

Multi-scale simulation of paperboard edge wicking using a fiber-resolving virtual paper model

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ABSTRACT: 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. The ability to make a priori predictions about the edge wicking properties of a certain paperboard material is therefore of great interest to the paper industry, as well as to packaging manufacturers. In this paper, a multi-scale framework is proposed that allows for detailed simulation of the edge wicking process.

On the fiber micro-scale, virtual paper models are generated based on input from tomographic and scanning electron microscope (SEM) images. A pore morphology method is used to calculate capillary pressure curves, and on the active pores, one-phase flow simulations are performed for relative permeabilities. The results as functions of saturation and porosity are stored in a database. The database is used as input for two-phase flow simulations on the paper macro-scale. The resulting fluid penetration is validated against pressurized edge wick measurements on paper lab sheets with very good agreement. The proposed multi-scale approach can be used to increase the understanding of how edge wicking in paperboard packages depends on the micro-structure.

Application: A unique modeling approach for multi-scale simulation of liquid penetration in package paperboard is proposed to increase the fundamental understanding of edge wicking and how it depends on the paper micro-structure.

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 may soak the material to some extent. 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, edge wicking that is too high may result in aesthetic and functional defects.

Four mechanisms are proposed in the literature for water transport in paper [1,2,3]: 1) diffusion transport of vapor in the pores, 2) capillary transport of liquid in the pores, 3) surface diffusion in the pores, and 4) 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. Hubbe [4] reviewed the effect of internal sizing chemicals on the paper's resistance to wetting. Roberts [5] provided an extensive review of theories for fluid flow in paper [5]. The majority of the earlier work is based on simplified models such as the Lucas-Washburn equation. Salminen [2] stated that this classical model did not adequately describe water transport in the pore system of paper and that it is necessary to take into account the external pressure, capillary

pressure, counter pressure of air, swelling of the fiber network, and liquid transport through the vapor phase.

Åvitsland et al. [6] studied how the paperboard inner structure affects the flow resistance by performing pore volume distribution measurements and concluded that chemithermo-mechanical pulp (CTMP) sheets resist flow to a much less extent than kraft sheets. The ability to make a priori predictions regarding the edge wicking properties of a certain paperboard material is of great interest to the 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, we propose a multi-scale framework.

On the micro-scale, virtual paper models are generated in PaperGeo, the virtual paper structure generator in GeoDict [7], based on input from tomographic and scanning electron microscope (SEM) images. Simulations are performed on these models to calculate the pressure drop and relative permeabilities as a function of saturation and porosity. The capillary pressure curves are efficiently obtained through a pore morphology method [8], and on the active pores, one-phase flow simulations are performed in IBOFlow (Immersed Boundary Octree Flow Solver) [9,10,11] for relative permeabilities. 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 results from the macro simulations are the liquid saturation level and pressure as a function of time.

Similar work on the micro-scale has been done by Hyv  luoma et al. [12,13] using a Lattice-Boltzmann method for the flow simulation. However, to the best of the authors' knowledge, a multi-scale approach, as proposed in this paper, has previously not been applied for prediction of edge wicking properties. The objective of this work is to present the novel approach and validate it to pressurized edge wick experiments.

THEORY

Due to the large difference in scales from the fiber to the paper level, a multi-scale ansatz for simulation of edge wicking is proposed. On the macro-scale, the fluid flow is modeled by a porous mixture model, where Darcy's [14] law is employed to derive a pressure equation. The resulting velocity field transports the saturation. To close the model, the permeability and capillary pressure as a function of saturation are required, which makes the model non-linear. The permeability and capillary pressure are calculated on the fiber micro-scale for a virtual model of the paper. On this scale, the fluid flow is modeled by the full Navier-Stokes equation. The simulation framework is the incompressible Navier-Stokes software, IBO-Flow, developed at Fraunhofer-Chalmers Centre. IBOFlow is a segregated solver that utilizes the SIMPLEC method [15] for coupling of the velocity and pressure fields. All variables are stored in a collocated arrangement, and Rhie-Chow interpolation [16] 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 is resolved, and immersed boundary methods [9,10] are used to model the presence of fibers in the flow.

