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Numerical simulation of flow through absorbing porous media; Part 1: Rigid porous media

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Abstract

The performance of the absorbing porous media is an important factor in several practical applications such as hygiene industries. The primary goal of hygiene products is to absorb and retain a liquid. In these types of products, the liquid flow is often driven by a strong capillary force. Hence, computational modelling of the liquid absorption process within rigid porous media would be helpful to design or modify these products. This paper demonstrates the application of a newly proposed approach for modelling liquid absorption within rigid porous media. The proposed modelling approach uses fewer input parameters than previously used methods in literature which make it simple to implement. The wicking heights, predicted by computational fluid dynamics simulations, are in good agreement with the experimental and analytical data. The capability of the method to model the flow through absorbing porous media is explored by considering different flow cases. For the case where the flow front hits the walls of a porous domain, the results showed interesting patterns of the flow front under the action of gravity. It is observed that the nature of flow front propagation becomes 1D as time passes. Finally, the newly proposed cell zone condition to mimic the liquid hold up showed promising results by allowing only air to pass through the porous domain.

1   Introduction

Absorbing porous materials have revolutionised the market of disposable hygiene products since they became commercialized in the late seventies. Their major characteristic is that they can absorb and retain the maximum volume of the liquid while swelling. Absorbent porous materials are used in agricultural industries as well as in sanitary products, including diapers and towel napkins. Diapers are now designed with a combination of different thin layers whose main function is to uptake, distribute, and partition the liquid, and the core part that stores the liquid is composed of superabsorbent polymer particles (SAP) (Wein et al., 2019).

Wicking is the spontaneous absorption of liquid in a porous matrix under the action of capillary pressure. This flow scenario can be called the system of multiphase flow as it involves at least two phases: a wetting phase, which is the liquid that enters the porous domain, and a non-wetting phase, which gets displaced by the wetting phase. During the wicking process, the difference in surface energies of dry and wet porous matrix causes the generation of a capillary force at the fluid interface that moves the liquid or wetting phase into the porous matrix (Masoodi and Pillai, 2012). Wicking performance is an important factor in absorbent porous materials, where the primary goal of the products is to absorb and retain the maximum amount of liquid (Masoodi et al., 2012).

There are two main mathematical models available to study wicking. The first and oldest approach is the Lucas-Washburn approach, which assumes the porous media as the bundle aligned capillary tubes of the same radius. As a result of this model, a linear relationship is obtained between the absorbed liquid mass and the square root of the time when the gravity effect is negligible (Lucas, 1918). Szekely et al. (1971) proposed a modified version of the Lucas-Washburn equation based on the energy balance to include the gravitational and inertial

2

effects and developed an ordinary differential equation that predicts wicking rate. Further, Masoodi et al. (2008) proposed a method to improve the wicking predictions of polymer wicks by showing that the hydraulic and capillary radii should be measured separately when using the capillary model. Research has shown that the suggested equation is also valid for absorbing porous media (Masoodi et al., 2011). Although the Washburn equation is important for modelling absorption in porous media, it is limited to one-dimensional flow cases along the direction of capillary tubes. Furthermore, the equation relies on the assumption of straight flow paths of liquid and is not accurate for real porous media, which have complicated and random paths (Masoodi et al., 2011).

Another approach in mathematical modelling of the wicking flow in porous media is based on Darcy's law, which proposes a simple relationship between pressure drop and averaged velocity of liquid while modelling the flow of water through a sand column. Darcy's law is a well-established approach and it has been widely used to model the single-phase flow through porous media (Bear, 2013). To do so, first, Darcy's law is coupled with the continuity equation to obtain the velocity and pressure fields. Masoodi et al. (2007) used Darcy's law-based approach to model the wicking flow in porous media by imposing the capillary pressure at the liquid front. The capillary pressure is calculated using two different approaches. The First approach is based on the balance of viscous dissipation and surface energy, whereas the second approach assumes porous media as a bundle of capillary tubes. Zarandi et al. (2018) proposed a new theoretical model for the transversely isotropic porous media to predict the flow front locations using Darcy's law approach. The results showed that the proposed model works best for the assumption of a fully saturated region behind the moving liquid front, but it fails to account for partial saturation effects due to the inhomogeneity of the porous media. Zarandi and Pillai (2021) in their latest efforts, investigated the effects of microstructure on the wicking performance of porous media by considering the three different types of wick structures; a) Sintered bed b) Fibrous wick (low porosity) and c) Fibrous (high porosity). The wicking

3

predictions from the previously proposed analytical model for highly porous wicks observed to be inaccurate due to assumption of sharp-liquid front. As a result, they highlighted the need to numerical modelling of the wicking flow to study time-dependant wicking.

