INFLUENCE OF FILTER DOMAIN SIZE ON THE SIMULATION OF GAS-LIQUID FILTRATION IN NONWOVEN AND FOAM MEDIA

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ABSTRACT

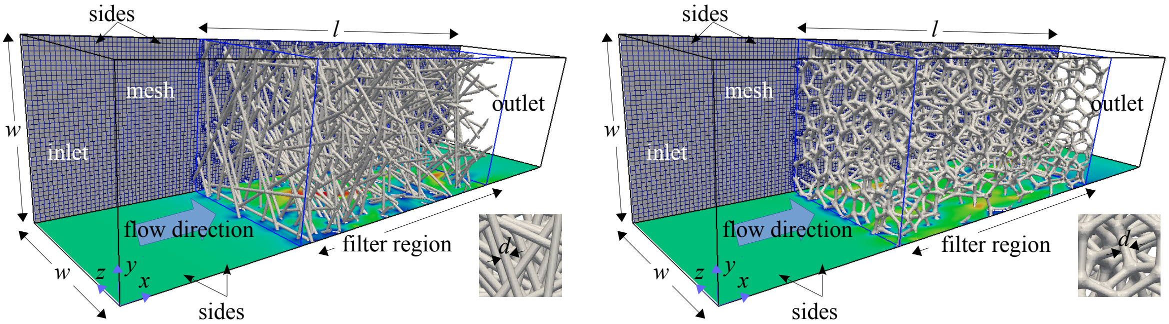
The process of coalescence mist filtration in liquid- or gas-liquid systems is strongly controlled by the dynamics of the multi-component fluid transport at the pore- or fibre-scales and its interactions with the filter media. However, current designs of mist filters are largely based on empirical data or on single-fibre filtration theory, primarily because of the complexity and difficulty in making accurate measurements at such (small) length scales. Current advancements in high performance computing provide a unique possibility to understand the dynamics of such flows using highly resolved droplet and interface capturing computational fluid dynamics (CFD) simulations - which can provide vital data for application-specific optimization of filter media. However it is important that the spatio-temporal resolutions required to accurately numerical model the fluid dynamics of micro or nano-fibre filtration processes at full size of the filters may typically demand simulations to be run with several hundred million (to over a billion) computational cells and long run-times. Hence, for reduced design lead times as well as computational cost, it is desirable to keep the size of the filter domain to a minimum, while ensuring that the largest fluid structures and scales are captured in the simulations. A review of the (limited) literature on CFD simulations of the mist-filtration process reveals that the size of the filtration domain have been predominantly chosen rather arbitrarily based on the a set multiple of the Brinkman screening length or by the computing power available - and no reported studies are yet available that address conditions of high levels of fluid saturation that involve large fluid structures. In the present study, a series of systematic computational simulations using successively larger domain sizes are carried out to identify the relationship between the characteristics of the two phase flow (such as saturation, thickness of liquid layer, pressure drop, etc.) and the size of the filter domains considered. Two vastly different types of filter media, nonwoven and foam, with similar properties such as packing density, fibre (or element of foam) diameters are chosen to additionally infer the influence of filter structures at the pore-scales to the domain size. The transient simulations are carried out using the interface capturing volume-of-fluid (VOF) solver available within the open-source CFD framework OpenFOAM.

KEYWORDS

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

1 INTRODUCTION

Several natural and anthropogenic processes including industrial gas compression, oil and gas production and distribution, lubricated manufacturing and in engine crankcases produce liquid mists that are either valuable products or undesirable byproducts which may pose a risk to health and the environment. Recovery of such mists for reuse or treatment is typically accomplished through coalescence filtration, employing highly porous fibrous (nonwoven) [1], knitted stainless steel [2] or foam [3] filter media, which are regarded to provide high filtration efficiencies and low pressure drops. Due to difficulties in accurate measurement and characterization of the complex multiphase fluid dynamics at the pore-scale and its correlation with the full-scale filtration process, design for most existing filters are based on empirical models, many of which are extrapolations of single-fibre filtration theory. Several studies [1] have pointed out that mist filters operate most of their life-time under dynamic conditions involving partial fluid saturation and redistribution, non-homogeneous drainage or re-entrainment, etc., that make the operating environments far from that considered by the single-fibre theories. The incomplete understanding of the pore-scale dynamics can often result in sub-optimal filtration efficiencies. Computational simulations using advanced droplet- and interface-tracking techniques provide a unique insight into the physics of the filtration process and droplet-filter dynamics at the different scales, which can provide vital data for application-specific optimization. However, the level of spatio-temporal resolutions that are required to accurately numerically model the fluid dynamics of filtration processes typically demand simulations to be carried out on several million grids per unit cell of the filter geometry, and over long computational times. Hence, even with the present-day high performance computing resources, it is desirable to keep the size of the computational domain as small as possible while ensuring the largest relevant scales of the flow and fluid structures are captured.