Macro-scale model

A porous media model for a two-phase fluid system of water and air is developed partly based on work in [17]. The model utilizes Darcy's law [14] and mass conservation of water and air to derive a pressure equation. Mass conservation of air and water is given by the continuity equation:

$$\Phi \frac{\partial \rho_\alpha S_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \vec{u}_\alpha) = q_\alpha \quad (1)$$

where $\Phi = \Phi(x)$ is the porosity of the porous medium ($\Phi = 1$ corresponds to all volume is water), ρ_α is the density, S is the saturation, $\vec{u}_\alpha$ is the velocity, and q_α is the source mass flow rate, for water $\alpha = w$ and for air $\alpha = a$. Darcy's law [17,14] for each phase relates the velocity to the gradient of the pressure linearly:

$$\vec{u}_\alpha = -\frac{\kappa_{kr}}{\mu_\alpha} \vec{\kappa} (\nabla p_\alpha - \rho_\alpha \vec{g}) \quad (2)$$

where $\vec{\kappa}_{i,j}$ is the absolute permeability tensor of the porous medium with only the diagonal components nonzero, κ_{kr} is the relative permeability, μ_α is the viscosity, P_α is the pressure, and $\vec{g}$ is the gravitational acceleration. The fluid fills the voids of the porous medium, represented by Φ , $S_a + S_w = 1$ 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:

$$p_c = \Delta p = \frac{2\gamma \cos \Theta}{r} \quad (3)$$

where Θ is the contact angle, γ is the surface tension, and r is the radius of the tube.

We introduce a weighted pressure, $p = S_w P_w + S_a P_a$, which is continuous between the phases and neglects gravity, as the length and time-scales are small. This, along with the capillary pressure definition, gives a reformulated Darcy's law:

$$\vec{u} = -\vec{\kappa} \left(\tilde{\lambda} \nabla p + [S \tilde{\lambda} - \lambda_w] \nabla p_c + \tilde{\lambda} p_c \nabla S \right) \quad (4)$$

where λ_w is the water mobility, $\tilde{\lambda}$ is the total mobility, and S is the water saturation. Darcy's law and the assumption of a divergence free fluid velocity field (incompressible flow) then gives an equation for the weighted pressure:

$$-\nabla \cdot (\vec{\kappa} \tilde{\lambda} \nabla p) = \nabla \cdot \left[\vec{\kappa} \left\{ (S \tilde{\lambda} - \lambda_w) \nabla p_c + \tilde{\lambda} p_c \nabla S \right\} \right] \quad (5)$$

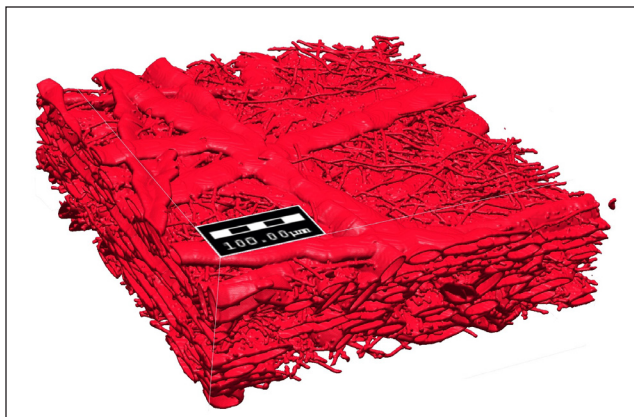
Now let the saturation be transported by the Darcy's velocity:

$$\Phi \frac{\partial S}{\partial t} + \vec{u} \cdot \nabla S = 0 \quad (6)$$

where the convective term is discretized by the shock capturing CICSAM scheme [18]. One should note 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 in Eq. (5) and Eq. (6) is completed by incorporating the micro simulations of permeability and capillary pressure.

