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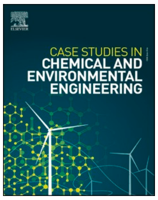

Case Report

A computational fluid dynamics approach to predict the scale-up dimension of a water filter column

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ABSTRACT

A bench-scale filter consisting of sand media was tested for hydrodynamic parameters (velocity and pressure) using ANSYS-CFX (computational fluid dynamics or CFD software) to further determine the ‘subjective minimum scale-up’ (SMS) filter dimension. The purpose of this study is to relate the hydrodynamics property of the bench scale column and the scale-up column for a porous fluid flow using CFD to understand the scale-up limitations. The poor flow regime in bench-scale filter was observed because of a high variance in the pressure gradient as obtained for a plane perpendicular to the direction of fluid flow (orthogonal plane). The flow regime pattern was analyzed by structural modelling and in-built programming using the concept of CFD. Using CFD, a SMS filter dimension was obtained that was found free of high-pressure gradient (on orthogonal plane near the column exit) that might have incurred due to a ‘bad’ flow regime in case of the bench-scale filter. This could sort operational issues caused due to pressure-velocity parameters and would help researchers to step-up with scale-up dimension (from bench-scale) more confidently and credibly. The simulation was obtained for the scale-up reactor using the intrinsic properties to validate the model. An error of 4.1% was reported between the experimental velocity of the bench-scale filter vs simulated value from ANSYS-CFX. Also, a better plug flow condition was obtained for the scale-up column using CFD (Morill dispersion index or MDI = 3) as compared to that of bench-scale filter (MDI = 2.2).

1. Introduction

A bench-scale filter column provides a baseline study for any adsorbent material to understand its feasibility for the removal of pollutants before progressing towards a scale-up study. Bench-scale filters have shown an effective removal in the past for various water pollutants such as organic matter, dyes, metals and pharmaceutical compounds [1,2]. Bench-scale columns have even proven to accurately predict the hydrodynamic behavior of the fluid flow [3]. However, the boundary conditions and wall effects in a small diameter column are majorly responsible for a non-uniform flow regime in a continuous fluid flow condition as compared to a larger dimension column where latter possess an insignificant wall effect [4,5]. These non-uniform flow regimes could possibly be linked to a change in the adsorption efficiency of the contaminant removal. Hence, it is required to understand the hydrodynamics of a bench-scale filter before it can be applied at a higher scale for studying the removal of various pollutants [6].

The head loss parameter plays an important role in an overall filter operation which is mainly responsible for the change in the flow rate and hence flow regime [7]). For a porous media biofilter operation studied using small diameter column, problems such as clogging, air-entrapment (due to biofilm growth), often escalate maintenance issues and requires frequent backwashing [8]. Due to a limited degree of freedom for the fluid movement in a bench-scale filter column (generally water), and a persisting capillary action due to low diameter column, the velocity and pressure distribution does not follow a smooth head loss pattern. This leads to an unavoidable consequence of ‘misjudgment’ during filter dimensioning for the scale-up study. Many researchers even perform a scale-up study by choosing a random column diameter without assessing the hydrodynamic behavior of the fluid. In such cases, adsorption efficiency of the studied pollutants, may show an underperformance when translated to a higher scale than bench-scale. Hence, proper flow regime

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must be understood for a chosen bench scale column to determine the degree of 'poor flow regime' and then a step forward to eradicate it.

Herein, the bench scale column filter dimensioning 22 mm square side, 650 mm length and 1 mm thickness was chosen and was studied for a sand-based porous media to understand the flow regime using two governing parameters: pressure and velocity. Computational fluid dynamics (CFD) was used to evaluate the numerical analysis involved in the fluid flow with respect to the adsorbent properties (porous sand media) including density, porosity, head loss coefficient, permeability constant, etc. After analyzing the contour mapping (flow regime) for the bench-scale columns based upon the pressure gradient values, various scale-up dimensions were hit and trialed (n = 71) to obtain a radial and more uniform distribution pattern of the pressure gradient for a plane chosen perpendicular to the direction of the fluid flow. For simplicity, only one scale-up dimension was shown in this study out of 71 trailed simulation that offered the best flow regime. The major hypotheses of the work are a) Scale-up dimension might improve the morill dispersion index (MDI) of the existing bench-scale filter column, b) A more radial and symmetric flow pattern (based on pressure gradient values) might improve the plug-flow conditions (related to MDI) in the porous bench-scale columns. It is to be noted that the present study does not present any result on operational or functional parameters related to environmental fluid reactor such as hydraulics retention time or contaminants concentration or its removal.