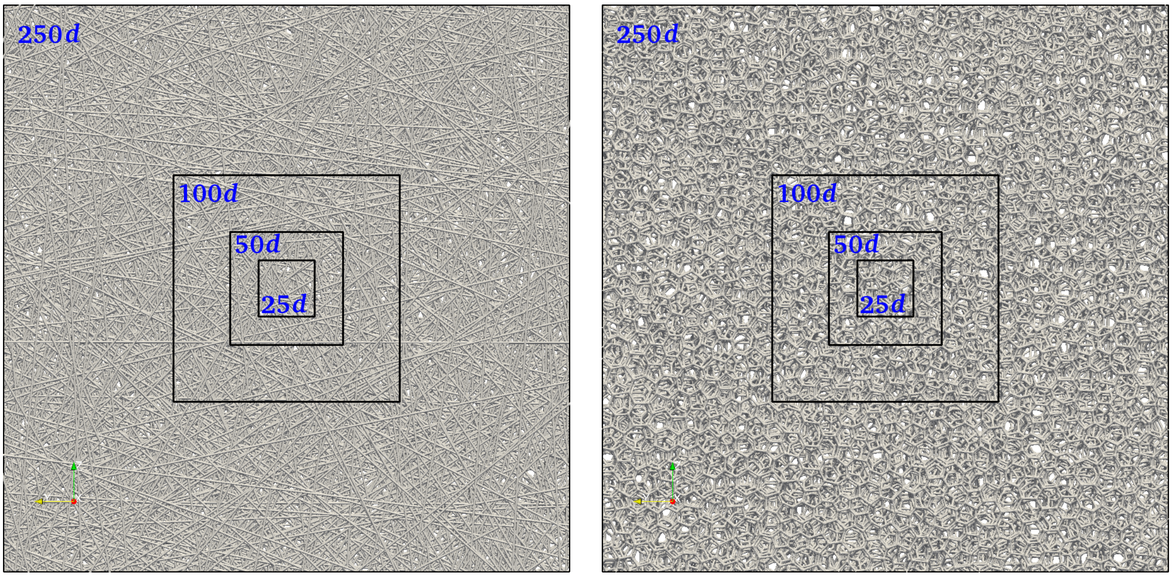


(a) nonwoven media (b) foam media

Figure 1: Schematic of the computational domains and representative structure of the nonwoven and foam media used in the present study

A review of the literature reveals that, of the limited studies available to-date on CFD simulation of mist-filtration in real or virtually developed filter media, most studies have chosen the domain size rather arbitrarily based on a multiple of the Brinkman screening length or limited by the computing power. More recently Lehmann et al. [4, 5] provided a new expression for the domain size needed for solid particle filtration, by tracking the change in pressure drop and particle capture with successively larger filter domains. It was also pointed out [5] that for the domain sizes that were considered in their study (on dust filtration in fibrous cellulose media), the macroscopic filter (and filtration) parameters such as packing density and pressure drop (single phase) remain relatively insensitive to the domain size, while the percolation path (of large dust particles) varied upto 50% across the domain sizes considered. They also pointed out that percolation path, rather than pressure drop would be a better indicator for choosing a fitler domain size for CFD simulations. To the best of the authors' knowledge, there is no reported study of mist filtration at the pore scales, and particularly involving conditions of large fluid saturations, that are representative of most mist filters operating at (pseudo) steady state.

In the present study, the effect of domain size on the two-phase flow through the filter is investigated using Diethylhexyl Sebacate (DEHS) and air as working fluids. Considering that the expected length scales of the large fluid structures at steady state (during filtration) for any given flow rate can be expected at high levels of fluid saturation, the simulations for the present study consider an initially fully saturated (with oil, i.e. DEHS) which is flushed using air (at constant flow rate). Two structurally different types filter media, nonwoven and foam, with similar properties such as fibre (or element of foam) diameter, packing density, surface-texture (which influences the fluid-surface contact angles) are used for the present study to additionally compare the influence of domain size across types of filter media.