The approaches mentioned above assume a single-phase formulation where only the liquid phase is considered. In the cases where wicking flow through porous media is considered as a multiphase flow scenario, the existence of several phases leads to the formulation of a momentum balance equation that considers the multiphase effects on the fluid dynamics (Santagata et al., 2020). The Richards equation, which describes the motion of liquid in porous media, has been widely used in modelling soil mechanics problems, such as the moisture distribution in soil. The Richards equation is a reduced form of a complex two-phase fluid problem that uses variable capillary pressure in a partial differential equation (Wein et al., 2019). The Richards equation can be derived by applying the general Darcy's law for two different fluids simultaneously; hence such an approach can also be termed as Darcy's law-based approach. Note that in Darcy's equation, the pressure is a single variable, but the Richards equation includes a term involving the moisture content. For a given porous material, the important term in the context of multiphase flow assumption is the saturation curve, which must be measured experimentally for different fluid combinations and fitted using non-linear empirical expressions. The Richards approach is hard to use if these parameters are not known, as complex experiments need to be done to measure the relative permeability, capillary pressure, and value of moisture diffusion coefficient (Diersch et al., 2011).

Computational fluid dynamics (CFD) is an effective tool for predicting the performance of porous materials. CFD solvers, based on some mathematical models mentioned above, have been successfully used to model the wicking flow through a porous medium. Different methods are used to solve the sets of equations numerically, and many examples can be found in the literature. Among all methods, finite element-based methods (FEM and FE-CV) are widely used to model wicking flow through the porous medium. The homogenized porous media

4

approach has proven to have the capability to simulate complex flow processes in porous media, such as the ability to include swelling effects.

Masoodi et al. (2011) developed Darcy's law-based single-phase model using the finite element control volume method (FE-CV) to model the 3-D liquid imbibition into polymer wicks. The simulation results were validated against the experimental data as well as analytical solutions of Washburn and Darcy's law. Although the predicted results showed the capability of the method, this study only considered a one-dimensional flow case. In another effort, Masoodi et al. (2012) adopted the same approach to model the wicking flow in paper-like swelling porous media, where the swelling effect was included by assuming permeability to be time-dependant. Mendez et al. (2010) also modelled imbibition in a fan-shaped porous membrane by considering a 2-D flow scenario, adopting Darcy's law-based approach, and using the finite element method. The main purpose of their study was to identify the limits of the Lucas-Washburn approach due to an increase in non-wetted pore volume.

Most recently, Santagata et al. (2020) modelled 3-D absorption of liquid in swelling porous media using finite scaling size method. The developed model was based on an approach developed by Diersch et al. (2011), where Richard's equation was used to solve mass and momentum. The flow was assumed to be multiphase, where three different phases (gas, liquid, and solid) coexist in the porous domain. The interesting thing about this work is the modelling of changes in dimensions of the porous domain because of swelling action. This flow condition has been modelled by solving the mass equations for the solid phase that considers a term related to the swelling. The numerically predicted liquid acquisition time and liquid distribution were in good agreement with the experimental data. As mentioned previously, to develop such a model, parameters like relative permeability, viscosity, and swelling ratio need to be measured and included in the model. F. Zarandi and Pillai (2018) developed a model based on Richard's Equation to predict the distribution of saturation along the length of wick. They adopted a pore scale simulation-based approach to determine the traditional properties of the

porous media such as capillary pressure and relative permeability. Later, based on these properties the numerical simulations based on Richard's equations were performed in 1D with Mathematica and in 2D with COMSOL. These efforts demonstrated the applicability of Richard's equation in modelling the liquid imbibition process in dry porous media. The motivation behind this work is to overcome the shortcomings of their previous work i.e. prediction of flow front locations under partially saturated porous media (Zarandi et al., 2018).

The Finite Volume Method (FVM) is rarely used while modelling the wicking flow in porous media using the homogenised porous media approach. Li et al. (2016) modelled the multiphase flow in porous media using the Eulerian approach. The main objective of their study was to analyse the performance of a reservoir and wells. The study presented 1-D, 2-D, and 3-D cases that mimicked actual reservoir conditions. The different models, such as Brookes-Corey and Buckley-Leverette models, were used to model the capillary pressure. Recently, Salokhe et al. (2020) developed a model based on a combination of FVM and the Volume of Fluid method to model the flow through porous media under swelling conditions. The study included the investigation of flow front advancement through isotropic and orthotropic porous media under swelling conditions. FVM is mostly used in pore-scale simulations where flow is simulated through a real structure of the porous medium. These types of simulations are used to study the details of flow and to determine relative permeability curves. Ashari and Tafreshi (2009) used the FVM and Eulerian multiphase modelling approach to study the rate of fluid transport in a partially saturated fibrous porous medium. They used a 3-D microscale model of 750 ×750 ×750 voxel with a single voxel size of 2 μm and selected the Leverette J model for capillary pressure estimation with proper values of empirical coefficients. As a result of the conducted simulations, a set of general mathematical relationships for capillary pressure and relative permeability is proposed which is valid for a range of fibre diameters (10-25 μm) and solid volume fraction (5-12.5%). In another effort, Ashari et al. (2010) used a similar approach to

model and study the radial spreading of liquid in a fibrous porous medium and motion-induced fluid release.