2. Material and methods

2.1. Materials

A column dimensioning 22 mm square sides, 650 mm length and 1 mm thickness was used as the representative bench scale filter column. Sand was used as the porous filter adsorbent based on the grain size distribution as described in our previous study [9]. For the analysis of hydrodynamic conditions, computational fluid dynamics was studied using ANSYS 2019 R2 software.

2.2. Column set-up and operation

A glass column was set-up (vertically) similar to what is represented in Fig. 1 and was continuously fed with lake water at a linear velocity equal to 0.00025 m/sec (0.9 m/h) which is approx. 40 mL discharge in 8.5 minutes under constant flow rate and at a constant water head of 12.5 cm maintained above the filter bed media. A constant head of 12.5 cm was chosen to determine the experimental flow velocity of the fluid in a bench-scale column. It is to be noted that the velocity can further be increased by changing the pressure head up to some extent, depending on the quality of water to be delivered at the expense of compromising the water quality. However, in the current study, flow velocity was determined at a fixed water head (i.e., 12.5 cms) based on a nominal water quality of the effluent.

2.3. Morrill dispersion index or MDI

The Morrill dispersion index or MDI is a widely used parameter to determine the amount or degree of diffusion and mixing in the contact system [10]. It was calculated based on the residence time distribution analysis where KCl was used as the tracer compound. 200 mg/L KCl was found equivalent to 67.7 μS/cm. MDI was calculated based on the following equation:

$MDI = T_{90}/T_{10}$

Where,

T_{90} = time taken to reach 90% of the conductivity value in the filtered effluent (proportional to tracer element concentration).

T_{10} = time taken to reach 10% of the conductivity value in the filtered effluent (proportional to tracer element concentration).

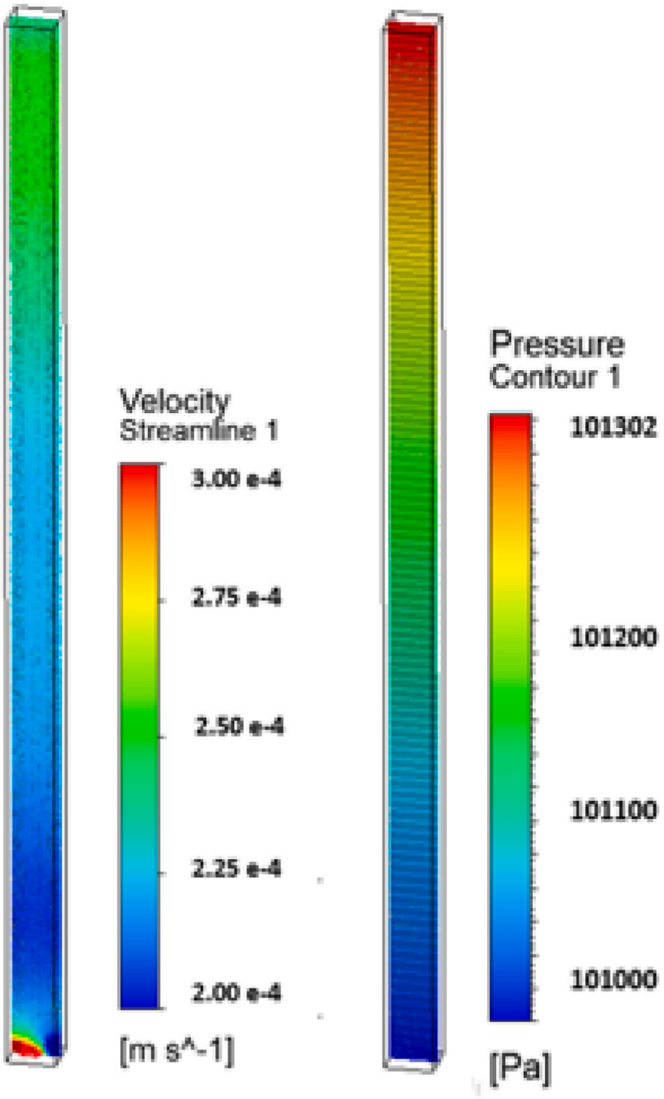

Fig. 1. Velocity and Pressure distribution along its length in bench-scale filter column.

MDI value close to 1 defines a perfect plug flow condition while value of 23 defines a completely mixed/stirred reactor [11]. Hence, for a porous packed bed column, value closer to 1 was more desirable.

