GENERATION OF REALISTIC NONWOVEN AND FOAM FILTER GEOMETRY AND MESH FOR FILTRATION SIMULATIONS USING OPEN-SOURCE TOOLS

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ABSTRACT

Recovery of liquid aerosols (mists) from industrial processes is typically accomplished through coalescence filtration, employing highly porous nonwoven (fibrous), knitted or foam media which are regarded to potentially provide high collection efficiencies. Highly resolved pore-scale computational fluid dynamics (CFD) analysis of mist filtration processes is increasingly becoming an important tool for design and optimization of such filter media. A key to efficient application-specific optimization of filter media is the ability to generate CFD-suitable virtual filter geometries with controllable geometric parameters including solidity, fibre diameters, morphology, etc. - yet, a review of the literature suggests that the current designs are heavily reliant on computed tomography (CT) scans of available filter media for accurate representation of the pore-scale structures in a computational simulation. In the present study, a novel methodology is presented for generating realistic virtual nonwoven (fibrous) and foam filter geometries with parametric customizability, using open-source tools including Python, OpenFOAM libraries, Gmsh and Blender. Further, a methodology for the generation of a computational mesh suitable for multiphase CFD at the pore-scale is delineated for the two types of filter media generated using the present technique, $viz.$ nonwoven and foam, using open-source tools available within the OpenFOAM framework. The proposed methodology for the generation of virtual filter media and computational mesh is validated by qualitative comparison against with images from electron-microscopy (SEM) scans of real filters as well as comparison of the single-phase pressure drops predicted from CFD simulations using the generated fibrous and foam media with different solidities, fibre (or strand of foam) diameters, filter thicknesses, against the literature. The excellent agreement between the predicted pressure drops and the literature and its consistency over the several different geometric conditions considered for comparison reaffirms the validity of the proposed methodology for efficient virtual filter media development, which can eventually lead to enhanced parametric optimization capabilities and reduced design costs and lead times.

KEYWORDS

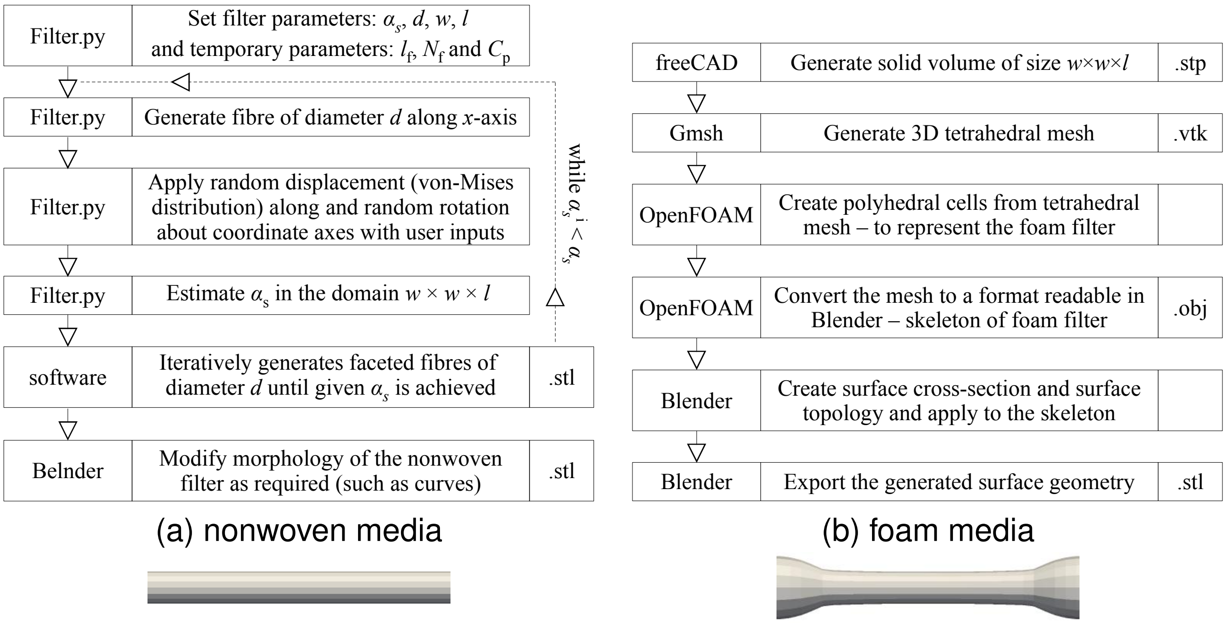
Aerosol, Mist filtration, Foam, Fibre, CFD, VOF

1 INTRODUCTION

Liquid mists are generated by several natural and anthropogenic processes including industrial compressors, production and distribution of petroleum and natural gas, lubricated manufacturing processes and internal combustion engine operation. Coalescence filtration using highly porous fibrous (nonwoven) [1], knitted stainless steel [2] or foam [3] media is widely regarded to provide high efficiency in recovery of such mists which are either valuable products or undesirable byproducts which may pose a risk to health and the environment. However, the complexity in accurate measurement and characterization of the complex multiphase flow physics inside the porous filter media during real operating conditions has to-date limited advances in the development of optimization equations for filtration systems. Most currently available design methodologies for coalescence filters are based on classical single-fibre models which, although provide acceptable predictions for clean filters, deteriorate when applied to dynamic filtration conditions (partial fluid saturation and redistribution, non-homogeneous drainage or re-entrainment, etc.), which best describes most of the operational life of such filters.