Micro-scale model

On the micro-scale, we first need to construct virtual paper models that have the same properties as the manufactured lab sheets, which were created as described in a section that follows on "Manufacturing of lab sheets." Tomographic and SEM images of the lab sheets are analyzed to extract information about the fiber network. The software GeoDict [7] is then used to generate a stochastic realization of the network (**Fig. 1**). Each fiber is considered to be a hollow non-



1. Stochastic realization of the micro-structure of a chemithermomechanical pulp (CTMP) lab sheet in PaperGeo.

straight slender body with an ellipsoidal cross-section. 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 $0.3125 \times 0.3125 \text{ mm}^2$ 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:

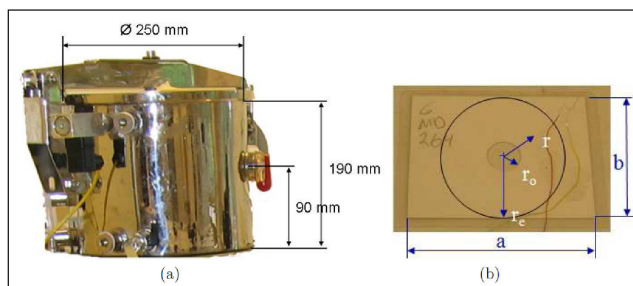
$$\begin{aligned} \nabla \cdot \vec{u} &= 0, \\ \rho_f \frac{\partial \vec{u}}{\partial t} + \rho_f \vec{u} \cdot \nabla \vec{u} &= -\nabla p + \mu \nabla^2 \vec{u}, \end{aligned} \quad (7)$$

where $\vec{u}$ is the fluid velocity, ρ_f is the fluid density, p is the pressure, and μ 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 tension model in IBOFlow. However, these direct numerical simulations of the problem 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 [8]. In the geometrical model, spheres with different radius, representing different capillary pressures according to Eq. (3), are 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 capil-



2. A scanning electron microscope (SEM) image of a CTMP lab sheet performed at Albany International.



3. (a) The pressurized edge wick equipment, and (b) a test sample of size of $a = 62 \text{ mm}$ and $b = 50 \text{ mm}$. The punched hole has radius $r_o = 6 \text{ mm}$.

lary 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.

EXPERIMENTS

Manufacturing of lab sheets

Paper lab sheets are manufactured using a STFI dynamic sheet former with circulating pulp, moving head box, and a stationary forming fabric. CTMP with and without alkylketene dimer (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 about 60 g/m^2 . **Fig. 2** provides an SEM image of the sheet.

Pressurized edge wick experiment

In **Fig. 3**, 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 is set to a predefined level. The paper samples (**Fig. 4**) consist of a punched hole with radius $r_o = 6 \text{ mm}$ where the liquid is free to penetrate into the polyethylene laminated paperboard. Paper samples of sizes $62 \times 50 \text{ mm}^2$ and $41 \times 33 \text{ mm}^2$ are used. The outer edge is also covered with laminated polyethylene. In the beginning of the test, the sample holder is lowered in the water and the lid is closed. The pressure inside the vessel is instantly increased to 15 kPa and held constant for the 20 s test time. Thereafter, the pressure is turned off and the rod lifts up the sample holder above the water level. Then 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,



4. A sample from the pressurized edge wick experiments.

Δm , divided by the area of the open edge of the hole:

$$EWI = \frac{\Delta m}{2\pi r_0 h} \left[\text{kg} / \text{m}^2 \right] \quad (8)$$

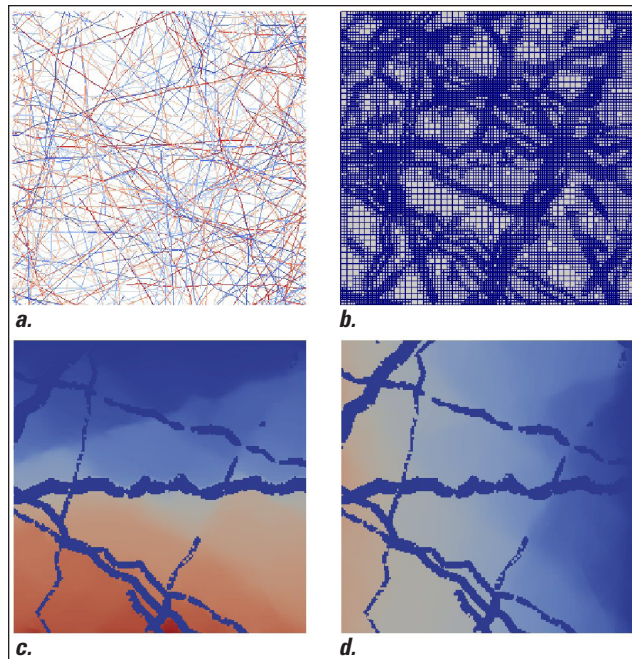
where h is the thickness of the paper. In this work, the pressurized edge wick experiment is performed on a number of constructed CTMP lab sheets of two different sizes, with and without AKD.