In summary, a variety of approaches have been used to model the liquid imbibition process in absorbing rigid and swelling porous media. Some researchers have used a single-phase flow formulation whereas others have used a multiphase flow formulation to model the flow. The most popular method for modelling flow is the finite element method based on Darcy's law, where the liquid imbibition is viewed as a single-phase flow. Methods based on the single-phase formulation consider the one-dimensional flow scenario only for both rigid and swelling porous media. When imbibition is considered as a system of multiphase flow, the methods based on Richard's equation and Eulerian methods have been used. Finite Volume and Volume of Fluid based models are rarely used to model the liquid imbibition process. Mostly, this method is used for pore-scale simulations. There is evidence that the FVM can be applied along with the Eulerian method to model the liquid absorption process. However, in this case, a lot of fitting parameters needs to be estimated with a series of experiments or simulations, and it might become difficult to model the liquid absorption process accurately if these parameters are not known correctly (Diersch et al., 2011) (Li et al., 2016).

The present work focuses on modelling the flow in liquid absorbing porous media using a combination of Finite Volume and Volume of fluid method. This novel combination is used for the first time to model liquid absorption within porous media under rigid conditions. If the values of porosity, permeability and capillary pressure is known for a given porous media, then the flow through absorbing porous media can be modelled easily and accurately. Note the capillary pressure is applied at the liquid front location, which varies over time. Furthermore, this method enables visualization and analysis of the location of the interface and the pressure distribution throughout the porous domain during the liquid absorption process. Generally, these parameters have been hard to analyse with experiments.

7

This work is split into two parts. Part 1 (the current paper) focuses on the modelling of the flow-through absorbing rigid porous media and Part 2 (a separate paper) focuses on the modelling of the flow-through absorbing swelling porous media.

2 Mathematical modelling

The system for the analysis is assumed as the isotropic and homogeneous porous domain with constant permeability and porosity. For the capillary pressure estimation, the effective bead radius is considered for the case of porous wicks. The wicking flow of liquid through a porous medium is usually slow, which can be taken as the inertia-less viscous flow (Stokes's flow). The wicking process is usually viewed as the mobile liquid front. It is common to assume that the wick is fully saturated behind the moving liquid front. As stated in the literature, the imbibition process requires the presence of at least two fluids, and the flow is taken as the multiphase flow with liquid as the wetting phase and air as the non-wetting phase. The process is considered to be isothermal, hence the interfacial tension between liquid and air is constant, and both fluids are Newtonian with constant viscosity (Carciofi et al., 2011).

2.1 Liquid flow during wicking process

The mathematical model for the wicking flow through porous media was developed based on the Volume of Fluid method (Salokhe et al., 2020). The continuity and momentum equations for this process can be expressed as,

$$\nabla.(\vec{u}) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho_e \vec{u}) + \nabla.(\rho \vec{u}\vec{u}) = -\nabla p + \nabla.(\bar{\bar{\tau}}) + \rho g - \left(\frac{\mu_e}{K}\vec{u}\right) + f_{\ Capillary} \tag{2}$$

Where, $\vec{u}$ is Darcy's velocity (Salokhe et al., 2020), p is pressure, g is the gravitational acceleration, ρ and μ are density, and dynamic viscosity, respectively, and $f_{\ Capillary}$ is the capillary force at liquid-air interface.

In the Volume of Fluid method, both the wetting phase (liquid) and non-wetting phase (air) are defined by a factor called volume fraction (α). The value of the volume fraction always falls between 0 and 1. The volume fraction is defined as,

$$\alpha = \begin{cases} 0 & Non\ wetting\ phase\ (air) \\ 1 & Wetting\ phase\ (liquid) \\ 0 < \alpha < 1 & Interface \end{cases} \tag{3}$$

The volume fraction follows the conservation law as,

$$\frac{\partial \alpha}{\partial t} + \nabla.(\vec{u}\alpha) = 0 \tag{4}$$

where α indicates the volume fraction of the corresponding secondary or wetting phase. The effective physical properties of the fluid ϕ (*viscosity μ_e, density ρ_e*) in a computational cell are expressed as a volume-weighted average, where, *a* and *w* refer to air and water respectively (Salokhe et al., 2020).

$$\phi_e(s,t) = \alpha(s,t).\phi_w + [1 - \alpha(s,t)].\phi_a \tag{5}$$

2.2 Capillary pressure modelling

As mentioned in the previous section, the suction pressure due to capillary action is created at the flow front. The basic expression for the capillary pressure is given by the well-known Young equation (Masoodi and Pillai, 2012).

$$P_c = \frac{2.\gamma.\cos(\theta)}{R_e} \tag{6}$$

The biggest challenge while using the Young equation is the estimation of the real or correct capillary radius. This equation assumes that the porous media is a bundle of identical aligned capillary tubes of radius R_e. However, in real porous media, the fluid path is tortuous in nature, hence the applicability of equation (6) is limited. According to Masoodi and Pillai (2012), the equivalent capillary radius is given by,

$$R_e = 2\frac{r_{sp}}{3}\frac{\varepsilon}{1-\varepsilon} \tag{7}$$

Where r_{sp} is the effective spherical radius of solid particles. Note that equation (7) is based on the geometry of the solid particles in the porous medium. For the present study, to validate the numerical method, experimental results for a wick made up of spherical particles are considered (Masoodi and Pillai, 2012), The corresponding capillary pressure is given by,

$$p_c = \frac{3\,(1-\varepsilon).\,\gamma.\cos(\theta)}{\varepsilon.\,r_{sp}} \tag{8}$$

where γ is the surface tension of the liquid and θ is the dynamic contact angle. Note that the above formula changes according to the microstructure of porous medium; a detailed analysis is presented in Masoodi and Pillai (2012).