2.4. Details on ANSYS-CFX and velocity-pressure determination

The effluent flow (in mL) of the bench scale column was measured experimentally and converted into m/sec. After that, the flow velocity was crosschecked with the flow velocity value obtained from modelling and simulation program using ANSYS-CFX solver. The simulation program came in-built in the software for example: steady-state flow condition, isotropic loss model to name a few while the user inputs related to fluid and adsorbent properties such as fluid density porosity of the adsorbent media (here sand), head loss coefficient (L) and permeability constant (P) were fed to the program. Some trials were done using L and K values to land up to a flow velocity near to the experimental value. Table 1 tabulate these values which were used to achieve a similar observation flow velocity. The error in velocity was reported by the Equation as follows:

(Experimental velocity – Velocity observed after ANSYS-CFX simulation)/ Experimental velocity) x 100%

Table 1
Parameters used in the ANSYS/CFX solver.

Parameters	Value
Volume porosity	0.43
Loss model	Isotropic loss
Permeability constant (m^2)	10,145,873,265 m^2
Loss coefficient	11,500,000 m^{-1}
Heat transfer coefficient	1.0 $W/m^2/K$
Pressure drop (from equation (1))	302 Pa
Velocity from the experiment (m/s)	0.000265 m/s
Velocity from ANSYS-CFX simulation (m/s)	0.000254 m/s (4.1% error)

Volume porosity was calculated experimentally using a fixed volume column (approximately 10 cm^3) where distilled water was used to fill the void space until brim (V_w). The bed porosity was then calculated using the formula as below:

Bed porosity = volume of void/volume of column (fixed)

where the volume of the void is V_w and the volume of the fixed column was determined by the graduation marked outside the column, which was approximately 10 cm^3.

The value of permeability constant and loss coefficient was known from the loop trial (as discussed above) based on the error reported in experimental velocity and velocity obtained after ANSYS/CFX solver for the bench-scale filter. The error of less than 5% was desired to confirm the model preciseness) and hence the value of 4.1% error reported in this study was accepted. The permeability constant and loss coefficient value were determined by few trials (5-10) (at error <5% as mentioned above) and reported to be 1.01e10 m^2 and 1.15e7 m^{-1}, respectively (Table 1). The pressure loss calculated with the Kozeny-Carman equation was found to be 302 Pa as mentioned below.

$$\Delta p = \left(kVs\mu\,(1-\varepsilon)^2 L\right) / \varnothing s^2 Dp^2 \varepsilon^3 \qquad \text{Equation 1}$$

Where, ΔP is the pressure loss or head loss.

k is a parametric value inversely proportional to ($6/D_p^2$).

L is the length of filter bed media in a column.

Vs is the superficial velocity

μ is the viscosity of the fluid

ε is the bed porosity.

Φ_s is the sphericity of the particles in the packed bed.

D_p is the diameter of the spherical particle (here sand).

Based on the head loss reported, the ‘flow regime’ needed to be analyzed in order to obtain the ‘*minimum subjective scale-up dimension*’ free of wall effect and capillary action. For this, another module (CFX-post) of the software was used which programmed all the data obtained from CFX simulation from CFX solver manager and created a flow regime contour plot (based on the pressure gradient values). This contour plot was obtained only after validating the velocity and head loss (pressure) response. Figs. 1 and 2 depict the velocity and pressure distribution along the length of the bench-scale filter.

After obtaining the velocity (at <5% error) and head loss distribution inside the column, the pressure gradient was obtained using post-CFX solver. To remove any effect of sudden pressure change (fluid flow inside the column to atmospheric pressure at the exit), the plane (orthogonal to fluid flow direction) was chosen at an offset height of 10% from the bottom (at 600 mm) and not exactly at the bottom of the filter column. All the trials were simulated for no less than 25 iterations or root mean square error of <0.001, whichever was reached first (latter preferable though).

3. Results

3.1. *ANSYS-CFX contour mapping*

After crosschecking the experimental flow velocity of the fluid for the bench-scale filter with one obtained from ANSYS-CFX simulation, the CFX-post was run to get the contour plot of the pressure distribution along the length of the filter (as mentioned above). Fig. 2 shows the pressure distribution along the length of the bench-scale filter. As can be observed, the effluent pressure was set to 101,001 Pa (atmospheric pressure) while the pressure at the influent to the column was set to 101,302 Pa (difference was calculated using equation (1) as discussed above). On the other hand, velocity distribution was maximum (2.6 e−4 m/s) at the top and minimum (2.09 e−4 m/s) at the bottom. However, at the bottom, a sudden decrease in the pressure flow to atmospheric pressure, the velocity peaked a bit (2.54 e−4 m/s) and was reported as the effluent linear flow velocity. It was obvious from the velocity pressure relation (relationship curve not shown here), that higher the pressure head, more is the flow velocity and vice-versa.