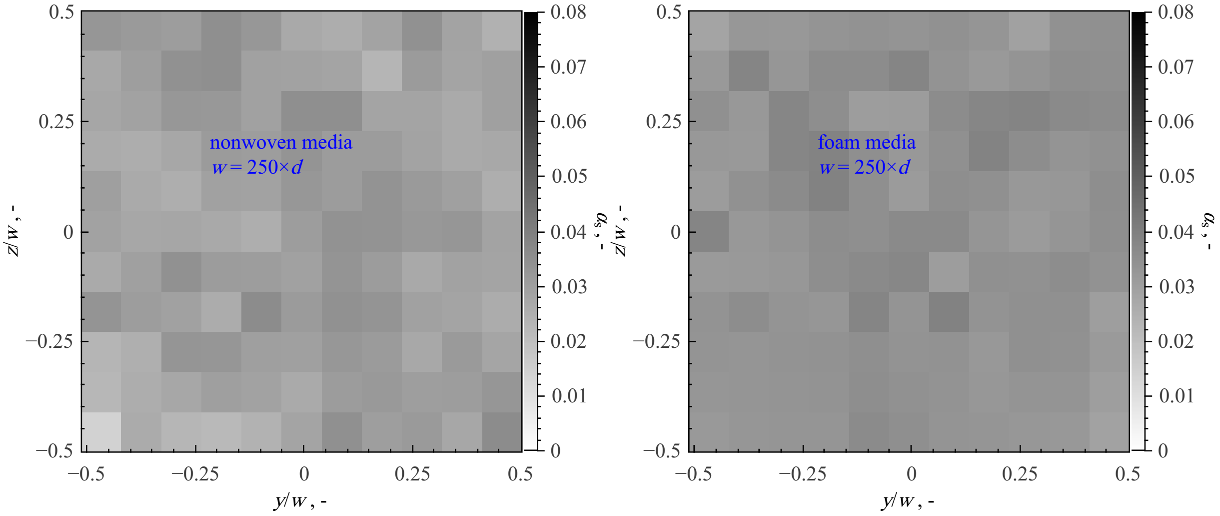


(a) nonwoven media (b) foam media

Figure 2: Sizes of the nonwoven and foam filter media chosen for the present study; fibre (and element of foam) diameters for both media are $d = 20$ μm

2 COMPUTATIONAL METHODOLOGY

The present study employs realistic filter geometries that are generated virtually using a novel in-house technique. The procedures for generating the nonwoven and foam geometries and computational mesh suitable for CFD are discussed in detail elsewhere [6] and hence omitted here for brevity. The schematic of the computational geometry used for the simulations is illustrated in Fig. 1, where representative sections of the nonwoven and foam media are shown in Fig. 1(a) and Fig. 1(b) respectively. Two types of simulations are carried out - (i) with air alone through dry filter media, and (ii) air flow with filter medium pre-saturated with DEHS oil. For the latter,the section of the computational domain indicated as 'filter region' in the figure (blue-box) is initially ($t = 0$) filled with DEHS to represent a 'dipped filter', while the rest of the domain is filled by air. A constant flow of air is imposed at the 'inlet' of the domain for all times $t > 0$ until steady state is reached - which is ascertained by monitoring the transience of: (i) pressure drop ($\triangle p_{\text{air-oil}}$), (ii) oil saturation in the filter region (α_{oil}), (iii) location of the centre of mass of oil in the filter region (x_{com}) and equivalent thickness of oil at the downstream face of the filter (λ_{eq}) calculated as $(V_{\text{oil}} - V_{\text{oil, filter}})/w^2$ where, w is the width of the filter cross-section (and computational domain). The fibre (and element of foam) diameter, length of the fibre along the direction of mean flow, and oil-filter contact angle are considered constant as d = 20 μm, l = 0.002 m and θ_{e} = 20°, respectively. The mean air flow velocity applied at the inlet for both, the single phase as well as the multiphase experiments, is fixed at u_{o} = 0.6 m/s, corresponding to a Reynolds number Re$= \rho_{\text{air}} u_{\text{o}} d/\mu_{\text{air}} = 0.8$ and a capillary number $Ca = \mu_{\text{air}} u_{\text{o}}/\sigma = 3.375 \times 10^{-4}$. The effect of domain size is studied by using successively larger domains for both, the nonwoven and the foam media, - as shown in Fig. 2.



(a) nonwoven media (b) foam media

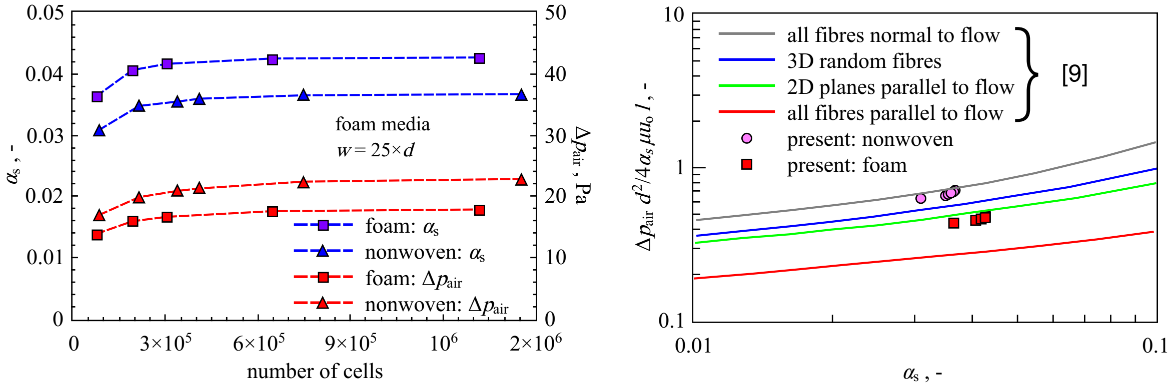
Figure 3: Contours of local packing density in the cross-section (averaged along the direction of flow) for representative nonwoven and foam filter media, calculated based on 11×11 divisions in the $y - z$ plane