2.3   Analytical models

2.3.1   1-D Flow cases

The analytical model developed by Masoodi et al. (2007) for the upward wicking case is used to validate the present approach for a 1-D flow. If the location of the flow front is known, then this equation can be used to estimate the corresponding time. The analytical model is given by Masoodi et al. (2007),

$$\ln\left|\frac{p_s}{p_s \mp \rho g h_f}\right| \mp \rho g h_f = \frac{\rho^2 g^2 K}{\varepsilon\mu}t \tag{9}$$

In the present study, the case where flow in the direction along with gravity (liquid draining case) is considered as well. To model such a condition, the effect of hydrostatic pressure is reversed. It is taken negative in the case of an upward wicking case and as a positive in the case of a draining case as shown in Figure 1.

2.3.2   3-D flow scenario

To validate the method for the 3-D case, the input data and analytical equation from Xiao et al. (2012) is used to develop and validate the CFD model. Following are the assumptions

considered to develop the model: 1). As shown in Figure 2, the analytical model assumes a point source from which the liquid is absorbed within the spherical porous media. 2) The shape of flow front advancement for this case is assumed to be hemispherical and the porous medium is isotropic. 3). The effect of the hydrostatic pressure on the flow front advancement is neglected. Xiao et al. (2012) considered the physical velocity when deriving the model. In this work, the analytical model developed by Xiao et al. (2012) is modified by using the Darcy velocity instead of the physical velocity.

The liquid flow rate through advancing flow front is given by,

$$Q = u2\pi r_f^2 \tag{10}$$

where r_f is the advancing front and u is the superficial velocity (Darcy velocity) of liquid and it is given by,

$$u = u_r \varepsilon_o \tag{11}$$

where u_r is the physical velocity of the liquid flow and ε_o is the porosity of the porous media.

From equations (10) and (11), the expression for the radial velocity is given as a function of pressure gradient according to well-known Darcy's law,

$$\nabla p = \frac{\mu}{k} \cdot \left(\frac{Q}{2\pi r_f^2} \right) \tag{12}$$

Assuming the atmospheric conditions at the source *(p_atm)*, and suction pressure at the interface or liquid flow front. Hence pressure at $r=r_f$ will be $p_{atm} - p_s$ (Masoodi and Pillai, 2012). Equation (12) can be integrated with respect to the radius of the wetted region to get the pressure by assuming the initial flow front to be $r = r_o$ to obtain the expression for the pressure.

$$p_s = \frac{\mu Q}{2\pi k_o} \left(\frac{1}{r_o} - \frac{1}{r_f} \right) \tag{13}$$

By combining the equations (13), (11), and (10), we get

$$r_f^2 \frac{dr_f}{dt}\left(\frac{1}{r_o} - \frac{1}{r_f}\right) = \frac{k_o p_s}{\varepsilon \mu} \tag{14}$$

Upon integrating equation (14) by assuming the wetting front to be $r = r_o$, an expression for wetting front can be derived. This equation can be used to calculate the time by assuming the values of the initial flow front radius and the corresponding range of wetting front radius values.

$$\frac{1}{3r_o}(r_f^3 - r_o^3) - \frac{1}{2}(r_f^2 - r_o^2)\frac{\mu\varepsilon}{p_s k_o} = t \tag{15}$$

Where r_f is the flow front radius, r_o is the initial flow front, k_o is permeability in rigid conditions, p_s is capillary suction pressure given by equation (8).

3 Numerical Simulations

Figure 3 shows the numerical algorithm of the proposed method in which equations (1) and (2) are solved to obtain the velocity fields (Fluent, 2011). The source term (S_i) is added to the momentum equations. For the case of liquid-absorbing porous media, the flow is mainly driven by the capillary forces. Hence, the capillary pressure calculated by equation (8) is added to the momentum equation as a source term via user-defined functions in Ansys Fluent. The air is considered as a primary phase, and water is considered as a secondary phase. The details of the fluid properties, input parameters, solution method, and boundary conditions are summarised in the next sub-section.

