Modeling and simulation of paperboard edge wicking


KEYWORDS: Multi-scale simulation, Edge soaking, Immersed Boundary Methods, Porous flow, Pore-morphology methods

SUMMARY: When liquid packaging board is made aseptic in the filling machine the unsealed edges of the board are exposed to hydrogen peroxide. A high level of liquid penetration may lead to aesthetic as well as functional defects. To be able to make a priori predictions of the edge wicking properties of a certain paperboard material is therefore of great interest to paper industry as well as to packaging manufacturers. The aim of this paper is to present a new analytical theory for prediction of the edge wicking properties of paperboard. The theory is based on Darcy’s law and the ideal gas law to describe the physical behavior of water flow in paperboard. The theory is compared to a recently published multi-scale framework and with pressurized edge wick experiments. The agreement is very good for paperboard samples of different sizes. The conclusion from the work is that both analytical theory and detailed simulations are useful to predict edge wicking properties of paperboard material.

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The resistance to in-plane edge penetration, or edge wicking, is one of the most important properties for liquid packaging board. In the filling machine the unsealed edges of the paperboard are exposed to hydrogen peroxide that to some extent may soak the material. A high-level of edge wicking could lead to a tube burst in the filling machine that destroys the aseptic environment and causes an expensive production loss. For the final paperboard package, too high edge wicking may result in aesthetic and functional defects.

Four mechanisms are proposed in the literature for water transport in paper (Bristow 1986; Salminen 1988; Tufvesson 2006): Diffusion transport of vapor in the pores, capillary transport of liquid in the pores, surface diffusion in the pores and water transport through the fibers. The importance of each mechanism depends on the temperature, the chemical composition, the vapor pressure of the liquid, the fiber structure and the chemical properties of the fibers. The majority of the earlier work is based on simplified models such as the Lucas-Washburn equation. Salminen (1988) stated that this classical model did not adequately describe water transport in the pore system of paper and that it is necessary to take the external pressure, capillary pressure, counter pressure of air, swelling of the fiber network and liquid transport through the vapor phase, into account. An extensive review of theories for fluid flow in paper is found in Roberts (2004). Roberts et al. (2003) experimentally studied the fluid penetration in unsized paper. They propose that when capillary forces govern penetration, fluid transport occurs by film flow along channels formed by fiber overlaps; they also discuss how sizing agents affect the flow. The effect of internal sizing chemicals on the paper’s resistance to wetting was also extensively reviewed by Hubbe (2006).

Åvitsland and Wågberg (2005) studied how the paperboard inner structure affects the flow resistance by performing pore volume distribution measurements and concluded that CTMP sheets resist flow to much less extent than Kraft sheets. To be able to make a priori predictions of the edge wicking properties of a certain paperboard material is of great interest to paper industry as well as to packaging manufacturers. Since the fluid penetration on the macro-scale depends heavily on the physical properties of the fiber network micro-scale a multi-scale framework was recently proposed by Mark et al. (2012). On the micro-scale simulations are performed on virtual paper models to calculate the pressure drop and relative permeabilities as a function of saturation and porosity. The results are stored in a database which is used as input for dynamic two-phase flow simulations on a homogenized macro-scale model of a virtual paper with varying anisotropic porosity.

The aim of this work is to present a new analytical theory for prediction of edge wick penetration. The theory is based on Darcy’s law and the ideal gas law to describe the physical behavior of water flow in paperboard. The theory is verified through comparison with the recently developed multi-scale framework (Mark et al. 2012) and measurements on paperboard samples of different sizes.