Fully resolved computational analysis of such systems could abate the difficulties in experimentation and provide a greater insight into the pore-scale flow physics thereby yielding vital data for design optimization. In addition, CFD helps in offsetting costs for trial based performance tests and reducing development lead time for any specific application. In recent years, X-ray micro-tomography, magnetic resonance imaging (MRI) and synchrotron imaging of filter media are increasingly being used for generation of virtual geometries for computational simulations [4, 5]. However, the best spatial resolution of most current are synchrotron: $\approx$0.5-1 μm), MCRI: $>$10-15 μm and micro-CT: $\approx$1-10 μm [6, 7] which implies that the resolution of the virtual media generated from such scans can be expected to deteriorate in accuracy for most micro-/ nano-fibre filter media. The deterioration in structural representation at the pore-scale will significantly affect the accuracy of any representative computational simulation, particularly those intended for liquid-liquid or gas-liquid mist filtration processes, due to the inaccurate representation of the surface topology of the fibres and their morphology which are critical for evaluation of the dynamics of wetting, and particle (mist) collection or liquid drainage.

The ability to generate virtual but realistic filter media with fully controllable user-specified geometric or topographic parameters including porosity, pore-size, fibre diameter, fibre orientations and microstructure make the generation of CFD-suitable virtual filter geometries effective and scale (length)-independent, and hence, ideal for CFD based design of filtration media. Commercial packages such as GeoDict [8, 9, 10] offer some possibilities for generation of such filter media with restricted customization options, and at a cost. Exploiting the random but statistically deterministic nature (for the purposes of its application in filtration-CFD) of the nonwoven filter structure, models based on filter solidity, fibre diameter, orientation and arrangement (such as layers) for the generation of virtual filter media have been proposed in the literature [10, 11]. Similar techniques have also been reported to be successful for the generation of fibrous filter geometries with bi-/ multi-modal distributions [8]. One of the earliest techniques for the generation of virtual foam media was developed by Lautensack et al. [12] based on a two stage approach - first, by fitting a random Laguerre tessellation to a polyurethane foam to form the core of the geometry, and subsequently using spheres with locally varying sizes to generate the solid strands of the foam in the gaps of the spheres in each pore. More recently, Redenbach et al. [9] proposed an improved (from [12]) technique for the generation of virtual foam filter media incorporating methods to introduce intensity and orientations of the closed strands (walls) of the foam. However, both the methodologies required CT scans of real foam media as starting points for the generation of a CFD suitable geometries.



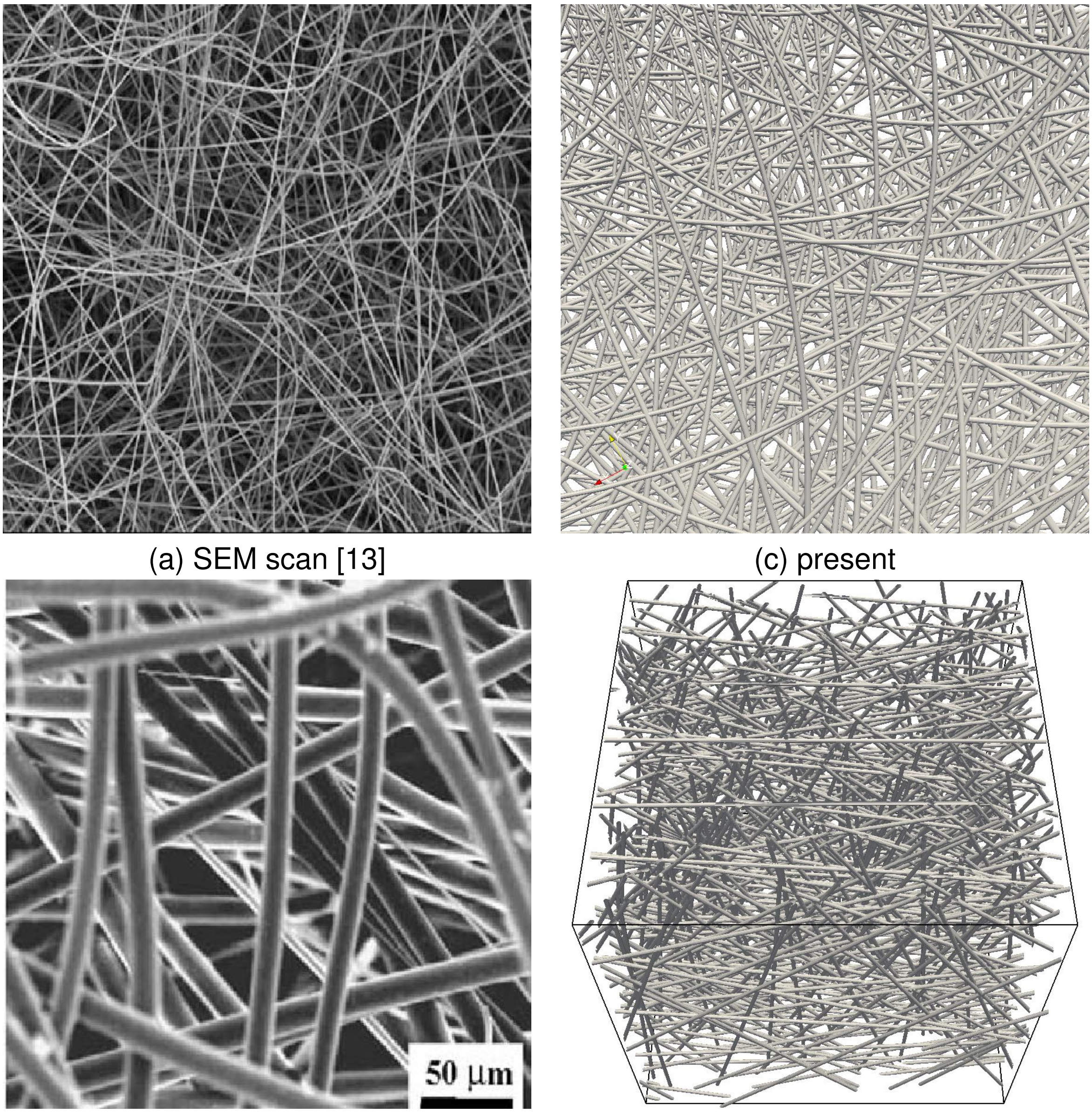
(c) single element of nonwoven media (d) single element (strand) of foam media