3.1 Validation of the CFD approach

3.1.1 Validation of CFD approach for 1-D flow

The obtained CFD simulation results were compared with the experimental and analytical data for the upward wicking case from Masoodi et al. (2011). The computational domain and important boundary conditions are shown in Figure 4. The computational domain was a cylindrical wick with 76 mm length and 7.2 diameter. The bottom part of the wick was specified as an inlet, which is assumed to be in contact with the liquid reservoir at atmospheric

conditions. To model the wicking process, the momentum source terms were added to the solver via a user-defined function based on the equation (8), which gave the value of capillary pressure as 206.46 Pa. The values of permeability, porosity and fluid properties appear in Table 1

Figure 5 shows a comparison between the experimental data and CFD predictions for the wicking height in the case of upward wicking flow conditions. It can be seen that the CFD results are in good agreement with the experimental, analytical, and numerical predictions by Masoodi et al. (2011). The present CFD predictions show an average percentage error of 3.92%. compared to experimental data. The following is the case of upward wicking flow where flow is mainly driven by the capillary forces. The flow front advancement slows down as the capillary forces start to get balanced when the height of the liquid column rises within the porous domain. This effect is clearly observed after 5 seconds. The flow front advancement is slow at the beginning and finally becomes negligible.

To test the capability of the method, the developed model is also used to predict the liquid front advancement for downward flow where all the forces i.e., capillary, and gravitational are in the same direction. To do so, only the position of the inlet and outlet is reversed (Figure 4 a&b) in the existing model of upward wicking case and simulations are done. As there is no such data available in literature where this type of flow condition is considered, the CFD results are validated against the analytical predictions by equation (9). As mentioned in the mathematical modelling section, the existing equation developed by Masoodi and Pillai (2012) for the upward wicking flow case is modified such that the effect of gravity on flow front advancement will be opposite to that of the upward wicking case. As shown in Figure 6, the analytical and CFD predictions are in excellent agreement.

3.1.2 Validation of CFD approach for 2-D flow scenario (Imbibition in the annular porous membrane)

For a 2-D flow, liquid absorption into a porous membrane is considered. In recent years, interest in the medical utility of paper substrates has resulted in the development of two-dimensional lateral flow assays and three-dimensional microfluidics. These lateral flow devices are used in medical applications that are fabricated to meet the need of users in poor areas (Mendez et al., 2010) (Songok and Toivakka, 2017).

To validate the CFD approach, the obtained CFD simulation results are compared with the experimental and analytical data from Mendez et al. (2010). Figure 7 shows the computational domain, important boundary conditions, and mesh used to develop this model. The values of permeability, porosity and fluid properties appear in Table 2. The capillary pressure is applied at the interface using the user-defined functions in x and y directions. The boundary conditions at the inlet and outlet are the same as that of 1-D simulations. The effect of gravity is neglected in this simulation, which is the same as Mendez et al. (2010).

Figure 8 shows a comparison between CFD and experimental data for flow front locations in an annular porous zone. As seen from Figure 8, the CFD predictions are in excellent agreement with experimental data from Mendez et al. (2010). Further, Figure 9 shows the transient contours of variation of the liquid flow front, pressure, and velocity with time. Consistent with liquid volume fraction contours, the pressure contours show the value of capillary pressure precisely at the interface. Further, the velocity contours are clipped in the range for better visualization, which shows a sharp line at the interface. There is evidence of some velocity field beyond that line. This can be related to the velocity of air approaching the outlet.

3.1.3 Validation of CFD approach for 3-D flow (Imbibition from a point source in a semi-infinite porous domain)

The predictions for the flow front locations from the 3-D CFD model are validated against the analytical predictions from equation (15). To do so, all the input parameters are taken from Xiao et al. (2012). Details of the computational domain, boundary conditions, and mesh are shown in Figure 10. The values of permeability, porosity and fluid properties appear in Table 3.

Figure 11 shows a comparison between CFD predictions and analytical predictions for flow front advancement. The CFD predictions are in good agreement with analytical predictions by equation (15). As mentioned earlier, the flow front advances at the same rate in all directions, which is expected as the material is isotropic. For the validation purpose, equation (15) is used to calculate the time for the pre-defined flow front radius values. The corresponding contours are shown in Figures 12 and 13.

4 Case studies

To explore the ability of the proposed modelling approach, two different scenarios are studied here. The first scenario focuses on the behaviour of the liquid flow front when it hits the walls of a porous domain (i.e., during the experiments, the porous samples are usually held in a container). The second scenario is different and focuses on the newly proposed cell-zone condition that mimics the liquid hold up within the porous domain, which is usually found in real-world applications (e.g., diapers, paper napkins). To do so, another porous zone with higher viscous resistance to the wetting phase is modelled (Figure 14 a). Hence, the outcomes from these case studies would help engineers design and optimise products that use absorbing porous materials by examining the pressure and velocity field at different locations within the porous domain. As cited in the literature, the analytical method is valid until the flow front

reaches the walls of a porous domain. These case studies show the details of flow front behaviour that an analytical method fails to describe.