NUMERICAL RESULTS

Micro simulations

On the micro-scale, two different types of simulations are performed to calculate the in-plane permeabilities and capillary pressure curves. The in-plane permeabilities are simulated in IBOFlow for different virtual realizations of small pieces $0.3125 \times 0.3125 \text{ mm}^2$ of the paper structure. The fibers are treated as immersed boundaries and a grid is automatically generated with a number of refinements around the fibers (Fig. 5). The permeabilities are simulated in both the machine (MD) and cross (CD) directions. Fig. 5 shows the pressure drop for the different directions.

By using the techniques described in the previous “Micro-scale model” section of this paper, the capillary pressure curves are calculated geometrically using a pore-morphology model and Laplace’s law. Based on the results from the pore morphology model, the relative permeabilities as a function of porosity and water saturation are calculated by one-phase Navier-Stokes simulations on the open pores. The capillary pressure as a function of porosity and water saturation for a given contact angle $\Phi = 95^\circ$ is shown in Fig. 6a, and the relative permeabilities are shown in Fig. 6b. The results are



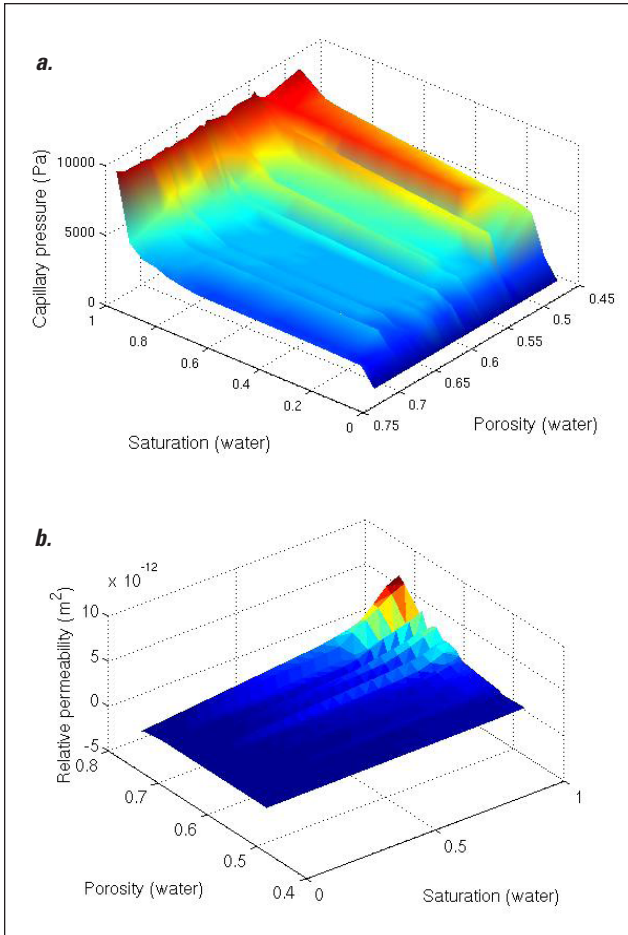
5. A micro simulation on a virtual paper sample. (a): Centerlines of fibers in the sample. (b): Adaptive computational grid with two refinements around the fibers. (c): Visualization of the pressure distribution over the paper in the machine direction. (d): Visualization of the pressure distribution in the cross direction.

stored in a database, which is used as input for the macro simulations.