Fig. 3 shows the pressure gradient contour at the defined plane (as mentioned in material and method section). It can be clearly observed that a non-uniform flow pattern existed where the pressure gradient (can be related to velocity of water flow) changes dynamically within the same plane as indicated by a dashed arrow (Fig. 2). Each color depicts an arc-shaped flow line with different pressure gradient and could possibly be because of a restricted degree of freedom caused due to wall resistance and high capillary condition. Since the diameter of the column is small (20 mm), the eddy current in the flow rises towards one end of the plane (shown by red color in Fig. 2). The MDI value of the bench-scale column was found to be > 3 (for graph, refer supplementary figure, Figure F1 (A)) which might raise and be responsible for some issues such as air entrapment, negative pressure built-up and reduced flow through velocity than normal.

3.2. *Finding minimum subjective scale-up dimension*

The next objective was to use the derived parameters from ANSYS-CFX, i.e., permeability constant and loss coefficient, to determine the ‘subjective minimum scale-up’ dimension (SMS) which could eradicate the poor flow regime condition (Fig. 2) and develop a more channelized

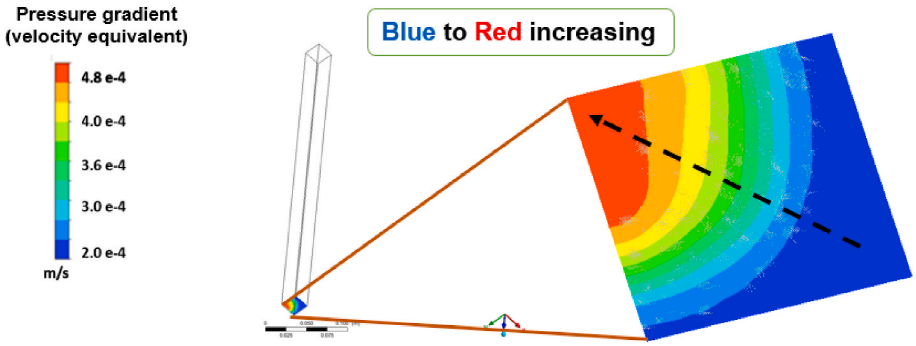

Fig. 2. Velocity contour of bench-scale filter taken at an orthogonal plane at 600 mm height.

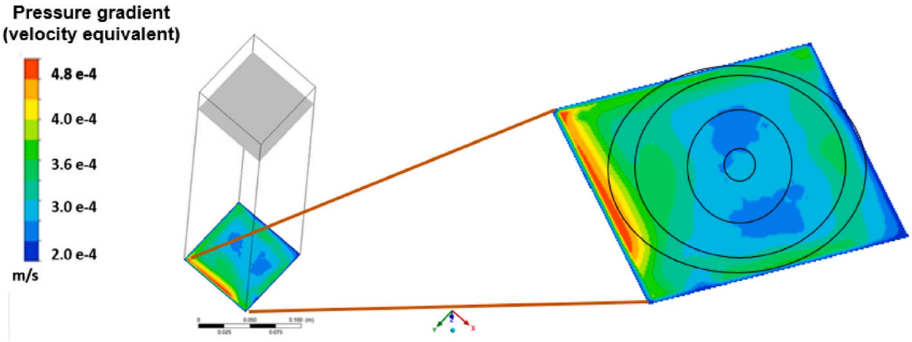

Fig. 3. Velocity contour of scale-up filter taken at an orthogonal plane at 270 mm height.

and radial pressure gradient pattern so that more bed surface can be utilized for the fluid flow. Different dimensions were trialed and simulated (not shown here) for sand media and the SMS was found to be 9 cm × 9 cm x 30 cm. This filter dimension was judged based on the flow-through velocity value which was meant to be at least similar if not lower than what was obtained experimentally for the bench-scale column. However, it should be noted that the requirement of a similar velocity value for the scale-up filter is less desirable than obtaining a uniform pressure gradient pattern. Fig. 3 shows the obtained pressure gradient plot for the trialed scale-up dimension (9 cm × 9 cm x 30 cm) which offered a radial distribution pattern of the pressure gradient on the plane (chosen at 10% offset from the bottom and orthogonal to the fluid direction).