Theory

Due to the large difference in scales from the fiber to the paper level a multi-scale ansatz for simulation of edge wicking was proposed by Mark et al. (2012). On the macro-scale, the fluid flow is modeled by a porous mixture model, where Darcy’s law (Bird et al. 1960) is...
where $\Theta$ is the contact angle, $\gamma$ is the surface tension, and $r$ is the radius of the tube. We introduce a weighted pressure, $p = S_0 p_w + S_a p_a$, which is continuous between the phases and neglect gravity as the length and time scales are small. This along with the capillary pressure definition gives a reformulated Darcy’s law

$$\vec{u} = -\vec{k}(\lambda \vec{V} p + \{S_{0w} \lambda_w - \lambda_w \} \nabla p_c + \lambda \vec{p}_c \nabla S)$$  

where $\lambda_w$ is the water mobility and $\lambda$ is the total mobility. Darcy’s law and the assumption of a divergence free fluid velocity field (incompressible flow) then gives an equation for the weighted pressure

$$-\nabla \cdot (\vec{k} \lambda \vec{V} p) = \nabla \cdot [\vec{k} \{(S_{0w} \lambda_w - \lambda_w \} \nabla p_c + \lambda \vec{p}_c \nabla S_w)]$$  

Now let the saturation be transported by the Darcy’s velocity

$$\Phi \frac{\partial S}{\partial t} + \vec{u} \cdot \nabla S_w = 0$$  

where the convective term is discretized by the shock capturing CICSAM scheme (Ubbink 1997). One should notice that the capillary pressure, permeabilities and phase mobilities are also dependent on the local porosity, which is captured in the micro models. The two-phase porous flow model Eqs [5] and [6] is completed by incorporating the micro simulations of permeability and capillary pressure.

### Macro-scale model

A porous media model for a two-phase fluid system of water and air is developed partly based on work by Chen et al. (2006). The model utilizes Darcy’s law and mass conservation of water and air to derive a pressure equation. Mass conservation of air and water is given by the continuity equation,

$$\Phi \frac{\partial \alpha S_w}{\partial t} + \nabla \cdot (\rho_a \vec{u}_a) = q_a$$  

where $\Phi = \Phi(x)$ is the porosity of the porous medium ($\Phi = 1$ corresponds to all volume is water), $\rho_a$ is the density, $S_a$ is the saturation, $\vec{u}_a$ is the velocity, and $q_a$ is the source mass flow rate, for water $\alpha = w$ and for air $\alpha = a$. Darcy’s law for each phase relates the velocity to the gradient of the pressure linearly,

$$\vec{u}_\alpha = -\frac{k_{kr}}{\mu_\alpha} (\nabla p_a - \rho_a \vec{g})$$  

where $k_{kr}$ is the absolute permeability tensor of the porous medium with only the diagonal components nonzero, $k_{kr}$ is the relative permeability, $\mu_\alpha$ is the viscosity, $p_a$ is the pressure, $\vec{g}$ is the gravitational acceleration. The fluid fills the voids of the porous medium, represented by $\Phi$, $S_a + S_w = 1$ and the pressure difference between the two phases is given by the capillary pressure $p_c(S, \vec{x}) = p_a - p_w$. The capillary pressure under capillary equilibrium is for a narrow tube or a pore of circular cross-section given by the Young Laplace equation

$$p_c = \Delta p = \frac{2\gamma \cos \Theta}{r}$$  

where $\Delta p$ is the absolute capillary pressure, $\gamma$ is the surface tension and $r$ is the radius of the tube.

In addition we also present a new analytical theory for predicting the edge wicking properties of paperboard.

### Micro-scale model

On the micro-scale we first need to construct realistic virtual paper models that have the same properties as the manufactured lab sheets. Tomographic and SEM images are analyzed to extract information about the fiber network. The software GeoDict (www.geodict.com) is then used to generate a stochastic realization of the network, see Fig 1. Each fiber is considered to be a hollow non-straight slender body with an ellipsoidal cross-section, where the minor and major axes in the cross-section are adjusted to take the partial collapsing during pressing into account. Statistical distributions of fiber size, shape and orientation, as well as solid volume fraction and paper height are used as input. These input parameters are fine-tuned by comparing air permeability simulations and measurements both in the paper plane and the out of plane direction. A number of different small samples of size 0.3125x0.3125 mm² are generated to represent the different parts of the lab sheets.