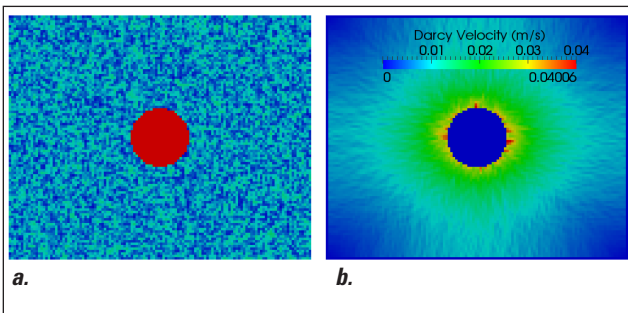
Macro simulations

On the macro-scale, the pressurized edge wick experiment is simulated in IBOFlow. The corresponding dimensions and a smoothed random paper porosity between 0.6 and 0.75 are set (Fig. 7). 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 is contained inside the paper. From the pressurized edge wick experiments, we have estimated that approximately 80% of the air is compressed and the other part leaves the domain. The simulated Darcy’s velocity field is shown in Fig. 7, where the velocity is higher in the regions of high porosity.

Measurements of the contact angle with and without AKD have been performed on the lab sheets. For the sheets with AKD, the contact angle was roughly 110° . The average porosity of the manufactured lab sheets was 0.75. To determine the required time and spatial resolution to obtain grid and time step independent solutions, a convergence study is performed. In Fig. 8, the edge wick index is plotted as a function of time for three different grid sizes, with time step of 1 ms. To see the difference between the grid sizes, only the first two

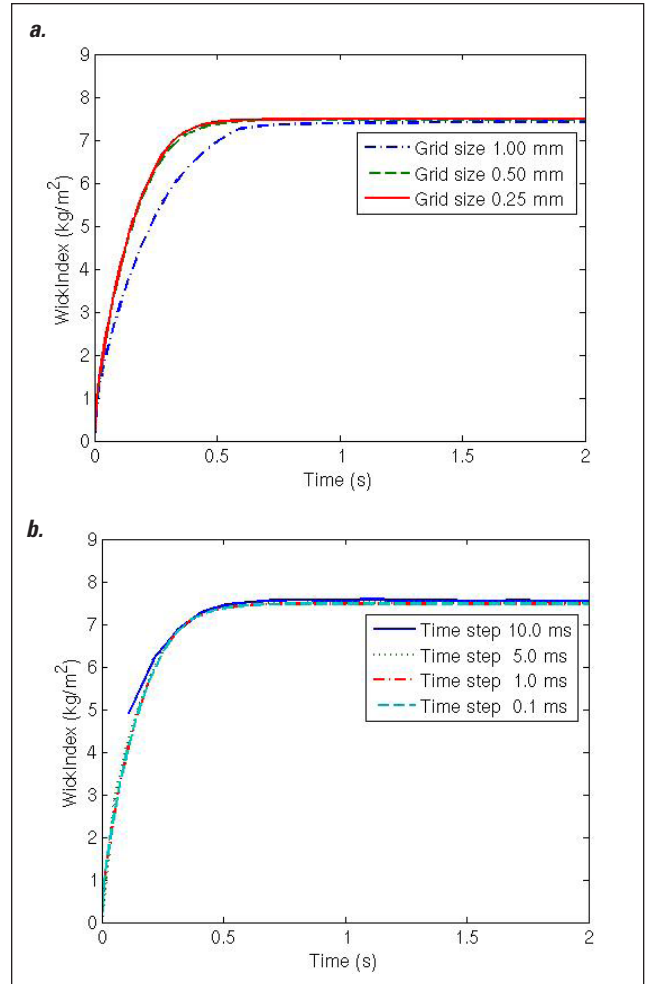


6. (a): The capillary pressure as a function of porosity and water saturation for the contact angle 95° . **(b):** The relative permeability as a function of porosity and water saturation.



7. Macro-scale simulation of the pressurized edge wick experiment. (a) Paper porosity between 0.6 and 0.75. The hole has porosity one. **(b)** The Darcy velocity field showing the anisotropic porosity dependency.

seconds are displayed. Similarly, simulations are also done for different time step lengths where the grid size is held constant at 0.5 mm. From Fig. 8, it is concluded that a grid size of 0.5 mm and a time step length of 1 ms are sufficiently small to reach a grid size and time step independent solution. Hence, this is the numerical resolution that is used in the experimental validation in the next section.