Figure 1: Methodology for generation of nonwoven and foam filter geometries

In the present study, novel techniques and work-flow for the the generation of realistic virtual nonwoven (fibrous) and foam filter media are presented. The proposed methodology enables full parametric customizability and employs open-source tools including Python, OpenFOAM libraries, Gmsh and Blender for the generation of the filter geometries. Subsequently, a methodology for the generation of a computational mesh suitable for multiphase CFD at the pore-scale is delineated for the two types of filter media, using open-source tools available within the OpenFOAM framework.

2 GENERATION OF VIRTUAL NONWOVEN AND FOAM FILTER MEDIA

The work-flow for the generation of virtual nonwoven and foam filter geometries is illustrated in Fig. 1(a,b) and representative smallest elements of the filters (fibre or strand of foam) are shown in Fig. 1(c,d). The nonwoven geometry is generated in three stages, using a combination of Python subroutines and the open-source 3D modeling software Blender. Firstly, user-specified inputs for filter solidity (α_s), fibre diameter (d), computational domain size in the cross-section (w), filter depth along the direction of flow (l), length of filter elements (l_f), resolution of filter cross-section (N_f) and layer-index (C_p) which specifies the level to which filters are to be generated in parallel planes, perpendicular to the direction of flow (layered media), are read into the Python script. In an iterative fashion, single line elements (centerline of fibres) are generated at each iteration, with the user-specified characteristics (l_f) and are randomly displaced



(a) SEM scan [13]

