05M13 (AniS), the Center for Mathematical and Computational Modelling (CM)\(^2\) and the Deutsche Forschungsgemeinschaft (DFG) within the RTG GrK 1932 “Stochastic Models for Innovations in the Engineering Sciences”, project area P3.

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