The primary porous zone is the main domain in which liquid absorption due to capillary forces takes place. The secondary porous zone is so defined that it only allows air to pass through it while blocking the flow of liquid. This cell-zone condition act as a wall to the wetting phase (liquid), whereas for air it acts similar to the primary porous zone. This was simply done by defining the higher resistance for the wetting phase (liquid) in a secondary porous zone. For the present case, the permeability ratio $\left({k_{pz1}}/{k_{pz2}} \right)$ was taken as 10. We considered two cases with different values of capillary pressure along with the new type of cell-zone condition. The shape of the flow front for all case studies is represented by radius in orthogonal directions *(x and z-direction)* and height *(y-direction)* as shown in Figure 14 (b).

4.1 Case 1: When flow front reaches the wall.

To check the applicability of the model for the case when flow front reaches the walls, where the analytical models fail, the domain with a smaller width was taken into consideration. For this case, the input data and boundary conditions for the model are taken the same as for the 3-D validation case as given by Table 3.

Figure 15 shows the variation of the flow front in the *x, y,* and *z*-direction. As shown in Figure 15, the flow front advancement in the *x* and *z* direction becomes almost constant when the flow front hits the walls around 20 sec of simulation time. On the other hand, the flow front continues to advance in the *y*-direction. From the trend of the graph, it can be seen that the flow front advancement in the *y*-direction is not affected by the termination of flow front advancements in other directions.

Figure 16 shows the transient contours of the volume fraction, pressure, and iso-surfaces. By observing the volume fraction contours and iso-surfaces, it can be seen that the shape of the

16

interface starts to change from a purely hemispherical nature when the flow front hits the walls. It is expected that for the longer times, the nature of the flow front would start to become 1-D. The blue-painted sphere-like area shows the position of the interface, and the volume-rendered red region shows the air volume fraction within the domain.

4.2 Case 2: Results for a newly proposed wall boundary condition with gravitational effects

As discussed in the previous sections, a new approach to model liquid retention in the porous media is proposed. To develop the model, the inputs (porosity, permeability) from the 1-D validation case are used. For the secondary porous zone, the permeability for the wetting phase (liquid) is set to be 10 times lower than the primary porous zone. Two different values of capillary pressure (400Pa and 1000Pa) are used for the study.

Figure 17 shows the evolution of flow front locations in the *x, y* and *z*-direction for two values of capillary pressure. For both cases, the effect of the gravity can be clearly seen on the flow front propagation in the *y*-direction, whose trend is similar to the 1-D validated case of upward wicking. Further, it is seen that the flow front advancement in the other two directions (*x* and *y*) stop after the flow front hits the interface of the porous zones, which demonstrates the capability of the proposed cell-zone condition.

For the capillary pressure values of 400 Pa and 1000 Pa, the flow front hits the interface around 6 sec and 4 sec, respectively. Also, it can be seen that the wicking height of the liquid is hardly affected by the value of capillary pressure, as the wicking height in the case of 1000 Pa capillary pressure did not vary significantly compared to the 400 Pa case. This can be related to the size of the porous domain. As the capillary force lifts the weight of the rising liquid column against gravity, it is expected that the wicking height would be higher for the same capillary pressure for the smaller sizes of the porous domain. To test this idea, the domain size is halved for the 400 Pa capillary pressure case and found the difference in the wicking height of the liquid.

Figure 18 clearly shows the effect of the porous domain size on the wicking height of the liquid. Further, Figures 19 and 20 show the transient contours of the liquid volume fraction, pressure, and iso-surfaces, showing the position of the interface. From volume fraction and pressure contours, it can be seen that the capillary pressure is being applied at the interface. Hence, this type of results related to the flow front location (liquid volume fraction contours), pressure could be helpful while designing and optimising the sanitary products according to performance constraints.

5   Summary and conclusion

The majority of the methods for modelling liquid absorption are based on the single-phase assumption within the porous domain. When a multiphase approach is assumed, the resulting model needed a lot of fitting parameters related to relative permeability, relative viscosity, and the relation between liquid saturation and capillary pressure. The multiphase approach suggested in this study is easier to implement as it only requires the values of porosity, permeability, and capillary pressure to predict the flow front locations during liquid imbibition. This approach is totally different than the previously used methods like Richard's equation as they require more input parameters such as saturation-capillary pressure curves and relative permeability.

In this study, the liquid absorption in rigid porous media is modelled using the Volume of Fluid method. This is the first time that such a method in combination with the Finite Volume Method has been used to model liquid absorption within porous media under rigid conditions. A good agreement between the CFD, experimental data, and available analytical expressions is obtained for all the developed models. Furthermore, an analytical model for the liquid draining case is proposed and for the case where the flow front is assumed to be hemispherical (3D imbibition), through which an existing model from the literature is modified. A new approach to model the liquid holdup within porous media is proposed in this research. The 3D transient results showed the ability of the model to track the interface during the liquid absorption process. The results also showed that a numerical model based on the combination of the Finite Volume Method and Volume of Fluid (FVM-VOF) can be used to model the liquid absorption process when the basic parameters, such as permeability, porosity, and capillary pressure, are known for any porous medium.