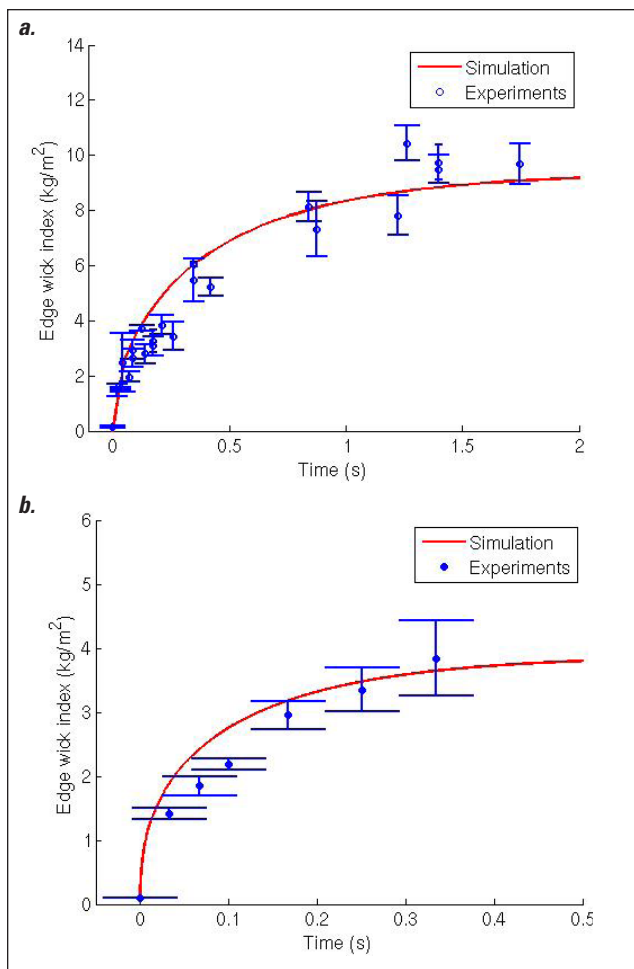


8. (a): Grid study where the edge wick index is plotted as a function of time for three different grid sizes. **(b):** Time step study where the edge wick index is shown for four different time step lengths. The contact angle equals 110° and the porosity equals 0.75.

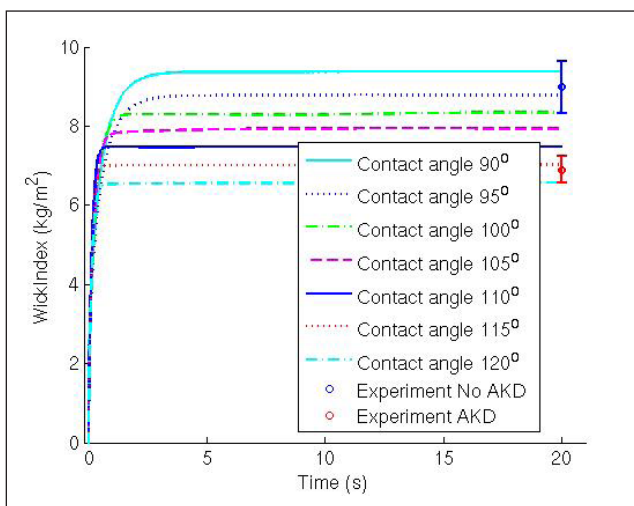
Experimental validation and contact angle study

To validate the multi-scale model, the pressurized edge wick experiment is simulated for two different sample sizes ($62 \times 50 \text{ mm}^2$ and $41 \times 33 \text{ mm}^2$) with contact angle of 110° and a constant porosity 0.75. In Fig. 9, the resulting transient edge wick indices are compared with the experiments. The experimental error bars show one standard deviation. For both sizes, the simulations show good agreement with the transient behavior of the edge wick index.