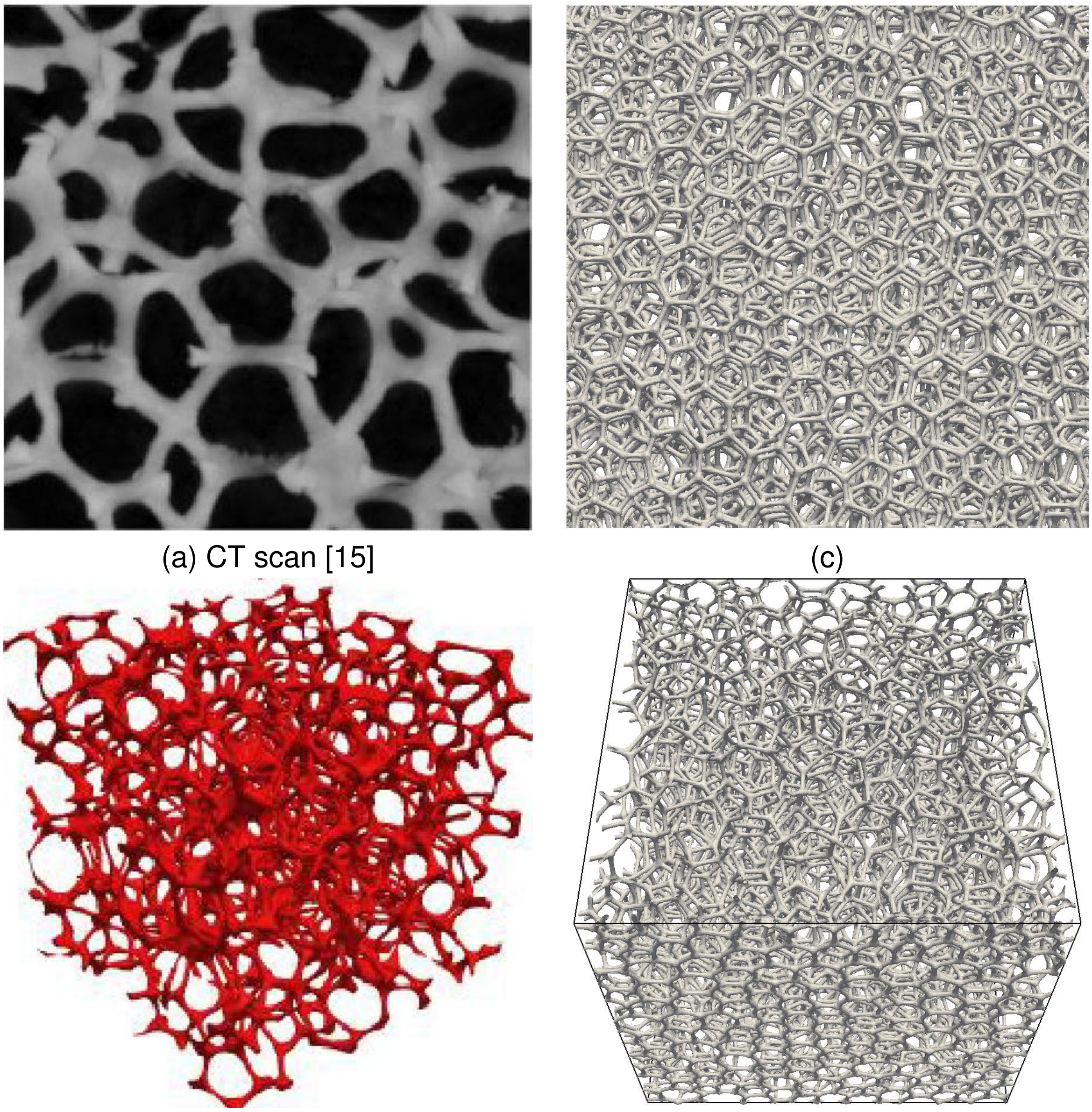
(c) present

(b) SEM scan [14]

(d) present

Figure 2: Comparison of nonwoven filter media generated using the present methodology (d =20 μm and w = 100$\times d$) against scans of similar real media

(von-Mises distribution) and rotated (uniform distribution) along the three coordinate directions and three angular directions, respectively, within the bounding box ($w \times w \times l$) to conform with the specified layer-index. Subsequently, based on the specified resolution (N_f, the shape converges to a circle with increasing N_f) and fibre diameter (d), cylindrical (faceted) fibres are generated around each line element. The procedure is repeated until the required solidity is reached within the bounding box (parts of some fibre elements may lie outside the bounding box to ensure conformance with α_s). For certain nonwoven filter media or depending on the length-scale of the filter required for the simulation, it may be necessary to modify the morphology of the fibres (curves instead of straight lines) which is carried out using the extensive functionalities available within Blender. The generated filter media is represented as a Stereo-lithography (.stl) file suitable for mesh generation and CFD. Representative nonwoven media generated



(a) CT scan [15]

(c)

(b) CT scan [16]

(d)

Figure 3: Comparison of foam filter media generated using the present methodology (d =20 μm and $w = 100 \times d$) against scans of similar real media

using the present methodology are shown in Fig. 2; scanning electron microscope images of real stainless steel ([13]) and glass fibre ([14]) media from the literature are also shown for comparison. It is seen from the figure that the fibrous media obtained using present methodology are in excellent qualitative agreement with the SEM images.

As shown in Fig. 1, the foam filter media is generated in four stages using open-source packages: FreeCAD, Gmsh, OpenFOAM and Blender. It is pointed out that unlike the other techniques in the literature discussed in the preceding section, the present methodology is able to generate the virtual foam geometry independent of any inputs from CT scans of real foams. In the present technique, a bounding box ($w \times w \times l$) volume is generated using FreeCAD and exported to the meshing software Gmsh. Here, tetrahedral cells are created within the bounding box using a Delaunay triangulations of user specified size and exported as .vtk mesh file. The tetrahedral

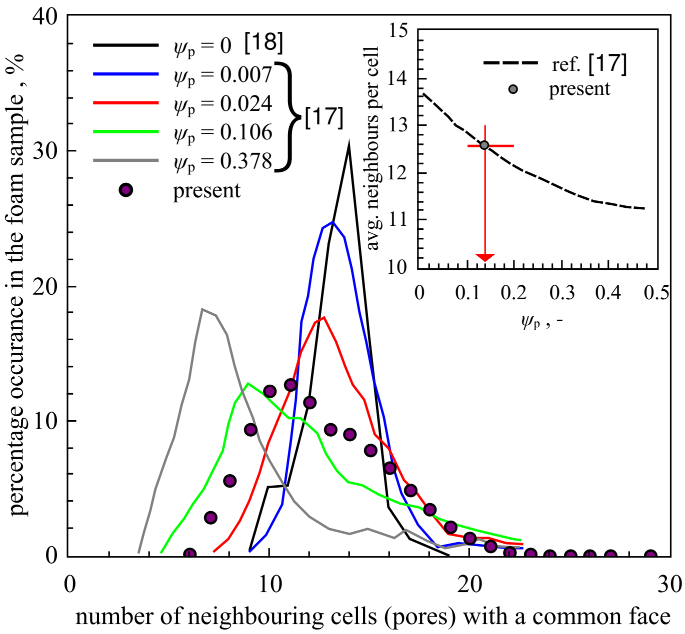


Figure 4: Comparison of the polydispersity index and the distribution in the number of neighboring cells (pores) in a representative foam filter generated using the present methodology, against the literature [17, 18]

mesh is subsequently read into OpenFOAM using in-built libraries and converted to a polyhedral mesh using user-specified inputs for a polyhedral feature angle. The edges of the polyhedral mesh now represent the strands of the foam filter geometry. A check for the polydispersity index [17] is carried out at this stage before exporting the edges into Blender, where the filter surface topology (such as circular for high density foams) and edge-structure are imposed using the advanced in-built functionalities therein. The generated geometry is subsequently exported as a faceted .stl file suitable for mesh generation and CFD. Representative sections of a foam filter geometries generated using the present methodology are shown in Fig. 3; scanning electron microscope and CT images of real foam media from the literature ([15, 16]) are also shown for comparison. It is seen from the figure that the foam media obtained using present methodology are in excellent qualitative agreement with the real media.