As can be observed from Fig. 3, the flow regime on the selected plane is much more radial and uniform in the pattern which allowed a better plug flow condition too (MDI <2.2, refer supplementary section, Figure F1 (B)) as compared to bench-scale case (MDI >3). The experiment to determine the MDI value for the chosen SMS dimension was done using plexi-glass column. A lower MDI value ($>26\%$) for the scale-up filter column signifies a better plug-flow condition as compared to the bench-scale filter. This change was obvious because of a better flow regime condition (Fig. 3) that was developed in the scale-up column filter. It should be noted that a higher MDI value for the scale-up filter as compared to the bench-scale filter can be compromised only if a radial flow regime is obtained for the former. However, an ideal condition would be to obtain a lower MDI as well as better pressure gradient (flow regime) distribution. Fig. 4 summarizes the overall process (8-step) that was performed to determine the SMS dimension from bench-scale column filter that depicted a radial and uniform pressure gradient pattern.

4. Discussion

Previous studies on CFD have shown the importance of hydrodynamics in a column reactor (Baten and Krishna 2004, [12]. An important benefit of the CFD approach to the column reactors is that the geometry and scale effects are automatically accounted for simulation. However, the success of the scale-up strategy depends on proper modelling of the fluid and media properties (Baten et al., 2003). In the present study, CFD model was validated using only two intrinsic properties of the porous media (sand): permeability constant and loss coefficient. After that, the simulation was obtained for the scale-up reactors. Though the above-mentioned studies failed to form a discussion on the scale-up size limit, a scale-up ratio of 20 was found to demonstrate a strong influence on the column hydrodynamics (Baten et al., 2003). Such influence was confirmed even at the scale-up factor of 4.5 in present study. This was attributed mainly due to the boundary limit at low scale columns which was evident from the flow pattern as observed from the planer contour diagram (Figs. 2 and 3). This was also confirmed by a decrease in the MDI value suggesting a better plug-flow condition regime when the reactor was scale-up. Such flow regime becomes an important aspect when it comes to an actual scale-up practice. Above mentioned idea may formulate a user desirable approach using a prototype or model (pilot scale) filter. However, for the technological feasibility this study still needs some important validation as the flow regime was only understood using two variables (pressure and velocity) and two intrinsic properties in form of head loss coefficient and permeability constant.

Nevertheless, the flow regime pattern is required to understand so as to not allow the excess pressure to build up inside a big or actual scale-up filter unit. Only after a successful scale-up validation based on the flow regime, a scale-up feasibility should be made rather than prioritizing the

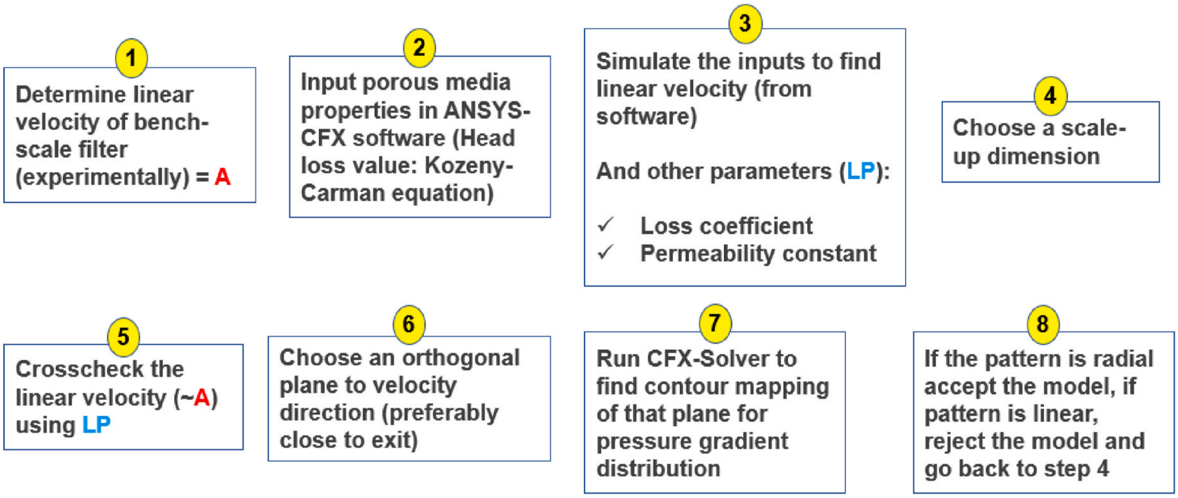

Fig. 4. A 8-step approach to determine subjective minimum scale-up dimension.