Further, to show the capillary pressure dependency of the model, the standard sample size $62 \times 50 \text{ mm}^2$ is simulated for different contact angles. The resulting edge wick index is compared to steady state values in the performed experiments with and without AKD. The lower and upper bound for contact angles are found by experiments to be 90° and 120° . In Fig. 10, the edge wick index is plotted as function of time for different contact angles in the range between 90° ,



9. Comparison between the transient part of the simulated and experimental edge wick indices for two different sample sizes: (a) 62 x 50 mm² and (b) 41 x 33 mm². The experimental error bars show one standard deviation.



10. The pressurized edge wick experiment is simulated for different contact angles. The transient simulation of the edge wick indices are compared to the final values of the experiments, with and without alkylketene dimer (AKD). The experimental error bars show one standard deviation.

where no capillary pressure is present, and 120°, where the lab sheet is highly hydrophobic. Contact angle experiments on the test sheet verify this range with values in the lower part without AKD and in the higher part with AKD. The experimental wick index for the lab sheet without AKD is higher compared to the one with AKD, which is expected due to the properties of the AKD sizing chemical [4]. The simulations show a qualitatively correct behavior of how the edge wick index depends on contact angle. For contact angles supported by experiments, we obtain a good agreement with final values obtained from the pressurized edge wick experiments.

SUMMARY

To calculate the penetration of fluid in the open edge of paperboard, a multi-scale framework is developed. On the fiber micro-scale, virtual paper models are generated in PaperGeo. In the fluid flow software IBOFlow, a pore-morphology method is used to calculate capillary pressure curves, and on the active pores, one-phase flow simulations are performed for relative permeabilities. The results as functions of saturation and porosity are stored in a database. The database is used as input for a two-phase flow simulation on a 2D virtual macro sheet to calculate the penetration of fluid in the paper. To generate a database with micro-structure information, including simulation of 25 different representations, takes approximately one day. The pressurized edge wick macro simulations take 10 min. The validation against pressurized edge wick measurements shows a good agreement. The conclusion from this work is therefore that the proposed multi-scale framework makes it possible to simulate accurately, and in a reasonable timeframe, how edge wicking in paperboard packages depends on the micro-structure.

In future work, the simulations will be used to gain an understanding of how the pore size distribution and sizing affect the edge wicking performance. Improved models for the contact angles, which possibly depend on saturation and time, will be developed. The general framework will be extended such that a multi-layer board consisting of single layer sheets can be handled, including a diffusion model for the layer interaction. The goal of the extended framework is to enable a priori predictions of the edge wicking properties of a certain paperboard material, which is of great interest to the paper industry, as well as to packaging manufacturers. **TJ**

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ABOUT THE AUTHORS

Resistance to in-plane edge penetration is one of the most important properties of liquid packaging board, so the ability to use detailed simulations for making a priori predictions regarding this resistance is of great interest to paper and packaging manufacturers. Here, we have developed a unique multi-scale modeling approach that can be used to calculate the edge wicking properties of paperboard and how it depends on the paper micro-structure.

The most challenging aspect of this research was the coupling of the micro- and macro-scales. This must be done carefully in order to capture the dependency of the micro-structure on the edge wicking performance.

The most interesting result from our work is the very good agreement between simulations and experiments. This agreement suggests many far reaching possibilities in using computers to perform more product and process development.

Mills can use this research to increase their understanding of how edge wicking properties of the final paperboard depend on sizing chemicals and process parameters that determine the paper micro-structure. We will next explore a more detailed analysis of how pore size distribution and sizing affect the edge wicking performance. The model will be generalized to multi-layer board, with the aim of enabling a priori predictions of edge wicking properties for a specific paperboard material.

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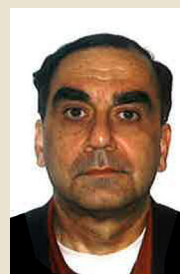
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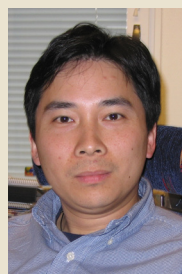
Fredlund



Amini



Rentzhog



Lai



Martinsson



Nyman



Tryding

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