The governing equations of mass and momentum for the single phase simulations are solved at steady state using the finite volume based computational solver $simpleFOAM$, available within OpenFOAM. The second series of simulations involving both air and DEHS are carried out using the transient $interFOAM$ solver which uses an algebraic volume-of-fluid (VOF) approach [7] for tracking the air-oil interface. Sufficient interface compression was used (> 1) for the simulations based on the mesh resolution for each case for accurate representation of the local interface curvature with minimal numerical smearing. The general set of governing equations are included in [7, 8] and hence omitted here for brevity. To ensure no spatial anomalies (at the pore-scale) exist in the virtual media, which may adversely influence the simulations, a check is carried out to evaluate the local packing density distribution in the largest domains of the foam and nonwoven media; the smaller domains are sub-sets of the largest domain, as shown in the figure. The local packing density distribution, evaluated by averaging the solid volume fraction in the direction parallel to mean flow along segmented locations in a plane perpendicular to the mean flow, is shown in Fig. 3 for the two media. It can be seen that the media are spatially consistent with minimal variation in the local packing density, reinforcing the confidence in the virtual filter geometries generated for the present research.

All computational simulations reported in this paper were carried out using 48-620 cores on the supercomputing facility Magnus with a Cray XC40 system at Pawsey Supercomputing Centre, Perth, Australia.

3 RESULTS AND DISCUSSION

To isolate the influence of domain size alone on the predictions from the computational studies and avoid any artifacts from the mesh resolution influencing the computations, it is important to first identify a suitable meshing configuration - or number of cells per unit cell of a filter structure - that can subsequently be consistently be scaled for the larger domains. This is carried out using several hybrid mesh configurations comprising of hexagonal, prism and polyhedral meshes that were generated using a standardized procedure elucidated in [6].



(a) (b)

Figure 4: Effect of mesh refinement on the (a) resolved packing density of the filters and single phase (air) pressure drop across the filter, and (b) comparison of the predicted dimensionless pressure drop against Spielman and Goren [9]

Figure 4(a-b) illustrate the influence of mesh refinement on the resolved packing density of the foam and nonwoven filter, and the single phase (air) pressure drop, for a representative domain size of $w = 25 \times d$. It is pointed out that with an increase in mesh resolution (and mesh size), a greater fraction of the filter surface is resolved, leading to an asymptotic limit of the real packing density for successively finer mesh. It can be seen from Fig. 4(a) that for both the types of filter media considered, the filter packing densities as well as the pressure drops become fairly mesh independent ($<$5%)beyond a mesh size of about 3×10^5-4×10^5 cells for the cases considered. It can also be seen from Fig. 4(b) that the nonwoven media, which was generated with a high layer-index (=1000) [6] corresponding to represent most fibres to be aligned perpendicular to the mean flow are in good agreement with the theoretical model of Spielman and Goren

[9]. It is also seen that as expected, the dimensionless pressure drop for the foam media - which consist of elements 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.