importance of other follow-up objectives. For example, adsorption of contaminant 'X' using adsorbent media 'Y' can be studied later but first thing first is to assure that the hydrodynamics of the matrix fluid is validated. In general, this could also account for a lower adsorption efficiency when translating any bench-scale condition to a scale-up condition. Many studies have also successfully predicted the breakthrough time of a bench-scale packed bed column [13]. However, the scale-up reactor could possess a different hydrodynamics property as compared to the bench-scale reactor, making all these matching experimental and simulation data null and void [14]. Hence, the CFD application can form a preliminary approach for the bench-scale filters to understand their scale-up feasibility and deciphering a SMS dimension that can avoid any hydrodynamic issues during the filter operation.

4.1. Limitations and future gaps of the above study

1. No Contaminant Transportation Phenomenon (CTP) was analyzed or studied in the present study using ANSYS-CFX. Hence, it would be interesting to observe the CTP along with the fluidic behavior in the porous bed column.
2. The value of permeability constant and loss coefficient were obtained from several hit and trials (arbitrary values) using ANSYS-CFX solver and hence these values could vary depending on other added parameters to the system (e.g.: CTP, change in filtration rate, change in influent velocity or change in the porous media).
3. Various other orthogonal planes and their related contour mapping at various length of the column could be analyzed and needs to be studied in future to establish a more concrete relationship between the pressure-velocity distribution.
4. In future, the CFD approach could be utilized to study porous media 'suitability' for a specific or mixture of emerging contaminants present in the polluted water. However, the initial concentration of pollutant in polluted water (influent to filter column) should be linked to the CTP to further understand any change in behavior of the fluidic or other specific properties related to the porous media column.
5. The convergency graph providing an information on residual values cannot be used as an only concrete tool to study the fluidic properties in the porous media columns. The residual value tool is only a small part of a complete assurance system that a true or a valid solution is obtained. Hence, to obtain a steady-state simulation, other factors should also satisfy the solution that comprise a) residual error values of below 10^{-4} or 10^{-5}), b) domain imbalance is less than 1% and c) monitoring points of interest has reached a steady solution.
6. In future, the CFD utility could also be explored in the field of water or wastewater treatment via artificial intelligence. Modelling of water quality parameters and its removal in water treatment can be improved using CFD simulation where a proper calibration could help in achieving a state-of-the-art research work [15,16].

4.2. Eco-friendly and sustainable green nano-technologies for the mitigation of emerging environmental pollutants

The current study could be handy in understanding the minimum subjective dimension of the column filter for a porous media. In this study, sand was used as the porous media. However, it is to be noted that the hydrodynamic parameters, properties, and flow regime can change if an advanced, efficient, and more eco-friendly adsorbent media (e.g., graphitized sand) is utilized instead of conventional media (such as sand) for the mitigation purpose of emerging pollutant present in the contaminated water. The present study could also benefit the researchers to decide the SMS dimensions with different porous media composition (hybrid) and would provide them a precise data on the variability of hydrodynamic parameters that could potentially be affected by a specific pollutants in a long-term filter operation. In this way, CFD approach could indirectly help in mitigating emerging pollutants for both conventional as well as advanced porous media (nanotechnology-based media) and help in maintaining a smooth flow regime which can be monitored periodically.

5. Conclusion

The use of computational fluid dynamics (CFD) using ANSYS-CFX (software) can help to understand the hydrodynamic fluid properties such as pressure and flow velocity for a porous adsorbent filter media in a tubular column. A non-uniform and non-radial asymmetric flow condition were observed for the bench-scale filter from the pressure gradient contour plot. It helped in understanding the limitation of the bench-scale filter with respect to the flow regime producing a low plug-flow condition inside the filter (Morrill dispersion index, MDI >3). The derived properties comprising permeability constant and loss coefficient from bench-scale computational analysis helped to find the scale-up dimension at which the flow regime showed a more radial and uniform pressure gradient contour. Also, a better plug-flow condition (MDI = 2.2) was observed as compared to the bench-scale filter that suggested the importance and significance of CFD for determining the scale-up dimension of a filter column. In future, CFD approach may be beneficial to lay a foundation for the scale-up studies.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.cscee.2022.100201.

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