The results demonstrated the ability of the model to capture the interface when the propagating liquid front hit the walls. The shape of the interface slowly starts to become 1D in nature when

the gravitational effects are neglected. Further, the model captured the interface when gravitational effects are considered. The effect of hydrostatic pressure was clearly seen on the flow front advancement. The newly proposed approach to mimic the liquid hold up within porous media demonstrated its applicability. The results demonstrating the position of the interface clearly showed the liquid retention within the porous domain. Further, the results showed that the size of the porous domain has a considerable effect on the wicking height of the liquid.

The combination of the Finite Volume Method and Volume of Fluid method (FVM-VOF) provided an efficient approach to model the liquid absorption within rigid porous media. It is expected that this approach can serve as an alternative to the other multiphase methods, such as Eulerian models or models based on the Richards equation, for analysing the flow front locations and pressure distribution within the porous media. The CFD analysis of the flow front locations using simulations would help to design and optimize the sanitary and personal hygiene products, such as diapers, paper napkins and wipes, and tampons. The results showed that the method is capable of modelling and tracking the liquid-air interface under different working conditions. For our current scenario, the flow was assumed to be isothermal, but this method can be further extended to model the non-isothermal effects within porous media, such as heat pipe modelling where heat is being transferred within the wick (porous region). Finally, the use of the FVM adds flexibility to model the flow within complex geometries that cannot be modelled using other methods such as FEM. This method can be applied where the relationship between the capillary pressure and the liquid saturation is not known. Future work could extend this method further to the applications where the swelling effects of porous media need to be considered.

6   References

Ashari, A. & Tafreshi, H. V. General capillary pressure and relative permeability expressions for through-plane fluid transport in thin fibrous sheets. *Colloids and Surfaces A: Physicochemical and Engineering Aspects,* 346**,** 114-122, 2009.

Ashari, A., Bucher, T., Tafreshi, H. V., Tahir, M. & Rahman, M. Modeling fluid spread in thin fibrous sheets: Effects of fiber orientation. *International journal of heat and mass transfer,* 53**,** 1750-1758, 2010.

Bear, J. *Dynamics of fluids in porous media*, Courier Corporation, 2013.

Carciofi, B. A., Prat, M. & Laurindo, J. B. Homogeneous volume-of-fluid (VOF) model for simulating the imbibition in porous media saturated by gas. *Energy & fuels,* 25**,** 2267-2273, 2011.

Diersch, H.-J. G., Clausnitzer, V., Myrnyy, V., Rosati, R., Schmidt, M., Beruda, H., Ehrnsperger, B. J. & Virgilio, R. Modeling unsaturated flow in absorbent swelling porous media: Part 2. numerical simulation. *Transport in porous media,* 86**,** 753-776, 2011.

F. Zarandi, M. A. & Pillai, K. M. Spontaneous imbibition of liquid in glass fiber wicks, Part II: Validation of a diffuse-front model. *AIChE Journal,* 64**,** 306-315, 2018.

Fluent, A. Ansys fluent theory guide. *ANSYS Inc., USA,* 15317**,** 724-746, 2011.

Li, H., Vasquez, S. A. & Azhar, M.Published. Modeling of multiphase flows in porous media with applications to reservoir and well performance analysis. Fluids Engineering Division Summer Meeting. American Society of Mechanical Engineers, V01BT21A003, 2016

Lucas, R. Rate of capillary ascension of liquids. *Kolloid Z,* 23**,** 15-22, 1918.

Masoodi, R. & Pillai, K. A general formula for capillary suction-pressure in porous media. *Journal of Porous Media,* 15**,** 775-783, 2012.

Masoodi, R., Pillai, K. M. & Varanasi, P. P. Darcy's law-based models for liquid absorption in polymer wicks. *AIChE journal,* 53**,** 2769-2782, 2007.

Masoodi, R., Pillai, K. M. & Varanasi, P. P.Published. Role of hydraulic and capillary radii in improving the effectiveness of capillary model in wicking. Fluids Engineering Division Summer Meeting. 251-259, 2008

Masoodi, R., Tan, H. & Pillai, K. M. Darcy's law–based numerical simulation for modeling 3D liquid absorption into porous wicks. *AIChE journal,* 57**,** 1132-1143, 2011.

Masoodi, R., Tan, H. & Pillai, K. M. Numerical simulation of liquid absorption in paper-like swelling porous media. *AIChE journal,* 58**,** 2536-2544, 2012.

Mendez, S., Fenton, E. M., Gallegos, G. R., Petsev, D. N., Sibbett, S. S., Stone, H. A., Zhang, Y. & López, G. P. Imbibition in porous membranes of complex shape: quasi-stationary flow in thin rectangular segments. *Langmuir,* 26**,** 1380-1385, 2010.

Salokhe, S., Rahmati, M. & Masoodi, R. Numerical modelling of the flow in a swelling preform during LCM mould filling. *Journal of Reinforced Plastics and Composites,* 40**,** 490-504, 2020.