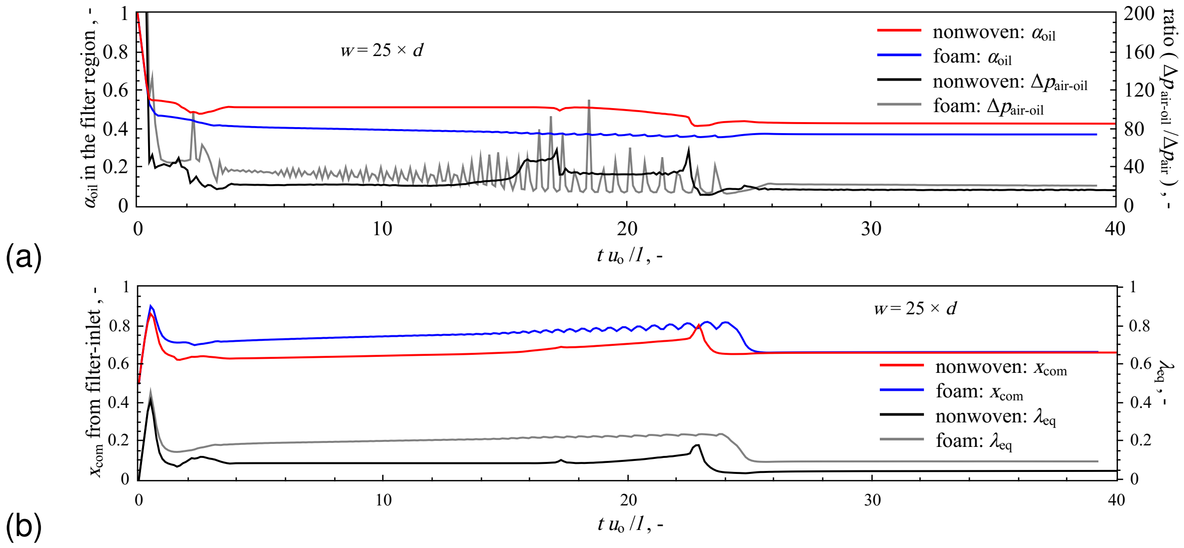
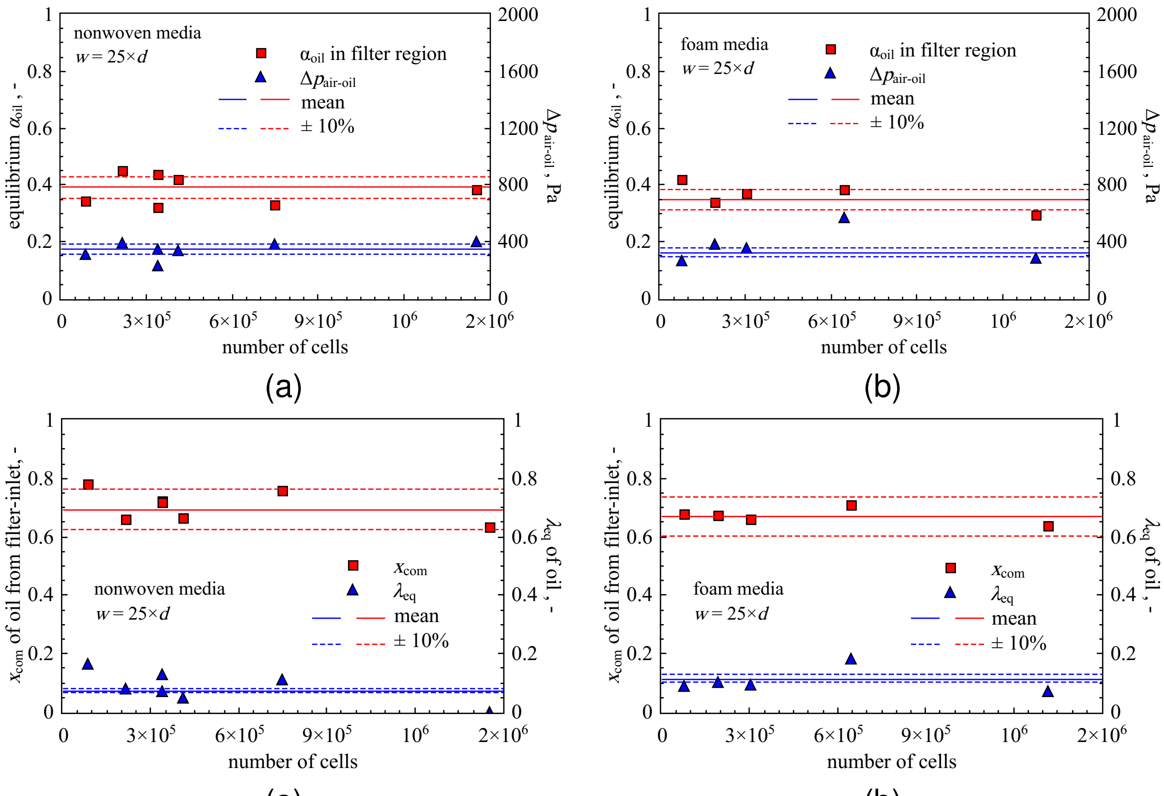


Figure 5: Transient evolution of oil saturation, pressure drop, centre of mass of oil retained in the filter and equivalent thickness of oil on the downstream face of the filter

The second set of simulations carried out to study the influence of mesh refinement, involves air flow through a filter media pre-saturated with DEHS. As mentioned in the preceding section, unlike the single phase simulations that are carried out at steady state, the two-phase simulations are carried out as transient simulations until steady state is deemed to be attained. Figure 5 shows the typical transient evolution of the quantities that are monitored to establish that steady state condition is reached for any case. The oscillations in the quantities correspond to events such as droplets detaching from the downstream face of the filter or liquid leaving the domain, which were visually observed from graphical representations at different times.