It is pointed out that the proposed methodology for the generation of foam media, unlike that for the nonwoven media, relies on the triangulation technique for the generation of the tetrahedral mesh which underpins the polyhedral structure of the open-cell foam. Considering that there are numerous polyhedral cell structures that can be generated using the current methodology, it is important to ensure that the pore-structure of the foam conforms to the structures that are relevant to filtration applications. This is carried out by check for polydispersity index and number of faces per pore of foam (or number of neighboring pores for each pore in the foam) as outlined earlier. Figure 4 shows such a distribution for a representative foam media generated using the present methodology, and compares the same with that in the literature. It is seen from the figure that the polydispersity index (ψ_p) for the case shown is approximately 0.14 based on the average number of faces per pore, and that distribution of the number of neighboring pores per pore lie entirely within the expected distribution (as per [17, 18]) for the calculated polydispersity index.

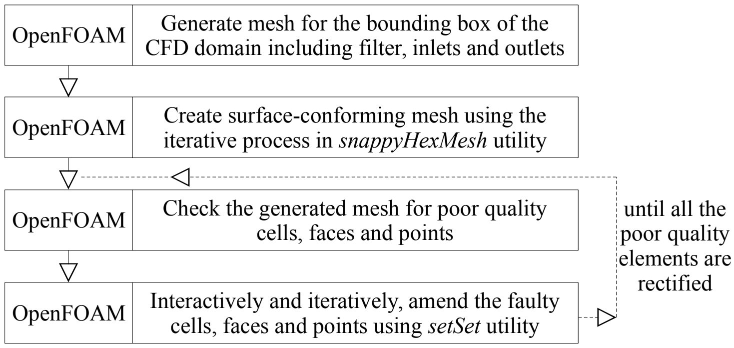
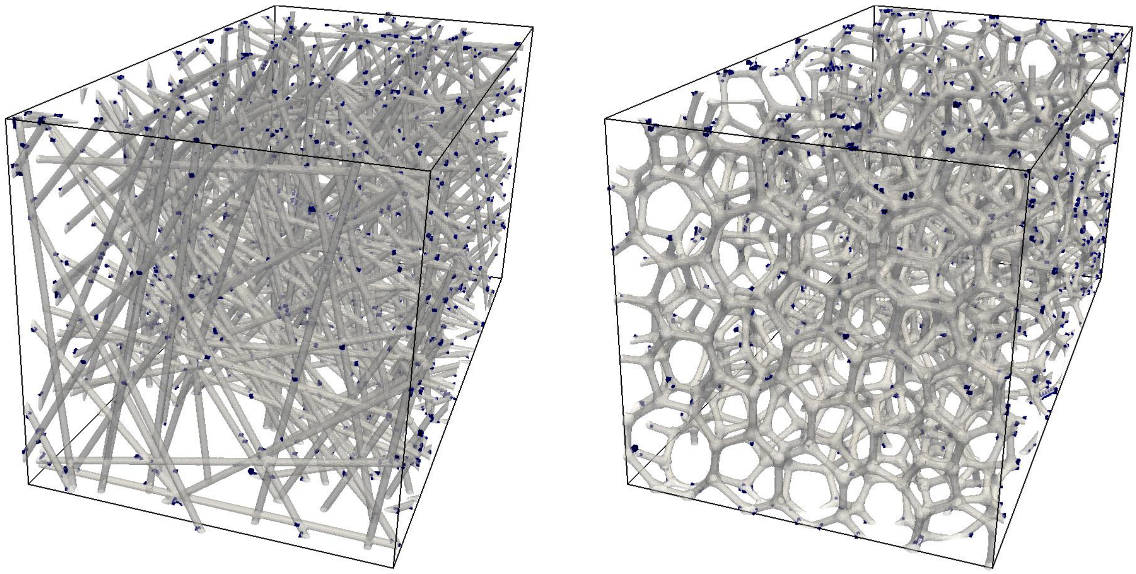


Figure 5: Methodology for generation of computational mesh suitable for multiphase CFD at the pore-scale



(a) (b)

Figure 6: Poor quality computational cells (blue) after generation of initial mesh, that would be rectified using the present methodology; d =20 μm and $w = 50 \times d$