Santagata, T., Solimene, R., Aprea, G. & Salatino, P. Modelling and experimental characterization of unsaturated flow in absorbent and swelling porous media. *Chemical Engineering Science,* 134**,** 725-753, 2020.

Songok, J. & Toivakka, M. Modelling of capillary-driven flow for closed paper-based microfluidic channels. *Journal of Micromechanics and Microengineering,* 27**,** 065001, 2017.

Szekely, J., Neumann, A. & Chuang, Y. The rate of capillary penetration and the applicability of the Washburn equation. *Journal of Colloid and Interface Science,* 35**,** 273-278, 1971.

Wein, F., Chen, N., Iqbal, N., Stingl, M. & Avila, M. Topology optimization of unsaturated flows in multi-material porous media: Application to a simple diaper model. *Communications in Nonlinear Science and Numerical Simulation,* 78**,** 104871, 2019.

Xiao, J., Stone, H. A. & Attinger, D. Source-like solution for radial imbibition into a homogeneous semi-infinite porous medium. *Langmuir,* 28**,** 4208-4212, 2012.

Zarandi, M. a. F. & Pillai, K. M. Investigating liquid-fronts during spontaneous imbibition of liquids in industrial wicks. Part I: Experimental studies. *AIChE Journal***,** e17324, 2021.

Zarandi, M. a. F., Pillai, K. M. & Kimmel, A. S. Spontaneous imbibition of liquids in glass-fiber wicks. Part I: Usefulness of a sharp-front approach. *AIChE Journal,* 64**,** 294-305, 2018.

Figure 1 Schematic view of 1D flow for a) an upward wicking case and b) a draining case

Figure 2 Details of the hemispherical imbibition process in a semi-infinite porous domain. The liquid is absorbed from the point source of diameter d.

Figure 3 Numerical algorithm employing user-defined functions for the present method.

Figure 4 Details of the computational domain for validation activity for a) an upward wicking flow case and b) a downward flow case

Figure 5 The comparison between experimental analytical and CFD predictions for the wicking height for an upward wicking flow case.

Figure 6 Comparison between CFD predictions and predictions from newly proposed analytical for a downward flow case

Figure 7 Details of Computational domain, Boundary conditions, and Mesh with central angle as 90° (The domain is symmetric about Y-axis)

Figure 8 Transient contours of liquid volume fraction, pressure, and velocity for liquid imbibition in an annular section.

Figure 9 Comparison between CFD and experimental [13] predictions for flow front displacement versus time for imbibition in a porous membrane of an annular sector shape.

Figure 10 Sectional view and mesh of the computational domain and details of the initial interface for a 3D simulation of liquid imbibition.

Figure 11 Transient contours of liquid volume fraction, pressure, and velocity on an ZX

Figure 12 Comparison between the CFD and analytical predictions from Eq (15) for flow front displacement versus time for imbibition in a 3-D porous domain

Figure 13 Transient contours of liquid volume fraction, pressure, and velocity on an XY and YZ plane.

Table 1 Input parameters for 1-D validations

CFD setup condition		
General	Solver:	Pressure-based transient
Fluid materials	Air	**Viscosity**: 0.0179 Kg/m. s
		Density: 1.225Kg/m^3
	Liquid	**Viscosity:** 0.00334 Kg/m. s
		Density: 773 Kg/m^3
		Surface tension :0.02224N/m
Cell zone condition	Permeability	$Kxx=Kyy$=4.84×10^{-10} m^2
	Porosity	**0.4**
Boundary conditions	Inlet (constant inlet pressure)	**Atmospheric pressure. P=0**
	Outlet (Pressure outlet	**Atmospheric pressure. P=0**
	Operating density	**Density of lighter phase (air):**1.225Kg/m^3
Model	Viscous flow model:	Laminar
	Multiphase model:	**Phase 1:** Air (non-wetting phase)
	Volume of Fluid	**Phase 2:** liquid (wetting phase)
		Surface tension :0.02224 N/m

Table 2 Input parameters for 2-D validation case

Input parameters		
Fluid materials	Air (Phase-1)	**Viscosity**: 0.0179 Kg/m. s
		Density: 1.225Kg/m^3
	Water (Phase-2)	**Viscosity:** 8.9×10^{-4} Kg/m. s
		Density: 998.2 Kg/m^3
		Surface tension :0.0728N/m
Cell zone condition	Permeability	*Kxx=Kyy*=6.83×10^{-13} m^2
	Porosity	**0.81**
Gravity		**Neglected**

Table 3 Input parameters for 3D validations

Input parameters		
Fluid materials	Air (Phase-1)	**Viscosity**: 0.0179 Kg/m. s
		Density: 1.225Kg/m^3
	Water (Phase-2)	**Viscosity:** 0.0010016 Kg/m. s
		Density: 998.2 Kg/m^3
		Capillary pressure:3480 N/m^2
Cell zone condition	Permeability	*Kxx=Kyy= Kzz:* 1.21×10^{-11} m^2
	Porosity	0.36
Gravity		**Neglected**