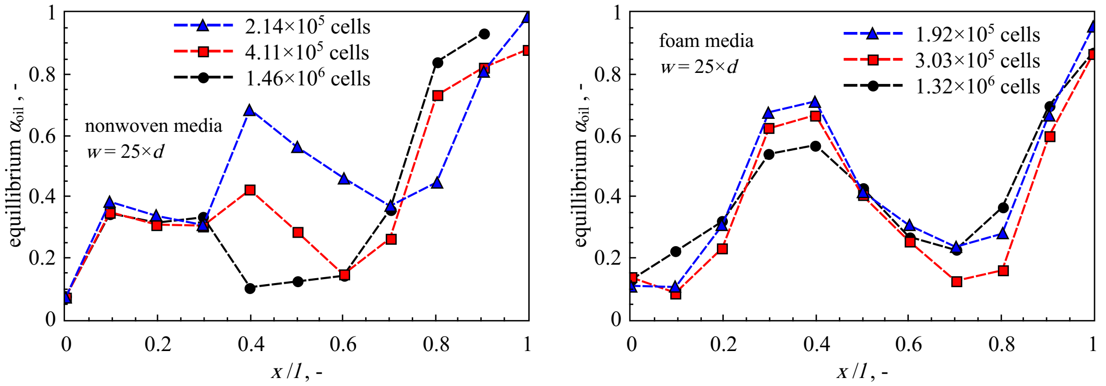
The steady state values of the pressure drop, oil saturation, centre of mass of oil in the filter region and the equivalent thickness of oil on the downstream face of the filter obtained for the different mesh sizes for the representative cases with $w = 25 \times d$ for both, foam and nonwoven media are illustrated in Fig. 6. It can be seen that unlike packing density or single phase pressure drop which converge to an asymptotic limit well with an increase in mesh resolution, the results from the two-phase simulations exhibit relatively greater scatter. This is indicative that unlike single phase flows through the porous filter, the contact-line dynamics at the pore-scale is significantly more complicated and highly sensitive to even small variations in local mesh configuration that can lead to relatively greater consequences in the steady state results. Confidence limits of +/- 90 % (excluding the data for the coarsest mesh) is also shown in the figure for the purposes of comparison. It can however be seen that the except for the λ_{eq} the overall trends in steady state magnitudes of all the other quantities remain within the 90 % confidence level. It is also seen from Fig. 7 that the distribution in the local oil saturation (along the direction of flow) in the two filter media converge relatively well with an increase in mesh refinement, however vairability exist ins ome regions of the nonwoven media.



(a) (b)

(a) (b)

Figure 6: Influence of mesh refinement on the equilibrium oil saturation, two-phase pressure drop, centre of mass of oil retained in the filter and equivalent thickness of oil on the downstream face of the filter

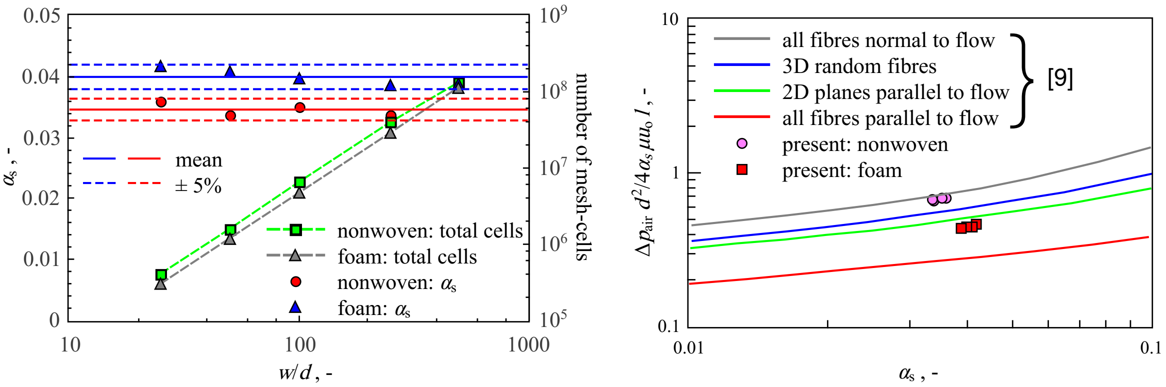


(a) (b)

Figure 7: Influence of mesh refinement on the local (along direction of flow) equilibrium oil saturation inside the filter media