3 GENERATION OF COMPUTATIONAL MESH FOR FILTRATION SIMULATIONS

Considering the irregular nature and complex structure of the filter geometries, the generation of a computational mesh suitable for CFD can often be a challenging task; and more so for interface tracking approaches that are required for liquid-liquid or gas-liquid filtration simulations with pore-scales resolved. In the present study, a work flow is developed using open-source tools available within OpenFOAM for generating a base mesh, and an iterative strategy for modifying the mesh to rectify any poor quality cells that are generated based on a series of mesh-quality control checks. This is particularly important to ensure stability and accuracy of the simulations that are being carried out using a coupled multi-grid Lagrangian-VOF simulation technique [19] employed for the larger scope of the research (not presented in the current paper). The general procedure is for mesh generation is illustrated in Fig. 5. An advanced and fully customizable functionality within OpenFOAM ($snappyHexMesh$) is employed to generate surface conforming mesh around the filter geometry and inside user-specified computational domain (bounding box for CFD) by truncating cells in the fluid domain that

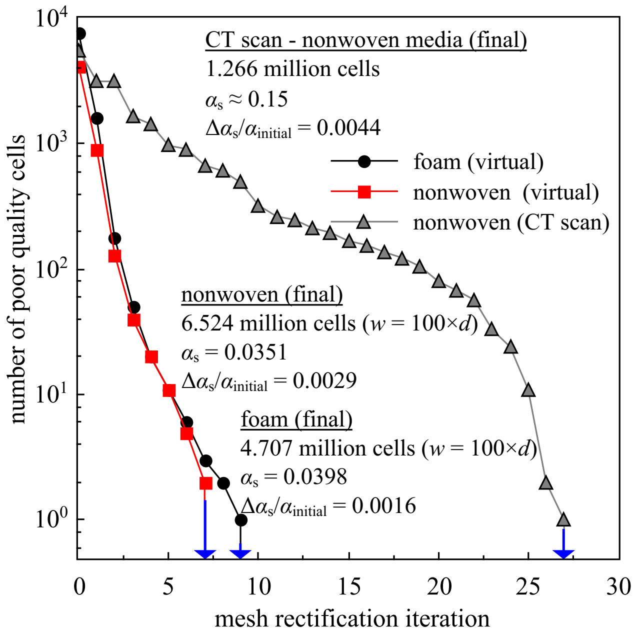


Figure 7: Representative statistics of poor quality cells with the present iterative mesh-rectification procedure

intersect with the triangulations on the faceted filter surface. The resolution/ size of the computational grids (or cells) is entirely determined by the user-specified resolution (or smaller than) of the bounding computational domain and hence can be controlled as required for any specific flow condition (such as velocity) chosen for the simulations. The generated base-mesh is checked for conformance against several cell-, face- and edge-quality control parameters including skewness, orthogonality, volume, area, twist, aspect ratio, etc. In many occasions, computational cells around the locations where the boundaries of the computational domain intersects with a filter structure may result in poor quality cells (shown in Fig. 6 for a representative case each for nonwoven and foam media) that may not conform to the imposed quality standards, and hence have to be corrected. This is carried out iteratively using another interactive functionality within OpenFOAM where the poor cells are either rectified or removed from the computational domain with a quality check carried out at each iteration. It is pointed out that the same procedure is extensible to filter media generated using other techniques such as from reconstructed CT scans of real media. The cumulative statistics of the reduction in poor quality cells with the present mesh-correction iteration for three representative cases (virtual foam, nonwoven and CT scan nonwoven) is shown in Fig. 7, where it can be seen that the change in solidity from the deletion of poor-quality cells is less than 0.1% - reinforcing the validity of the meshing technique. Representative final computational mesh for a chosen pair of 20 μm diameter fibre and foam media is shown in Fig. 8 - where both, the geometries as well as the mesh are generated using the present methodology.

A further quality check is carried before deeming the computational mesh to be suitable for CFD, by evaluating the spatial consistency in the local solidity of the filter through the entire domain - this is with the aim to identify any local irregularities or anomalies that may have resulted from some of the random-number controlled stages in the geometry generation stage. The statistics of the local solidity is evaluated by av-

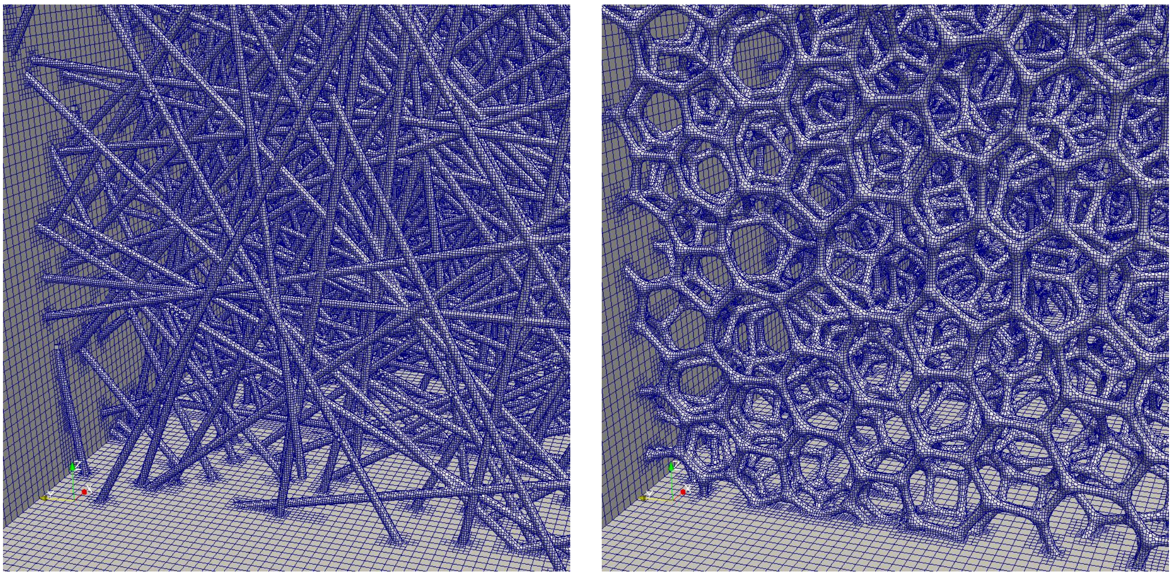


Figure 8: Representative computational mesh on for nonwoven and foam filter media; (only surface mesh is shown for clarity); d =20 μm and $w = 100 \times d$