The macro-scale model requires the relative permeabilities and capillary pressure curves as an input. These flow properties are simulated for each virtually generated paper sample. This is accomplished by solving the incompressible Navier-Stokes equations:

$$\nabla \cdot \vec{u} = 0$$

$$\rho_f \frac{\partial \vec{u}}{\partial t} + \rho_f \vec{u} \cdot \nabla \vec{u} = -\nabla p + \mu \nabla^2 \vec{u}$$

where $\vec{u}$ is the fluid velocity, $\rho_f$ is the fluid density, $p$ is the pressure and $\mu$ is the dynamic viscosity. A possible approach would be to solve these equations for the two-phase flow of water penetrating the fiber structure, e.g. by the Volume of Fluid (VOF) method with a surface

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**Fig 1.** Stochastic realization of the paper micro-structure in PaperGeo.
tension model. However, these direct numerical simulations would be computationally very expensive and we adopt a different strategy for which a series of one-phase flow simulations are done instead.

For each virtual sample the flow properties are simulated. The capillary pressure curve is determined by a pore-morphology model (Becker et al. 2008). In the geometrical model spheres with different radius, representing different capillary pressures according to Eq [3], is propagated through the structure. For each sphere radius different parts of the volume between the fibers can be reached from the inlet. In this way the reached volume or saturation level is related to the capillary pressure. As a result we get a capillary pressure curve for each virtual paper sample. To calculate the relative permeabilities, we perform one-phase flow simulations of the full Navier-Stokes equations for channels that are accessible for a certain capillary pressure. For each paper sample this results in a relationship between permeability and saturation. By simulating different paper samples with varying porosity, the porosity dependency is also captured.

The simulation framework for the one-phase flow simulations is the incompressible Navier-Stokes software, IBOFlow (www.iboflow.com), developed at Fraunhofer-Chalmers Centre. IBOFlow is a segregated solver that utilizes the SIMPLEC method (van Doormaal, Raithby 1984) for coupling of the velocity and pressure fields. All variables are stored in a collocated arrangement and Rhie-Chow interpolation (Rhie, Chow 1983) is used to prevent pressure oscillations. It is based on a finite volume discretization on a Cartesian octree grid that can be dynamically refined and coarsened. The flow around the fibers are resolved and immersed boundary methods (Mark, van Wachem 2008; Mark et al. 2011) are used to model the presence of fibers in the flow.

**Pressurized edge wick theory**

To understand the dominating phenomena determining the edge wicking process an analytical theory has been derived in parallel to the multi-scale framework. The starting point is the volumetric flow \( Q(t) \) that can be expressed as the product between the cross-sectional area and the velocity of the flow in a radial coordinate as \( Q = A(r)v(r,t) \), where \( v = dr/dt \) is the radial velocity and \( r \) denotes the position of the (fictitious) water meniscus. The cross-section area \( A(r) \) depends on the radius, i.e. \( A(r)=2\pi r \Phi h \). Note that \( \Phi h \) can be interpreted as an effective thickness. Hence, \( Q(t)=2\pi \Phi hr v(r,t) \) is constant with respect to the flow path \( r \). Insertion into Darcy’s law, Eq [2], and assuming zero gravity gives together with a variable separation

\[
-P(r) = \frac{\mu}{k} \frac{d}{dr} \left( \frac{Q(t)}{2\pi r \Phi h} \right)
\]

where \( k = \kappa_v \Phi \). Integration of the pressure side (left side) from an initial pressure \( P(r_0) \) to an arbitrary pressure \( P(r) \) and the radius side (right side) from \( r_o \) to \( r \) in Eq [8] gives

\[
P(r) - P(r_0) = -\frac{\mu}{k} \frac{Q(t)}{2\pi \Phi h} \ln \left( \frac{r}{r_0} \right)
\]

where \( k = \kappa_v \Phi \). Integration of the pressure side (left side) from an initial pressure \( P(r_0) \) to an arbitrary pressure \( P(r) \) and the radius side (right side) from \( r_o \) to \( r \) in Eq [8] gives

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\]

Note that our definition of \( \kappa \) differs from the one used by Muskat (1946). The initial pressure at the hole \( r = r_0 \) at \( t = 0 \) is equal to the driving pressure, i.e. \( P(r_0) = P_d \). The driving pressure \( P_d \) is equal to the sum of the applied outer pressure \( P_{atm} \), the atmospheric pressure \( P_{atm} \) and the capillary pressure \( p_c \).