With the quantified limits in variations obtained from mesh sensitivity analysis, the influence of domain size is carried out using the scaled (from $w = 25 \times d$) mesh configurations corresponding to 4.11×10^5 cells for the nonwoven filter and 3.03×10^5 for the foam filter. Figures 8(a,b) shows the variation in the resolved packing density of the two types of media, total computational mesh size (count) and dimensionless single phase (air) pressure drops obtained for the different domain sizes considered for the study. It is pointed out that the "smallest" domain size considered for the present study

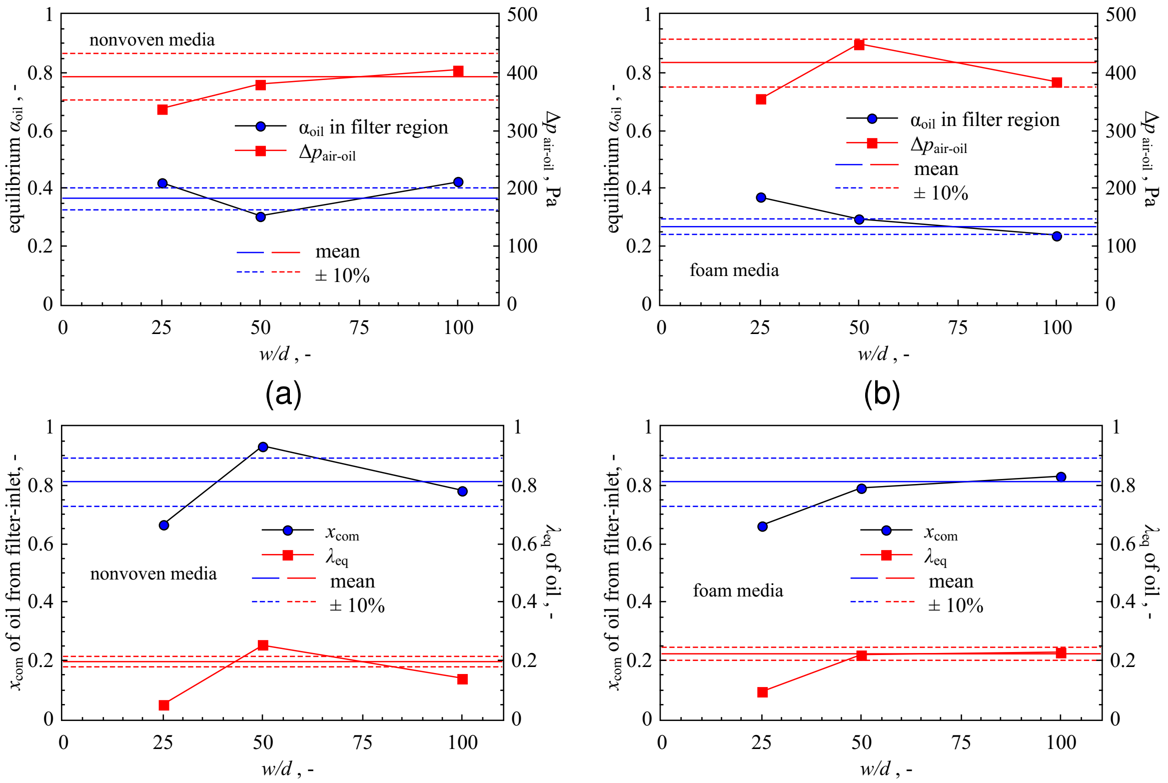
($w = 25 \times d$) is about 15 × the permeability based brinkman length scale for each media -which is the “largest” domain size recommended by other studies in the literature for statistical independence of CFD results. For a geometry with a cross-section $w = 1$ cm, that is comparable with the order of magnitude of the size of most filters used in laboratory experiments, the total mesh size increases to an overwhelming 135 million cells for the packing densities considered. It is however seen from Fig. 8(a) figure that α_s of both filters converge to an asymptotic limit of approximately 0.034 for the nonwoven and 0.039 for the foam filter media, within +/- 5%. It is also seen from Fig. 8(b) that the single phase pressure drops are in good agreement with the expected ranges as compared to Spielman and Goren [9].



(a) (b)

Figure 8: Influence of domain size on (a) filter packing density and total computational cells (mesh), and (b) single phase (air) pressure drop (compared against Spielman and Goren [9]), in nonwoven and foam media