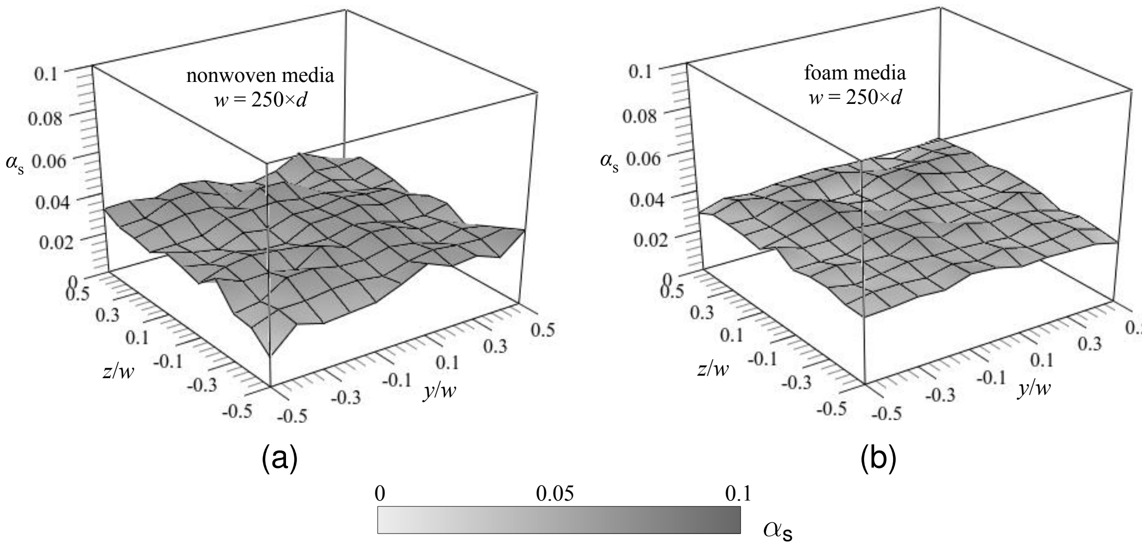


Figure 9: Contours of local solidity in the cross-section (averaged along the direction of flow) for representative fibrous and foam filter media, calculated based on 11×11 divisions in the y-z plane; $d = 20$ μm

eraging the solid volume fraction in the direction parallel to mean flow along segmented locations in a plane perpendicular to the mean flow. Figure 9 shows the distribution of the local solidities for two representative geometries (foam and nonwoven; $d = 20$ μm) generated using he present methodology for cross-sectional size $w = 250 \times d$; it can be seen that the local solidities are consistent across the entire domain reaffirming that the generated geometries as representative of a real media.

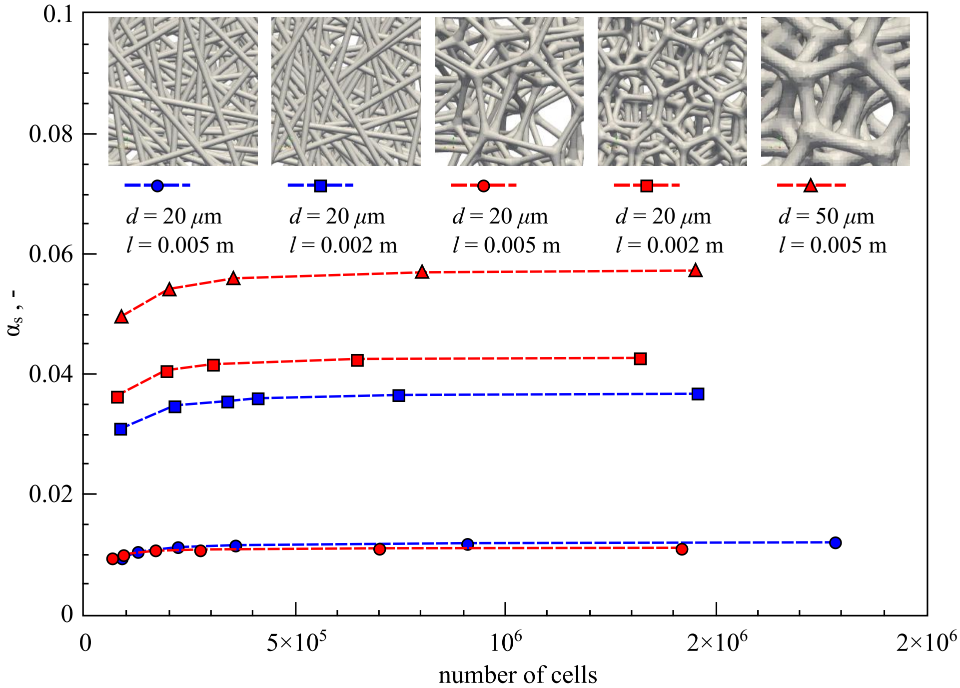


Figure 10: Effect of mesh refinement on the resolved filter solidity in the virtually generated nonwoven and foam media