Insertion of the volumetric flow \( Q(t) = 2\pi \Phi hr dr / dt \) into Eq [9] gives

\[
P(r) - P_d = -\frac{\mu}{k} \frac{d}{dr} \ln \left( \frac{r}{r_0} \right)
\]

Note, that in Eq [10] the effective thickness \( \Phi h \) is cancelled out. Hence, Eq [10] gives us only information on how the liquid meniscus front is penetrated into the sample, no information is gained about the amount of liquid mass which is penetrating into the sample.

The pressure \( P(r) \) in Eq [10] at the liquid meniscus is equal to the air counter pressure. The decreasing air volume is calculated from the ideal gas law. The experiments in the pressurized edge wick (PEW) equipment are done under a constant temperature. Hence, the pressure increase due to a decreasing volume can be calculated from the relation \( P(r)V(r) = P_{atm} V(r_0) \). The air volume is \( V(r) = h \pi r_c^2 (r_c^2 - r^2) \), where \( r_c \) is the outer radius of the sample. Insertion of \( V(r) \) into the gas law gives the air counter pressure as

\[
P(r) = P_{atm} \left( \frac{r_c^2 - r_0^2}{r_c^2 - r^2} \right)
\]


\[
p_o \left( \frac{r_c^2 - r^2}{r_c^2 - r_0^2} \right) = \frac{1}{P_{atm}} \frac{\mu}{k} \frac{d}{dr} \ln \left( \frac{r}{r_0} \right)
\]

where \( p_o = P_d / P_{atm} \). Introduce a normalized area

\[
z = \frac{r^2}{r_0^2}
\]

and a geometry-material time

\[
\tau = \frac{1}{2} \frac{r_0^2}{P_{atm}} \frac{\mu}{k}
\]


\[
p_o \left( 1 - a^{-1}(z-1)^{-1} \right) = \frac{1}{2} \ln(z) \frac{dz}{d(t/\tau)}
\]

where \( a = (r_c^2 / r_0^2 - 1) \). The geometry variable \( a \) can physically be interpreted as the ratio between the sample area \( \pi (r_c^2 - r_0^2) \) and the hole area, \( \pi r_0^2 \).

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An analytical solution of Eq \([15]\), using the Maple™ software with the initial condition that at time zero the meniscus of the fluid is at \(r = r_o\), is given by

\[
2 p_o^2 \frac{t}{r} = \ln(z) \left[ z_p o - a \ln \left( \frac{z p o}{a (p_o - 1) + p o} \right) \right] \\
- (z-1) p o \\
- a \text{dilog} \left( 1 - \frac{z p o}{a (p_o - 1) + p o} \right) \\
+ a \text{dilog} \left( 1 - \frac{p o}{a (p_o - 1) + p o} \right)
\]

[16]

where \(\text{dilog}[\ ]\) is the Dilogarithm function.

The mass penetration in a sample as a function of the penetrated radius, \(r\), is given as

\[
\Delta m = \pi \rho (\Phi h) (r^2 - r_o^2) = \pi \rho (\Phi h) r_o^2 (z-1)
\]

[17]

where we used Eq \([13]\).

Experiments

Manufacturing of lab sheets

Paper lab sheets were manufactured using an STFI dynamic sheet former with circulating pulp, moving head box and a stationary forming fabric. CTMP (Chemo Thermo Mechanical Pulp) pulp with AKD sizing chemicals was used. The lab sheets were dried and pressed by a rotating cylinder. The grammage of the resulting CTMP lab sheet was ~60g/m².

Pressurized edge wick experiment

In Fig 2 the pressurized edge wick equipment is shown. The purpose of the equipment is to simulate the environmental conditions in the deep bath of a filling machine. The diameter of the pressure-vessel is 250 mm and its height is 190 mm. The vessel is filled with water to a height of 90 mm. The water temperature can be controlled. The cardboard samples (see Fig 2b) have a punched hole with radius \(r_o = 6\) mm through which the liquid can freely penetrate into the polyethylene laminated paperboard.