The steady state quantities from the simulations carried out with the different domain sizes are illustrated in Fig. 9. It is seen from the figures that as observed in the preceding discussion on the effect of mesh resolution, the steady state values for the oil saturation, two-phase pressure drop, oil centre of mass and equivalent liquid thickness to vary by about +/- 10% despite a much lower variation in the filter packing densities as seen Fig. 8. The inherent irregularities in the structure of the porous filter media and the sensitivity of the two-phase flow at the pore-scale can be attributed as large contributors to such variations. The distributions in the corresponding local oil saturations inside the nonwoven and foam media are illustrated in Fig. 10 for the different domain sizes considered. It is seen that the locally averaged packing densities however appear to converge fairly well with an increase in domains size, indicating that the variations of +/- 10% observed in the steady state quantities observed in Fig. 8 are an accumulated effect of such local inhomogeneities. It is also interesting to note that the qualitative effect of the domain size on the steady state quantities is similar in both the types of filter media used. It is well known by experimentalists that local variations in filter media properties can significantly influence small-scale laboratory results. Such an effect can also be observed in the present results, despite relatively more idealised geometries are considered for the study. The results obtained from the present research indicates that, as pointed out Lehmann et al. [5] for dust filtration simulations, single phase pressure drop alone may not be an indicator for the accuracy of simulations involving mist filtration with significant fluid saturation. It is also pointed out that further simulations with larger domain sizes are required for a conclusive comment



(a) (b)

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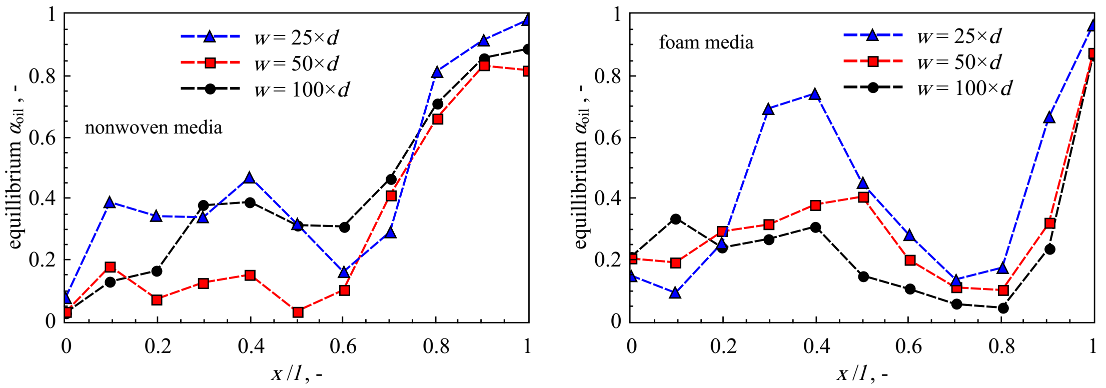
Figure 9: Influence of domain size on the equilibrium oil saturation, two-phase pressure drop, centre of mass of oil retained in the filter and equivalent thickness of oil on the downstream face of the filter



(a) (b)

Figure 10: Influence of mesh refinement on the local (along direction of flow) equilibrium oil saturation inside the filter media

on the appropriate domain size that may be required for accurate design of mist filters using CFD. As it is inferred from the present study that the multi-phase flow physics and its sensitivity underpins the size of the representative domain sizes that may be required for accurate CFD of such systems, and as the size of the liquid structures are also expected to be influenced significantly by the flow conditions (velocity), fluid properties and surface (and implicitly the contact angles), further research as a direct extension of the present analysis is required to characterize the domain size that can be used for design and optimization of mist filters.

4 CONCLUSIONS

Fully resolved computational fluid dynamics simulations of filtration processes are increasingly becoming an important tool for efficient design of dust and mist filters. However, the spatio-temporal resolutions that are required to accurately resolve different multi-phase fluid dynamics scales for full-size filters pose significant challenges on computing powers for such CFD simulations. Hence it is important to identify the minimum domain sizes that can accurately represent the multi-phase fluid dynamics interactions in the filter media, while capturing the dynamics of the largest fluid structures that are present, particularly at high saturations that are representative of the conditions in which mist filters operate most of their intended life-time. Considering that no such comprehensive study is yet available, in the present paper, a systematic analysis is carried out to illustrate the influence of the size of the computational domain (and filter) considered on the transient and steady state characteristics of air-oil transport in two different types of filter media (nonwoven and foam). It is found that unlike indicators that have been used in the literature to-date, single phase pressure (or permeability) - which converge to an asymptotic limit with an increase domain size - alone cannot be an accurate indicator for the representative domain size for gas-liquid or liquid-liquid filtration simulations. It is also found that the two-phase flow physics is highly sensitive to the resolution of the mesh at the pore-scales as well as the inherent randomness in the filter structures. For the domain sizes considered, the overall variation in the steady state macroscopic quantities including pressure drop (air-oil), oil saturation, equivalent thickness at the downstream face of the filter and the centre of mass of oil is about +/- 10%. Further research with larger domain sizes, and simulations with more fluid properties and flow conditions are required for a conclusive comment on the domain sizes that may be required for accurate CFD based designs of mist filtration systems.

5 ACKNOWLEDGEMENTS

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