4 MESH INDEPENDENCE AND VALIDATION

A detailed methodology for the generation of fully virtual nonwoven and foam filter media and computational mesh was presented in the preceding sections of this paper. To ensure that the results from any CFD carried out using the generated mesh are reliable and independent of mesh resolution, a thorough mesh-independence study is necessary. An interesting characteristic of pore-scale CFD on filter media is that an increase mesh size would consequently result in a greater fraction of the filter surface to be resolved - leading to an asymptotic limit corresponding to true solidity at high levels of mesh resolution. Figure 10 shows the influence of mesh resolution for a representative domain size of $w = 25 \times d$ for nonwoven and foam media with five different combinations of fibre (or strand of foam) diameters and filter thicknesses. It is seen that the solidity becomes independent of mesh resolution ($<$ 5%) at about 5×10^5 computational cells for the case shown.

To further demonstrate the validity and consistency of the filter geometries and mesh generated using the present methodology, single phase CFD simulations are carried out for the five different foam and nonwoven media discussed in Fig. 10, to compare the overall pressure drops across the filter against theoretical models in the literature. Figure 11 shows the dimensionless pressure drop obtained from the present computational simulations using air against the classical models of Spielman and Goren [20] which encapsulate filter media where: (i) all fibres are parallel to flow, (ii) all fibres are in 2D planes parallel to flow, (iii) all fibres are normal to flow, (iv) 3D randomly distributed fibres. All the simulations are carried out at steady state using the single phase solver $simpleFoam$ within OpenFOAM, for a given superficial flow velocity u_o = 0.6 m/s. For the purpose of comparison, the results obtained from using successively finer meshes are also shown for two cases (foam and nonwoven d = 20

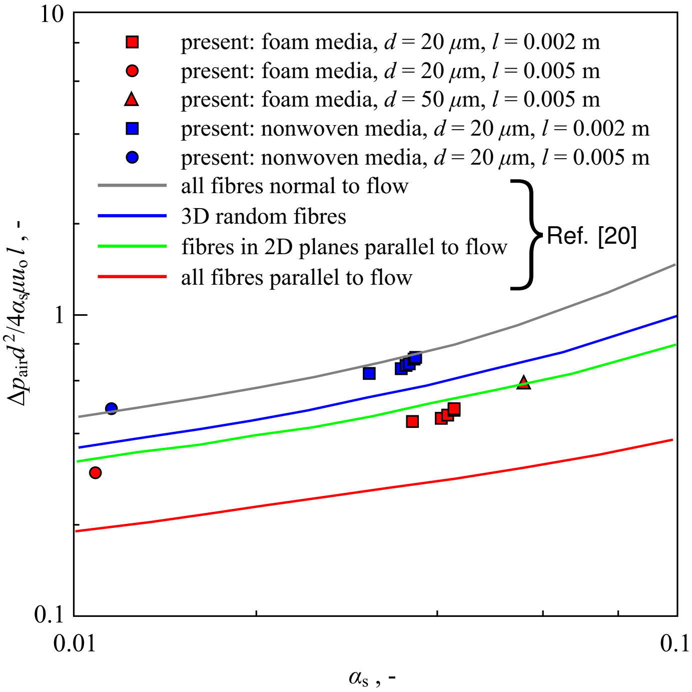


Figure 11: Comparison of the predicted dimensionless pressure drop against Spielman and Goren [20]; data obtained using different meshes are included for a representative case each for foam and nonwoven media (d =20 μm, l =0.002 m)

μm and l = 0.002 m). It is seen from the figure that the nonwoven media, which were generated with a high layer-index (=1000) corresponding to represent most fibres to be aligned perpendicular to the mean flow are in excellent agreement with the literature. It is also seen that as expected, the dimensionless pressure drop for the foam media - which consist of strands (or edges) partially aligned and partially normal to the mean flow - lie between the corresponding theoretical predictions reinforcing the validity of the present approach for the generation of nonwoven and foam media.

5 CONCLUSIONS

Computational fluid dynamics simulations of the filtration at the pore-scale is becoming an important tool for design and optimization of gas-liquid and liquid-liquid filtration media. However, most current CFD based designs rely heavily on scans of real media for simulations, which in many cases may deviate from accurately representing the pore-scale structures due to the limitations in measurement resolutions. In the present study, novel and fully customizable methodologies for the generation of nonwoven and foam filter media using open-source tools are presented. Subsequently, a generalized work-flow for the generation of computational mesh suitable for CFD is presented and strategies for improving the quality of the generated mesh are outlined. The validity of the present technique for the generation of nonwoven and foam filter media is established through qualitative comparison of the generated structures against SEM and CT scans of real media, as well as quantitative comparison of the pore-scale structures against the literature. The quality and consistency of the generated mesh is also verified through a thorough mesh independence test and comparison of the single phase pressure drops against theoretical models in the literature.

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