Samples with dimensions \(50\times62\) mm² and \(33\times41\) mm² from a commercial paperboard were used. The outer edge was also sealed with laminated Polyethylene. The test sequence is as follows: First the sample holder is lowered into water and the lid is closed. Then the pressure inside the vessel is instantaneously increased to 15 kPa and held constant for the 20 s test time. Subsequently the pressure is turned off and a rod lifts the sample holder above the water level. Finally the lid is opened and the sample is removed and weighed again. The edge wick index for the sample is defined as the difference in weight before and after the test, \(\Delta m\), divided by the area of the open edge of the hole,

\[
EWI = \frac{\Delta m}{2 \pi r_o h} \left[ \text{kg/m}^2 \right]
\]

[18]

where \(h\) is the thickness of the paper.

Results

In Mark et al. (2012) the multi-scale framework was validated and a contact angle study was performed. It was shown that a contact angle of 110° gave a good correspondence between measurements and simulations for the sheets that included AKD chemicals. Here we will use that same contact angle and compare the analytical PEW theory with the multi-scale simulations and measurements for different paper sample sizes. In order to compare measurement results from commercial paperboard with the simulation results for the lab sheets the measurements are scaled with the PEW theory in Figs 4 and 5. The scaling is based on the capillary pressure and permeability constants given in Fig 3.

A constant porosity 0.75 is used in all simulations. The pressure in the hole is set to 15 kPa and for the external boundaries ambient pressure outlet boundary conditions are used. To capture the compression of the air when the water enters the paper, the pressure on the outlet is increased according to the ideal gas law. It is unknown how much of the air that remains trapped inside the paper. From the pressurized edge wick experiments we have estimated that approximately 80% of the air is compressed while the remainder leaves the domain.

Comparison between PEW theory and simulations

To compare the results obtained with the PEW theory and the multi-scale simulations we investigate three different paper sample sizes (33×41 mm², 50×62 mm², 100×124 mm²). In Fig 3 the resulting edge wick indices are compared. A very good agreement is obtained for all three sizes.

Experimental validation

Furthermore, we also compare the theory and multi-scale simulations with pressurized edge wick experiments on a commercial board by using the equipment in Fig 2. Experiments are unfortunately only available for the two smaller paper sample sizes and the results are shown in Figs 4 and 5. The experimental error bars show one standard deviation. Both the theory and the simulations show a good correspondence with the experiments.
Fig 3. Comparison of edge wick indices from simulation and analytical PEW theory for different paper sample sizes. The wick index is normalized with $\alpha$ and the time is normalized with $\alpha r$. The parameters $\kappa$ and $P_c$ used in Eq [16] are obtained through a nonlinear least squares regression analysis of the PEW simulation.

**Discussion**

The derivation of the PEW theory contains several tacit simplifications: penetration being quasi-stationary, the medium being isotropic, saturated flow (with a distinct meniscus at $r = r_m$) and effective porosity being equal to the geometrical porosity (absence of dead-end pores). In the light of these assumptions and considering that in the theoretical PEW approximation the micro-structure is only taken into account through Darcy’s law, the correspondence between the PEW theory and the multi-scale simulations is surprisingly good. Both approaches capture the first-order phenomena and agree well with the experiments. However, since the multi-scale approach takes also the micro-structure properties into account it is a more detailed model that includes the pore-size distribution and sizing effects on edge wicking performance.

In future work, improved models for the contact angle, which may depend on saturation and time, will be developed. The general framework will be extended in such a way that a multi-layer board consisting of single layer sheets can be handled, and a diffusion model will be used to capture the layer interaction. The goal of the extended framework is to enable a priori predictions of the edge wicking properties of a given paperboard material. This is relevant to paper industry as well as to packaging manufacturers.

**Conclusions**

The conclusion from this work is that both the proposed analytical theory and the multi-scale framework are useful tools for increasing the fundamental understanding of the important phenomena that determine the edge wicking properties of paperboard.

**Acknowledgements**

This work is part of the ISOP (Innovative Simulation of Paper) project which is performed by a consortium consisting of Albany International, Eka Chemicals, Stora Enso, Tetra Pak, Fraunhofer ITWM and Fraunhofer-Chalmers Centre.

**Literature**


